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A remarkable connection has been established for antiferromagnetic 2-spin systems, including the Ising and hard-core models, showing that the computational complexity of approximating the partition function for graphs with maximum degree Δ undergoes a phase transition that coincides with the statistical physics uniqueness/nonuniqueness phase transition on the infinite Δ -regular tree. Despite this clear picture for 2-spin systems, there is little known for multispin systems. We present the first analog of this in approximability results for multispin systems.

The main difficulty in previous inapproximability results was analyzing the behavior of the model on random Δ -regular bipartite graphs, which served as the gadget in the reduction. To this end, one needs to understand the moments of the partition function. Our key contribution is connecting: (i) induced matrix norms, (ii) maxima of the expectation of the partition function, and (iii) attractive fixed points of the associated tree recursions (belief propagation). The view through matrix norms allows a simple and generic analysis of the second moment for any spin system on random Δ -regular bipartite graphs. This yields concentration results for any spin system in which one can analyze the maxima of the first moment. The connection to fixed points of the tree recursions enables an analysis of the maxima of the first moment for specific models of interest.

For *k*-colorings we prove that for even *k*, in a tree nonuniqueness region (which corresponds to $k < \Delta$) there is no FPRAS, unless NP = RP, to approximate the number of colorings for triangle-free Δ -regular graphs. Our proof extends to the antiferromagnetic Potts model, and, in fact, to every antiferromagnetic model under a mild condition.

1. INTRODUCTION

1.1. Background

Spin systems are a general framework from statistical physics that captures classical physics models, including the Ising and Potts models, and models of particular combinatorial interest, including k-colorings and the hard-core lattice gas model defined on independent sets. We define these combinatorial models more precisely before presenting the context of our results.

The hard-core lattice gas model is an example of a 2-spin system. For a graph G = (V, E), configurations of the model are the set Ω of independent sets of G. The model is parameterized by an activity $\lambda > 0$, and a configuration $\sigma \in \Omega$ is assigned weight $w(\sigma) = \lambda^{|\sigma|}$. The Gibbs distribution is $\mu(\sigma) = w(\sigma)/Z$ where the normalizing factor is known as the partition function and is defined as $Z = \sum_{\sigma \in \Omega} w(\sigma)$. In the hard-core model, the spins correspond to occupied/unoccupied. Multispin systems are models with more than two spins, an example being the k-colorings problem. In the colorings problem, for a graph G = (V, E), configurations are the set Ω of assignments of a set of k colors to vertices so that neighboring vertices receive different colors. The Gibbs distribution is the uniform distribution over Ω , and in this case the partition function $Z = |\Omega|$ is the number of k-colorings in G.

The hard-core model and colorings are examples of antiferromagnetic systems – neighboring vertices "prefer" to have different spins. In contrast, in ferromagnetic systems neighboring spins tend to align. We defer the formal definition of antiferromagnetic spin systems to Section 1.2.3 (see Definition 1.3), where we also discuss how our results extend to general spin systems.

The focus of this article is the computational complexity of computing the partition function. Exact computation of the partition function is typically #P-complete, even for very restricted classes of graphs [Greenhill 2000]. Hence, our focus is on the existence of a fully polynomial approximation scheme – either a deterministic FPTAS or randomized FPRAS – for estimating the partition function. For any spin system, (approximate) sampling from the Gibbs distribution implies an FPRAS for estimating the partition function, and hence our hardness results also apply to the associated sampling problem.

The computational complexity of approximating the partition function is now wellunderstood for 2-spin systems, such as the Ising and hard-core models. For all ferromagnetic 2-spin systems, there is an FPRAS for estimating the partition function [Goldberg et al. 2003]. The picture is more intricate (and fascinating) for antiferromagnetic 2-spin systems. We will detail the picture after introducing the statistical physics notion of a phase transition.

Let $\mathbb{T}_{\Delta,\ell}$ denote the complete Δ -regular tree of depth ℓ with root r. The question of interest is whether or not we can fix a configuration on the leaves of $\mathbb{T}_{\Delta,\ell}$ so that the root is influenced by this boundary configuration in the limit $\ell \to \infty$. For the example of colorings, fix a coloring σ_{ℓ} of the leaves (such that there is at least one coloring of the rest of the tree that is consistent with σ_{ℓ}). Look at a random coloring of the tree $\mathbb{T}_{\Delta,\ell}$ conditioned on the leaves having coloring σ_{ℓ} . For all sequences (σ_{ℓ}) of fixed leaf colorings, if in the limit $\ell \to \infty$, the marginal at the root is uniform over the k colors, then we say uniqueness holds, and otherwise we say nonuniqueness holds. (The terminology comes from statistical physics where the focus is on the set of infinite-volume Gibbs measures, see Georgii [2011].)

For the hard-core model the critical activity is $\lambda_c(\Delta) = (\Delta - 1)^{\Delta-1}/(\Delta - 2)^{\Delta}$ [Kelly 1991]. Weitz [2006] presented an FPTAS for estimating the partition function in the tree uniqueness region (i.e., when $\lambda < \lambda_c(\Delta)$). On the other side, Sly [2010] (extended in Sly and Sun [2012] and Galanis et al. [2014, 2012]) proved that, unless NP = RP, it is NP-hard to obtain an FPRAS for Δ -regular graphs in the tree non-uniqueness

region (i.e., when $\lambda > \lambda_c(\Delta)$). These results were extended to all symmetric 2-spin antiferromagnetic models by Li et al. [2013] (see also Sinclair et al. [2012]) and Sly and Sun [2012]. For 2-spin antiferromagnetic models, this establishes a beautiful picture connecting the computational complexity of approximating the partition function to statistical physics phase transitions in the infinite tree.

1.2. Main Results

The picture for multispin systems (systems with q > 2 possible spins for vertices) is much less clear; these approaches for 2-spin systems do not extend to multi-spin models in a straightforward manner. We aim to establish the analog of this inapproximability results for the colorings problem, namely, NP-hardness in the tree nonuniqueness region. Our techniques and results generalize to a broad class of antiferromagnetic spin systems.

1.2.1. Results for Colorings. For the colorings problem, even understanding the uniqueness threshold is challenging. Jonasson [2002] established uniqueness when $k \ge \Delta + 1$, and it is easy to show nonuniqueness when $k \le \Delta$ since a fixed coloring on the leaves can "freeze" the internal coloring. For 2-spin systems, nonuniqueness can be characterized by the existence of multiple solutions of a certain system of Eq. (22), called tree recursions, see Section 4 for additional explanation. In statistical physics terminology the solutions to these equations correspond to semitranslation-invariant measures on the infinite tree \mathbb{T}_{Δ} . For colorings, the uniqueness threshold and the semitranslation-invariant uniqueness threshold no longer coincide. In particular, Brightwell and Winkler [2002] established, for semitranslation-invariant measures, uniqueness when $k \ge \Delta$ and nonuniqueness when $k < \Delta$.

We prove, for even k, that it is NP-hard to approximate the number of colorings (in other words, NP-hard to approximate the partition function) when there is nonuniqueness of semitranslation-invariant Gibbs measures on \mathbb{T}_{Δ} , that is, when $k < \Delta$. Moreover, our result proves hardness for the class of triangle-free Δ -regular graphs. Hence, our result is particularly interesting in the region $k = \Omega(\Delta/\log \Delta)$ since a seminal result of Johansson [1996] (see also Molloy and Reed [2002]) shows that all triangle-free graphs are colorable with $O(\Delta/\log \Delta)$ colors. His proof, which uses the nibble method and the Lovász Local Lemma, can be made algorithmic using the constructive proof of Moser and Tardos [2010]. For general graphs with maximum degree Δ , the interesting region is $k = \Delta - O(\sqrt{\Delta})$, since Molloy and Reed [2001] showed, for sufficiently large constant Δ , a polynomial-time algorithm to determine if a graph with maximum degree Δ is k-colorable when $k \geq \Delta - \sqrt{\Delta} + 3$. We note that most parts of the proof extend to the odd k case as well, modulo the technical condition described in the end of Section 1.2.3.

Here is the formal statement of our inapproximability result for colorings.

THEOREM 1.1. For all even $k \ge 4$, all $\Delta \ge 3$, for the k-colorings problem, when $k < \Delta$, unless NP = RP, there is no FPRAS that approximates the partition function for triangle-free Δ -regular graphs. Moreover, there exists $\varepsilon = \varepsilon(k, \Delta)$ such that, unless NP = RP, one cannot approximate the partition function within a factor $2^{\varepsilon n}$ for triangle-free Δ -regular graphs (where n is the number of vertices).

1.2.2. Results for Antiferromagnetic Potts. Our result also extends to the antiferromagnetic Potts model. In the *q*-state Potts model, there is a parameter B > 0 which corresponds to the "temperature" and controls the strength of the interactions along an edge. For a graph G = (V, E), the set Ω of configurations are assignments σ where $\sigma : V \to [q]$. Each configuration has a weight $w(\sigma) = B^{m(\sigma)}$ where $m(\sigma)$ is the number of monochromatic edges in σ . The Gibbs distribution is $\mu(\sigma) = w(\sigma)/Z$ where $Z = \sum_{\tau \in \Omega} w(\tau)$ is the

partition function. The case B > 1 is the ferromagnetic Potts model, and B < 1 is the antiferromagnetic Potts model. Colorings corresponds to the B = 0 case, and the Ising model is the q = 2 case.

The uniqueness/nonuniqueness threshold for the infinite tree \mathbb{T}_{Δ} is not known for the antiferromagnetic Potts model. We prove that the uniqueness/nonuniqueness threshold for semitranslation-invariant Gibbs measures on \mathbb{T}_{Δ} occurs at $B_c(\Delta) = \frac{\Delta - q}{\Delta}$. We believe this threshold coincides with the uniqueness/nonuniqueness threshold, unlike in the case of colorings. We prove, for even q, that approximating the partition function is NP-hard in the nonuniqueness region for semitranslation-invariant measures.

THEOREM 1.2. For all even $q \ge 4$, all $\Delta \ge 3$, for the antiferromagnetic q-state Potts model, for all $B < \frac{\Delta-q}{\Delta}$, unless NP = RP, there is no FPRAS that approximates the partition function for triangle-free Δ -regular graphs. Moreover, there exists $\varepsilon = \varepsilon(q, \Delta)$ such that, unless NP = RP, one cannot approximate the partition function within a factor $2^{\varepsilon n}$ for triangle-free Δ -regular graphs (where n is the number of vertices).

1.2.3. Results for General Antiferromagnetic Models. Our approach applies in much more generality and yields inapproximability of the partition function for any antiferromagnetic model when there is nonuniqueness of semitranslation-invariant measures on \mathbb{T}_{Δ} and mild additional conditions.

We first need to define general antiferromagnetic models. A general q-spin system is specified by a symmetric $q \times q$ interaction matrix $\mathbf{B} = (B_{ij})_{i,j \in [q]}$ with nonnegative entries, which specify the strength of the interaction between the spins. For example, the interaction matrix for the Potts model has off-diagonal entries equal to 1 and its diagonal entries equal to B. For a finite undirected graph G = (V, E), a q-spin system is a probability distribution μ_G over the space Ω_G of all *configurations*, that is, spin assignments $\sigma : V \rightarrow [q]$. The weight of a configuration $\sigma \in \Omega_G$ is the product of neighboring spin interactions, that is,

$$w_G(\sigma) = \prod_{(u,v)\in E} B_{\sigma(u)\sigma(v)}.$$

The Gibbs distribution μ_G is defined as $\mu_G(\sigma) = w_G(\sigma)/Z_G$ where the partition function Z_G is $Z_G = \sum_{\sigma \in \Omega_G} w_G(\sigma)$. We drop the subscript *G* when the graph under consideration is clear.

We use the following definition of antiferromagnetic models in terms of the signature of the interaction matrix **B**, that is, the signs of its eigenvalues. The interaction matrix **B** is assumed to be symmetric and have nonnegative entries. These are standard assumptions since we are interested in undirected graphs and the Gibbs distribution should be a probability distribution. Without loss of generality, we will also assume that **B** is irreducible. Otherwise, by a suitable permutation of the spins, **B** can be put into block diagonal form (which coincides with the normal form of the reducible **B**) where each of the blocks is either irreducible or zero. Effectively, this says that the original spin model can be studied by considering the induced submodels of each block which correspond to irreducible symmetric matrices (where our results apply). For connected graphs G, the partition function for the original model is simply the sum of the partition functions of each submodel.

We are now ready to give the definition of antiferromagnetism we use.

Definition 1.3. Let **B** be the interaction matrix of a q-state spin system. Since **B** is symmetric all of its eigenvalues are real. Also note that it has nonnegative entries and by irreducibility, the Perron-Frobenius theorem implies that one of the eigenvalues of **B** with the largest magnitude is positive and simple, that is, the associated eigenspace

is one-dimensional. The model is called *antiferromagnetic* if all the other eigenvalues are negative. Note that no eigenvalue is allowed to be zero and hence \mathbf{B} is nonsingular.

This definition generalizes antiferromagnetism for 2-spin systems (see Goldberg et al. [2003], Li et al. [2013], and Sly and Sun [2012]), and captures colorings as well as the antiferromagnetic region for the Potts models. Moreover, this definition seems natural in that it implies that neighboring vertices prefer to have different spin assignments (see Corollary 6.4 in Section 6.2). Another nice feature of Definition 1.3 is that it does not depend on the presence of external fields. Specifically, for Δ -regular graphs, any external field can be pushed into the interaction matrix **B** with a congruence transformation of the matrix **B**. The resulting interaction matrix, by Sylvester's law of inertia, has the same number of positive, zero, and negative eigenvalues and in particular remains antiferromagnetic.

We conclude this discussion by pointing out that some of our results for general models are more easily stated when **B** is further assumed to be aperiodic. We shall refer to such matrices **B** (irreducible and aperiodic) as *ergodic*. Note that if **B** is periodic, its period must be two, since **B** is symmetric. Such a model is only interesting on bipartite graphs (otherwise the partition function is zero). Note that the spectrum of a symmetric and periodic matrix is symmetric around 0, so Definition 1.3 implies that the interaction matrix **B** of an antiferromagnetic model is ergodic whenever $q \ge 3$ (observe that it is trivial to compute the partition function on periodic models with q = 2).

We need several additional definitions concerning the moments of the partition function. For antiferromagnetic models on a random Δ -regular bipartite graph G = (V, E) with bipartition $V = V_1 \cup V_2$, the goal is to understand the Gibbs distribution μ_G by looking at the distribution of spin values in V_1 and V_2 . Let $n = |V_1| = |V_2|$. For a configuration $\sigma : V \to [q]$, we shall denote the set of vertices assigned spin *i* by $\sigma^{-1}(i)$. Denote by Δ_q the simplex $\Delta_q = \{(x_1, x_2, \ldots, x_q) \in \mathbb{R}^q \mid \sum_{i=1}^q x_i = 1 \text{ and } x_i \ge 0 \text{ for } i = 1, \ldots, q\}$. For $\alpha, \beta \in \Delta_q$, let

$$\Sigma^{\alpha,\beta} = \left\{ \sigma : V \to \{1, \dots, q\} \, \middle| \, |\sigma^{-1}(i) \cap V_1| = \alpha_i n, \, |\sigma^{-1}(i) \cap V_2| = \beta_i n \text{ for } i = 1, \dots, q \right\},$$

that is, configurations in $\Sigma^{\alpha,\beta}$ assign $\alpha_i n$ and $\beta_i n$ vertices in V_1 and V_2 the spin value i, respectively.¹ We will be interested in the total weight $Z_G^{\alpha,\beta}$ of configurations in $\Sigma^{\alpha,\beta}$, namely,

$$Z_G^{\boldsymbol{\alpha},\boldsymbol{\beta}} = \sum_{\boldsymbol{\sigma} \in \Sigma^{\boldsymbol{\alpha},\boldsymbol{\beta}}} w(\boldsymbol{\sigma}).$$

We study $Z_G^{\alpha,\beta}$ by looking at the moments $\mathbf{E}_{\mathcal{G}}[Z_G^{\alpha,\beta}]$ and $\mathbf{E}_{\mathcal{G}}[(Z_G^{\alpha,\beta})^2]$, where the expectation is over the distribution of the random Δ -regular bipartite graph, from hereon denoted by \mathcal{G} .

For $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \triangle_q$, denote the leading term of the first and second moments as

$$\Psi_1(\boldsymbol{\alpha},\boldsymbol{\beta}) = \Psi_1^{\mathbf{B}}(\boldsymbol{\alpha},\boldsymbol{\beta}) := \lim_{n \to \infty} \frac{1}{n} \log \mathbf{E}_{\mathcal{G}} [Z_G^{\boldsymbol{\alpha},\boldsymbol{\beta}}], \tag{1}$$

$$\Psi_{2}(\boldsymbol{\alpha},\boldsymbol{\beta}) = \Psi_{2}^{\mathbf{B}}(\boldsymbol{\alpha},\boldsymbol{\beta}) := \lim_{n \to \infty} \frac{1}{n} \log \mathbf{E}_{\mathcal{G}}[(Z_{G}^{\boldsymbol{\alpha},\boldsymbol{\beta}})^{2}].$$
(2)

(The limits in (1) and (2) exist, see Section 2 for pointers to the literature.)

¹Technically we need to define $\Sigma^{\alpha,\beta} = \{\sigma : V \to [q] \mid |\sigma^{-1}(i) \cap V_1| = \hat{\alpha}_i, |\sigma^{-1}(i) \cap V_2| = \hat{\beta}_i \text{ for } i \in [q]\}$, where $\{\hat{\alpha}_i\}$ are $\{\alpha_i n\}$ rounded in a canonical fashion so that their sum is preserved (e.g., using "cascade rounding") and in the same way $\{\hat{\beta}_i\}$ are $\{\beta_i n\}$ rounded.

We will refer to α , β that maximize Ψ_1 as *dominant phases*. Moreover, we say that a dominant phase (α, β) is *Hessian dominant* if the Hessian of Ψ_1 at (α, β) is negative definite. (Note this is a sufficient condition for α , β to be a local maximum.) In the uniqueness, region, there is a unique dominant phase and it has $\alpha = \beta$. In contrast, for 2-spin antiferromagnetic models and for colorings in the semitranslation-invariant nonuniqueness region, the dominant phases have $\alpha \neq \beta$, and one expects this would hold for all antiferromagnetic models. In our reduction, we will need this additional condition that the dominant phases are not symmetric (i.e., $\alpha \neq \beta$).

Our main technical result relates the second moment to the first moment, for any model on random bipartite regular graphs.

THEOREM 1.4. For any spin system, for all $\Delta \geq 3$,

$$\max_{\boldsymbol{\alpha},\boldsymbol{\beta}}\Psi_2(\boldsymbol{\alpha},\boldsymbol{\beta})=2\max_{\boldsymbol{\alpha},\boldsymbol{\beta}}\Psi_1(\boldsymbol{\alpha},\boldsymbol{\beta}).$$

Crucially, Theorem 1.4 implies that $\Psi_2(\alpha, \beta) = 2\Psi_1(\alpha, \beta)$ for dominant phases, which is key for our arguments, since it will eventually allow us to find the asymptotic distribution of the random variables $Z_G^{\alpha,\beta}$ (as $n \to \infty$). We do this by applying the so-called small subgraph conditioning method. The asymptotic convergence is utilized to prove the properties of the gadget we use in the reduction. The gadget is a slight modification of a random Δ -regular bipartite graph and its properties are described in Section 6.4. The precise formulation of these properties does not matter at this stage, but rather that we can prove them when the dominant phases (α, β) satisfy the following conditions: (i) each dominant phase is Hessian dominant, (ii) the dominant phases are permutation symmetric, that is, obtainable from one another by a suitable permutation of the set of spins (we clarify here that the permutations must be automorphisms of the interaction matrix **B**),² and (iii) each dominant phase (α, β) has $\alpha \neq \beta$. Condition (iii) implies that the model is in the nonuniqueness region of \mathbb{T}_{Δ} and, further, that a typical configuration in the Gibbs distribution of the random graph is "unbalanced" between the two sides, which allows to encode a CSP (in our case MAX-CUT). Condition (i) ensures the asymptotic convergence of $Z_G^{\alpha,\beta}$. Condition (ii) ensures that the asymptotic distribution of $Z_G^{\alpha,\beta}$ is identical for all the dominant phases. We want to remark why the permutation symmetry condition arises naturally. A

We want to remark why the permutation symmetry condition arises naturally. A generic multispin system in the semitranslational nonuniqueness region will have exactly two maxima of Ψ_1 and hardness (assuming NP = RP) follows easily. Models coming from statistical physics (e.g., Potts model or Widom-Rowlinson model) are not generic since they usually come with permutation symmetries of the same type as condition (ii) in the previous paragraph. (The symmetries make the hardness result more difficult to state and prove.)

We now state our general inapproximability result.

THEOREM 1.5. Let $q \ge 2, \Delta \ge 3$. For an antiferromagnetic q-spin system whose interaction matrix **B** is ergodic, if the dominant phases (α, β) of Ψ_1 are permutation symmetric and all of them are Hessian dominant and satisfy $\alpha \ne \beta$, then, unless NP = RP, there is no FPRAS for approximating the partition function for triangle free Δ regular graphs. Moreover, there exists $\varepsilon = \varepsilon(q, \Delta)$ such that, unless NP = RP, one cannot

²More precisely, the permutation symmetric property can be stated as follows: for any two dominant phases, say (α_1, β_1) and (α_2, β_2) , there exists a $q \times q$ permutation matrix **P** such that **B** = **PBP**^{\intercal} and $(\alpha_1, \beta_1) = (\mathbf{P}\alpha_2, \mathbf{P}\beta_2)$ or $(\alpha_1, \beta_1) = (\mathbf{P}\beta_2, \mathbf{P}\alpha_2)$. In other words, the dominant phases can be obtained from each other by interchanging α and β , by permuting the spins in a way that **B** is left invariant, or a combination of the previous two operations.

approximate the partition function within a factor $2^{\varepsilon n}$ for triangle-free Δ -regular graphs (where n is the number of vertices).

We remark here that, whenever the hypotheses of Theorem 1.5 are satisfied, the spin system with interaction matrix **B** is in the tree nonuniqueness region of \mathbb{T}_{Δ} , see Section 4 for more details. However, the reverse direction is not necessarily true, that is, an antiferromagnetic spin system in the tree nonuniqueness region of \mathbb{T}_{Δ} does not necessarily have multiple dominant phases, an example is the k-colorings model when $k = \Delta$ (see Theorem 1.6).

For illustrative purposes, we first note that the inapproximability results for antiferromagnetnic 2-spin systems in the tree nonuniqueness region [Sly 2010; Sly and Sun 2012; Galanis et al. 2012] follow as corollaries of Theorem 1.5. In particular, for antiferromagnetic 2-spin systems it is well known that for any $\Delta \geq 3$, in the nonuniqueness region of \mathbb{T}_{Λ} , the maximizers of Ψ_1 are exactly two pairs $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ and $(\boldsymbol{\beta}, \boldsymbol{\alpha})$ with $\alpha \neq \beta$. Note that these two dominant phases satisfy trivially the permutation symmetric property. Moreover, it can also be verified that they are Hessian dominant and hence the hypotheses of Theorem 1.5 are satisfied.

As a more indicative application of Theorem 1.5, let us deduce Theorems 1.1 and 1.2. To do this, we need the following theorem (proved in Section 7) which describes the dominant phases for the colorings and antiferromagnetic Potts models.

THEOREM 1.6. Let $q \geq 3$, $0 \leq B < 1$ and $\Delta \geq 3$. For the antiferromagnetic q-state Potts model with parameter B on a random Δ -regular bipartite graph (note that the k-colorings model corresponds to B = 0 and q = k in the following), it holds that

- (1) When $B \geq \frac{\Delta-q}{\Delta}$, there is a unique dominant phase (α, β) which satisfies $\alpha = \beta$.
- (2) For all even $q \ge 4$, for all $\Delta \ge 3$, when $0 \le B < \frac{\Delta q}{\Delta}$, the dominant phases (α, β) are in one-to-one correspondence with subsets $T \subseteq [q]$ with |T| = q/2. Moreover, there exist $a(q, \Delta, B), b(q, \Delta, B)$ with $a \neq b$ such that for $T \subseteq [q]$ with |T| = q/2, the dominant phase (α, β) corresponding to T satisfies

$$\begin{aligned} \alpha_i &= a \text{ if } i \in T, \quad \alpha_i = b \text{ if } i \notin T, \\ \beta_i &= b \text{ if } i \in T, \quad \beta_i = a \text{ if } i \notin T. \end{aligned}$$

$$(3)$$

Moreover, the dominant phases are Hessian.

PROOF OF THEOREMS 1.1 AND 1.2. We just need to verify the hypotheses of Theorem 1.5. Equation (3) of Theorem 1.6 establishes that the dominant phases (α, β) are permutation symmetric and each of them satisfies $\alpha \neq \beta$. Thus, the hypotheses of Theorem 1.5 hold in the regime $q < \Delta$ and $0 \le B < \frac{\Delta - q}{\Lambda}$. \Box

Note that the restriction of even k, q in Theorems 1.1 and 1.2, respectively, is a technical one and comes from the second part of Theorem 1.6. For odd q, we are unable to establish whether the dominant phases are supported on vectors with two or three different entries, see Section 7 for more details. Classifying the dominant phases for odd q would also extend the inapproximability results of Theorems 1.1 and 1.2.

1.3. Proof Approach

The key gadget in the inapproximability results for 2-spin models is a random Δ regular bipartite graph. The rough idea for the hard-core model is that in the tree nonuniqueness region, on a random Δ -regular bipartite graph, an independent set from the Gibbs distribution is "unbalanced" with high probability (the fraction of occupied vertices in the two parts of the bipartition differ by a constant). To analyze random regular bipartite graphs, the original inapproximability result of Sly [2010] relied on a second moment analysis of Mossel et al. [2009], which Sly called a technical tour-deforce. The optimization at the heart of that analysis was difficult enough that his result only held for λ close to the uniqueness threshold.

We present a new approach for the associated optimization problem which is at the heart of the second moment analysis. Our approach yields a simple, short analysis that holds for *any model* on random Δ -regular bipartite graphs. The key idea is to define a new function Φ , which is represented as an induced matrix norm, and has the same critical points as the first moment. We can then use the fact that induced matrix norms are multiplicative over tensor product to analyze the second moment.

1.4. Article Outline

In Section 2, we derive some basic expressions for the first and second moments. Then, in Section 3, we analyze the second moment using matrix norms and thereby prove Theorem 1.4. In Section 4, we analyze the maxima of the function Ψ_1 . There, we further prove a connection between local maxima of Ψ_1 and stable fixpoints of the so-called tree recursions which is used in later sections.

The reduction for the inapproximability results uses an intermediate problem, which we call the *phase labeling problem*. Our inapproximability results hinge on showing that the phase labeling problem is hard to approximate. In Section 5, we give the main elements of this reduction for the colorings model to introduce the relevant concepts. The hardness of approximating the phase labeling problem for general antiferromagnetic models is proved in Section 6, where we also fill in the details which were omitted in the simplified exposition for the colorings model.

We show how the phase labeling problem reduces to the approximation of the partition function in Section 6.4, based on arguments in Sly and Sun [2012]. The reduction uses gadgets whose existence and construction are based on a slight variation of the random Δ -regular bipartite graph distribution. At this point, to establish the properties of the gadgets, we use the small subgraph conditioning method. The application of the method is fairly standard though technically intensive due to its use of precise asymptotics for the first and second moments. The technical details of applying the method in our case are given in Appendix A, while the asymptotics for the first and second moments are derived in Appendix B.

The proof of our general inapproximability result (Theorem 1.5) is given in Section 6.1. We saw in Section 1.2.3 how to deduce the inapproximability results for the colorings and Potts models (Theorems 1.1 and 1.2) from Theorem 1.5 using the classification of the dominant phases in Item 2 of Theorem 1.6. The proof of Item 2 in Theorem 1.6 is given in Section 7.

Finally, in Appendix C, we extend the argument of Brightwell and Winkler [2002] to prove Item 1 of Theorem 1.6, that is, show uniqueness for semitranslation-invariant Gibbs measures for the antiferromagnetic Potts model when $B \ge (\Delta - q)/\Delta$.

2. EXPRESSIONS FOR THE FIRST AND SECOND MOMENTS

In this section, we derive the expressions for the first and second moments of $Z_G^{\alpha,\beta}$ and, in particular, the expressions for Ψ_1 and Ψ_2 .

Let $\mathcal{G}_n(\Delta)$ be the probability distribution over bipartite graphs with n + n vertices formed by taking the union of Δ random perfect matchings. We will use the simplified notation $\mathcal{G}_n := \mathcal{G}_n(\Delta)$ or even $\mathcal{G} := \mathcal{G}_n(\Delta)$ when n is clear from context. Strictly speaking, this distribution is over bipartite multigraphs. However, since our results hold asymptotically almost surely (a.a.s.) over \mathcal{G}_n , as noted in Mossel et al. [2009], by contiguity arguments they also hold a.a.s. for the uniform distribution over bipartite Δ -regular graphs. For a complete account of contiguity, we refer the reader to Janson et al. [2000, Chapter 9]. Let $G \sim \mathcal{G}$. We will denote the two sides of the bipartition of G as V_1, V_2 . We first compute the first moment $\mathbf{E}_{\mathcal{G}}[Z_G^{\alpha,\beta}]$. For $\sigma \in \Sigma^{\alpha,\beta}$ and a uniform matching between V_1 and V_2 , let nx_{ij} denote the number of edges matching vertices in $\sigma^{-1}(i) \cap V_1$ and $\sigma^{-1}(j) \cap V_2$. Under the convention that $0^0 \equiv 1$, we then have

$$\mathbf{E}_{\mathcal{G}}[Z_{G}^{\boldsymbol{\alpha},\boldsymbol{\beta}}] = \binom{n}{\alpha_{1}n,\ldots,\alpha_{q}n} \binom{n}{\beta_{1}n,\ldots,\beta_{q}n} \times \left(\sum_{\mathbf{x}} \frac{\prod_{i} \binom{\alpha_{i}n}{(x_{i1}n,\ldots,x_{iq}n)} \prod_{j} \binom{\beta_{j}n}{(x_{1j}n,\ldots,x_{qj}n)} \prod_{i,j} B_{ij}^{nx_{ij}}}{\binom{n}{(x_{11}n,\ldots,x_{qq}n)}}\right)^{\Delta},$$
(4)

where the sum ranges over $\mathbf{x} = (x_{11}, \ldots, x_{qq})$ with $n\mathbf{x} \in \mathbb{Z}^{q^2}$ satisfying the following constraints:

$$\sum_{j} x_{ij} = \alpha_i \quad (\forall i \in [q]), \quad \sum_{i} x_{ij} = \beta_j \quad (\forall j \in [q]),$$

$$x_{ij} \ge 0 \quad (\forall (i, j) \in [q]^2).$$
(5)

The first line in (4) accounts for the cardinality of $\Sigma^{\alpha,\beta}$, while the second line is $\mathbf{E}_{\mathcal{G}}[w_G(\sigma)]$ for an arbitrary $\sigma \in \Sigma^{\alpha,\beta}$. Since the weight of a configuration is multiplicative over the edges and the matchings are independent, $\mathbf{E}_{\mathcal{G}}[w_G(\sigma)]$ is the Δ -power of the expected contribution of a single matching. The latter is completely determined by \mathbf{x} and is equal to $\prod_{i,j} B_{ij}^{n_{x_{ij}}}$, scaled by the probability that the matching induces the prescribed \mathbf{x} .

We next calculate the second moment of $Z_G^{\alpha,\beta}$. To do this, for $(\sigma_1, \sigma_2) \in \Sigma^{\alpha,\beta} \times \Sigma^{\alpha,\beta}$, we need to compute $\mathbf{E}_{\mathcal{G}}[w_G(\sigma_1)w_G(\sigma_2)]$. Let $\gamma_{ik} = |\sigma_1^{-1}(i) \cap \sigma_2^{-1}(k) \cap V_1|$, $\delta_{jl} = |\sigma_1^{-1}(j) \cap \sigma_2^{-1}(l) \cap V_2|$. The vectors $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ capture the overlap of configurations in V_1 and V_2 , respectively. For a uniform matching between V_1 and V_2 , let y_{ikjl} denote the number of edges matching vertices in $\sigma_1^{-1}(i) \cap \sigma_2^{-1}(k) \cap V_1$ and $\sigma_1^{-1}(j) \cap \sigma_2^{-1}(l) \cap V_2$. Under the convention $0^0 \equiv 1$, we then have

$$\mathbf{E}_{\mathcal{G}}[(Z_{G}^{\alpha,\beta})^{2}] = \sum_{\boldsymbol{\gamma},\boldsymbol{\delta}} \binom{n}{\gamma_{11}n, \dots, \gamma_{qq}n} \binom{n}{\delta_{11}n, \dots, \delta_{qq}n} \times \left(\sum_{\mathbf{y}} \frac{\prod_{i,k} \binom{\gamma_{ikn}}{y_{ik11}n, \dots, y_{ikqq}n} \prod_{j,l} \binom{\delta_{jl}n}{\binom{y_{11jl}n, \dots, y_{qqjl}n} \prod_{ikjl} (B_{ij}B_{kl})^{ny_{ikjl}}}{\binom{n}{\gamma_{1111}n, \dots, \gamma_{qqqq}n}}\right)^{\Delta},$$
(6)

where the sums range over $\boldsymbol{\gamma} = (\gamma_{11}, \ldots, \gamma_{qq}), \, \boldsymbol{\delta} = (\delta_{11}, \ldots, \delta_{qq}), \, \mathbf{y} = (y_{1111}, \ldots, y_{qqqq})$ with $n\boldsymbol{\gamma}, n\boldsymbol{\delta} \in \mathbb{Z}^{q^2}$ and $n\mathbf{y} \in \mathbb{Z}^{q^4}$ satisfying

$$\begin{split} \sum_{k} \gamma_{ik} &= \alpha_{i} \quad (\forall i \in [q]), \quad \sum_{l} \delta_{jl} = \beta_{j} \quad (\forall j \in [q]), \quad \sum_{j,l} y_{ikjl} = \gamma_{ik} \quad (\forall (i,k) \in [q]^{2}), \\ \sum_{i} \gamma_{ik} &= \alpha_{k} \quad (\forall k \in [q]), \quad \sum_{j} \delta_{jl} = \beta_{l} \quad (\forall l \in [q]), \quad \sum_{i,k} y_{ikjl} = \delta_{jl} \quad (\forall (j,l) \in [q]^{2}), \quad (7) \\ \gamma_{ik} &\geq 0 \quad (\forall (i,k) \in [q]^{2}), \quad \delta_{jl} \geq 0 \quad (\forall (j,l) \in [q]^{2}), \quad y_{ikjl} \geq 0 \quad (\forall (i,k,j,l) \in [q]^{4}). \end{split}$$

The first line in (6) accounts for the cardinality of $\Sigma^{\alpha,\beta} \times \Sigma^{\alpha,\beta}$, while the second line is $\mathbf{E}_{\mathcal{G}}[w_G(\sigma_1)w_G(\sigma_2)]$ for $(\sigma_1, \sigma_2) \in \Sigma^{\alpha,\beta} \times \Sigma^{\alpha,\beta}$ with the prescribed $\boldsymbol{\gamma}, \boldsymbol{\delta}$. Since the weight of a configuration is multiplicative over the edges and the matchings are independent, $\mathbf{E}_{\mathcal{G}}[w_G(\sigma_1)w_G(\sigma_2)]$ is the Δ -power of the expected weight of a single matching. The latter is completely determined by \mathbf{y} and is equal to $\prod_{i,k,j,l} (B_{ij}B_{kl})^{y_{ikjl}}$, scaled by the probability that the matching induces the prescribed \mathbf{y} .

Remark 2.1. Note that (6) shows that the second moment can be interpreted as the first moment of a paired-spin model with interaction matrix $\mathbf{B} \otimes \mathbf{B}$. Indeed, we can

interpret $B_{ij}B_{kl}$ as the activity between the paired spins (i, k) and (j, l), thus giving the desired alignment.

The sums in (4) and (6) are typically exponential in *n*. The most critical component of our arguments is to find the quantitative structure of configurations which determine the exponential order of the moments. Formally, we study the limits of $\frac{1}{n} \log \mathbf{E}_{\mathcal{G}}[Z_G^{\alpha,\beta}]$ and $\frac{1}{n} \log \mathbf{E}_{\mathcal{G}}[(Z_G^{\alpha,\beta})^2]$ as $n \to \infty$. Under the usual conventions that $\ln 0 \equiv -\infty$ and $0 \ln 0 \equiv 0$, standard application of Stirling's approximation yields the following:

$$\Psi_{1}(\boldsymbol{\alpha},\boldsymbol{\beta}) := \lim_{n \to \infty} \frac{1}{n} \log \mathbf{E}_{\mathcal{G}} [Z_{G}^{\boldsymbol{\alpha},\boldsymbol{\beta}}] = \max_{\mathbf{x}} \Upsilon_{1}(\boldsymbol{\alpha},\boldsymbol{\beta},\mathbf{x}), \tag{8}$$
where $\Upsilon_{1}(\boldsymbol{\alpha},\boldsymbol{\beta},\mathbf{x}) := (\Delta - 1) f_{1}(\boldsymbol{\alpha},\boldsymbol{\beta}) + \Delta g_{1}(\mathbf{x})$

$$f_{1}(\boldsymbol{\alpha},\boldsymbol{\beta}) := \sum_{i} \alpha_{i} \ln \alpha_{i} + \sum_{j} \beta_{j} \ln \beta_{j}$$

$$g_{1}(\mathbf{x}) := \sum_{i,j} x_{ij} \ln B_{ij} - \sum_{i,j} x_{ij} \ln x_{ij}.$$

And for the second moment:

$$\Psi_{2}(\boldsymbol{\alpha},\boldsymbol{\beta}) := \lim_{n \to \infty} \frac{1}{n} \log \mathbf{E}_{\mathcal{G}} \Big[\big(Z_{G}^{\boldsymbol{\alpha},\boldsymbol{\beta}} \big)^{2} \Big] = \max_{\boldsymbol{\gamma},\boldsymbol{\delta}} \max_{\mathbf{y}} \Upsilon_{2}(\boldsymbol{\gamma},\boldsymbol{\delta},\mathbf{y}), \tag{9}$$
where $\Upsilon_{2}(\boldsymbol{\gamma},\boldsymbol{\delta},\mathbf{y}) := (\Delta - 1) f_{2}(\boldsymbol{\gamma},\boldsymbol{\delta}) + \Delta g_{2}(\mathbf{y})$

$$f_{2}(\boldsymbol{\gamma},\boldsymbol{\delta}) := \sum_{i,k} \gamma_{ik} \ln \gamma_{ik} + \sum_{j,l} \delta_{jl} \ln \delta_{jl}$$

$$g_{2}(\mathbf{y}) := \sum_{i,k,j,l} y_{ikjl} \ln(B_{ij}B_{kl}) - \sum_{i,k,j,l} y_{ikjl} \ln y_{ikjl}.$$

The functions Υ_1 and Υ_2 are defined on the regions (5) and (7), respectively. We also relax the integrality constraints of the vectors $\boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{x}$ and $\boldsymbol{\gamma}, \boldsymbol{\delta}, \mathbf{y}$ which were imposed by the expressions (4) and (6). This does not affect our considerations in the limit $n \to \infty$. Moreover, note that the function Υ_2 depends on $\boldsymbol{\alpha}, \boldsymbol{\beta}$ due to the linear constraints (7). This dependence is omitted here since we are going to study the second moment for $\boldsymbol{\alpha}, \boldsymbol{\beta}$ fixed to some well-chosen vectors.

The limits (8) and (9) can be justified using standard Laplace arguments (see, e.g., de Bruijn [1981, Chapter 4]).

Remark 2.2. The maximization in the first moment depends only on the function $g_1(\mathbf{x})$ which is strictly concave in the convex region where it is defined. Hence, for any fixed $\boldsymbol{\alpha}, \boldsymbol{\beta}$, the global maximum of $\Upsilon_1(\boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{x})$ with respect to \mathbf{x} is achieved at a unique point. Similarly, for any fixed $\boldsymbol{\gamma}, \boldsymbol{\delta}$, the maximum of $\Upsilon_2(\boldsymbol{\gamma}, \boldsymbol{\delta}, \mathbf{y})$ with respect to \mathbf{y} is achieved at a unique point. Crucially for the calculation of the asymptotics of the second moment in Appendix B, if $\boldsymbol{\alpha}, \boldsymbol{\beta}$ are global maximizers of Ψ_1 , the global maximum of $\Upsilon_2(\boldsymbol{\gamma}, \boldsymbol{\delta}, \mathbf{y})$ with respect to $\boldsymbol{\gamma}, \boldsymbol{\delta}, \mathbf{y}$ is also achieved at a unique point, see Lemma 3.2 in Section 3.4.

A notational convention that we have adopted silently so far is perhaps useful to allude: the indices i, k "point" to the set V_1 , while indices j, l "point" to the set V_2 .

3. SECOND MOMENT ANALYSIS

In this section, we prove Theorem 1.4. We first present some basic definitions concerning matrix norms. We then show that the maximum of the first moment function Ψ_1 can be reformulated in terms of matrix norms. This then enables a short proof of Theorem 1.4.

3.1. Basic Definitions: Matrix Norms

We will reformulate the maxima of the first and second moments in terms of matrix norms. We first recall the basic definitions regarding matrix norms. The usual vector norms are denoted as

$$\|\mathbf{x}\|_p = \left(\sum_{i=1}^n x_i^p\right)^{1/p}.$$

We will use the subordinate matrix norm (also known as the induced matrix norm) which will be denoted as $\|\cdot\|_{p\to q}$ and is defined as.

$$\|\mathbf{A}\|_{p \to q} = \max_{\|\mathbf{x}\|_p = 1} \|\mathbf{A}\,\mathbf{x}\|_q.$$

Note that if **A** has nonnegative entries then one can restrict the maximization to **x** with nonnegative entries. A well-known example of an induced norm is the spectral norm $\|\cdot\|_{2\to 2}$.

3.2. Reformulating the First Moment in Terms of Matrix Norms

A key component in the analysis of the second moment is the following function Φ . Let $p = \Delta/(\Delta - 1)$. For nonnegative **r**, **c**, define $\Phi(\mathbf{r}, \mathbf{c})$ by

$$\exp\left(\Phi(\mathbf{r},\mathbf{c})/\Delta\right) = \frac{\mathbf{r}^{\mathsf{T}}\mathbf{B}\mathbf{c}}{\|\mathbf{r}\|_{p}\|\mathbf{c}\|_{p}}.$$

We will show that the critical points of Φ and Ψ_1 match in the sense that there is a oneto-one correspondence between them and their values are equal at the corresponding critical points. The full statement is contained in Theorem 4.1 in Section 4.1, but the important element for the current discussion is captured in the following lemma.

Lemma 3.1.

$$\max_{\boldsymbol{\alpha},\boldsymbol{\beta}\in \Delta_q}\Psi_1(\boldsymbol{\alpha},\boldsymbol{\beta})=\max_{\mathbf{r},\mathbf{c}}\Phi(\mathbf{r},\mathbf{c}).$$

Therefore, to determine the dominant phases of Ψ_1 it suffices to study Φ . The maximum of Φ can be compactly expressed in terms of matrix norms as follows:

$$\max_{\mathbf{r},\mathbf{c}} \exp\left(\Phi(\mathbf{r},\mathbf{c})/\Delta\right) = \max_{\mathbf{c}} \max_{\mathbf{r}} \frac{\mathbf{r}^{\mathsf{T}} \mathbf{B} \mathbf{c}}{\|\mathbf{r}\|_{p} \|\mathbf{c}\|_{p}} = \max_{\mathbf{c}} \frac{\|\mathbf{B}\mathbf{c}\|_{\Delta}}{\|\mathbf{c}\|_{p}} = \|\mathbf{B}\|_{p \to \Delta}, \quad (10)$$

where the second equality follows from norm duality.

Hence, the dominant phases of Ψ_1 can be expressed in terms of matrix norms:

$$\max_{\boldsymbol{\alpha},\boldsymbol{\beta}\in\Delta_q} \exp\left(\Psi_1(\boldsymbol{\alpha},\boldsymbol{\beta})/\Delta\right) = \|\mathbf{B}\|_{\frac{\Delta}{\Delta-1}\to\Delta}.$$
(11)

3.3. Analyzing the Second Moment: Proof of Theorem 1.4

To analyze the second moment function Ψ_2 , we will reduce it to the first moment optimization in the following manner. The key observation is that the associated optimization for the second moment is equivalent to a first moment optimization of a "paired-spin" model which is specified by the tensor product of the original interaction matrix with itself. This property enables us to relate the maximum for the second moment calculations with the maximum of the first moment calculations.

PROOF OF THEOREM 1.4. The second moment considers a pair of configurations, say σ and σ' , which are constrained to have a given phase α for V_1 and β for V_2 , where $V = V_1 \cup V_2$. We capture this constraint using a pair of vectors $\boldsymbol{\gamma}, \boldsymbol{\delta}$ corresponding to

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the overlap between σ and σ' , in particular, γ_{ij} (and δ_{ij}) is the number of vertices in V_1 (and V_2 , respectively) with spin *i* in σ and spin *j* in σ' . Recall, $\Psi_1^{\mathbf{B}}$ indicates the dependence of the function Ψ_1 on the interaction matrix **B**;

Recall, $\Psi_1^{\mathbf{B}}$ indicates the dependence of the function Ψ_1 on the interaction matrix **B**; to simplify the notation we will drop the exponent if it is **B**. We have (see Remark 2.1 in Section 2 for more details on this connection)

$$\Psi_2(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \max_{\boldsymbol{\gamma}, \boldsymbol{\delta}} \Psi_1^{\mathbf{B} \otimes \mathbf{B}}(\boldsymbol{\gamma}, \boldsymbol{\delta}), \tag{12}$$

where the optimization in (12) is constrained to γ and δ such that

$$\sum_{i} \gamma_{ik} = \alpha_k, \qquad \sum_{k} \gamma_{ik} = \alpha_i, \qquad \sum_{j} \delta_{j\ell} = \beta_\ell, \quad \text{and} \quad \sum_{\ell} \delta_{j\ell} = \beta_j. \tag{13}$$

Ignoring the four constraints in (13) can only increase the value of (12) and hence

$$\max_{\boldsymbol{\alpha},\boldsymbol{\beta}} \exp\left(\Psi_2(\boldsymbol{\alpha},\,\boldsymbol{\beta})/\Delta\right) \le \max_{\boldsymbol{\gamma},\boldsymbol{\delta}} \exp\left(\Psi_1^{\mathbf{B}\otimes\mathbf{B}}(\boldsymbol{\gamma},\,\boldsymbol{\delta})/\Delta\right) = \|\mathbf{B}\otimes\mathbf{B}\|_{\frac{\Delta}{\Delta-1}\to\Delta}.$$
 (14)

The key fact we now use is that for induced norms $\|\cdot\|_{p\to q}$ with $p \leq q$, it holds (cf., Bennett [1977, Proposition 10.1]) that

$$\|\mathbf{B} \otimes \mathbf{B}\|_{p \to q} = \|\mathbf{B}\|_{p \to q} \|\mathbf{B}\|_{p \to q}.$$
(15)

Therefore,

$$\max_{\boldsymbol{\alpha},\boldsymbol{\beta}} \Psi_{2}(\boldsymbol{\alpha},\boldsymbol{\beta}) \leq 2\Delta \log \|\mathbf{B}\|_{\frac{\Delta}{\Delta-1} \to \Delta} = 2 \max_{\boldsymbol{\alpha},\boldsymbol{\beta}} \Psi_{1}(\boldsymbol{\alpha},\boldsymbol{\beta}).$$
(16)

To complete the proof of Theorem 1.4, it just remains to prove the reverse inequality, which follows from the fact that $\mathbf{E}[X^2] \ge \mathbf{E}[X]^2$. \Box

3.4. Optimal Second Moment Configuration

We will need more detailed information about the γ , δ which achieve equality in Theorem 1.4 and Eq. (12). The following lemma is true whenever **B** is nonsingular (and hence for antiferromagnetic models as well, cf. Definition 1.3). Roughly, the lemma captures that the major contribution to the second moment comes from pairs of configurations which are uncorrelated. This is crucial to calculate the asymptotics of the second moment in Appendix B.

LEMMA 3.2. Assume that **B** is nonsingular. The γ , δ for which the equality in

$$\max_{\boldsymbol{\alpha},\boldsymbol{\beta}} \max_{\boldsymbol{\gamma},\boldsymbol{\delta}} \max_{\text{satisfying (13)}} \Psi_1^{\mathbf{B}\otimes\mathbf{B}}(\boldsymbol{\gamma},\boldsymbol{\delta}) = 2 \max_{\boldsymbol{\alpha},\boldsymbol{\beta}} \Psi_1^{\mathbf{B}}(\boldsymbol{\alpha},\boldsymbol{\beta}), \tag{17}$$

is achieved satisfy (for all $i, j, k, l \in [q]$)

$$\gamma_{ik} = \alpha_i \alpha_k \quad and \quad \delta_{il} = \beta_i \beta_l. \tag{18}$$

PROOF. We will have to dig in to the proof of (15) and use (13). Bennett's proof of (15) is the following (our particular values are $q' = \Delta$ and $p = \Delta/(\Delta - 1)$), we will explain

shortly the derivation of the intermediate steps:

$$\begin{split} \|(\mathbf{B} \otimes \mathbf{B})\mathbf{r}\|_{q'} &= \left(\sum_{k} \sum_{i} \left|\sum_{j} B_{ij} \sum_{l} B_{kl} R_{jl}\right|^{q'}\right)^{1/q'} \\ &\leq \|\mathbf{B}\|_{p \to q'} \left(\sum_{k} \left(\sum_{j} \left|\sum_{l} B_{kl} R_{jl}\right|^{p}\right)^{q'/p}\right)^{1/q'} \\ &\leq \|\mathbf{B}\|_{p \to q'} \left(\sum_{j} \left(\sum_{k} \left|\sum_{l} B_{kl} R_{jl}\right|^{q'}\right)^{p/q'}\right)^{1/p} \\ &\leq \|\mathbf{B}\|_{p \to q'}^{2} \left(\sum_{j,l} R_{jl}^{p}\right)^{1/p}. \end{split}$$

Note that in the last inequality one uses $\|\mathbf{B} \mathbf{r}\|_{q'} \leq \|\mathbf{B}\|_{p \to q'} \|\mathbf{r}\|_p$, applied to the vectors $\mathbf{r}'_j := (R_{j1}, R_{j2}, \ldots, R_{jq})$, for $j = 1, \ldots, q$. Thus, if \mathbf{r} is a maximizer of

$$\max_{\mathbf{r}} \frac{\|(\mathbf{B} \otimes \mathbf{B})\mathbf{r}\|_{q'}}{\|\mathbf{r}\|_{p}},\tag{19}$$

then the vectors \mathbf{r}'_i are maximizers of

$$\max_{\mathbf{r}'} \frac{\|\mathbf{B}\,\mathbf{r}'\|_{q'}}{\|\mathbf{r}'\|_{p}}.$$
(20)

The same, by symmetry, applies to $\mathbf{r}_l' := (R_{1l}, R_{2l}, \dots, R_{ql})$, for $l = 1, \dots, q$.

The second inequality in Bennett's proof is Minkowski's inequality for the (q'/p)norm (note that q' > p) applied to the q vectors which are obtained from $\mathbf{Br}'_1, \ldots, \mathbf{Br}'_q$ by raising each of their entries to the pth power. The equality is achieved only if $\mathbf{Br}'_1, \ldots, \mathbf{Br}'_q$ generate a space of dimension one, and since \mathbf{B} is nonsingular we have also that $\mathbf{r}'_1, \ldots, \mathbf{r}'_q$ generate a space of dimension one. Hence, for a maximizer \mathbf{r} of (19) we have $\mathbf{r} = \mathbf{r}' \otimes \mathbf{r}''$, where \mathbf{r}' and \mathbf{r}'' are maximizers of (20). By Theorem 4.1 (Eq. (23)), we then have

$$\gamma_{ik} = \alpha'_i \alpha''_k \tag{21}$$

for the corresponding maximizers of $\Psi_1^{\mathbf{B}\otimes\mathbf{B}}(\boldsymbol{\gamma},\boldsymbol{\delta})$ and $\Psi_1^{\mathbf{B}}(\boldsymbol{\alpha},\boldsymbol{\beta})$. Equation (21) together with constraints

$$\sum_{i} \gamma_{ik} = \alpha_k \quad \text{and} \quad \sum_{k} \gamma_{ik} = \alpha_i,$$

from (13) imply $\gamma_{ik} = \alpha_i \alpha_k$ (since $\alpha_k = \sum_i \gamma_{ik} = \sum_i \alpha'_i \alpha''_k = \alpha''_k$ and similarly $\alpha_i = \alpha'_i$). The proof of $\delta_{jl} = \beta_j \beta_l$ is analogous. \Box

4. TREE RECURSIONS, FIRST MOMENT, AND MATRIX NORMS

The second moment results of the previous section will be used to establish that, with probability 1 - o(1) over the choice of a random Δ -regular bipartite graph, the Gibbs distribution has most of its mass on configurations whose spin frequencies on the two sides of the graph are (close to) dominant phases. To do this, it will be important to

examine dominant phases, that is, the maxima of $\Psi_1(\alpha, \beta)$ and, further, to characterize the local maxima. We will use this information to connect the functions Φ and Ψ_1 and thus prove Lemma 3.1 which was the critical component in the second moment analysis; in fact, Lemma 3.1 is an immediate corollary of the upcoming Theorem 4.1 which details further the connection between Φ and Ψ_1 .

For a spin system with interaction matrix **B**, the following recursions are relevant for the analysis of the critical points of Ψ_1 .

$$\hat{R}_i \propto \left(\sum_{j=1}^q B_{ij}C_j\right)^{\Delta-1}$$
 and $\hat{C}_j \propto \left(\sum_{i=1}^q B_{ij}R_j\right)^{\Delta-1}$. (22)

We refer to (22) as *tree recursions* since they emerge naturally in the analysis of spin systems on the infinite Δ -regular tree \mathbb{T}_{Δ} . More precisely, the fixpoints of the tree recursions correspond to semitranslation-invariant Gibbs measures on \mathbb{T}_{Δ} (fixpoints of (22) are those R_i 's and C_j 's such that $\hat{R}_i \propto R_i$ and $\hat{C}_j \propto C_j$, for all $i, j \in [q]$). The fixpoints of the tree recursions correspond to critical points of Ψ_1 , as was first observed in Mossel et al. [2009], see Section 4.1.2 for a derivation in our setting.

We prove the following result which connects tree recursions, the function Φ and the function Ψ_1 . Lemma 3.1 is a corollary of the following more general theorem.

THEOREM 4.1. There is a one-to-one correspondence between the fixpoints of the tree recursions and the critical points of Φ (both considered for $R_i \ge 0, C_j \ge 0$ in the projective space, that is, up to scaling by a constant).

The following transformation $(\mathbf{r}, \mathbf{c}) \mapsto (\boldsymbol{\alpha}, \boldsymbol{\beta})$ given by

$$\alpha_i = \frac{R_i^{\Delta/(\Delta-1)}}{\sum_i R_i^{\Delta/(\Delta-1)}} \quad and \quad \beta_j = \frac{C_j^{\Delta/(\Delta-1)}}{\sum_j C_j^{\Delta/(\Delta-1)}}$$
(23)

yields a one-to-one-to-one correspondence between the critical points of Φ and the critical points of Ψ_1 (in the region defined by $\alpha_i \ge 0$, $\beta_j \ge 0$, and $\sum_i \alpha_i = 1$, $\sum_j \beta_j = 1$).

Moreover, for the corresponding critical points (\mathbf{r}, \mathbf{c}) and (α, β) , one has

$$\Phi(\mathbf{r}, \mathbf{c}) = \Psi_1(\boldsymbol{\alpha}, \boldsymbol{\beta}). \tag{24}$$

Finally, for spin systems whose interaction matrix **B** is ergodic, the local maxima of Φ and Ψ_1 happen at the critical points (i.e., there are no local maxima on the boundary).

To argue that the Gibbs distribution places most of its mass on configurations whose spin frequencies are given by dominant phases, we need a more explicit handle on *local* maxima of Ψ_1 . The latter will also be crucial to analyze the global maxima of Ψ_1 for specific models of interest.

We connect local maxima of Ψ_1 to attractive fixpoints of the associated tree recursions. Specifically, we call a fixpoint x of a function f a Jacobian attractive fixpoint if the Jacobian of f at x has spectral radius less than 1. We say that a critical point α , β is a Hessian local maximum if the Hessian of Ψ_1 at α , β is negative definite (note this is a sufficient condition for α , β to be a local maximum).

We prove the following theorem in Section 4.2.

THEOREM 4.2. Jacobian attractive fixpoints of the tree recursions (22) (considered as a function $(R_1, \ldots, R_q, C_1, \ldots, C_q) \mapsto (\hat{R}_1, \ldots, \hat{R}_q, \hat{C}_1, \ldots, \hat{C}_q)$) correspond to Hessian local maxima of Ψ_1 .

Theorem 4.2 is important for analyzing the global maxima of Ψ_1 for colorings and antiferromagnetic Potts model (see Section 7). Moreover, it will be used to apply the small subgraph conditioning method (see Appendix A.2).

4.1. Connection between Φ and Ψ_1

In this section, we prove Theorem 4.1.

4.1.1. Preliminaries on Maximum-Entropy Distributions. Let α and β be nonnegative vectors in \mathbb{R}^q such that

$$\sum_{i} \alpha_{i} = 1 \quad \text{and} \quad \sum_{j} \beta_{j} = 1.$$
(25)

For α and β that satisfy (25), let

$$g(\alpha_1, \dots, \alpha_q, \beta_1, \dots, \beta_q) = \max \sum_{i=1}^q \sum_{j=1}^q x_{ij} (\ln(B_{ij}) - \ln x_{ij}),$$
 (26)

where the maximum is taken over nonnegative x_{ij} 's such that

$$\alpha_i = \sum_j x_{ij} \quad \text{and} \quad \beta_j = \sum_i x_{ij}.$$
(27)

LEMMA 4.3. The maximum of the right-hand-side of (26) is achieved at unique x_{ij} . The x_{ij} are given by

$$x_{ij} = B_{ij} R_i C_j, \tag{28}$$

where \mathbf{r} and \mathbf{c} satisfy

$$R_i \sum_{j=1}^q B_{ij} C_j = \alpha_i \quad and \quad C_j \sum_{i=1}^q B_{ij} R_i = \beta_j,$$
(29)

and

$$\sum_{j=1}^{q} B_{ij}C_j = 0 \implies R_i = 0;$$

$$\sum_{i=1}^{q} B_{ij}R_i = 0 \implies C_j = 0.$$
(30)

The value of g, in terms of R_i 's and C_j 's, is given by

$$g(\alpha_1, \dots, \alpha_q, \beta_1, \dots, \beta_q) = -\sum_{i=1}^q \sum_{j=1}^q B_{ij} R_i C_j \ln(R_i C_j).$$
 (31)

PROOF. From strict concavity of $-x \ln x$, it follows that the right-hand side of (26) has a unique critical point (if there were two critical points, then the segment between the points lies in the linear space defined by (27); the function has a zero derivative on both ends of the segment; and the second derivative of the function is negative on the segment; a contradiction).

Using the method of Lagrange multipliers, we obtain that the critical points of the right-hand side of (26) are x_{ij} given by (28) where R_i 's and C_j 's are solutions of (29). We can make any solution of (29) satisfy (30): if $\sum_{j=1}^{q} B_{ij}C_j = 0$, then set $R_i = 0$ (and

symmetrically, if $\sum_{i=1}^{q} B_{ij} R_i = 0$, then set $C_j = 0$). We now argue that this change does not violate (29). Suppose that, after the change for some $k \in [q]$, we have

$$R_k \sum_{j=1}^q B_{kj} C_j \neq \alpha_k.$$
(32)

Then i = k (since only R_i changed) and since $\sum_{j=1}^q B_{ij}C_j = 0$, we also have $\alpha_i = 0$, a contradiction (with (32)). Now suppose that, after the change for some $j \in [q]$, we have

$$C_j \sum_{k=1}^{q} B_{kj} R_k \neq \beta_j.$$
(33)

Then $B_{ij} > 0$ and $C_j > 0$ (otherwise, changing R_i would not violate (33)). This then implies $\sum_{j=1}^{q} B_{ij}C_j > B_{ij}C_j > 0$, a contradiction. Thus, the change does not violate (29). Equation (31) is obtained by substituting (29) into (26). \Box

Remark 4.4. Scaling all the R_i 's up by the same factor while scaling all the C_j 's down by the same factor preserves (28) and (29). Modulo such scaling the R_i 's and C_j 's are unique, since the x_{ij} 's are unique and (28) determines the R_i 's and C_j 's once one value (say R_1) is fixed (here we use the fact that the matrix of the model is ergodic).

Remark 4.5. Note that the condition (25) translates (using (29)) into the following condition on R_i 's and C_j 's

$$\sum_{i=1}^{q} \sum_{j=1}^{q} B_{ij} R_i C_j = 1.$$
(34)

Our goal now is to see how the value of (26) changes when we perturb α_i 's and β_j 's. We are going to view them as functions of a new variable *z*. All differentiation in this section will be with respect to *z*. Note that, to stay in the subspace defined by (25), we should have, in particular,

$$\sum_{i} \alpha'_{i} = \sum_{i} \alpha''_{i} = 0 \quad \text{and} \quad \sum_{j} \beta'_{j} = \sum_{j} \beta''_{j} = 0.$$
(35)

Differentiating (29), we obtain

$$\sum_{j=1}^{q} B_{ij}(R_i C_j)' = \alpha_i' \quad \text{and} \quad \sum_{i=1}^{q} B_{ij}(R_i C_j)' = \beta_j'.$$
(36)

The following ratio of (29) and (36) will be useful later:

$$\frac{\alpha'_i}{\alpha_i} = \frac{R'_i}{R_i} + \frac{\sum_{j=1}^q B_{ij} C'_j}{\sum_{j=1}^q B_{ij} C_j} \quad \text{and} \quad \frac{\beta'_j}{\beta_j} = \frac{C'_j}{C_j} + \frac{\sum_{i=1}^q B_{ij} R'_i}{\sum_{i=1}^q B_{ij} R_i}.$$
(37)

Scaling all the R_i 's up by the same factor while scaling all the C_j 's down by the same factor (also discussed in Remark 4.4) is equivalent to increasing all R'_i/R_i 's by the same (additive) amount and decreasing all C'_i/C_i by the same (additive) amount. We are going to remove this freedom by requiring

$$\sum_{i=1}^{q} \alpha_i \frac{R'_i}{R_i} = \sum_{j=1}^{q} \beta_j \frac{C'_j}{C_j}.$$
(38)

(Recall that we study the effect of perturbing g when we change α_i 's and β_j 's; Equation (38) just fixes the corresponding change in R_i 's and C_j 's.)

Now we compute the derivatives of *g*.

LEMMA 4.6. We have

$$g' = -\sum_{i=1}^{q} (\ln R_i) \alpha'_i - \sum_{j=1}^{q} (\ln C_j) \beta'_j,$$
(39)

$$g'' = -\sum_{i=1}^{q} \frac{R'_i}{R_i} \alpha'_i - \sum_{j=1}^{q} \frac{C'_j}{C_j} \beta'_j - \sum_{i=1}^{q} (\ln R_i) \alpha''_i - \sum_{j=1}^{q} (\ln C_j) \beta''_j.$$
(40)

PROOF. Using $(f \ln f)' = (1 + \ln f)f'$ and Eq. (31), (35), and (36), we obtain

$$g' = -\sum_{i=1}^{q} \sum_{j=1}^{q} B_{ij} (1 + \ln(R_i C_j)) (R_i C_j)' = -\sum_{i=1}^{q} (\ln R_i) \alpha'_i - \sum_j (\ln C_j) \beta'_j.$$

Differentiating (39), we obtain (40). \Box

Note the expressions (39) and (40) are independent of the choice of scaling of R_i 's and C_j 's (this follows from (35)). The particular tying of R'_i/R_i 's and C'_j/C_j 's to α'_i and β'_j (given by (38)) will be useful later.

4.1.2. Critical Points of Ψ_1 and the Tree Recursions. In this section, we establish the connection between the critical points of Ψ_1 and the fixpoints of the tree recursions.

LEMMA 4.7. Let α , β be a critical point of $\Psi_1(\alpha, \beta)$ in the subspace defined by (25). Let \mathbf{r}, \mathbf{c} be given by (29). Then

$$\alpha_i \propto R_i^{\Delta/(\Delta-1)} \quad and \quad \beta_j \propto C_j^{\Delta/(\Delta-1)}.$$
(41)

Consequently, \mathbf{r}, \mathbf{c} satisfy the tree recursions stated in Section 4:

$$R_i \propto \left(\sum_{j=1}^q B_{ij}C_j\right)^{\Delta-1}$$
 and $C_j \propto \left(\sum_{i=1}^q B_{ij}R_i\right)^{\Delta-1}$. (22)

PROOF. At the critical points of Ψ_1 , the first derivative of Ψ_1 has to vanish for all α'_i 's and β'_i 's from the subspace defined by (35), that is,

$$\Psi_{1}' = (\Delta - 1) \left(\sum_{i=1}^{q} (1 + \ln \alpha_{i}) \alpha_{i}' + \sum_{j=1}^{q} (1 + \ln \beta_{j}) \beta_{j}' \right) - \Delta \left(\sum_{i=1}^{q} (\ln R_{i}) \alpha_{i}' + \sum_{j=1}^{q} (\ln C_{j}) \beta_{j}' \right)$$
$$= \sum_{i=1}^{q} ((\Delta - 1)(1 + \ln \alpha_{i}) - \Delta \ln R_{i}) \alpha_{i}' + \sum_{j=1}^{q} ((\Delta - 1)(1 + \ln \beta_{j}) - \Delta \ln C_{j}) \beta_{j}' = 0, \quad (42)$$

where the R_i 's and C_j 's are given by (29). Inspecting (42), we see that $(\Delta - 1)(1 + \ln \alpha_i) - \Delta \ln R_i$ have the same value. Indeed, if two of them, say with indices i_1, i_2 , had different values, then we could increase α_{i_1} and decrease α_{i_2} by the same infinitesimal amount and violate (42). Similarly, $(\Delta - 1)(1 + \ln \beta_j) - \Delta C_j$ have the same value and hence we have (41). Plugging (41) into (29) one obtains (22). \Box

LEMMA 4.8. Let (\mathbf{r}, \mathbf{c}) be a solution of the tree recursions (22). Let $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ be given by (23). Then, $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ is a critical point of $\Psi_1(\boldsymbol{\alpha}, \boldsymbol{\beta})$ in the subspace defined by (25).

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PROOF. Let

$$Z_R := (\Delta - 1)(1 + \ln \alpha_i) - \Delta \ln R_i = (\Delta - 1) \left(1 - \ln \sum_{i=1}^q R_i^{\Delta/(\Delta - 1)} \right),$$

where the second equality follows from (23). Note that Z_R is independent of the choice of *i*. Similarly, let

$$Z_C := (\Delta - 1)(1 + \ln \beta_j) - \Delta \ln C_j = (\Delta - 1) \left(1 - \ln \sum_{j=1}^q C_j^{\Delta/(\Delta - 1)} \right).$$

For perturbations of α , β in the subspace given by (25), we have

$$\begin{split} \Psi_1'(\boldsymbol{\alpha},\boldsymbol{\beta}) &= \sum_{i=1}^q \left((\Delta - 1)(1 + \ln \alpha_i) - \Delta \ln R_i \right) \alpha_i' + \sum_{j=1}^q ((\Delta - 1)(1 + \ln \beta_j) - \Delta \ln C_j) \beta_j' \\ &= Z_R \sum_{i=1}^q \alpha_i' + Z_C \sum_{j=1}^q \beta_j' = 0, \end{split}$$

and hence (α, β) is a critical point. \Box

4.1.3. Value of Ψ_1 at the Critical Points

LEMMA 4.9. Let (α, β) be critical point of $\Psi_1(\alpha, \beta)$. Let (\mathbf{r}, \mathbf{c}) be given by (23). Then

$$\Phi(\mathbf{r}, \mathbf{c}) = \Psi_1(\boldsymbol{\alpha}, \boldsymbol{\beta}). \tag{24}$$

Moreover, (\mathbf{r}, \mathbf{c}) *is a critical point of* $\Phi(\mathbf{r}, \mathbf{c})$ *.*

PROOF. From Eq. (8) and (31), we have

$$\Psi_1(\boldsymbol{\alpha},\boldsymbol{\beta}) = (\Delta - 1) \left(\sum_{i=1}^q \alpha_i \ln \alpha_i + \sum_{j=1}^q \beta_j \ln \beta_j \right) - \Delta \sum_{i=1}^q \sum_{j=1}^q B_{ij} R_i C_j \ln(R_i C_j).$$
(43)

where the R_i , C_j in (43) are given by (29). At the critical points α , β of Ψ_1 , in addition to (29), it also holds that (see Eq. (41))

$$\alpha_{i} = \frac{R_{i}^{\Delta/(\Delta-1)}}{\sum_{i=1}^{q} R_{i}^{\Delta/(\Delta-1)}} \quad \text{and} \quad \beta_{j} = \frac{C_{j}^{\Delta/(\Delta-1)}}{\sum_{j=1}^{q} C_{j}^{\Delta/(\Delta-1)}}.$$
(44)

Plugging (29) into (43), we obtain

$$\Psi_{1}(\boldsymbol{\alpha},\boldsymbol{\beta}) = (\Delta - 1) \left(\sum_{i=1}^{q} \alpha_{i} \ln \alpha_{i} + \sum_{j=1}^{q} \beta_{j} \ln \beta_{j} \right) - \Delta \left(\sum_{i=1}^{q} \alpha_{i} \ln R_{i} + \sum_{j=1}^{q} \beta_{j} \ln C_{j} \right)$$
$$= \sum_{i=1}^{q} \alpha_{i} \ln \frac{\alpha_{i}^{\Delta - 1}}{R_{i}^{\Delta}} + \sum_{j=1}^{q} \beta_{j} \ln \frac{\beta_{j}^{\Delta - 1}}{C_{j}^{\Delta}} = -(\Delta - 1) \left[\ln \left(\sum_{i=1}^{q} R_{i}^{\Delta / (\Delta - 1)} \right) + \ln \left(\sum_{j=1}^{q} C_{j}^{\Delta / (\Delta - 1)} \right) \right],$$
(45)

where, in the last equality, we used (44) and the fact that α_i 's and β_j 's sum to 1. Recall that

$$\sum_{i=1}^{q} \sum_{j=1}^{q} B_{ij} R_i C_j = \sum_{i=1}^{q} \alpha_i = 1,$$
(46)

and hence the following is obtained by adding zero to the right-hand side of (45):

$$\Psi_{1}(\boldsymbol{\alpha},\boldsymbol{\beta}) = \Delta \ln \left(\sum_{i=1}^{q} \sum_{j=1}^{q} B_{ij} R_{i} C_{j} \right) - (\Delta - 1) \left[\ln \left(\sum_{i=1}^{q} R_{i}^{\Delta/(\Delta - 1)} \right) + \ln \left(\sum_{j=1}^{q} C_{j}^{\Delta/(\Delta - 1)} \right) \right]$$

= $\Phi(\mathbf{r}, \mathbf{c}).$

Now we argue that (\mathbf{r}, \mathbf{c}) is a critical point of $\Phi(\mathbf{r}, \mathbf{c})$. We have

$$\frac{\partial}{\partial R_i} \Phi(\mathbf{r}, \mathbf{c}) = \Delta \frac{\sum_{j=1}^q B_{ij} C_j}{\sum_{i=1}^q \sum_{j=1}^q B_{ij} R_i C_j} - (\Delta - 1) \frac{\frac{\Delta}{\Delta - 1} R_i^{1/(\Delta - 1)}}{\sum_{i=1}^q R_i^{\Delta/(\Delta - 1)}} = \Delta \frac{\alpha_i}{R_i} - \Delta \frac{\alpha_i}{R_i} = 0, \quad (47)$$

where we used (44), (25), and (29). The same argument yields

$$\frac{\partial}{\partial C_j} \Phi(\mathbf{r}, \mathbf{c}) = \Delta \frac{\sum_{i=1}^q B_{ij} R_i}{\sum_{i=1}^q \sum_{j=1}^q B_{ij} R_i C_j} - (\Delta - 1) \frac{\frac{\Delta}{\Delta - 1} C_j^{1/(\Delta - 1)}}{\sum_{j=1}^q C_j^{\Delta/(\Delta - 1)}} = 0.$$
(48)

and hence \mathbf{r}, \mathbf{c} is a critical point of Φ . \Box

LEMMA 4.10. Let (\mathbf{r}, \mathbf{c}) be a critical point of $\Phi(\mathbf{r}, \mathbf{c})$. Let $\boldsymbol{\alpha}, \boldsymbol{\beta}$ be given by (23). Then $\boldsymbol{\alpha}, \boldsymbol{\beta}$ is a critical point of $\Psi_1(\boldsymbol{\alpha}, \boldsymbol{\beta})$ in the subspace defined by (25).

PROOF. At a critical point of Φ , we have that (47) is zero for $i \in [q]$. Note that the denominators do not depend on i and hence we have

$$R_i^{1/(\Delta-1)} \propto \sum_{j=1}^q B_{ij} C_j.$$

Similarly, from (48), we obtain

$$C_j^{1/(\Delta-1)} \propto \sum_{i=1}^q B_{ij} R_i.$$

Hence, (\mathbf{r}, \mathbf{c}) satisfy the tree recursions. Now, we use Lemma 4.8 to conclude that (α, β) is a critical point of $\Psi_1(\alpha, \beta)$ in the subspace defined by (25). \Box

4.1.4. Local Maxima of Ψ_1 are in the Interior. In this section, we show that, for models with ergodic (irreducible and aperiodic) interaction matrix **B**, the maximum of $\Phi(\mathbf{r}, \mathbf{c})$ is achieved in the interior. A symmetric matrix is irreducible if the graph whose edges correspond to nonzero edges of **B** is connected. A symmetric matrix is aperiodic if the graph whose edges correspond to nonzero edges of **B** has an odd cycle.

LEMMA 4.11. Assume that **B** is ergodic. Let $(\mathbf{r}, \mathbf{c}) \neq 0$ be a local maximum of Φ in the region $\mathbf{r}, \mathbf{c} \geq 0$. Then, $R_i > 0$ for all $i \in [q]$ and $C_j > 0$ for all $j \in [q]$.

PROOF. Suppose not, that is, we have a maximum that has a zero on some coordinate of **r** or **c**. From the ergodicity of **B**, we have that there exist $i, j \in [q]$ such that (i) $R_i = 0, C_j > 0$, and $B_{ij} > 0$ or (ii) $R_i > 0, C_j = 0$, and $B_{ij} > 0$. (To see this, suppose that, for all i, j, neither (i) nor (ii) happens. Let $Z_R \subseteq [q]$ be the set of i such that $R_i = 0$ and, similarly, let $Z_C \subseteq [q]$ be the set of j such that $C_j = 0$. By the assumption that neither (i) nor (ii) happens, the only entries B_{ij} which can be nonzero must satisfy either $i \in Z_R$, $j \in Z_C$ or $i \in [q] \setminus Z_R$, $j \in [q] \setminus Z_C$. Using that **B** is symmetric, we obtain that in \mathbf{B}^2 the only nonzero $(B^2)_{ij}$ must satisfy either $i, j \in Z_R$ or $i, j \in [q] \setminus Z_R$. Thus, \mathbf{B}^2 is reducible and hence not ergodic, from where it follows that **B** is not ergodic, contradiction.) Without loss of generality assume that it is the case (i), case (ii) can be handled analogously.

The derivative of Φ with respect to R_i is (we are using $R_i = 0$)

$$rac{\partial}{\partial R_i} \Phi(\mathbf{r},\mathbf{c}) = \Delta rac{\sum_{j=1}^q B_{ij}C_j}{\sum_{i=1}^q \sum_{j=1}^q B_{ij}R_iC_j} > \Delta rac{B_{ij}C_j}{\sum_{i=1}^q \sum_{j=1}^q B_{ij}R_iC_j} > 0,$$

and hence we are not at a maximum, a contradiction. \Box

LEMMA 4.12. Assume that **B** is ergodic. Let α , $\beta \ge 0$ be a local maximum of $\Psi_1(\alpha, \beta)$ in the subspace defined by (25). Then, $\alpha_i > 0$ for all $i \in [q]$ and $\beta_j > 0$ for all $j \in [q]$.

PROOF. It will be useful to view Ψ_1 as a function of (\mathbf{r}, \mathbf{c}) , where \mathbf{r}, \mathbf{c} are given by (29). Because of Lemma 4.3, we have (\mathbf{r}, \mathbf{c}) satisfying (46) and (30) (and any such (\mathbf{r}, \mathbf{c}) yields $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ satisfying (25)). We have (from (43))

$$\Psi_1(\boldsymbol{\alpha},\boldsymbol{\beta}) = \sum_{i=1}^q \sum_{j=1}^q B_{ij} R_i C_j \left((\Delta - 1) \left(\ln \left(\sum_{j=1}^q B_{ij} C_j \right) + \ln \left(\sum_{i=1}^q B_{ij} R_i \right) \right) - \ln R_i - \ln C_j \right)$$

=: $\hat{\Psi}_1(\mathbf{r}, \mathbf{c}).$

If **r** or **c** has a zero coordinate, then, by ergodicity of **B**, there exists $k, \ell \in [q]$ such that (i) $R_k = 0, C_\ell > 0$, and $B_{k\ell} > 0$ or (ii) $R_k > 0, C_\ell = 0$, and $B_{k\ell} > 0$ (see the argument in the proof of Lemma 4.11). Without loss of generality, it is the case (i).

Note that we have

$$\frac{\partial}{\partial R_k} \sum_{i=1}^q \sum_{j=1}^q B_{ij} R_i C_j = \sum_{j=1}^q B_{kj} C_j \ge B_{k\ell} C_\ell > 0.$$

$$\tag{49}$$

We have

$$\frac{\partial}{\partial R_k} \hat{\Psi}_1 = \sum_{j=1}^q B_{kj} C_j \left((\Delta - 1) \ln \left(\sum_{i=1}^q B_{ij} R_i \right) - \ln C_j \right) \\ + \left((\Delta - 1) \ln \left(\sum_{j=1}^q B_{kj} C_j \right) - \ln R_k \right) \left(\sum_{j=1}^q B_{kj} C_j \right) + (\Delta - 2) \sum_{j=1}^q B_{kj} C_j.$$
(50)

The first sum in (50) is finite since if $C_j > 0$, then $\sum_{i=1}^q B_{ij}R_i > 0$, (using (30)); if $C_j = 0$, then the contribution of the term to the sum is zero (we are using the usual convention $0 \ln 0 = 0$). The second term in (50) has value $+\infty$ since $\ln R_k = -\infty$ and (49). Finally, the last term in (50) is finite and hence we have $\frac{\partial}{\partial R_k}\hat{\Psi}_1 = +\infty$.

Recall that $C_{\ell} > 0$ and hence (using (30)):

$$\frac{\partial}{\partial C_{\ell}} \sum_{i=1}^{q} \sum_{j=1}^{q} B_{ij} R_i C_j = \sum_{i=1}^{q} B_{i\ell} R_i > 0.$$
(51)

Finally, we argue that $\frac{\partial}{\partial C_{\ell}}\hat{\Psi}_1$ is finite. We have (analogously to (50))

$$\frac{\partial}{\partial C_{\ell}} \hat{\Psi}_{1} = \sum_{i=1}^{q} B_{i\ell} R_{i} \left((\Delta - 1) \ln \left(\sum_{j=1}^{q} B_{ij} C_{j} \right) - \ln R_{i} \right) + \left((\Delta - 1) \ln \left(\sum_{i=1}^{q} B_{i\ell} R_{i} \right) - \ln C_{\ell} \right) \left(\sum_{i=1}^{q} B_{i\ell} R_{i} \right) + (\Delta - 2) \sum_{i=1}^{q} B_{i\ell} R_{i}.$$
(52)

The first and third term in (52) are finite by the same argument as for (50). In the second term, we use (51) and $C_{\ell} > 0$.

Now we increase R_k by an infinitesimal amount and change C_ℓ to maintain (34) (and hence (25)). (This is possible because both C_ℓ and R_k change the value of (34), see Eqs. (49) and (51).) This change will increase Ψ_1 and hence Ψ_1 contradicting the local maximality of α , β . \Box

4.1.5. Proof of Theorem 4.1

PROOF OF THEOREM 4.1. Lemmas 4.7 and 4.8 give the connection between the critical points of Ψ_1 and the fixpoints of the tree recursions. Lemmas 4.9 and 4.10 give connection between the critical points of Ψ_1 and Φ and show that the values agree on the corresponding critical points. Finally, Lemmas 4.11 and 4.12 show that the maxima happen in the interior (that is, for $R_i > 0$, $C_j > 0$ in the case of Φ and for $\alpha_i > 0$, $\beta_j > 0$ in the case of Ψ_1). \Box

4.2. Connecting Local Maxima and Stability of Tree Recursions

In this section, we prove Theorem 4.2.

4.2.1. Maximum Entropy Configurations on Random \triangle -Regular Bipartite Graphs. We analyze the critical points by looking at the second derivative. Using $(f \ln f)'' = (f')^2/f + (1 + \ln f)f''$ we have

$$\begin{split} \Psi_{1}^{\prime\prime}(\boldsymbol{\alpha},\boldsymbol{\beta}) &= (\Delta-1)\sum_{i=1}^{q} \left((\alpha_{i}^{\prime})^{2}/\alpha_{i} + (1+\ln\alpha_{i})\alpha_{i}^{\prime\prime} \right) - \Delta\sum_{i=1}^{q} \left(\alpha_{i}^{\prime}\frac{R_{i}^{\prime}}{R_{i}} + (\ln R_{i})\alpha_{i}^{\prime\prime} \right) \\ &+ (\Delta-1)\sum_{j=1}^{q} \left((\beta_{j}^{\prime})^{2}/\beta_{j} + (1+\ln\beta_{j})\beta_{j}^{\prime\prime} \right) - \Delta\sum_{j=1}^{q} \left(\beta_{j}^{\prime}\frac{C_{j}^{\prime}}{C_{j}} + (\ln C_{j})\beta_{j}^{\prime\prime} \right) \\ &= (\Delta-1)\sum_{i=1}^{q} (\alpha_{i}^{\prime})^{2}/\alpha_{i} - \Delta\sum_{i=1}^{q} \alpha_{i}^{\prime}\frac{R_{i}^{\prime}}{R_{i}} + \sum_{i=1}^{q} \alpha_{i}^{\prime\prime}((\Delta-1)(1+\ln\alpha_{i}) - \Delta\ln R_{i}) \\ &+ (\Delta-1)\sum_{j=1}^{q} (\beta_{j}^{\prime})^{2}/\beta_{j} - \Delta\sum_{j=1}^{q} \beta_{j}^{\prime}\frac{C_{j}^{\prime}}{C_{j}} + \sum_{j=1}^{q} \beta_{j}^{\prime\prime}((\Delta-1)(1+\ln\beta_{j}) - \Delta\ln C_{j}) \\ &= (\Delta-1)\sum_{i=1}^{q} (\alpha_{i}^{\prime})^{2}/\alpha_{i} - \Delta\sum_{i=1}^{q} \alpha_{i}^{\prime}\frac{R_{i}^{\prime}}{R_{i}} + (\Delta-1)\sum_{j=1}^{q} (\beta_{j}^{\prime})^{2}/\beta_{j} - \Delta\sum_{j=1}^{q} \beta_{j}^{\prime}\frac{C_{j}^{\prime}}{C_{j}}, \end{split}$$

where the last equality follows from (42) (replacing α'_i by α''_i and β'_j by β''_j ; note that they are both from the same subspace (35)).

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Plugging (37) into (53) we obtain

$$\Psi_{1}^{\prime\prime}(\boldsymbol{\alpha},\boldsymbol{\beta}) = \sum_{i=1}^{q} \alpha_{i}^{\prime} \left((\Delta - 1) \frac{\sum_{j=1}^{q} B_{ij} C_{j}^{\prime}}{\sum_{j=1}^{q} B_{ij} C_{j}} - \frac{R_{i}^{\prime}}{R_{i}} \right) + \sum_{j=1}^{q} \beta_{j}^{\prime} \left((\Delta - 1) \frac{\sum_{i=1}^{q} B_{ij} R_{i}^{\prime}}{\sum_{i=1}^{q} B_{ij} R_{i}} - \frac{C_{j}^{\prime}}{C_{j}} \right).$$
(54)

We are going to use the second partial derivative test (which gives a sufficient condition) to establish maxima of Ψ_1 . We will use the following terminology for local maxima established using this method.

Definition 4.13. A critical point x of a function $f : \mathcal{M} \to \mathbb{R}$ is called *Hessian local* maximum if the Hessian of f at x is negative definite.

Let **L** be the (matrix of the) linear map $(r_1, \ldots, r_q, c_1, \ldots, c_q) \mapsto (\hat{r}_1, \ldots, \hat{r}_q, \hat{c}_1, \ldots, \hat{c}_q)$ given by

$$\hat{r}_i = \sum_j \frac{B_{ij} R_i C_j}{\sqrt{\alpha_i \beta_j}} c_j \quad \text{and} \quad \hat{c}_j = \sum_i \frac{B_{ij} R_i C_j}{\sqrt{\alpha_i \beta_j}} r_i.$$
(55)

In the following, we denote by **I** the identity matrix of dimension $2q \times 2q$.

LEMMA 4.14. A critical point $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ is a Hessian local maximum of $\Psi_1(\boldsymbol{\alpha}, \boldsymbol{\beta})$ in the subspace defined by (35) if and only if $\mathbf{w}^{\mathsf{T}}(\mathbf{I} + \mathbf{L})((\Delta - 1)\mathbf{L} - \mathbf{I})\mathbf{w} < 0$ for all $\mathbf{w} = (r_1, \ldots, r_q, c_1, \ldots, c_q)^{\mathsf{T}}$ such that

$$\sum_{i=1}^{q} \sqrt{\alpha_i} r_i = 0 \quad and \quad \sum_{j=1}^{q} \sqrt{\beta_j} c_j = 0.$$
(56)

PROOF. To check whether we are at a Hessian local maximum of $\Psi_1(\alpha, \beta)$, we have to have (54) negative for nonzero α'_i 's and β'_j 's from the subspace defined by (35) and (38). Let $r_i = \sqrt{\alpha_i} R'_i / R_i$ and $c_j = \sqrt{\beta_j} C'_j / C_j$. Using (37) in (54), we have

$$\begin{split} \Psi_1'' &= \sum_i \alpha_i \bigg(\frac{R_i'}{R_i} + \frac{\sum_j B_{ij} C_j'}{\sum_j B_{ij} C_j} \bigg) \bigg((\Delta - 1) \frac{\sum_j B_{ij} C_j'}{\sum_j B_{ij} C_j} - \frac{R_i'}{R_i} \bigg) \\ &+ \sum_j \beta_j \bigg(\frac{C_j'}{C_j} + \frac{\sum_i B_{ij} R_i'}{\sum_i B_{ij} R_i} \bigg) \bigg((\Delta - 1) \frac{\sum_i B_{ij} R_i'}{\sum_i B_{ij} R_i} - \frac{C_j'}{C_j} \bigg) \\ &= \sum_i \bigg(r_i + \sum_j \frac{B_{ij} R_i C_j}{\sqrt{\alpha_i \beta_j}} c_j \bigg) \bigg(\sum_j (\Delta - 1) \frac{B_{ij} R_i C_j}{\sqrt{\alpha_i \beta_j}} c_j - r_i \bigg) \\ &+ \sum_j \bigg(c_j + \sum_i \frac{B_{ij} R_i C_j}{\sqrt{\alpha_i \beta_j}} r_i \bigg) \bigg(\sum_i (\Delta - 1) \frac{B_{ij} R_i C_j}{\sqrt{\alpha_i \beta_j}} r_i - c_j \bigg), \end{split}$$

where the second equality follows by using (29) to substitute the expressions $\sum_j B_{ij}C_j$ and $\sum_i B_{ij}R_i$. Let $\mathbf{w} = (r_1, \ldots, r_q, c_1, \ldots, c_q)^{\intercal}$. In terms of **L** and **w** (recall that **L** is a symmetric 2 × 2 block matrix with zero blocks on the diagonal), we have

$$\Psi_1'' = \mathbf{w}^{\mathsf{T}} (\mathbf{I} + \mathbf{L}) ((\Delta - 1)\mathbf{L} - \mathbf{I}) \mathbf{w}.$$
(57)

We have to examine when (57) is in the subspace defined by (35) and (38), which in terms of r_i 's and c_j 's become

$$\sum_{i} \alpha'_{i} = \sum_{j} \beta'_{j} = \sum_{i} \sqrt{\alpha_{i}} r_{i} + \sum_{j} \sqrt{\beta_{j}} c_{j} = 0,$$
(58)

$$\sum_{i} \alpha_i \frac{R'_i}{R_i} - \sum_{j} \beta_j \frac{C'_j}{C_j} = \sum_{i} \sqrt{\alpha_i} r_i - \sum_{j} \sqrt{\beta_j} c_j = 0.$$
(59)

We give more detail on the derivation of (58). We have

$$\sum_{i} \alpha'_{i} = \sum_{i} \alpha_{i} \frac{\alpha'_{i}}{\alpha_{i}} = \sum_{i} \alpha_{i} \left(\frac{R'_{i}}{R_{i}} + \frac{\sum_{j} B_{ij}C'_{j}}{\sum_{j} B_{ij}C_{j}} \right) = \sum_{i} r_{i} \sqrt{\alpha_{i}} + \sum_{i} \sum_{j} B_{ij}R_{i}C'_{j}$$
$$= \sum_{i} r_{i} \sqrt{\alpha_{i}} + \sum_{j} \frac{c_{j}}{\sqrt{\beta_{j}}} \sum_{i} B_{ij}R_{i}C_{j} = \sum_{i} r_{i} \sqrt{\alpha_{i}} + \sum_{j} c_{j} \sqrt{\beta_{j}},$$

the derivation for $\sum_j \beta'_j$ is analogous (or, alternatively, use (35) to argue directly that $\sum_j \beta'_j = \sum_i \alpha'_i$). \Box

4.2.2. Attractive Fixpoints of Tree Recursions. The variables R_i , C_j , α_i , β_j in this section refer to a priori different quantities as the variables in Section 4.2.1. We feel that this conflict is justified since we will establish that they coincide.

For convenience we repeat the tree recursions as stated in the introduction:

$$\hat{R}_i \propto \left(\sum_{j=1}^q B_{ij}C_j\right)^{\Delta-1}$$
 and $\hat{C}_j \propto \left(\sum_{i=1}^q B_{ij}R_j\right)^{\Delta-1}$. (22)

We are interested in the *fixpoints* of the tree recursions, that is, R_i 's and C_j 's such that

$$\hat{R}_i \propto R_i$$
 and $\hat{C}_j \propto C_j$

for all $i, j \in [q]$. Note that the fixpoints correspond to the critical points of Ψ_1 (using Theorem 4.1)).

Next we examine the stability of fixpoints. For a continuously differentiable map a sufficient condition for a fixpoint to be attractive is if the spectral radius of the derivative is less than one at the fixpoint. We will use the following terminology for fixpoints whose attractiveness is established using this method.

Definition 4.15. A fixpoint x of a function $f : \mathcal{M} \to \mathcal{M}$ is called *jacobian attractive fixpoint* if the Jacobian of f at x has spectral radius less than 1.

LEMMA 4.16. Let (\mathbf{r}, \mathbf{c}) be a fixpoint of the tree recursions. Let $\alpha_i = \sum_{j=1}^q B_{ij}R_iC_j$ and $\beta_j = \sum_{i=1}^q B_{ij}R_iC_j$ and let \mathbf{L} be the (matrix of the) map defined by (55). We have that (\mathbf{r}, \mathbf{c}) is Jacobian attractive if and only if $(\Delta - 1)\mathbf{L}$ has spectral radius less than 1 in the subspace of $\mathbf{w} = (r_1, \ldots, r_q, c_1, \ldots, c_q)$ that satisfies

$$\sum_{i=1}^{q} \sqrt{\alpha_i} r_i = 0 \quad and \quad \sum_{j=1}^{q} \sqrt{\beta_j} c_j = 0.$$
(56)

PROOF. Without loss of generality, we can assume that (\mathbf{r}, \mathbf{c}) is scaled so that

$$\sum_{i=1}^{q} \sum_{j=1}^{q} B_{ij} R_i C_j = 1.$$
(60)

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Note that the scaling does not affect the value of L nor does it affect the constraint (56).

When we perturb the R_i 's and C_j 's and apply one step of the tree recursion, we obtain

$$\frac{\hat{R}'_{i}}{\hat{R}_{i}} = (\Delta - 1) \frac{\sum_{j=1}^{q} B_{ij} C_{j} \frac{C_{j}}{C_{j}}}{\sum_{j=1}^{q} B_{ij} C_{j}} \quad \text{and} \quad \frac{\hat{C}'_{j}}{\hat{C}_{j}} = (\Delta - 1) \frac{\sum_{i=1}^{q} B_{ij} R_{i} \frac{R'_{i}}{R_{i}}}{\sum_{i=1}^{q} B_{ij} R_{i}}.$$
(61)

We can rewrite (61) as follows

$$\frac{\hat{R}'_{i}}{\hat{R}_{i}} = (\Delta - 1) \frac{\sum_{j=1}^{q} B_{ij} R_{i} C_{j} \frac{C_{j}}{C_{j}}}{\alpha_{i}} \quad \text{and} \quad \frac{\hat{C}'_{j}}{\hat{C}_{j}} = (\Delta - 1) \frac{\sum_{i=1}^{q} B_{ij} R_{i} C_{j} \frac{R'_{i}}{R_{i}}}{\beta_{j}}.$$
(62)

Note that Eq. (22) is invariant under scaling all the R_i 's by the same factor. Similarly scaling all C_j 's by the same factor does not change (22). We need to exclude this scaling freedom when studying the local stability of (61). More precisely, we will locate an invariant subspace of (62) whose complement corresponds to the scaling. We obtain the following subspace (it corresponds to preserving (60)):

$$\sum_{i=1}^{q} \alpha_i \frac{R'_i}{R_i} = 0 \quad \text{and} \quad \sum_{j=1}^{q} \beta_j \frac{C'_j}{C_j} = 0.$$
(63)

Now we check that (63) is invariant under the map (62), indeed,

$$\sum_{i=1}^{q} \alpha_i \frac{\hat{R}'_i}{\hat{R}_i} = (\Delta - 1) \sum_{i=1}^{q} \sum_{j=1}^{q} B_{ij} R_i C_j \frac{C'_j}{C_j} = (\Delta - 1) \sum_{j=1}^{q} \beta_j \frac{C'_j}{C_j} = 0;$$
(64)

the argument for $\sum_{j=1}^{q} \beta_j \frac{\hat{C}'_j}{\hat{C}_j} = 0$ is analogous.

The linear map (given by (61))

$$\left(\frac{R'_1}{R_1}, \dots, \frac{R'_q}{R_q}, \frac{C'_1}{C_1}, \dots, \frac{C'_q}{C_q}\right) \mapsto \left(\frac{\hat{R}'_1}{\hat{R}_1}, \dots, \frac{\hat{R}'_q}{\hat{R}_q}, \frac{\hat{C}'_1}{\hat{C}_1}, \dots, \frac{\hat{C}'_q}{\hat{C}_q}\right)$$
(65)

considered in the subspace defined by (63) is the linear map of the Jacobian of (22) at $(R_1, \ldots, R_q, C_1, \ldots, C_q)$ (in the projective space). A fixpoint $(R_1, \ldots, R_q, C_1, \ldots, C_q)$ of (22) is Jacobian attractive if the linear map (65) has spectral radius less than 1.

Let $r_i = \sqrt{\alpha_i} \hat{R}'_i / \hat{R}_i$, $c_j = \sqrt{\beta_j} \hat{C}'_j / \hat{C}_j$, $\hat{r}_i = \sqrt{\alpha_i} \hat{R}'_i / \hat{R}_i$, and $\hat{c}_j = \sqrt{\beta_j} \hat{C}'_j / \hat{C}_j$. This linear transformation of variables turns (62) into

$$\hat{r}_i = (\Delta - 1) \sum_{j=1}^q \frac{B_{ij} R_i C_j}{\sqrt{\alpha_i \beta_j}} c_j \quad \text{and} \quad \hat{c}_j = (\Delta - 1) \sum_{i=1}^q \frac{B_{ij} R_i C_j}{\sqrt{\alpha_i \beta_j}} r_i.$$
(66)

Note that (66) is $(\Delta - 1)L$ where L is the map defined by (55). The constraint (63) becomes (56). \Box

4.2.3. Connecting Attractive Fixpoints to Maximum Entropy Configurations. Now we are ready to prove Theorem 4.2.

PROOF OF THEOREM 4.2. Let S be the linear subspace defined by (56) (note that (58) together with (59) define the same subspace). The constraint for the fixpoint to be Jacobian attractive is that $(\Delta - 1)\mathbf{L}$ on S has spectral radius less than 1. The constraint for the critical point to be Hessian maximum is that the eigenvalues of $(\mathbf{I} + \mathbf{L})((\Delta - 1)\mathbf{L} - \mathbf{I})$ on S are negative (see Eq. (57)).

Note that **L** is a symmetric 2×2 block matrix (each of the blocks has dimension $q \times q$) with zero blocks on the diagonal. From this, we conclude³ that **L** has symmetric real spectrum (symmetry means that if $a \neq 0$ is an eigenvalue then so is -a by the same multiplicity). Note that *S* is invariant under **L** and hence the spectrum of **L** on *S* is a subset of the spectrum of **L** (it is still symmetric real; the restriction wiped out a pair of eigenvalues -1 and 1).

The constraint for the fixpoint to be Jacobian attractive, in terms of eigenvalues, is: for each eigenvalue x of **L** on *S*

$$-1 < (\Delta - 1)x < 1.$$
(67)

The constraint for the critical point to be Hessian maximum, in terms of eigenvalues, is: for each eigenvalue x of **L** on S

$$(1+x)((\Delta-1)x-1) < 0$$
 and $(1-x)(-(\Delta-1)x-1) < 0$, (68)

where the second constraint comes from the symmetry of the spectrum (thus -x is an eigenvalue). Note that conditions (67) and (68) are equivalent (since $(1+x)((\Delta - 1)x - 1)$ is negative for $-1 < x < 1/(\Delta - 1)$). \Box

5. REDUCTION FOR COLORINGS

In this section, we outline our proof of Theorem 1.1. We start by reviewing the main components of the reduction for 2-spin systems (as carried out in Sly [2010] and Sly and Sun [2012]) and in particular the hard-core model. This will allow us to isolate the parts of the argument which do not extend to the multispin case and motivate our reduction scheme. The first step is a reduction from max-cut to a so-called phase labeling problem that we introduce. To present the main ideas of this particular key reduction, we first present it in this section in the simplified setting of the colorings problem (see Lemma 5.1).

We begin by reviewing the reduction for the hard-core model. The basic gadget in the reduction is a bipartite random graph, which we denote by G. The sides of the bipartition have an equal number of vertices, and the sides are labeled with + and -. Most vertices in G have degree Δ but there is also a small number of degree $\Delta - 1$ vertices (to allow to make connections between gadgets without creating degree $\Delta + 1$ vertices). For $s = \{+, -\}$, let the vertices in the *s*-side be $U^s \cup W^s$ where the vertices in $U = U^+ \cup U^-$ have degree Δ and the vertices in $W = W^+ \cup W^-$ have degree $\Delta - 1$. The phase of an independent set I is + (respectively -) if I has more vertices in U^+ (respectively U^-). Note that the phase depends only on the spins of the "large" portion of the graph, that is, the spins of vertices in U.

In nonuniqueness regimes, the gadget G has two important properties (both of which can be obtained by building on the second moment analysis of Section 3). First, the phase of a random independent set I is equal to + or - with probability roughly equal to 1/2. Second, conditioned on the phase of a random independent set I, the spins of the vertices in W are approximately independent, that is, the marginal distribution on W is close to a product distribution. In this product distribution if the phase is +(respectively -), a vertex in W^+ is in I with probability p^+ (respectively p^-), while a vertex in W^- is in I with probability p^- (respectively p^+). The values p^{\pm} correspond

³Write $\mathbf{L} = \begin{bmatrix} \mathbf{0} & \mathbf{M} \\ \mathbf{0} & \mathbf{V} \end{bmatrix}$ where \mathbf{M} is a $q \times q$ matrix. Let $a \neq 0$ be an eigenvalue of \mathbf{L} with corresponding eigenvector \mathbf{v} . Note that \mathbf{v} has dimension 2q. Let $\mathbf{v}_1, \mathbf{v}_2$ be the q-dimensional vectors obtained by the first q and the last q coordinates of \mathbf{v} , respectively. It holds that $\mathbf{M}\mathbf{v}_2 = a\mathbf{v}_1$ and $\mathbf{M}^{\mathsf{T}}\mathbf{v}_1 = a\mathbf{v}_2$. Let \mathbf{v}' be the (2q)-dimensional vector whose first q coordinates are given by the coordinates of $-\mathbf{v}_1$ and the last q coordinates are given by the coordinates of $-\mathbf{v}_1$ and the last q coordinates are given by the coordinates of $-\mathbf{v}_1$ and the last q coordinates are given by the coordinates of \mathbf{v}_2 . Note that \mathbf{v}' is an eigenvector of \mathbf{L} with corresponding eigenvalue -a. Finally, observe that the map $\mathbf{v} \mapsto \mathbf{v}'$ as defined here preserves the linear independence of the eigenvectors corresponding to a (this is relevant if a has multiplicity greater than 1).

to maxima of the function Ψ_1 and, crucially (as we shall demonstrate shortly), they satisfy $p^+ \neq p^-$.

The conditional independence property is important in that it allows to quantify the effect of using vertices of W as terminals to make connections between copies of the gadget G. For example, consider the following type of connection, which we refer to as parallel. Let $v^+ \in W^+$, $v^- \in W^-$ and consider two copies of the gadget G, say G_1, G_2 . For i = 1, 2, denote by v_i^+, v_i^- the copies of v^+, v^- in G_i , respectively. Now add the edges (v_1^+, v_2^+) and (v_1^-, v_2^-) and denote the final graph by G_{12} . Thus, a parallel connection corresponds to joining the +, + and -, - sides of two copies of the gadget.

Random independent sets of G_{12} can be sampled from the hard-core measure by first sampling random independent sets I_1, I_2 from the hard-core measure of G_1, G_2 respectively and keeping $I_1 \cup I_2$ if it is a valid independent set in G_{12} . We thus have that the partition function of G_{12} is equal to $(Z_G)^2$ times the probability that v_1^{\pm}, v_2^{\pm} are not simultaneously in the independent set $I_1 \cup I_2$. The latter quantity can easily be computed if we condition on the phases of the independent sets I_1, I_2 in G_1, G_2 respectively. In particular, if the phases agree the desired quantity is given by $(1 - (p^+)^2)(1 - (p^-)^2)$, otherwise by $(1 - p^+p^-)^2$.

Crucially, since $p^+ \neq p^-$, observe that under a parallel connection neighboring gadgets prefer to have different phases, that is,

$$(1 - (p^+)^2)(1 - (p^-)^2) < (1 - p^+p^-)^2.$$
(69)

As we shall describe next, this property together with the fact that there are exactly two phases suffices to show hardness (i.e., using only parallel connections between gadgets in the reduction). In particular, assume that H is an instance of MAX-CUT and replace each vertex in H by a copy of the gadget G. Then, for each edge of H, connect the respective gadgets in parallel. The partition function of the final graph is dominated from phase assignments which correspond to large cuts in H. This intuition is the basis of the reduction in Sly [2010] and Sly and Sun [2012].

We now switch to the k-colorings model and describe the most significant obstacles for carrying out the previous reduction. First, let us describe the properties of the gadget G (defined identically as before). Using the second moment analysis of Section 3 and in particular Theorem 1.4, we can analyze the phases of a random coloring of Gin the semitranslation nonuniqueness regime (the precise statement of the gadget's properties are given in Lemma 6.9). The main difference from the hard-core model is that now the number of phases is much greater than two (equal to the number of maximizers of the function Ψ_1 , see Theorem 1.6). In particular, for k even, the phase of a coloring is determined by the dominant set of k/2 colors on U^+ , that is, the k/2colors with largest frequencies among vertices of U^+ . Each of the $\binom{k}{k/2}$ phases appears with roughly equal probability and given the phase, the marginal distribution on W is close to a product distribution, which we now describe. We can compute explicit values $a' = a'(k, \Delta), b' = b'(k, \Delta)$ such that for a phase $T \in \binom{[k]}{k/2}$ the probability mass function \mathbf{x} of a vertex in W^+ has its *i*th entry equal to a' if $i \in T$ and equal to b' if $i \notin T$. Similarly, the probability mass function \mathbf{y} of a vertex in W^- has its *i*th entry equal to b' if $i \in T$ and equal to a' if $i \notin T$. (The values a', b' correspond to the values a, b described in Item 2 of Theorem 1.6, the correspondence is obtained using (23) in Theorem 4.1.⁴)

Let Q be the union of the pairs (\mathbf{x}, \mathbf{y}) over all dominant phases. Hereafter, we will identify the phases with elements of Q. Note that if $(\mathbf{x}, \mathbf{y}) \in Q$, then $(\mathbf{y}, \mathbf{x}) \in Q$ as well. We also denote by Q' the union of unordered elements of Q. Elements of Q' are called

⁴In particular, a', b' can be readily obtained from a, b using the relations $a = a'^{\Delta/\Delta - 1}/S$, $b = a'^{\Delta/\Delta - 1}/S$, $\frac{q}{2}(a' + b') = 1$, where $S := \frac{q}{2}(a'^{\Delta/\Delta - 1} + b'^{\Delta/\Delta - 1})$.

unordered phases (we use **p** to denote unordered phases). Given a phase $\mathbf{p} = {\mathbf{x}, \mathbf{y}}$ an ordering of the pair will be called "assigning spin to the phase". The two ordered phases corresponding to the unordered phase **p** will be denoted by \mathbf{p}^+ and \mathbf{p}^- .

In our reduction, we will again use parallel connections between disjoint copies of the gadget (though we will need later to also consider other types of connections). Recall that the graph G_{12} is obtained by adding a parallel connection between two disjoint copies of G and that the edges (v_1^+, v_2^+) and (v_1^-, v_2^-) realize the connection between the + sides and - sides of the gadgets, respectively. We next quantify the effect of a parallel connection, and here we will use the conditional independence of vertices in $W^+ \cup W^-$ (conditioned on the phase). To do this, observe that random colorings of G_{12} can be generated by first generating random colorings of G_1 , G_2 and keeping the resulting coloring if v_1^{\pm}, v_2^{\pm} have different colors. We thus have that the partition function of G_{12} is equal to $(Z_G)^2$ times the probability that v_1^{\pm}, v_2^{\pm} have different colors in random colorings of G_1, G_2 . The latter quantity can easily be computed if we condition on the phases $(\mathbf{x}_1, \mathbf{y}_1), (\mathbf{x}_2, \mathbf{y}_2)$ of the colorings in G_1, G_2 , and is equal to $(1 - \mathbf{x}_1^{\dagger}\mathbf{x}_2)(1 - \mathbf{y}_1^{\dagger}\mathbf{y}_2)$.

By taking logarithms, we can assume a parallel connection between gadgets with phases $(\mathbf{x}_1, \mathbf{y}_1)$ and $(\mathbf{x}_2, \mathbf{y}_2)$ incurs an (additive) weight

$$w_p((\mathbf{x}_1, \mathbf{y}_1), (\mathbf{x}_2, \mathbf{y}_2)) = \ln\left(1 - \mathbf{x}_1^{\mathsf{T}} \mathbf{x}_2\right) + \ln\left(1 - \mathbf{y}_1^{\mathsf{T}} \mathbf{y}_2\right)$$

Let $\mathbf{p} = {\mathbf{x}, \mathbf{y}} \in \mathcal{Q}'$ be an arbitrary unordered phase and recall that (in the nonuniqueness regime) we have $\mathbf{x} \neq \mathbf{y}$. Using this, the forthcoming Lemma 6.3 shows (in a more general setting) that the weight function $w_p(\cdot, \cdot)$ satisfies

$$w_p(\mathbf{p}^+, \mathbf{p}^+) = w_p(\mathbf{p}^-, \mathbf{p}^-) < w_p(\mathbf{p}^+, \mathbf{p}^-).$$
 (70)

(We encountered an instance of (70) in the earlier discussion for the hard-core model, see (69).) Intuitively, (70) says that for two gadgets connected in parallel and which are assigned the same unordered phase \mathbf{p} , the optimal "spin" (or ordering) assignment is to give the gadgets opposite assignments \mathbf{p}^+ , \mathbf{p}^- (or vice versa).

For the colorings model, simply using parallel connections to reduce from MAX-CUT no longer suffices. A short calculation shows that the optimal configuration for a triangle of gadgets connected in parallel is to give all three gadgets different phases. To bypass this entanglement, we need to introduce some sort of ferromagnetism in the reduction to enforce gadgets corresponding to vertices of *H* to use a single (unordered) phase. To achieve this, we use *symmetric* connections, which correspond to having not only (+, +), (-, -) connections of the gadgets, but also (+, -) and (-, +). Thus, a symmetric connection whose endpoints have phases $(\mathbf{x}_1, \mathbf{y}_1), (\mathbf{x}_2, \mathbf{y}_2)$ incurs (additive) weight

$$w_s((\mathbf{x}_1, \mathbf{y}_1), (\mathbf{x}_2, \mathbf{y}_2)) = w_p((\mathbf{x}_1, \mathbf{y}_1), (\mathbf{x}_2, \mathbf{y}_2)) + w_p((\mathbf{x}_1, \mathbf{y}_1), (\mathbf{y}_2, \mathbf{x}_2)).$$

Symmetric connections will allow us to enforce a single unordered phase to all gadgets, while parallel connections will allow us to recover a maximum-cut partition. To have some modularity in our construction, rather than reducing from MAX-CUT directly, we use the following "phase labeling problem".

COLORINGS PHASE LABELING PROBLEM(\mathbf{B}, \mathcal{Q})

INPUT: undirected edge-weighted multigraph H = (V, E) and a partition of the edges $\{E_p, E_s\}$.

OUTPUT: MAXLWT(H) := max_{\mathcal{Y}} LWT_H(\mathcal{Y}), where the maximization is over all possible phase labelings $\mathcal{Y} : V \to \mathcal{Q}$ and

$$\operatorname{Lwr}_{H}(\mathcal{Y}) := \sum_{\{u,v\}\in E_{s}} w_{s}(\mathcal{Y}(u), \mathcal{Y}(v)) + \sum_{\{u,v\}\in E_{p}} w_{p}(\mathcal{Y}(u), \mathcal{Y}(v)).$$

Edges in E_p (respectively E_s) correspond to parallel (respectively symmetric) connections and we shall refer to them as parallel (respectively symmetric) edges. The arguments in Sly and Sun [2012], which we sketched earlier, can easily be adapted to show that an algorithm for approximating the partition function to an arbitrarily small exponential factor yields a PTAS for the phase labeling problem, see Lemma 6.1 and its proof in Section 6.4. It then remains to prove that a PTAS for the phase labeling problem yields a PTAS for MAX-CUT on 3-regular graphs. This is the scope of the next lemma, which we focus on proving in the remainder of this section.

LEMMA 5.1. A (randomized) algorithm that approximates the solution to the Color-INGS PHASE LABELING PROBLEM(**B**, Q) on bounded degree graphs within a factor of 1 - o(1)yields a (randomized) algorithm that approximates MAXCUT on 3-regular graphs within a factor of 1 - o(1).

Our reduction relies on the following construction of a gadget (Lemma 5.2) which "prefers" the unordered phase of two distinguished vertices u and v to agree. The key idea is that for the complete graph on |Q'| vertices (recall that |Q'| is the number of unordered phases) and whose edges are all symmetric, the optimal phase assignment is to give each vertex a distinct unordered phase (note that, in this graph, the "spins" of the phases do not matter since all of its edges are symmetric). Now, consider the complete graph on |Q'| + 1 vertices, all of whose edges are symmetric, where one edge, say (u, v), is removed. Vertices u, v now "prefer" to have the same unordered phase, that is, the optimal phase assignment in the resulting graph is to give u, v the same unordered phase \mathbf{p} and the remaining vertices a distinct unordered phase from $Q' \setminus \{\mathbf{p}\}$. (A modification of this gadget will also work for general antiferromagnetic \mathbf{B} .)

We will use the following notation: for a phase assignment \mathcal{Y} with *ordered* phases, we denote by \mathcal{Y}' the respective phase assignment with *unordered* phases.

LEMMA 5.2. A constant sized gadget J_1 with two distinguished vertices u, v can be constructed with the following property: all edges of J_1 are symmetric and the following is true:

$$\max_{\mathcal{Y}; \mathcal{Y}'(u) = \mathcal{Y}'(v)} \operatorname{Lwr}_{J_{1}}(\mathcal{Y}) > \varepsilon_{1} + \max_{\mathcal{Y}; \mathcal{Y}'(u) \neq \mathcal{Y}'(v)} \operatorname{Lwr}_{J_{1}}(\mathcal{Y}),$$
(71)

where $\varepsilon_1 > 0$ is a constant depending only on k and Δ .

We give the proof of the critical Lemma 5.2 after the (simpler) proof of Lemma 5.1.

Proof of Lemma 5.1. Let ε_1 be as in Lemma 5.2 and

$$t := 2 \lceil (\max_{\mathbf{p}_1, \mathbf{p}_2} w_p(\mathbf{p}_1, \mathbf{p}_2) - \min_{\mathbf{p}_1, \mathbf{p}_2} w_p(\mathbf{p}_1, \mathbf{p}_2)) / \varepsilon_1 \rceil.$$

Given a 3-regular instance H = (V, E) of Max-Cut, we first declare all edges of H to be parallel. Moreover, for every edge (u', v') of H, take t copies of gadget J_1 from Lemma 5.2, identify (merge) their u vertices with u', and identify (merge) their v vertices with v'. Let H' be the final graph.

To find the optimal phase labeling of H', we may focus on the phase assignment restricted to vertices in H, since each gadget J_1 can be independently set to its optimal value conditioned on the phases for its distinguished vertices u and v. We claim that

$$MaxLwT(H') = C_1 MaxCUT(H) + (C_2 + C_3 t)|E|,$$
(72)

for constants C_1, C_2, C_3 to be specified later (depending only on k, Δ). Using the bound $MaxCut(H) \ge |E|/2 = 3|V|/4$, the lemma follows easily from (72). We thus focus on proving (72).

The key idea is that for any phase labeling $\mathcal{Y} : V \to \mathcal{Q}$, changing the unordered phases of vertices in H to the same unordered phase $\mathbf{p} \in \mathcal{Q}'$, while keeping the spins, can only increase the weight of the labeling. Indeed, for $(u, v) \in E$ such that $\mathcal{Y}'(u) = \mathcal{Y}'(v)$, no change in the weight of the labeling occurs by the symmetry of the phases. For $(u, v) \in E$ such that $\mathcal{Y}'(u) \neq \mathcal{Y}'(v)$, the potential (weight) loss from the parallel edge (u, v) is compensated by the gain on the t copies of J_1 by (71) and the choice of t.

For phase labelings which assign vertices of H the same unordered phase \mathbf{p} (but perhaps different spins), to attain the maximum weight for a phase labeling, we only need to choose the spins, in order to maximize the contribution from parallel edges (the edges of H). By the same argument we discussed for the hard-core model, (70) yields that the optimal choice of spins to the phases induces a maximum-cut partition of H. For such a spin assignment, the contribution from parallel edges is $C_1 \text{MaxCut}(H) + C_2 |E|$, where

$$C_1 := w_p(\mathbf{p}^+, \mathbf{p}^-) - w_p(\mathbf{p}^-, \mathbf{p}^-) \text{ and } C_2 := w_p(\mathbf{p}^-, \mathbf{p}^-).$$

The contribution from symmetric edges is $C_3t|E|$, where

$$C_3 \coloneqq \max_{\mathcal{Y}; \mathcal{Y}'(u) = \mathcal{Y}'(v) = \mathbf{p}} \operatorname{Lwt}_{J_1}(\mathcal{Y}).$$

This proves (72). \Box

We conclude this section by giving the proof of Lemma 5.2.

PROOF OF LEMMA 5.2. Let $Q' := \{\mathbf{p}_1, \ldots, \mathbf{p}_Q\}$ be the collection of all unordered phases and set $\mathbf{p}_i := \{\mathbf{x}_i, \mathbf{y}_i\}$ for $i \in [Q']$. Denote by K the multigraph on Q' vertices b_1, b_2, \ldots, b_Q' with the following symmetric edges: self-loop on b_i for $i \in [Q]$ and two edges between b_i and b_j for every $i, j \in [Q]$ with $i \neq j$. We first prove that the optimal phase assignments \mathcal{Y} of K are those which assign each vertex b_i a distinct phase from Q' (note that the spins of the phases do not matter since all edges of K are symmetric). The desired gadget J_1 will be constructed afterwards.

Let \mathcal{Y} be a phase labeling of K and s_i be the number of vertices assigned phase \mathbf{p}_i . Denote by \mathbf{s} the vector $(s_1, \ldots, s_Q)^{\intercal}$. Note that $\mathbf{1}^{\intercal}\mathbf{s} = Q'$, where $\mathbf{1}$ is the all one vector with dimension Q'. Then

$$\operatorname{Lwt}_{K}(\mathcal{Y}) = \sum_{i,j \in [Q]} s_{i} s_{j} w_{s}(\mathbf{p}_{i}, \mathbf{p}_{j}) = \mathbf{s}^{\mathsf{T}} \mathbf{A} \mathbf{s},$$

where **A** is the $Q \times Q$ matrix whose (i, j) entry equals $w_s(\mathbf{p}_i, \mathbf{p}_j)$. Note that **A** is symmetric and **1** is an eigenvector of **A** (because of the transitive symmetry of phases). Moreover, if we let $\mathbf{s}' = \mathbf{s} - \mathbf{1}$, then $\mathbf{1}^{\mathsf{T}}\mathbf{s}' = 0$. It follows that

$$\mathbf{s}^{\mathsf{T}}\mathbf{A}\mathbf{s} = \mathbf{1}^{\mathsf{T}}\mathbf{A}\mathbf{1} + (\mathbf{s}')^{\mathsf{T}}\mathbf{A}\mathbf{s}'.$$
(73)

If **A** is negative definite, Eq. (73) shows that the all ones labeling, that is, $\mathbf{s} = \mathbf{1}$, is (strictly) better than any other labeling. Hence, the result will follow if we prove that **A** is negative definite.

Let $\mathbf{z}_1, \ldots, \mathbf{z}_Q := \mathbf{x}_1, \ldots, \mathbf{x}_Q, \mathbf{y}_1, \ldots, \mathbf{y}_Q$ and let $\hat{\mathbf{A}}$ be the $Q \times Q$ matrix whose *ij*-entry is $\ln(1 - \mathbf{z}_i^{\mathsf{T}} \mathbf{z}_j)$. Using the definition of the weights $w_s(\cdot, \cdot)$, it is easy to check that for any vector \mathbf{s} it holds that

$$\mathbf{s}^{\mathsf{T}}\mathbf{A}\mathbf{s} = (\mathbf{s}, \mathbf{s})^{\mathsf{T}}\hat{\mathbf{A}}(\mathbf{s}, \mathbf{s}),$$

so it suffices to prove that $\hat{\mathbf{A}}$ is negative definite. We will show here that $\hat{\mathbf{A}}$ is negative semi-definite; the proof that $\hat{\mathbf{A}}$ is nonsingular (and hence negative definite) is trickier and is given in the proof of the more general Lemma 6.5. Note that the entries of $\hat{\mathbf{A}}$

are obtained by applying $z \mapsto \ln(1-z)$ to each entry of the Gram matrix of the vectors $\mathbf{z}_1, \ldots, \mathbf{z}_Q$. Since, for |z| < 1, we have $\ln(1-z) = -z - z^2/2 - z^3/3 - \cdots$, by Schur's product theorem (see Corollary 7.5.9 in Horn and Johnson [2013]) we obtain that $\hat{\mathbf{A}}$ is negative semidefinite, as desired.

To construct the gadget J_1 , we overlay two copies of K as follows. Let K_u (respectively K_v) be a copy of K, where the image of b_Q is renamed to u (respectively v). Overlay K_u , K_v by identifying the images of b_1, \ldots, b_{Q-1} in the two copies. Thus, the resulting graph J_1 has two self loops on b_i for $i \in [Q-1]$, four edges between b_i and b_j for every $i, j \in [Q-1]$ with $i \neq j$, two edges between u and b_i for $i \in [Q-1]$, two edges between v and b_i for $i \in [Q'-1]$ and a self loop on u, v.

Note that, for every phase labeling \mathcal{Y} of J_1 , we have $\operatorname{Lwt}_{J_1}(\mathcal{Y}) = \operatorname{Lwt}_{K_u}(\mathcal{Y}) + \operatorname{Lwt}_{K_v}(\mathcal{Y})$ and hence $\operatorname{MaxLwt}(J_1) \leq 2\operatorname{MaxLwt}(K)$. Using that the optimal phase labelings for K are those which assign each vertex a distinct phase from \mathcal{Q}' , we obtain that the inequality holds at equality for those (and only those) phase labelings which assign u, v a common phase $\mathbf{p} \in \mathcal{Q}'$ and vertices b_1, \ldots, b_{Q-1} a distinct phase from $\mathcal{Q}' - \{\mathbf{p}\}$. This yields the ε_1 in the statement of the lemma. Note that ε_1 depends only on \mathcal{Q}' , which in turn is completely determined by k, Δ . \Box

6. GENERAL REDUCTION

6.1. Phase Labeling Problem

We first introduce the phase labeling problem for a general antiferromagnetic spin system (which satisfies the hypotheses of Theorem 1.5). As in the case for the colorings model (see Section 5), we let Q' be the union of $\{\mathbf{x}, \mathbf{y}\}$ over all dominant phases, that is,

$$\mathcal{Q}' = \{\{\mathbf{x}_1, \mathbf{y}_1\}, \ldots, \{\mathbf{x}_Q, \mathbf{y}_Q\}\}.$$

Henceforth, we will refer to elements of Q' as unordered phases. Note that for fixed q, Δ, \mathbf{B} the global maxima of Ψ_1 correspond to fixpoints of (22) and hence can be approximated to any desired polynomial accuracy of their values. The values of \mathbf{x}, \mathbf{y} may then be recovered using (23) (see Footnote 4 for an explicit description of the correspondence in the case of colorings). The assumption of Theorem 1.5 translates into $\mathbf{x}_i \neq \mathbf{y}_i$ for all $i \in [Q']$.

Given an unordered phase $\{x, y\}$ an ordering of the pair will be called "assigning spin to the phase". Let

$$\mathcal{Q} = \{(\mathbf{x}_1, \mathbf{y}_1), \dots, (\mathbf{x}_Q, \mathbf{y}_Q)\}$$

be the collection of ordered phases. Note that Q = 2Q'. We will denote unordered phases using **p**; the two ordered phases corresponding to the unordered phase **p** will be denoted by \mathbf{p}^+ and \mathbf{p}^- . Given a graph *H* with vertex set *V*, we will assign ordered phases to its vertices—the labeling (also called *phase assignment*) will be denoted by $\mathcal{Y}: V \to Q$. The corresponding labeling by *unordered* phases (where the ordering is removed) will be denoted by \mathcal{Y}' .

Now we define the weight of a phase assignment. We will have two types of edges in H: parallel or symmetric; the type of an edge will only impact the weight of a phase assignment. In particular, a parallel edge whose endpoints have labels $(\mathbf{x}_1, \mathbf{y}_1)$ and $(\mathbf{x}_2, \mathbf{y}_2)$ incurs weight

$$w_p((\mathbf{x}_1, \mathbf{y}_1), (\mathbf{x}_2, \mathbf{y}_2)) = \ln(\mathbf{x}_1^\mathsf{T} \mathbf{B} \mathbf{x}_2) + \ln(\mathbf{y}_1^\mathsf{T} \mathbf{B} \mathbf{y}_2),$$

while a symmetric edge incurs weight

$$w_s((\mathbf{x}_1, \mathbf{y}_1), (\mathbf{x}_2, \mathbf{y}_2)) = w_p((\mathbf{x}_1, \mathbf{y}_1), (\mathbf{x}_2, \mathbf{y}_2)) + w_p((\mathbf{x}_1, \mathbf{y}_1), (\mathbf{y}_2, \mathbf{x}_2)).$$

Note that if we flip $(\mathbf{x}_1, \mathbf{y}_1)$, that is, replace it by $(\mathbf{y}_1, \mathbf{x}_1)$, the weight of the symmetric edge does not change.

We will use the following problem in our reduction.

Phase Labeling Problem $(\mathbf{B}, \mathcal{Q})$

INPUT: undirected edge-weighted multigraph H = (V, E) and a partition of the edges $\{E_p, E_s\}$.

OUTPUT: MAXLWT(H) := max_{\mathcal{Y}} LWT_H(\mathcal{Y}), where the maximization is over all possible phase labelings $\mathcal{Y} : V \to \mathcal{Q}$ and

$$\mathrm{Lwt}_H(\mathcal{Y}) = \sum_{\{u,v\} \in E_s} w_s(\mathcal{Y}(u), \mathcal{Y}(v)) + \sum_{\{u,v\} \in E_p} w_p(\mathcal{Y}(u), \mathcal{Y}(v)).$$

The motivation for the PHASE LABELING PROBLEM is the following lemma. The proof roughly follows the lines of Sly and Sun [2012] and is given in Section 6.4.

LEMMA 6.1. In the setting of Theorem 1.5, the following holds. A (randomized) algorithm that approximates the partition function on triangle free Δ -regular graphs within an arbitrarily small exponential factor yields a (randomized) algorithm that approximates the solution to the Phase Labeling Problem with parameters **B**, Q on bounded degree graphs within a factor of 1 - o(1).

The following lemma requires more work in our setting and is proved in Section 6.3.

LEMMA 6.2. A (randomized) algorithm that approximates the solution to the phase labeling problem with parameters **B**, Q on bounded degree graphs within a factor of 1-o(1) yields a (randomized) algorithm that approximates MAXCUT on 3-regular graphs within a factor of 1-o(1).

Using Lemmas 6.1 and 6.2, we obtain Theorem 1.5.

PROOF OF THEOREM 1.5. Suppose that there exists a (randomized) algorithm to approximate the partition function on Δ -regular graphs with interaction matrix **B** up to an arbitrarily small exponential factor. Then, combinining Lemmas 6.1 and 6.2, we obtain a (randomized) algorithm to approximate MAXCUT on 3-regular graphs within a factor of 1 - o(1). This contradicts the result of Alimonti and Kann [1997]. \Box

6.2. Properties of Antiferromagnetic Spin Systems

In this section, we prove two basic properties of antiferromagnetic systems that will be used in our general reductions.

As a consequence of the Perron-Frobenius theorem and the antiferromagnetism definition (cf., Definition 1.3), we may decompose the interaction matrix \mathbf{B} of an antiferromagnetic model as

$$\mathbf{B} = \mathbf{u}\mathbf{u}^{\mathsf{T}} - \mathbf{P}^{\mathsf{T}}\mathbf{P},\tag{74}$$

where the vector **u** has positive entries and **P** is a square matrix. In (74), **u** corresponds to the Perron-Frobenius eigenvector of the matrix **B** and **P** is the Cholesky decomposition of $\mathbf{uu}^{\intercal} - \mathbf{B}$ (which is positive semidefinite by the assumption that **B** is antiferromagnetic). Using the decomposition (74), we prove the following two lemmas which are used in the reduction.

LEMMA 6.3. For antiferromagnetic **B**, and vectors $\mathbf{z}_1, \mathbf{z}_2 \in \mathbb{R}^q_{\geq 0}$ with $\|\mathbf{z}_1\|_1 = \|\mathbf{z}_2\|_1 = 1$, we have

$$(\mathbf{z}_1^{\mathsf{T}}\mathbf{B}\mathbf{z}_1)(\mathbf{z}_2^{\mathsf{T}}\mathbf{B}\mathbf{z}_2) \leq (\mathbf{z}_1^{\mathsf{T}}\mathbf{B}\mathbf{z}_2)^2.$$

Equality holds iff $\mathbf{z}_1 = \mathbf{z}_2$.

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PROOF. Set $\mathbf{w}_1 = \mathbf{P}\mathbf{z}_1$, $\mathbf{w}_2 = \mathbf{P}\mathbf{z}_2$, $a_1 = \mathbf{u}^{\mathsf{T}}\mathbf{z}_1$, $a_2 = \mathbf{u}^{\mathsf{T}}\mathbf{z}_2$. Then

$$\mathbf{z}_1^{\mathsf{T}}\mathbf{B}\mathbf{z}_1 = a_1^2 - \mathbf{w}_1^{\mathsf{T}}\mathbf{w}_1, \ \mathbf{z}_2^{\mathsf{T}}\mathbf{B}\mathbf{z}_2 = a_2^2 - \mathbf{w}_2^{\mathsf{T}}\mathbf{w}_2, \ \mathbf{z}_1^{\mathsf{T}}\mathbf{B}\mathbf{z}_2 = a_1a_2 - \mathbf{w}_1^{\mathsf{T}}\mathbf{w}_2.$$

Since **B**, \mathbf{z}_1 , \mathbf{z}_2 have nonnegative entries, these equalities imply $a_1^2 - \mathbf{w}_1^{\mathsf{T}} \mathbf{w}_1, a_2^2 - \mathbf{w}_2^{\mathsf{T}} \mathbf{w}_2, a_1 a_2 - \mathbf{w}_1^{\mathsf{T}} \mathbf{w}_2 \ge 0$. The inequality reduces to

$$(a_1^2 - \mathbf{w}_1^\intercal \mathbf{w}_1)(a_2^2 - \mathbf{w}_2^\intercal \mathbf{w}_2) \le (a_1 a_2 - \mathbf{w}_1^\intercal \mathbf{w}_2)^2.$$

This is known as Aczél's inequality. The fastest proof goes as follows: set $b_1^2 = a_1^2 - \mathbf{w}_1^{\mathsf{T}} \mathbf{w}_1$ and $b_2^2 = a_2^2 - \mathbf{w}_2^{\mathsf{T}} \mathbf{w}_2$, so that by Cauchy-Schwarz $a_1 a_2 \ge b_1 b_2 + \mathbf{w}_1^{\mathsf{T}} \mathbf{w}_2$, implying the inequality.

Equality can only hold if $a_1 = \lambda a_2$ and $\mathbf{w}_1 = \lambda \mathbf{w}_2$, yielding $\mathbf{u}^{\mathsf{T}}(\mathbf{z}_1 - \lambda \mathbf{z}_2) = 0$ and $\mathbf{P}(\mathbf{z}_1 - \lambda \mathbf{z}_2) = 0$. We easily obtain $\mathbf{B}(\mathbf{z}_1 - \lambda \mathbf{z}_2) = 0$ and since **B** is invertible, $\mathbf{z}_1 = \lambda \mathbf{z}_2$. The assumption $\|\mathbf{z}_1\|_1 = \|\mathbf{z}_2\|_1 = 1$ implies $\lambda = 1$, as wanted. \Box

COROLLARY 6.4. By plugging in the inequality of Lemma 6.3, the vectors with a single 1 in the positions i and j respectively, we obtain that any two spins i, j induce an antiferromagnetic two-spin system.

LEMMA 6.5. Let $\mathbf{z}_1, \ldots, \mathbf{z}_n \in \mathbb{R}^q$ be a collection of distinct nonnegative vectors such that $\|\mathbf{z}_i\|_1 = 1$ for $i \in [n]$. Let $a_i = \mathbf{z}_i^{\mathsf{T}} \mathbf{u}$, where \mathbf{u} is as in (74). Let \mathbf{A}' be the $n \times n$ matrix whose ijth entry is $\ln(\mathbf{z}_i^{\mathsf{T}} \mathbf{B} \mathbf{z}_j) - \ln(a_i) - \ln(a_j)$. Then \mathbf{A}' is negative definite.

PROOF. Let $\mathbf{w}_i = \frac{1}{a_i} \mathbf{P} \mathbf{z}_i$ and let \mathbf{W} be the $q \times n$ matrix whose columns are $\mathbf{w}_1, \ldots, \mathbf{w}_n$. We first argue $\mathbf{w}_i \neq \mathbf{w}_j$ for $i \neq j$. Suppose $\mathbf{w}_i = \mathbf{w}_j$. Let $\mathbf{z} = \frac{1}{a_i} \mathbf{z}_i - \frac{1}{a_j} \mathbf{z}_j$. We have $\mathbf{P} \mathbf{z} = \mathbf{w}_i - \mathbf{w}_j = 0$ and $\mathbf{u}^{\mathsf{T}} \mathbf{z} = 1 - 1 = 0$ and hence $\mathbf{B} \mathbf{z} = 0$. Since \mathbf{B} is nonsingular, we have $\mathbf{z} = 0$. Thus, $0 = \mathbf{z}^{\mathsf{T}} \mathbf{1} = \frac{1}{a_i} - \frac{1}{a_j}$ which implies $a_i = a_j$ which in turn implies $\mathbf{z}_i = \mathbf{z}_j$, a contradiction. Thus, $\mathbf{w}_i \neq \mathbf{w}_j$ for $i \neq j$.

Note that we have

$$\ln\left(1-\mathbf{w}_{i}^{\mathsf{T}}\mathbf{w}_{j}\right)=\ln\left(a_{i}a_{j}-\mathbf{z}_{i}^{\mathsf{T}}\mathbf{P}^{\mathsf{T}}\mathbf{P}\mathbf{z}_{j}\right)-\ln(a_{i}a_{j})=A_{ij}^{\prime}.$$

Thus the *ij*th entry in \mathbf{A}' is obtained by applying $z \mapsto \ln(1-z)$ to each entry of the Gramm matrix $\mathbf{W}^{\mathsf{T}}\mathbf{W}$. Note that for |z| < 1 we have $\ln(1-z) = -z - z^2/2 - z^3/3 - \cdots$ and hence by Schur product theorem \mathbf{A}' is negative semidefinite (see Corollary 7.5.9 in Horn and Johnson [2013]).

Now we argue that \mathbf{A}' is nonsingular (and hence negative definite). We have

$$-\mathbf{A}' = \sum_{k=1}^{\infty} \frac{1}{k} \mathbf{W}_k^{\mathsf{T}} \mathbf{W}_k, \tag{75}$$

where \mathbf{W}_k is the $q^k \times n$ matrix whose columns are $w_1^{\otimes k}, \ldots, w_n^{\otimes k}$. Note that if \mathbf{A}' is singular then there exists a nonzero vector v such that $\mathbf{v}^{\dagger}\mathbf{A}'\mathbf{v} = 0$ and for this to happen, we would have to have

$$\mathbf{W}_k \mathbf{v} = 0 \tag{76}$$

for all $k \ge 1$ (the terms on the right-hand side of (75) are nonnegative and if even one of them is positive then $\mathbf{v}^{\mathsf{T}} \mathbf{A}' \mathbf{v} < 0$).

There exists a vector $\mathbf{r} \in \mathbb{R}^q$ such that $\alpha_i = \mathbf{r}^{\mathsf{T}} \mathbf{w}_i, i = 1, \ldots, n$ are distinct real numbers (the \mathbf{w}_i 's are distinct and hence for any $i \neq j$ the measure of $r \in [0, 1]^q$ such that $\mathbf{r}^{\mathsf{T}} \mathbf{w}_i = \mathbf{r}^{\mathsf{T}} \mathbf{w}_j$ is zero). Note that $(\mathbf{r}^{\otimes k})^{\mathsf{T}} \mathbf{W}_k$ is $(\alpha_1^k, \ldots, \alpha_n^k)$. From (76) we obtain that for every integer $k \geq 1$ we have $(\alpha_1^k, \ldots, \alpha_n^k)\mathbf{v} = 0$ and hence $\mathbf{v} = 0$ (by considering the Vandermonde matrix $\{\alpha_i^k\}$), a contradiction. Hence \mathbf{A}' is nonsingular and negative definite. \Box

6.3. Reducing MaxCut to Phase Labeling

In this section, we prove Lemma 6.2.

6.3.1. An Intermediate Gadget. We will use the following gadget which, among the set of all ordered phase assignments, "prefers" the unordered phase of two vertices to agree.

LEMMA 6.6. A constant sized gadget J_1 with two distinguished vertices u, v can be constructed with the following property: all edges of J_1 are symmetric and the following is true,

$$\max_{\mathcal{Y}; \mathcal{Y}'(u) = \mathcal{Y}'(v)} \operatorname{Lwr}_{J_1}(\mathcal{Y}) > \varepsilon_1 + \max_{\mathcal{Y}; \mathcal{Y}'(u) \neq \mathcal{Y}'(v)} \operatorname{Lwr}_{J_1}(\mathcal{Y}),$$
(77)

where $\varepsilon_1 > 0$ is a constant depending only on the spin model and Δ .

Note that Lemma 5.2, which was proved in Section 5, is a special case of Lemma 6.6 in the case of the colorings model. The proof of Lemma 6.6 follows roughly the same lines with slightly more intricate technical details.

PROOF OF LEMMA 6.6. Let $\mathbf{z}_1, \ldots, \mathbf{z}_Q := \mathbf{x}_1, \ldots, \mathbf{x}_Q, \mathbf{y}_1, \ldots, \mathbf{y}_Q$. Let \mathbf{u} be defined as in Eq. (74). In Section 6.2, Lemma 6.5, it is proved that the $Q \times Q$ matrix $\hat{\mathbf{A}}$ whose *ij*th entry is $\ln(\mathbf{z}_i^{\mathsf{T}} \mathbf{B} \mathbf{z}_j) - \ln(\mathbf{z}_i^{\mathsf{T}} \mathbf{u}) - \ln(\mathbf{z}_j^{\mathsf{T}} \mathbf{u})$ is negative definite. Let \mathbf{A}' be the $Q' \times Q'$ matrix obtained by the following "folding" of $\hat{\mathbf{A}}$:

$$\mathbf{A}'_{ij} = \hat{\mathbf{A}}_{i,j} + \hat{\mathbf{A}}_{i+Q,j} + \hat{\mathbf{A}}_{i,j+Q} + \hat{\mathbf{A}}_{i+Q,j+Q}.$$

We have that \mathbf{A}' is also negative definite (since $\mathbf{x}^{\mathsf{T}}\mathbf{A}'\mathbf{x} = \mathbf{y}^{\mathsf{T}}\hat{\mathbf{A}}\mathbf{y}'$, where $\mathbf{y}^{\mathsf{T}} = (\mathbf{x}^{\mathsf{T}}, \mathbf{x}^{\mathsf{T}})$). Note that

$$\mathbf{A}_{ij}' = w_s((\mathbf{x}_i, \mathbf{y}_i), (\mathbf{x}_j, \mathbf{y}_j)) - a_i' - a_j',$$

where $a'_i := 2 \ln(\mathbf{x}_i^{\mathsf{T}} \mathbf{u}) + 2 \ln(\mathbf{y}_i^{\mathsf{T}} \mathbf{u})$.

Let λ_1 be largest eigenvalue of $-\mathbf{A}'$ and let λ_2 be the smallest eigenvalue of $-\mathbf{A}'$. Note that $0 < \lambda_2 \leq \lambda_1$. Define \mathbf{A} to be the $Q' \times Q'$ matrix with $A_{ij} = A'_{ij} + a'_i + a'_j$ and consider the following maximization problem

$$\max_{\mathbf{x};\mathbf{x}^{\intercal}\mathbf{1}=1,\mathbf{x}\geq0}\mathbf{x}^{\intercal}\mathbf{A}\mathbf{x}.$$
(78)

Note that, for **x** with $\mathbf{x}^{\mathsf{T}}\mathbf{1} = 1$, we have

$$\mathbf{x}^{\mathsf{T}}\mathbf{A}\mathbf{x} = 2\mathbf{a}^{\prime\mathsf{T}}\mathbf{x} + \mathbf{x}^{\mathsf{T}}\mathbf{A}^{\prime}\mathbf{x},\tag{79}$$

where \mathbf{A}' is negative definite. Note that, if \mathbf{x} and \mathbf{y} are distinct optimal solutions of (78), then $(\mathbf{x} + \mathbf{y})/2$ satisfies all the constraints, and from (79) and negative definiteness of \mathbf{A}' we have

$$((\mathbf{x} + \mathbf{y})/2)^{\mathsf{T}} \mathbf{A}((\mathbf{x} + \mathbf{y})/2) > (\mathbf{x}^{\mathsf{T}} \mathbf{A} \mathbf{x} + \mathbf{y}^{\mathsf{T}} \mathbf{A} \mathbf{y})/2,$$

a contradiction (with optimality of both **x** and **y**). Thus, (78) has a unique maximum; let \mathbf{x}^* be the value of **x** achieving it. Note, by the method of Lagrange multipliers, the local optimality of \mathbf{x}^* implies that the coordinates of $\mathbf{a}'^{\mathsf{T}} + (\mathbf{x}^*)^{\mathsf{T}} \mathbf{A}'$ are identical, that is, $\mathbf{a}'^{\mathsf{T}} + (\mathbf{x}^*)^{\mathsf{T}} \mathbf{A}' = \rho \mathbf{1}^{\mathsf{T}}$ for some $\rho \in \mathbb{R}$. Let O^* be $(\mathbf{x}^*)^{\mathsf{T}} \mathbf{A} \mathbf{x}^*$. Let S be the set of nonzero coordinates in \mathbf{x}^* .

Let $\mathbf{y} \in \mathbb{R}^{Q}$ be such that $\mathbf{y}^{\mathsf{T}}\mathbf{1} = 0$ and \mathbf{y} is zero on coordinates outside S. Then, from (local) optimality of \mathbf{x}^* , we have

$$(\mathbf{x}^* + \mathbf{y})^{\mathsf{T}} \mathbf{A} (\mathbf{x}^* + \mathbf{y}) = O^* + 2(\mathbf{a}^{\prime\mathsf{T}} + (\mathbf{x}^*)^{\mathsf{T}} \mathbf{A}') \mathbf{y} + \mathbf{y}^{\mathsf{T}} \mathbf{A}' \mathbf{y} = O^* + \mathbf{y}^{\mathsf{T}} \mathbf{A}' \mathbf{y} \ge O^* - \lambda_1 \|\mathbf{y}\|_2^2,$$
(80)

where, in the second equality, we used that $\mathbf{a}^{\prime \intercal} + (\mathbf{x}^*)^{\intercal} \mathbf{A}^{\prime}$ is a vector whose coordinates are identical and $\mathbf{y}^{\intercal} \mathbf{1} = 0$. Equation (80) tells us that moving slightly from the optimum the objective decreases at most quadratically in the length of \mathbf{y} .

Let $\mathbf{y} \in \mathbb{R}^{Q}$ be such that $\mathbf{y}^{\mathsf{T}}\mathbf{1} = 0$ and \mathbf{y} is nonnegative on coordinates outside S. Then, from (local) optimality of \mathbf{x}^* , we have

$$(\mathbf{x}^* + \mathbf{y})^{\mathsf{T}} \mathbf{A} (\mathbf{x}^* + \mathbf{y}) = O^* + 2(\mathbf{a}^{\mathsf{T}} + (\mathbf{x}^*)^{\mathsf{T}} \mathbf{A}^{\mathsf{T}}) \mathbf{y} + \mathbf{y}^{\mathsf{T}} \mathbf{A}^{\mathsf{T}} \mathbf{y} = O^* + \mathbf{y}^{\mathsf{T}} \mathbf{A}^{\mathsf{T}} \mathbf{y} \le O^* - \lambda_2 \|\mathbf{y}\|_2^2.$$
(81)

Equation (81) tells us that moving slightly from the optimum the objective decreases at least quadratically in the length of \mathbf{y} .

Let $Z \ge (4Q\lambda_1/\lambda_2)^Q$. Note that Z is a constant depending only on the model and Δ . Let $z_1/z, \ldots, z_Q/z$ be the optimal simultaneous Diophantine approximation of x_1^*, \ldots, x_Q^* with $z_1, \ldots, z_Q, z \in \mathbb{Z}$ and $1 \le z \le Z$. By Dirichlet's theorem, we have

$$|zx_i^* - z_i| \le Z^{-1/Q} < 1.$$
 (82)

Note that (82) implies

if
$$x_i^* = 0$$
, then $z_i = 0$. (83)

Also note that

$$\left|\sum_{i=1}^Q z x_i^* - \sum_{i=1}^Q z_i
ight| \leq \sum_{i=1}^Q \left| z x_i^* - z_i
ight| \leq Q' Z^{-1/Q'} < 1,$$

and since z and z_i 's are integers and $(\mathbf{x}^*)^{\mathsf{T}}\mathbf{1} = 1$, we have

$$\sum_{i=1}^{Q} \frac{z_i}{z} = 1.$$
(84)

From (83) and (84), we have that, for $\mathbf{y} := (z_1/z, \ldots, z_Q/z) - \mathbf{x}^*$, we can apply (80) and hence

$$(z_1/z, \dots, z_Q/z)\mathbf{A}(z_1/z, \dots, z_Q/z)^{\mathsf{T}} \ge O^* - \lambda_1 Q' Z^{-2/Q'} z^{-2}.$$
(85)

Now we are ready to construct the gadget J_1 . First, let K be the multigraph on z vertices b_1, b_2, \ldots, b_z with the following symmetric edges: self-loop on b_i for $i \in [z]$ and two edges between b_i and b_j for every $i, j \in [z]$ with $i \neq j$. To obtain J_1 , we overlay two copies of K as follows. Let K_u (respectively K_v) be a copy of K, where the copy of b_z in K_u is renamed to u (respectively v). Overlay K_u, K_v by identifying the copies of b_1, \ldots, b_{z-1} in the two copies. Thus, the resulting graph J_1 has z + 1 vertices and the following edges: two self loops on b_i for $i \in [z-1]$, four edges between b_i and b_j for every $i, j \in [Q-1]$ with $i \neq j$, two edges between u and b_i for $i \in [z-1]$, two edges between v and b_i for $i \in [z-1]$ and a self loop on u, v. Note that the weight of a phase assignment on J_1 is the sum of the induced phase assignments on K_u and K_v .

Consider an assignment of phases \mathcal{Y}_o such that in each complete graph z_i vertices get the unordered phase *i* (note that this forces the phases of *u* and *v* to be the same). The weight of the phase assignment \mathcal{Y}_o is

$$Lw_{T_{J_1}}(\mathcal{Y}_o) = \mathbf{S}_1 := 2(z_1, \dots, z_Q) \mathbf{A}(z_1, \dots, z_Q)^{\mathsf{T}} \ge 2z^2 O^* - 2\lambda_1 Q' Z^{-2/Q'}.$$
(86)

Now suppose that we have a phase assignment \mathcal{Y} for J_1 where the unordered phases of u and v are different. Let $\hat{\mathbf{u}}$ be the vector with \hat{u}_i counting the number of vertices with phase i in K_u and define similarly $\hat{\mathbf{v}}$. Note that $\|\hat{\mathbf{u}} - \hat{\mathbf{v}}\|_2^2 = 2$ (since $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$ differ in two coordinates—the phases of u and v in the assignment). By triangle inequality we have $\|\hat{\mathbf{u}}/z - \mathbf{x}^*\|_2 \ge 1/(z\sqrt{2})$ or $\|\hat{\mathbf{v}}/z - \mathbf{x}^*\|_2 \ge 1/(z\sqrt{2})$ (otherwise we would have

 $\|\hat{\mathbf{u}}/z - \hat{\mathbf{v}}/z\|_2 < \sqrt{2}/z$. Without loss of generality, assume that $\hat{\mathbf{u}}/z$ has the greater distance from \mathbf{x}^* . Using (81), we obtain

$$Lw_{T_{J_1}}(\mathcal{Y}_o) = \mathbf{S}_2 := \hat{\mathbf{u}}^{\mathsf{T}} \mathbf{A} \hat{\mathbf{u}} + \hat{\mathbf{v}}^{\mathsf{T}} \mathbf{A} \hat{\mathbf{v}} \le z^2 (2O^* - \lambda_2/(2z^2)) = 2z^2 O^* - \lambda_2/2.$$
(87)

By our choice of Z we have $S_1 > S_2$ and hence in an optimal phase assignment for J_1 we have that u and v get the same unordered phase. Note that we did not show which phase assignment is optimal; we only found a phase assignment in which u, v have the same unordered phase that is better than any assignment in which u, v have different unordered phases. \Box

6.3.2. The Reduction. In Section 6.2, Lemma 6.3, we proved that, for a parallel edge and any unordered phase \mathbf{p} , we have $w_p(\mathbf{p}^+, \mathbf{p}^+) = w_p(\mathbf{p}^-, \mathbf{p}^-) < w_p(\mathbf{p}^+, \mathbf{p}^-)$ and hence there exists a constant $\varepsilon_2 > 0$ depending only on the model and Δ such that, for every unordered phase $\mathbf{p} \in \mathcal{Q}'$, we have

$$w_p(\mathbf{p}^+, \mathbf{p}^+) = w_p(\mathbf{p}^-, \mathbf{p}^-) < w_p(\mathbf{p}^+, \mathbf{p}^-) - \varepsilon_2.$$
(88)

Combining Lemma 6.6 with Eq. (88), we can construct a gadget that "prefers" the unordered phase of two vertices to agree and also "prefers" the spin assignment to disagree.

LEMMA 6.7. A constant sized gadget J_2 can be constructed with two distinguished vertices u, v and the following property: there exists a phase $\mathbf{p} \in Q'$ satisfying simultaneously all of the following:

(1) $A_1(\mathbf{p}) = \text{MaxLwr}(J_2), where$ $A_1(\mathbf{p}) := \max_{\mathcal{Y}; \, \mathcal{Y}(u) = \mathbf{p}^+, \, \mathcal{Y}(v) = \mathbf{p}^-} \text{Lwr}_{J_2}(\mathcal{Y}) = \max_{\mathcal{Y}; \, \mathcal{Y}(u) = \mathbf{p}^-, \, \mathcal{Y}(v) = \mathbf{p}^+} \text{Lwr}_{J_2}(\mathcal{Y}).$ (89)

(2) Among **p** that satisfy Item 1, **p** maximizes

$$A_{2}(\mathbf{p}) := \max_{\mathcal{Y}; \mathcal{Y}(u) = \mathbf{p}^{+}, \mathcal{Y}(v) = \mathbf{p}^{+}} \operatorname{Lwr}_{J_{2}}(\mathcal{Y}) = \max_{\mathcal{Y}; \mathcal{Y}(u) = \mathbf{p}^{-}, \mathcal{Y}(v) = \mathbf{p}^{-}} \operatorname{Lwr}_{J_{2}}(\mathcal{Y}).$$
(90)

(3) The following inequalities hold

$$A_{1}(\mathbf{p}) > A_{2}(\mathbf{p}) + \varepsilon_{3} \quad and \quad A_{2}(\mathbf{p}) > \varepsilon_{3} + \max_{\mathcal{Y}; \mathcal{Y}'(u) \neq \mathcal{Y}'(v)} \operatorname{Lwr}_{J_{2}}(\mathcal{Y}), \tag{91}$$

where $\varepsilon_3 > 0$ is a constant (depending only on the model and Δ).

PROOF. To construct J_2 , we take $t := 3 \lceil (\max_{\mathbf{p}_1, \mathbf{p}_2} w_p(\mathbf{p}_1, \mathbf{p}_2) - \min_{\mathbf{p}_1, \mathbf{p}_2} w_p(\mathbf{p}_1, \mathbf{p}_2)) / \varepsilon_1 \rceil$ copies of gadget J_1 from Lemma 6.6, identify (merge) their u vertices, and identify (merge) their v vertices. Finally we add a parallel edge between u and v.

Let **p** be the unordered phase that is the common value of $\mathcal{Y}'(u)$ and $\mathcal{Y}'(v)$ for which the maximum on the left-hand side of (77) is achieved (note that **p** is not unique; we just take one such **p**). Let

$$A_4:=\max_{\mathcal{Y};\,\mathcal{Y}'(u)=\mathbf{p},\mathcal{Y}'(v)=\mathbf{p}}\mathrm{Lwr}_{J_2}(\mathcal{Y})\quad\text{and}\quad A_5:=\max_{\mathcal{Y};\,\mathcal{Y}'(u)\neq\mathcal{Y}'(v)}\mathrm{Lwr}_{J_2}(\mathcal{Y}).$$

Then, applying (77) on each copy of J_1 in J_2 we obtain

$$A_4 > A_5 + 2(\max_{\mathbf{p}_1, \mathbf{p}_2} w_p(\mathbf{p}_1, \mathbf{p}_2) - \min_{\mathbf{p}_1, \mathbf{p}_2} w_p(\mathbf{p}_1, \mathbf{p}_2)).$$
(92)

Thus, the maximizer of $\max_{\mathcal{Y}} \operatorname{Lwr}_{J_2}(\mathcal{Y})$ happens for \mathcal{Y} with $\mathcal{Y}'(u) = \mathcal{Y}'(v)$. Only the parallel edge is influenced by the spin and hence, by (88), we have

$$\max_{\mathcal{Y}} \operatorname{Lwr}_{J_2}(\mathcal{Y}) = \max_{\mathbf{p}} \max_{\mathcal{Y}: \mathcal{Y}(u) = \mathbf{p}^+, \mathcal{Y}(v) = \mathbf{p}^-} \operatorname{Lwr}_{J_2}(\mathcal{Y}).$$
(93)

Let **p** be the maximizer on the right-hand side of (93) that (secondarily) maximizes the second expression in (90). Note that **p** satisfies the first and second conditions of the lemma. The first part of the third condition is satisfied for any $\varepsilon_3 \leq \varepsilon_2$ (using the fact that the edges of J_1 are symmetric and inequality (88)). Recall that $\varepsilon_2 > 0$. The second part of the third condition is satisfied for $\varepsilon_3 \leq \max_{\mathbf{p}_1, \mathbf{p}_2} w_p(\mathbf{p}_1, \mathbf{p}_2) - \min_{\mathbf{p}_1, \mathbf{p}_2} w_p(\mathbf{p}_1, \mathbf{p}_2)$. Recall that $\max_{\mathbf{p}_1, \mathbf{p}_2} w_p(\mathbf{p}_1, \mathbf{p}_2) - \min_{\mathbf{p}_1, \mathbf{p}_2} w_p(\mathbf{p}_1, \mathbf{p}_2) > 0$. Thus, we can take $\varepsilon_3 > 0$ to be the smaller of the two upper bounds (each of which is a constant depending on the model and Δ only). \Box

LEMMA 6.8. Let **B** be the interaction matrix of an antiferromagnetic spin model. Let A_1, A_2 be the constants defined in Lemma 6.7. There exists constants D_1, D_2, D_3 depending only on the model and Δ such that the following is true. Given a cubic graph H, we can, in polynomial-time, construct a max-degree- D_1 graph G with $|V(G)| \leq D_2|V(H)|$ such that

$$MaxLwt(G) = (A_1 - A_2)MaxCut(H) + A_2|E(H)| + A_1D_3|V(H)|.$$

We can now go back and prove the inapproximability result for the phase labeling problem.

PROOF OF LEMMA 6.2. Let H be a cubic graph which is an input to MAXCUT. We have the standard bound $MaxCut(H) \ge 1/2|E(H)| = 3/4|V(H)|$. We apply Lemma 6.8. Since A_1, A_2, D_3 are constants depending only on the model and Δ , we obtain the result. \Box

PROOF OF LEMMA 6.8. Let H = (V, E) be a cubic graph which is an input to MAX-CUT. We construct the graph G as follows. For every edge (u', v') of H, take a copy of the gadget J_2 from Lemma 5.2, identify (merge) its u vertex with u', and identify (merge) its v vertex with v'. Also, for an integer $D_3 \ge 0$ which we will determine shortly, for each vertex $w \in V(H)$ add D_3 new vertices w_1, \ldots, w_{D_3} and add a gadget J_2 between w and w_i for $i \in [D_3]$ (i.e., identify the distinguished vertices u, v of J_2 with w, w_i respectively).

The purpose of the D_3 copies of J_2 is to force phase **p** (from Lemma 6.7) to be assigned on all vertices in V(H) in a labeling of G with maximum weight. A phase $\mathbf{r} \neq \mathbf{p}$ can have

$$\ell_1(\mathbf{r}) := \max_{\mathcal{Y}; \mathcal{Y}(u) = \mathbf{r}^+, \mathcal{Y}(v) = \mathbf{r}^+} \operatorname{Lwr}_{J_2}(\mathcal{Y}) - \max_{\mathcal{Y}; \mathcal{Y}(u) = \mathbf{p}^+, \mathcal{Y}(v) = \mathbf{p}^+} \operatorname{Lwr}_{J_2}(\mathcal{Y}) > 0,$$
(94)

but then by the choice of **p**

$$\ell_{2}(\mathbf{r}) := \max_{\mathcal{Y}; \, \mathcal{Y}(u) = \mathbf{p}^{+}, \, \mathcal{Y}(v) = \mathbf{p}^{-}} \operatorname{Lwr}_{J_{2}}(\mathcal{Y}) - \max_{\mathcal{Y}; \, \mathcal{Y}(u) = \mathbf{r}^{+}, \, \mathcal{Y}(v) = \mathbf{r}^{-}} \operatorname{Lwr}_{J_{2}}(\mathcal{Y}) > 0.$$
(95)

Let

$$D_3 = 4 + 3 \left\lceil \max_{\mathbf{r}} rac{\ell_1(\mathbf{r})}{\ell_2(\mathbf{r})}
ight
ceil,$$

where the maximum is taken over **r** such that (94) is satisfied (if no such **r** exists, we can take $D_3 = 0$). Note that D_3 is a constant depending on the model and Δ only.

Now we want to find the maximum weight labeling of G. The union of the distinguished vertices u, v of the J_2 gadgets in the graph G will be referred to as the distinguished vertices of G. Note, to find the maximum weight labeling of G, we may focus on labeling the distinguished vertices of G, since once those are fixed one just finds the optimal labeling in each gadget (conditioned on the labels of the distinguished vertices). Let W be a labeling of the distinguished vertices that leads to the maximum weight labeling of G. Let \hat{W} be the labeling obtained from W by changing the phase of each distinguished vertex to \mathbf{p} while (1) keeping the original spin on the vertices of H, and (2) making the spin of w_1, \ldots, w_{D_3} the opposite of the spin of w (for each $w \in V(H)$).

Now we compare W and \hat{W} for each J_2 gadget corresponding to an edge of H:

—if in W the unordered phases of u and v were different, then \hat{W} has greater weight than W on the gadget, using (91);

- —if in W the unordered phases of u and v are the same but the spins are different, then \hat{W} has greater or equal weight than W on the gadget, using (89);
- —if in W the unordered phases of u and v are the same and the spins are the same, then the loss of \hat{W} on the gadget (compared to W) is $\ell_1(\mathbf{r})$ (where \mathbf{r} is the phase of u, v in W).

For the J_2 gadgets connecting w to w_1, \ldots, w_{D_3} , we have

—if the (unordered) phase of w in W was \mathbf{r} such that $\ell_1(\mathbf{r}) > 0$, then the gain of \hat{W} on each gadget (compared to W) is at least $\ell_2(\mathbf{r})$;

—otherwise, by (89), then \hat{W} has greater or equal weight than W on the gadget.

For each vertex whose phase in W was \mathbf{r} such that $\ell_1(\mathbf{r}) > 0$, there are three edges where \hat{W} can lose $\ell_1(\mathbf{r})$ (compared to W) but there are D_3 edges where \hat{W} gains $\ell_2(\mathbf{r})$ (compared to W). Since $D_3\ell_2(\mathbf{r}) > 3\ell_1(\mathbf{r})$, we have that \hat{W} has at least as large weight as W (and hence is also optimal).

Now we just argue how the spins should be assigned. The largest number of J_2 gadgets with opposite spins on the distinguished vertices arises when we take the max-cut of H and assign the spin according to the cut. \Box

6.4. Connection between Approximating the Partition Function and the Phase Labeling Problem

In this section, we prove Lemma 6.1.

Let H = (V, E) be an instance of the phase labeling problem, where $\{E_p, E_s\}$ is a partition of the edges of H. Let |V| = m. The degree of a vertex $v \in V$ will be defined as $2d_s + d_p + 4l_s + 2l_p$, where d_s , d_p are the numbers of symmetric and parallel edges joining v to a distinct vertex u and l_s , l_p are the numbers of symmetric and parallel loops from v to itself. The bounded degree assumption means there is an absolute constant D (not depending on m) which bounds the degree of any $v \in V$.

To approximate the phase labeling problem on H with parameters \mathbf{B} , \mathcal{Q} , we will replace each vertex in the graph H by a suitable graph in a family of gadgets \mathcal{F} . The construction has a parameter k which roughly controls the accuracy of the approximation we want to achieve. The family \mathcal{F} will be of the form $\{G^d\}_{d\in[D]}$ and the gadget for a vertex v will be G^d where d is the degree of v. Note that the cardinality of \mathcal{F} is bounded by the absolute constant D. The gadgets G^d are selected from a graph distribution \mathcal{G}_n^{kd} for some appropriate n to be specified later. For integer r, n satisfying $n > r \ge 0$, we next describe the graph distribution $\mathcal{G}_n^r := \mathcal{G}_n^r(\Delta)$.

- (1) \mathcal{G}_n^r is supported on bipartite graphs. The two parts of the bipartite graph are labeled by +, - and each is partitioned as $U^s \cup W^s$ where $|U^s| = n$, $|W^s| = r$ for $s = \{+, -\}$. U denotes the set $U^+ \cup U^-$ and similarly W denotes the set $W^+ \cup W^-$.
- (2) To sample $G \sim \mathcal{G}_n^r$, sample uniformly and independently Δ matchings: (i) $(\Delta 1)$ perfect matchings between $U^+ \cup W^+$ and $U^- \cup W^-$, (ii) a *n*-matching between U^+ and U^- . The edge set of G is the union of the Δ matchings. Thus, vertices in U have degree Δ , while vertices in W have degree $\Delta 1$.

Note that, in the special case r = 0, the distribution \mathcal{G}_n^r is identical to the graph distribution \mathcal{G}_n defined in Section 2.

Before further specifying the family \mathcal{F} , we first describe the properties that a gadget in \mathcal{F} should have. We assume throughout that r is an arbitrarily large constant (independent of n). Let $G \sim \mathcal{G}_n^r$ and denote by μ_G the Gibbs distribution on G with interaction matrix **B**. Note that G is a random graph on 2(n + r) vertices.

For $\sigma : U \cup W \to [q]$, the footprint of σ is a pair of q-dimensional vectors $(\boldsymbol{\alpha}_{\sigma}, \boldsymbol{\beta}_{\sigma})$. The *i*th entry of $\boldsymbol{\alpha}_{\sigma}$ (respectively $\boldsymbol{\beta}_{\sigma}$) is equal to $|\sigma^{-1}(i) \cap U^+|/n$ (respectively $|\sigma^{-1}(i) \cap U^-|/n$). Let $\mathbf{p} \in \mathcal{Q}$ and recall that \mathbf{p} corresponds to a dominant phase $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ of Ψ_1 . The phase of a configuration $\sigma : U \cup W \to [q]$ will be denoted by $Y(\sigma)$ and equals \mathbf{p} if the closest⁵ dominant phase to the footprint $(\boldsymbol{\alpha}_{\sigma}, \boldsymbol{\beta}_{\sigma})$ of σ is $(\boldsymbol{\alpha}, \boldsymbol{\beta})$. Note that the phase of σ depends only on the spins of vertices in U.

We shall display shortly that, conditioned on $Y(\sigma) = \mathbf{p}$, the marginal distribution of μ_G on the vertices in W can be well approximated by an appropriate product measure $\nu_{\mathbf{p}}^{\otimes}(\cdot)$. To do this, recall that every phase $\mathbf{p} \in \mathcal{Q}$ corresponds to a fixpoint of the tree recursions (22). Let $(\hat{R}_1, \ldots, \hat{R}_q)$ be a scaled version of (R_1, \ldots, R_q) so that $\sum_i \hat{R}_i = 1$ (and define similarly $\hat{C}_1, \ldots, \hat{C}_q$). We now define a product measure $\nu_{\mathbf{p}}^{\otimes}(\cdot)$ on the space of spin assignments to vertices in W. For $\eta: W \to [q]$ and $\mathbf{p} \in \mathcal{Q}$, let

$$\nu_{\mathbf{p}}^{\otimes}(\eta) = \prod_{i \in [q]} (\hat{R}_i)^{|\eta^{-1}(i) \cap W^+|} \prod_{j \in [q]} (\hat{C}_j)^{|\eta^{-1}(j) \cap W^-|}.$$
(96)

For σ : $U \cup W \rightarrow [q]$, denote by σ_W the restriction of σ to vertices in W.

LEMMA 6.9. Let r be an arbitrarily large constant. In the setting of Theorem 1.5, for every $\varepsilon > 0$, there exists $N(\varepsilon)$ such that for $n \ge N$, a random graph $G \sim \mathcal{G}_n^r$ satisfies with positive probability the following.

- (1) The graph G is simple.
- (2) For each $\mathbf{p} \in \mathcal{Q}$, $(1 \varepsilon)/|\mathcal{Q}| \le \mu_G(Y(\sigma) = \mathbf{p}) \le (1 + \varepsilon)/|\mathcal{Q}|$. That is, the phases in \mathcal{Q} appear with roughly equal probability.
- (3) Let σ ~ μ_G. Then, μ_G(σ_W = η | Y(σ) = p)/ν[⊗]_p(η) ∈ [1 ε, 1 + ε] for all η : W → [q]. That is, conditioned on the phase p of the configuration, the spins of the vertices in W are roughly independent and the marginal distribution on them can be approximated by the distribution ν[∞]_p(·).
- (4) There is no edge between W^+ and W^- . Moreover, there is no vertex in G which has two neighbors in $W^+ \cup W^-$.

Lemma 6.9 is proved in Section 6.4.1. An immediate consequence of Lemma 6.9 is the following.

COROLLARY 6.10. Let k be an arbitrarily large constant. For $d \in [D]$, let $G^d \sim \mathcal{G}_n^{kd}$ and set $\mathcal{F} = \{G^d\}_{d \in [D]}$. Then, for all sufficiently large n, G^d satisfies Items (1), (2), (3), and (4) of Lemma 6.9 with positive probability for every $d \in [D]$.

Corollary 6.10 also yields a trivial randomized algorithm to construct the family \mathcal{F} for an arbitrary constant k. In fact, since all the parameters are constants, one can construct the family \mathcal{F} by brute force search. With the family \mathcal{F} in our hands, we can now give the details of the construction.

The first step consists of replacing each vertex $v \in H$ with degree d with a distinct copy of the gadget $G^d \in \mathcal{F}$. We will denote the gadget corresponding to vertex v by G_v and the images of the sets W, W^{\pm}, U^{\pm} in G_v by $W_v, W_v^{\pm}, U_v^{\pm}$. Further, denote by \hat{H} the graph obtained by the disconnected copies of the gadgets.

⁵See Appendix B, Eq. (161) for the precise definition.

The second step consists of encoding the edges of H in \hat{H} , that is, making connections between the gadgets. The final graph will be denoted by $H_{\mathcal{F}}$. The edges we are going to place will form a perfect matching on $\bigcup_{v \in H} W_v$ and as a result $H_{\mathcal{F}}$ will be Δ -regular. Every parallel edge of H corresponds to 2k edges in $H_{\mathcal{F}}$, while every symmetric to 4k. Roughly, parallel and symmetric indicate which parts of two gadgets get connected (recall that the gadgets are bipartite). Loops in H connect distinct vertices in \hat{H} .

In detail, let (u, v) be an edge e of H. Suppose first that $u \neq v$. If e is parallel, place k edges between W_u^s and W_v^s for $s \in \{+, -\}$. If e is symmetric, place k edges between W_u^s and W_v^{-s} for $s \in \{+, -\}$. Suppose now that u = v. If e is parallel, place k edges between distinct vertices in W_v^+ and k edges between distinct vertices in W_v^- . If e is symmetric, place 2k edges between W_v^+ and W_v^- , k edges between distinct vertices in W_v^- . The first step of the construction microstruction microstruction microstruction microstruction microstruction microstruction for k = 1.

The first step of the construction guarantees that the second step can be done in a (deterministic) way so that $H_{\mathcal{F}}$ is Δ -regular. Moreover, by Corollary 6.10 and item 4 of Lemma 6.9, $H_{\mathcal{F}}$ is a simple, triangle-free graph.

PROOF OF LEMMA 6.1. Using Corollary 6.10 and specifically items (2) and (3) of Lemma 6.9, the argument in Sly and Sun [2012, Lemma 4.3] almost verbatim gives

$$\frac{(1-\varepsilon)^{2m}}{|\mathcal{Q}|^m} \leq \frac{Z_{H_{\mathcal{F}}}/Z_{\widehat{H}}}{\exp(k\cdot \operatorname{MaxLwt}(H))} \leq (1+\varepsilon)^m.$$

This can be rearranged into

$$\frac{1}{k}\log\left(\frac{Z_{H_{\mathcal{F}}}}{Z_{\widehat{H}}}\right) - \frac{m}{k}\log(1+\varepsilon) \le \operatorname{MaxLwr}(H) \le \frac{1}{k}\log\left(\frac{Z_{H_{\mathcal{F}}}}{Z_{\widehat{H}}}\right) - \frac{m}{k}[2\log(1-\varepsilon) - \log|\mathcal{Q}|].$$
(97)

The argument in Sly and Sun [2012, Proof of Theorems 1 and 2] gives the desired result. We give the short details. The graph \widehat{H} consists of m disconnected subgraphs, each of constant size. Hence, we can compute $Z_{\widehat{H}}$ exactly in polynomial time. Assume now that $Z_{H_{\mathcal{F}}}$ can be approximated within a factor of $\exp(c|\widehat{H}|)$ in polynomial time for any c > 0. Since $\log(Z_{H_{\mathcal{F}}})$ is bounded above by $O(|\widehat{H}|)$, the ratio $\log(Z_{H_{\mathcal{F}}}/Z_{\widehat{H}})$ can be approximated within an additive $O(c|\widehat{H}|) = O[cm(n + kD)] = O(cnm)$ since n > kD. Thus, by (97), we obtain upper and lower bounds for MAXLWT(H) which differ by O[(cn + 1)m/k]. A random phase labeling yields the lower bound MAXLWT(H) $\geq \Omega(m)$. Thus, the final approximation is within a multiplicative factor O[(cn + 1)/k] of MAXLWT(H). To make the multiplicative factor arbitrarily small, we need to take k large. This might increase n, but we can compensate by taking c small. This concludes the proof. \Box

6.4.1. Proof of Lemma 6.9. Let $G \sim \mathcal{G}_n^r$. To get a handle on Items 2 and 3 of Lemma 6.9, we first define the partition functions conditioned on a phase $\mathbf{p} \in \mathcal{Q}$. Similar definitions appear in [Sly 2010]. Let $\Omega^{\mathbf{p}}$ be the configurations $\sigma \in \Omega$ whose phase $Y(\sigma)$ equals \mathbf{p} , that is,

$$\Omega^{\mathbf{p}} = \{ \sigma \in \Omega \mid Y(\sigma) = \mathbf{p} \}.$$
(98)

Similarly, for a configuration $\eta: W \to [q]$, let

$$\Omega^{\mathbf{p}}(\eta) = \{ \sigma \in \Omega \mid Y(\sigma) = \mathbf{p}, \sigma_W = \eta \}.$$
(99)

Note that $\Omega^{\mathbf{p}} = \bigcup_{\eta} \Omega^{\mathbf{p}}(\eta)$ and $\Omega = \bigcup_{\mathbf{p} \in \mathcal{Q}} \Omega^{\mathbf{p}}$. The conditioned partition functions $Z_G^{\mathbf{p}}$ and $Z_G^{\mathbf{p}}(\eta)$ are defined as

$$Z_{G}^{\mathbf{p}}(\eta) := \sum_{\sigma \in \Omega^{\mathbf{p}}(\eta)} w_{G}(\sigma), \quad Z_{G}^{\mathbf{p}} := \sum_{\sigma \in \Omega^{\mathbf{p}}} w_{G}(\sigma) = \sum_{\eta: W \to [q]} Z_{G}^{\mathbf{p}}(\eta).$$
(100)

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The following equalities display the relevance of these quantities to Lemma 6.9.

$$\mu_G(Y(\sigma) = \mathbf{p}) = \frac{Z_G^{\mathbf{p}}}{\sum_{\mathbf{p} \in \mathcal{Q}} Z_G^{\mathbf{p}}}, \quad \mu_G(\sigma_W = \eta | Y(\sigma) = \mathbf{p}) = \frac{Z_G^{\mathbf{p}}(\eta)}{Z_G^{\mathbf{p}}}.$$
 (101)

Note that the definition of $Z_G^{\mathbf{p}}$ also makes sense in the case r = 0. Note that for r = 0, there are no vertices of degree $\Delta - 1$ (and hence no set W), so the graph distribution \mathcal{G}_n^0 is identical to the graph distribution \mathcal{G}_n defined in Section 2.

To start, we are going to show that Items (2) and (3) of Lemma 6.9 hold in expectation. This is the scope of the following lemma which expresses $\mathbf{E}_{\mathcal{G}_n^r}[Z_G^{\mathbf{p}}], \mathbf{E}_{\mathcal{G}_n^r}[Z_G^{\mathbf{p}}(\eta)]$ in terms of $\mathbf{E}_{\mathcal{G}_n}[Z_G^{\mathbf{p}}]$. Note that o(1) refers to quantities that tend to 0 as $n \to \infty$.

LEMMA 6.11. Let r be a fixed constant and let **p** be a phase, that is, $\mathbf{p} \in Q$. There exists a constant $C(\mathbf{p})$ such that for every $\eta : W \to [q]$, it holds that

$$\mathbf{E}_{\mathcal{G}_{n}^{r}}\left[Z_{G}^{\mathbf{p}}(\eta)\right] = (1+o(1))C^{r}\nu_{\mathbf{p}}^{\otimes}(\eta)\mathbf{E}_{\mathcal{G}_{n}}\left[Z_{G}^{\mathbf{p}}\right], \text{ and thus } \max_{\eta:W \to [q]}\left|\frac{\mathbf{E}_{\mathcal{G}_{n}^{r}}\left[Z_{G}^{\mathbf{p}}(\eta)\right]}{\mathbf{E}_{\mathcal{G}_{n}^{r}}\left[Z_{G}^{\mathbf{p}}\right]} - \nu_{\mathbf{p}}^{\otimes}(\eta)\right| = o(1).$$
(102)

Moreover, when the phases Q are permutation symmetric, $\mathbf{E}_{\mathcal{G}_n}[Z_G^{\mathbf{p}}] = (1+o(1))\mathbf{E}_{\mathcal{G}_n}[Z_G^{\mathbf{p}'}]$ for any two phases $\mathbf{p}, \mathbf{p}' \in Q$ and the constant C in (102) does not depend on the particular phase \mathbf{p} . Consequently, for $\mathbf{p}, \mathbf{p}' \in Q$

$$\mathbf{E}_{\mathcal{G}_{h}^{r}}\left[Z_{G}^{\mathbf{p}}\right] = (1+o(1))\mathbf{E}_{\mathcal{G}_{h}^{r}}\left[Z_{G}^{\mathbf{p}'}\right], and thus \quad \frac{\mathbf{E}_{\mathcal{G}_{h}^{r}}\left[Z_{G}^{\mathbf{p}}\right]}{\sum_{\mathbf{p}\in\mathcal{Q}}\mathbf{E}_{\mathcal{G}_{h}^{r}}\left[Z_{G}^{\mathbf{p}}\right]} = (1+o(1))\frac{1}{|\mathcal{Q}|}.$$
(103)

PROOF. The second equalities in each of (102) and (103) follow immediately from the first. The equality $\mathbf{E}_{\mathcal{G}_n}[Z_G^{\mathbf{p}}] = (1 + o(1))\mathbf{E}_{\mathcal{G}_n}[Z_G^{\mathbf{p}'}]$ for permutation symmetric phases follows from Eq. (193) in the Appendix (see also Lemma A.4). Thus, the first equality in (103) follows by adding the first equality in (102) over all configurations η . The first equality in (102) may be proved by explicit calculations following the same arguments as in Sly [2010, Lemma 3.3]. The details can be found in Appendix D.1, see Lemma D.1 (where also the explicit value of the constant *C* is given).

It is worthy to note that (102) holds even if the phases are not permutation symmetric, which is not in general true for (103). \Box

In light of Eqs. (101), (102), and (103), the path to obtain Items (2) and (3) of Lemma (6.9) is now paved: it suffices to show that the conditioned partition functions $Z_G^{\mathbf{p}}(\eta)$ are (with positive probability) arbitrarily close to their expectations for large *n*. Note that we want this to be simultaneously true for all \mathbf{p} and η , that is, for the same graph *G*. This in turn requires using in full strength a theorem by Janson [1995], which is an extension of the small subgraph conditioning method introduced by Robinson and Wormald [1994].

We do an exposition of these theorems and their application in Appendix A. For satisfying the reader who is more interested in the proof of Lemma 6.9, the following lemma is a distilled version of the results in Appendix A, yet at the same point containing some important bits which will allow us to motivate it.

LEMMA 6.12. Let $G \sim \mathcal{G}_n^r$ and denote by X_{in} , $i = 1, 2, \ldots$, the number of cycles of length 2*i* in *G*. There exist random variables $W_{mn}^{\mathbf{p}}$, a deterministic function of $X_{1n}, X_{2n}, \ldots, X_{mn}$, such that for every $\varepsilon > 0$

$$\lim_{m \to \infty} \limsup_{n \to \infty} \Pr_{\mathcal{G}_n^r} \left(\bigcup_{\mathbf{p}} \bigcup_{\eta} \left[\left| \frac{Z_G^{\mathbf{p}}(\eta)}{\mathbf{E}_{\mathcal{G}_n^r}[Z_G^{\mathbf{p}}(\eta)]} - W_{mn}^{\mathbf{p}} \right| > \varepsilon \right] \right) = 0.$$
(104)

There also exists a positive constant c > 0 such that $W_{mn}^{\mathbf{p}} > c$ uniformly in m, n. Moreover, when the phases Q are permutation symmetric, the random variables $W_{mn}^{\mathbf{p}}$ do not depend on the phase \mathbf{p} .

Lemma 6.12 provides a straightforward proof of Lemma 6.9, so we shall elucidate its most important aspects in an attempt to demystify its rather unintuitive statement. Equation (104) says that for all sufficiently large m, n the random variables $Z_{G}^{\mathbf{p}}(\eta)/\mathbf{E}_{\mathcal{G}_{L}^{\mathbf{p}}}[Z_{G}^{\mathbf{p}}(\eta)]$ are well approximated by the variables $W_{mn}^{\mathbf{p}}$, with large probability. To get a feeling about this statement, it is a well-known fact that a random Δ -regular graph is locally tree-like and its girth diverges as $n \to \infty$. That is, as n grows large, for any positive integer t, for all but o(n) vertices, the t-depth neighborhood of a vertex is isomorphic to the first t levels of the infinite \triangle -regular tree. This is in alignment with the fact that $\mathbf{E}_{\mathcal{G}_n^r}[Z_G^{\mathbf{p}}(\eta)]$ is determined by the Gibbs measure on the infinite Δ -regular tree associated to the phase **p**. On the other hand, a graph $G \sim \mathcal{G}_n^r$ does have o(n) vertices which are contained in constant sized cycles. Thus, it is reasonable to expect that $Z_G^{\mathbf{p}}(\eta)$ fluctuates from its expectation. It is equally reasonable to expect the fluctuations to depend on the presence of small cycles which occur with small but nonzero probability. Equation (104) thus provides an explicit handle on these fluctuations, given by the variables W_{pn}^{p} , which are a deterministic function of the small cycle counts in G. Crucially for our proof of Lemma 6.9, when the phases are permutation symmetric, the fluctuations from the expectation are captured by a single random variable, which allows us to control them uniformly over all the phases **p** and configurations η .

We should point out that the notation $W_{mn}^{\mathbf{p}}$ should not be confused by any means to the labeling of the degree $\Delta - 1$ vertices in *G*, that is, the set of vertices *W*.

PROOF OF LEMMA 6.9. We assume that the ε in the statement of the lemma is fixed. Let $\varepsilon' > 0$ be sufficiently small, to be picked later.

By Lemma 6.12, we have that for all m, n sufficiently large the random variables $Z_{G}^{\mathbf{p}}(\eta)/\mathbf{E}_{\mathcal{G}_{n}^{r}}[Z_{G}^{\mathbf{p}}(\eta)]$ are well approximated by $W_{mn}^{\mathbf{p}}$ with large probability. That is, there exist $M(\varepsilon')$, $N(\varepsilon')$ such that for $m \geq M$ and $n \geq N$, it holds with probability $1 - \varepsilon'$ over the choice of the graph G that, for every phase \mathbf{p} and every configuration $\eta: W \to [q]$,

$$Z_G^{\mathbf{p}}(\eta) = (W_{mn}^{\mathbf{p}} \pm \varepsilon') \mathbf{E}_{\mathcal{G}_n^r} [Z_G^{\mathbf{p}}(\eta)].$$
(105)

We will show that whenever this is the case, Items (2) and (3) hold. To do this, sum (105) over η to obtain that for each phase **p**, it holds

$$Z_G^{\mathbf{p}} = \left(W_{mn}^{\mathbf{p}} \pm \varepsilon' \right) \mathbf{E}_{\mathcal{G}_n^r} [Z_G^{\mathbf{p}}], \tag{106}$$

Using the positive constant c in Lemma 6.12, we obtain that for ε' sufficiently smaller than c, the ratio $Z_G^{\mathbf{p}}(\eta)/Z_G^{\mathbf{p}}$ is within a multiplicative $(1 \pm \varepsilon)$ from $\mathbf{E}_{\mathcal{G}_n^r}[Z_G^{\mathbf{p}}(\eta)]/\mathbf{E}_{\mathcal{G}_n^r}[Z_G^{\mathbf{p}}]$. This gives Item (3) of the lemma, when used in conjuction with (101) and (102). Note that this part of the argument did not use that the phases \mathbf{p} are permutation symmetric.

To obtain Item (2), we have to use that the phases **p** are permutation symmetric. Then $W_{mn}^{\mathbf{p}} =: W_{mn}$ by the last assertion in Lemma 6.12. Thus, a summation of (106) over $\mathbf{p} \in \mathcal{Q}$ gives $Z_G = (W_{mn} \pm \varepsilon') \mathbf{E}_{\mathcal{G}_n^r}[Z_G]$. Exactly the same reasoning as before (using now (101) and (103)) yields the thesis.

It is a standard union bound to show that Item (4) holds with probability 1 - O(1/n) over the choice of the graph G, essentially because G is an expander. Perhaps the second assertion there requires a brief proof sketch. Let v be a vertex in the part of G labeled +, that is, $v \in U^+ \cup W^+$, and consider two vertices $w_1, w_2 \in W^-$. For i = 1, 2, let E_i be the event that (v, w_i) is an edge of G. The events E_1, E_2 are negatively correlated since v has a fixed number of edges incident to it, either Δ or $\Delta - 1$. It is also easy to see that $\Pr_{\mathcal{G}_{i}^{r}}(E_i) \leq 1 - (1 - 1/n)^{\Delta} = O(1/n)$, so that $\Pr_{\mathcal{G}_{i}^{r}}(E_1 \cap E_2) = O(1/n^2)$. A union bound over

the roughly $(n+r)r^2 = O(n)$ possibilities for the selection of the vertices v, w_1, w_2 gives the desired bound.

Thus, a graph $G \sim \mathcal{G}_n^r$ satisfies Items (2), (3), and (4) with large probability for all sufficiently large *n*. The first assertion in Item (1) of Lemma 6.12 can hence be guaranteed by contiguity, see Janson [1995, Section 2]. \Box

7. DOMINANT PHASES FOR POTTS MODEL AND COLORINGS

7.1. Proof Outline

In this section, we prove Theorem 1.6 which establishes the hypotheses of Theorem 1.5 for the dominant phases of the antiferromagnetic Potts and colorings models on random Δ -regular bipartite graphs (and, as we showed in Section 1.2.3, Theorems 1.1 and 1.2 follow as corollaries).

Recall, the interaction matrix **B** for the Potts model is completely determined by a parameter *B*, which is equal to $\exp(-\beta)$ where β is the inverse temperature in the standard notation for the Potts model. The antiferromagnetic regime corresponds to 0 < B < 1. The coloring model is the zero temperature limit of the Potts model and corresponds to the particular case B = 0 in what follows. We should note that in Statistical Physics terms, the arguments of this section are closely related to the phase diagrams of the models.

By Theorem 4.1 specialized to the antiferromagnetic Potts and colorings models, studying the global maxima of Ψ_1 is equivalent to studying the global maxima of Φ . Moreover, the global maxima of Φ and Ψ_1 occur at their critical points. Since there is a one-to-one correspondence between the critical points of Φ and the critical points of Ψ_1 (given by (23)), we will freely interchange our focus between critical points of Φ and Ψ_1 .

The critical points of Φ , by the first part of Theorem 4.1, are given by fixpoints of the tree recursions (22), which for the Potts model read as

$$R_i \propto \left(BC_i + \sum_{j \neq i} C_j\right)^d, \quad C_j \propto \left(BR_j + \sum_{i \neq j} R_i\right)^d,$$
 (107)

where i, j = 1, ..., q and d is the notational convenient substitution $d := \Delta - 1 \ge 2$. Given a fixpoint of the tree recursions (107), we will classify whether it is a Hessian local maximum of Ψ_1 using Theorem 4.2.

Once we find the global maxima of Ψ_1 , it will be simple to prove that they are Hessian and permutation symmetric. Finding however the global maxima of Ψ_1 is going to be more intricate, mainly because the number of local maxima varies according to the value of *B*. We will thus have to compare the values of Ψ_1 at the critical points. Rather than doing this directly (which seems to be a difficult task), we solve a relaxed optimisation problem, which for *q* even can be tied to the maximization of Ψ_1 . We next give the details.

We begin our considerations by examining when a fixpoint (107) is translation invariant, that is, satisfies $R_i \propto C_i$ for every $i \in [q]$.

LEMMA 7.1. Let $0 \leq B < 1$ and $\Delta \geq 3$. If a solution of (107) satisfies $R_i \propto C_i$ for $i \in [q]$, then it holds that $R_1 = \cdots = R_q$ and $C_1 = \cdots = C_q$.

PROOF OF LEMMA 7.1. By the symmetries of the model, we may assume an arbitrary ordering of the R_i 's. Since $0 \le B < 1$, (107) easily implies the reverse ordering of the C_i 's. Thus, $R_i \propto C_i$ for every $i \in [q]$ yields that the ordering must be trivial, that is, $R_1 = \cdots = R_q$ and $C_1 = \cdots = C_q$. \Box

COROLLARY 7.2. Translation-invariant fixpoints of (107) always exist and are unique up to scaling.

We next explore in which regimes of B, the critical points of Φ consist solely of translation-invariant fixpoints. In this regime, we immediately obtain by Theorem 4.1 that the global maximum of Ψ_1 (and hence the global maximum of Φ as well) is achieved at a translation-invariant fixpoint.

LEMMA 7.3. Let $0 \leq B < 1$ and $q, \Delta \geq 3$. When $B \geq \frac{\Delta - q}{\Delta}$, the solution of the system of Eq. (107) satisfies $R_1 = \cdots = R_q$ and $C_1 = \cdots = C_q$.

The proof of Lemma 7.3 is an extension of an argument in Brightwell and Winkler [2002] for colorings and is given in Appendix C. The next lemma states that in the complementary regime of Lemma 7.3, the translation-invariant fixpoint does not correspond to a local maximum of Ψ_1 and hence, by Theorem 4.1, the global maximum of Ψ_1 occurs at a fixpoint of (107) which is not translation invariant. In particular, in this regime, we have semitranslational nonuniqueness.

LEMMA 7.4. For $0 \leq B < \frac{\Delta-q}{\Delta}$, the global maximum of Ψ_1 is not achieved at the translation-invariant fixpoint.

PROOF OF LEMMA 7.4. We apply Theorem 4.2 by showing that the translationinvariant fixpoint is Jacobian unstable and hence not a local maximum of Ψ_1 . By Lemma 4.16, for a general interaction matrix **B**, the condition for Jacobian stability of a fixpoint of the tree recursions is related to the spectrum of $\mathbf{L} = \begin{bmatrix} 0 & \mathbf{A} \\ \mathbf{A}^T & \mathbf{0} \end{bmatrix}$, where **A** is the $q \times q$ matrix whose (i, j)-entry is given by $A_{ij} = B_{ij}R_iC_j/\sqrt{\alpha_i\beta_j}$ and α_i, β_j are given by (29). Recall that ± 1 are eigenvalues of **L** and the condition for Jacobian stability is that all the other eigenvalues have absolute value less than $1/(\Delta - 1)$ (for details, see the proof of Theorem 4.2 in Section 4.2.3).

In the setting of the lemma, the matrix **A** for the translation-invariant fixpoint has off-diagonal entries equal to 1/(B+q-1) and diagonal entries equal to B/(B+q-1). It follows that the eigenvalues of **L** are ± 1 by multiplicity 1 and $\pm (1-B)/(B+q-1)$ by multiplicity q-1. The absolute value of the latter is greater than $\frac{1}{\Delta-1}$ for $0 \le B < \frac{\Delta-q}{\Delta}$, as claimed. \Box

We summarize these results into the following corollary.

COROLLARY 7.5. Let $0 \leq B < 1$ and $q, \Delta \geq 3$. When $B \geq \frac{\Delta-q}{\Delta}$, Ψ_1 has a unique global maximum for $\alpha_1 = \cdots = \alpha_q = \beta_1 = \cdots = \beta_q = 1/q$ or, in other words, the global maximum of Ψ_1 is achieved by the fixpoint which corresponds to the (unique) translation-invariant Gibbs measure. In the complementary regime $0 \leq B < \frac{\Delta-q}{\Delta}$, the maximum of Ψ_1 is not achieved at the translation-invariant fixpoint, and hence it is achieved at a semitranslation-invariant fixpoint which is not translation invariant.

Corollary 7.5 is not sufficient to obtain Theorems 1.1 and 1.2, since we need to verify that the global maxima of Ψ_1 in semitranslational nonuniqueness are Hessian and permutation symmetric. We do this by identifying the critical points which are maxima of Ψ_1 .

To state the result, we first need the following structural statement for the solutions of Eq. (107), namely that solutions of (107) are supported on at most three values for the R_i 's and similarly for the C_i 's.

LEMMA 7.6. Let $(R_1, \ldots, R_q, C_1, \ldots, C_q)$ be a positive solution of the system (107). Let t_R be the number of values on which the R_i 's are supported and define similarly t_C . Then $t_R, t_C \leq 3$ and $t_R = t_C =: t$.

The proof of Lemma 7.6 is given in Section 7.5. Lemma 7.6 motivates the following definition.

Definition 7.7. From Lemma 7.6, the R_i 's and C_j 's of a fixpoint of (107) attain at most $t \leq 3$ different values. Let $\tilde{R}_1, \ldots, \tilde{R}_t$ and $\tilde{C}_1, \ldots, \tilde{C}_t$ be their values and let $q_1, \ldots, q_t \geq 1$ be their multiplicities. When t = 1, define $q_2 = q_3 = 0$; when t = 2, define $q_3 = 0$; when $q_i = 0$, define the values of \tilde{R}_i, \tilde{C}_i to be zero. The corresponding solution of (107) or equivalently the fixpoint of the tree recursions is then defined to be of type (q_1, q_2, q_3) . Note that $q_1 + q_2 + q_3 = q$ and the q_i 's are nonnegative integers. Call a (q_1, q_2, q_3) -type fixpoint to be t-supported if the number of q_i 's which are nonzero equals t.

Finding the types of fixpoints which correspond (via (23)) to global maxima of Ψ_1 is a nontrivial task. While 2-supported fixpoints are simple to handle for all $q \ge 2$, this is not the case for 3-supported fixpoints (this is the only reason we obtain Theorems 1.1 and 1.2 for even k and q, respectively). The main lemma we prove is the following, which identifies the type of fixpoints maximizing Ψ_1 .

LEMMA 7.8. For $0 \le B < \frac{\Delta-q}{\Delta}$ and even $q \ge 3$, the maximum of Ψ_1 over (q_1, q_2, q_3) -type fixpoints of (107) is attained (uniquely) at fixpoints of type (q/2, q/2, 0).

The final piece is to show that fixpoints of type (q/2, q/2, 0) correspond to Hessian maxima of Ψ_1 and are permutation symmetric. This is the scope of the next lemma, whose proof is given in Section 7.5.

LEMMA 7.9. For $0 \leq B < \frac{\Delta-q}{\Delta}$ and even $q \geq 3$, fixpoints of type (q/2, q/2, 0) are Jacobian stable and hence correspond to Hessian local maxima of Ψ_1 . The values of R_i 's and C_j 's for fixpoints of type (q/2, q/2, 0) are unique up to scaling and permutations of the colors.

We are now ready to prove Theorem 1.6.

PROOF OF THEOREM 1.6. Item (1) follows from Corollary 7.5 (see also Lemmas 7.3 and 7.4). Item (2) follows from Lemmas 7.8 and 7.9, after using the correspondence between fixpoints of the tree recursions (107) and dominant phases of Theorem 4.1 (Eq. (23)). \Box

7.2. Proof of Lemma 7.8

In this section, we outline the proof of Lemma 7.8. We need to find the type(s) of the fixpoints of (107) which maximize Ψ_1 .

Let $\mathbf{q} = (q_1, q_2, q_3)$ specify the type of a fixpoint of (107) and let $\mathbf{r} = (\tilde{R}_1, \tilde{R}_2, \tilde{R}_3)$, $\mathbf{c} = (\tilde{C}_1, \tilde{C}_2, \tilde{C}_3)$ be the respective values of the R_i 's and C_j 's, see Definition 7.7. Henceforth, we will use for simplicity the notation $\mathbf{r} = (R_1, R_2, R_3)$, $\mathbf{c} = (C_1, C_2, C_3)$. Note that the q_i 's are nonnegative integers satisfying $q_1 + q_2 + q_3 = q$.

Using Theorem 4.1, we obtain that the value of $\Psi_1(\alpha, \beta)$ corresponding to such a fixpoint of (107) is given by the value of the function $\overline{\Phi^S}$, where

$$\overline{\Phi^{S}}(\mathbf{q}, \mathbf{r}, \mathbf{c}) := (d+1) \ln \left(\sum_{i=1}^{3} q_{i} R_{i} \sum_{j=1}^{3} q_{j} C_{j} + (B-1) \sum_{i} q_{i} R_{i} C_{i} \right)
- d \ln \left(\sum_{i=1}^{3} q_{i} R_{i}^{(d+1)/d} \right) - d \ln \left(\sum_{j=1}^{3} q_{j} C_{j}^{(d+1)/d} \right),$$
(108)

and $d = \Delta - 1$. We remark here that in the derivation of (108), we used that if a solution of (107) satisfies $R_i = R_j$ for some *i*, *j* then also $C_i = C_j$ (and vice-versa).

It is a nontrivial task to directly compare the values of $\overline{\Phi^S}$ over fixpoints of (107). Instead, we will solve a relaxed version of the problem, seeking to maximize $\overline{\Phi^S}$ over nonnegative q_i 's which satisfy $q_1 + q_2 + q_3 = q$. If this maximum happens to occur for integer **q** and the respective values of R_i 's and C_j 's satisfy (107), then we have also found the solution to the original maximization problem. It turns out that all of these conditions are satisfied if and only if q is even.

To formalize the argument, for nonnegative q_i 's such that $q_1 + q_2 + q_3 = q$, define

$$\overline{\Phi}(\mathbf{q}) := \max_{\mathbf{r}, \mathbf{c}} \overline{\Phi^S}(\mathbf{q}, \mathbf{r}, \mathbf{c}), \tag{109}$$

where the maximum is over $\mathbf{r} = (R_1, R_2, R_3)^{\mathsf{T}}$, $\mathbf{c} = (C_1, C_2, C_3)^{\mathsf{T}}$ which satisfy

$$\sum_{i=1}^{3} q_i R_i \sum_{j=1}^{3} q_j C_j + (B-1) \sum_{i=1}^{3} q_i R_i C_i > 0,$$

$$R_1, R_2, R_3, C_1, C_2, C_3 \ge 0.$$
(110)

It is simple to see that $\overline{\Phi^S}$ is well defined in the region (110). It is not completely immediate that the maximum in (109) is well defined since the region (110) is not compact. Nevertheless, the maximum turns out to be well defined as a consequence of the following scale-free property of $\overline{\Phi^S}$ with respect to **r** and **c**:

for every
$$c_1, c_2 > 0$$
 it holds that $\Phi^S(\mathbf{q}, c_1 \mathbf{r}, c_2 \mathbf{c}) = \Phi^S(\mathbf{q}, \mathbf{r}, \mathbf{c}).$ (111)

Using (111), it is simple to obtain the following (see Section 7.5).

LEMMA 7.10. Let $B \ge 0$ and $q \ge 2$. For all $q_1, q_2, q_3 \ge 0$ which satisfy $q_1 + q_2 + q_3 = q$, the maximum in (109) is well defined. Moreover, the maximum of $\overline{\Phi}(q_1, q_2, q_3)$ over all such q_1, q_2, q_3 is attained.

We next seek to connect the maximizers of (109) with solutions of (107). To do this, we first need to consider whether the maximum in (109) happens on the boundary of the region (110); it turns out that the maximum can happen at the boundary $R_i = 0$ or $C_i = 0$ if q_i is close to zero. While the boundary cases are an artifact of allowing q_i 's to be noninteger, we will need to treat them explicitly to find the maximum of $\overline{\Phi}$.

Definition 7.11. A triple $\mathbf{q} = (q_1, q_2, q_3)$ is good if the \mathbf{r}, \mathbf{c} which achieve the maximum in (109) satisfy: for $i = 1, 2, 3, q_i > 0$ implies $R_i, C_i > 0$. A triple $\mathbf{q} = (q_1, q_2, q_3)$ is bad if it is not good.

To complete the connection, we need to further restrict the set of triples **q**. To motivate this restriction, note that if we consider the region (110) in the subspace $R_1 = R_2$ and $C_1 = C_2$, we obtain $\overline{\Phi}(q_1 + q_2, q_3, 0) \leq \overline{\Phi}(q_1, q_2, q_3)$. To avoid degenerate cases, roughly, we consider only triples **q** where such simple inequalities do not hold at equality.

Definition 7.12. Let t = 2 or 3. A triple $\mathbf{q} = (q_1, q_2, q_3)$ is called *t*-maximal if exactly *t* of the q_i 's are nonzero and there exist $\mathbf{r} = (R_1, R_2, R_3)$ and $\mathbf{c} = (C_1, C_2, C_3)$ which achieve the maximum in (109) such that, for all distinct $i, j \in \{1, 2, 3\}$ with $q_i q_j > 0$, it holds that $R_i \neq R_j$ and $C_i \neq C_j$.

Remark 7.13. In general, determining whether a triple $\mathbf{q} = (q_1, q_2, q_3)$ is maximal is a difficult task. For example, if the q_i 's are positive integers, it is conceivable that \mathbf{q} being maximal relates to whether a 3-supported fixpoint of (107) of type (q_1, q_2, q_3) exists. Our use of the notion of maximality is going to be roughly along the following lines: if for some q, B it holds that $\max \Psi_1 = \max \overline{\Phi}$ and a fixpoint of (107) of type (q_1, q_2, q_3) is assumed to maximize Ψ_1 , then the triple (q_1, q_2, q_3) has to be maximal. (Recall that for q even, we will be able to show that $\max \Psi_1 = \max \overline{\Phi}$.)

Our interest is in maximal good triples $\mathbf{q} = (q_1, q_2, q_3)$. This is justified by the following lemma, whose proof is given in Section 7.5.

LEMMA 7.14. Suppose that q_1, q_2, q_3 are nonnegative integers and the triple $\mathbf{q} =$ (q_1, q_2, q_3) is t-maximal and good. Then, there exist \mathbf{r}, \mathbf{c} which achieve the maximum in (109) and specify a t-supported fixpoint of (107) of type (q_1, q_2, q_3) .

Roughly, to prove Lemma 7.8, it will suffice to prove that the triple (q/2, q/2, 0) is 2-maximal and good and that the maximum of $\overline{\Phi}(\mathbf{q})$ is achieved at (q/2, q/2, 0).

The next lemma examines which maximal good triples can be maximizers of $\overline{\Phi}$ (proved in Section 7.3).

LEMMA 7.15. Let q > 3 and 0 < B < 1. There do not exist 3-maximal good triples **q** which maximize $\Phi(\mathbf{q})$. The only 2-maximal good triples **q** where a maximum of $\Phi(\mathbf{q})$ can occur are (q/2, q/2, 0) or its permutations.

Lemma 7.15 is not sufficient to yield Lemma 7.8 because the maximum of $\Phi(\mathbf{q})$ can occur at a bad triple **q**. This possibility is excluded by the following lemma (proved in Section 7.4).

LEMMA 7.16. Let $q \ge 3$ and $0 \le B < \frac{\Delta - q}{\Delta}$. There do not exist bad triples **q** which maximize $\overline{\Phi}(\mathbf{q})$.

We will also need the following property of good triples (proved in Section 7.5).

LEMMA 7.17. Let $\mathbf{q} = (q_1, q_2, q_3)$ be a good triple and suppose that $i, j \in \{1, 2, 3\}$ are such that $q_i, q_j > 0$. Let $\mathbf{r} = (R_1, R_2, R_3), \mathbf{c} = (C_1, C_2, C_3)$ achieve the maximum in (109). Then $R_i = R_j$ iff $C_i = C_j$.

Using Lemmas 7.15, 7.16, and 7.17, we can now give the proof of Lemma 7.8.

PROOF OF LEMMA 7.8. Let q be an even integer ≥ 4 and $0 \leq B < \frac{\Delta - q}{\Delta}$. Recall that the maximizers of Ψ_1 correspond to a fixpoint of (107). Recall that for a fixpoint \mathbf{r}, \mathbf{c} of type $\mathbf{q} = (q_1, q_2, q_3)$, the corresponding value of Ψ_1 is given by $\overline{\Phi^S}(\mathbf{q}, \mathbf{r}, \mathbf{c})$.

Let $MAX := \max_{\mathbf{q}} \overline{\Phi}(\mathbf{q})$ (recall that the maximum of $\overline{\Phi}(\mathbf{q})$ over triples \mathbf{q} is attained by Lemma 7.10). Since $\overline{\Phi}(\mathbf{q}) = \max_{\mathbf{r},\mathbf{c}} \overline{\Phi^S}(\mathbf{q},\mathbf{r},\mathbf{c})$, we also have that MAX = $\max_{\mathbf{q},\mathbf{r},\mathbf{c}} \overline{\Phi^S}(\mathbf{q},\mathbf{r},\mathbf{c})$. It follows that $MAX \ge \max \Psi_1$. Let $\widehat{\mathbf{q}} := (q/2, q/2, 0)$. We will show that⁶

$$MAX = \Phi(\widehat{\mathbf{q}}) \text{ and } \widehat{\mathbf{q}} \text{ is } 2\text{-maximal and good.}$$
 (112)

Assuming (112) for the moment, let us conclude the lemma. Since $\hat{\mathbf{q}}$ is 2-maximal and good, by Lemma 7.14, there exist $\hat{\mathbf{r}}, \hat{\mathbf{c}}$ such that $\overline{\Phi}(\hat{\mathbf{q}}) = \Phi^S(\hat{\mathbf{q}}, \hat{\mathbf{r}}, \hat{\mathbf{c}})$ and $\hat{\mathbf{r}}, \hat{\mathbf{c}}$ specify a 2-supported fixpoint of (107) of type $\widehat{\mathbf{q}}$ (here we used that q is even). It follows that $MAX = \max \Psi_1$.

Now, let \mathbf{r}^* , \mathbf{c}^* be a *t*-supported fixpoint of type \mathbf{q}^* (cf., Definition 7.7) which achieves the maximum of Ψ_1 (note that the entries of \mathbf{q}^* are integers). Since $MAX = \max \Psi_1$, we have that \mathbf{q}^* also achieves the maximum of $\overline{\Phi}(\mathbf{q})$ and $\mathbf{r}^*, \mathbf{c}^*$ achieve the maximum of $\Phi^{S}(\mathbf{q}^{*}, \mathbf{r}, \mathbf{c})$. It follows that the triple \mathbf{q}^{*} is both good (Lemma 7.16) and *t*-maximal (by definition, using the maximizers $\mathbf{r}^*, \mathbf{c}^*$). By Lemma 7.14, it must be the case that $\mathbf{q}^* = (q/2, q/2, 0)$ and hence the only fixpoints of (107) which correspond to maximizers of Ψ_1 are of type (q/2, q/2, 0), yielding the statement of the lemma.

It remains to prove (112). The following hold for any maximizer \mathbf{q}^* of $\Phi(\mathbf{q})$.

⁶In fact, the proof of (112) holds for all integer $q \ge 3$ (not just even).

- (1) \mathbf{q}^* is a good triple. This is an immediate consequence of Lemma 7.16.
- (2) **q**^{*} has at least two positive entries, that is, $\mathbf{q}^* \neq (q, 0, 0)$, and thus $MAX > \Phi(q, 0, 0)$. Otherwise, $MAX = \overline{\Phi}(q, 0, 0)$, in which case the global maximum of Ψ_1 is achieved at a translation-invariant fixpoint which is excluded by Lemma 7.4 (in the regime $0 \leq B < \frac{\Delta - q}{\Delta}$).
- (3) If \mathbf{q}^* has exactly two nonzero entries, then \mathbf{q}^* is 2-maximal. For the sake of contradiction, assume that this is not the case for some $\mathbf{q}^* = (q_1, q_2, 0)$ with $q_1, q_2 > 0$. Consider a maximizer \mathbf{r}^* , \mathbf{c}^* of $\overline{\Phi^S}(\mathbf{q}^*, \mathbf{r}, \mathbf{c})$. Since \mathbf{q}^* is not 2-maximal, it holds either that $R_1 = R_2$ or $C_1 = C_2$. Since \mathbf{q}^* is good (by Item (1)), from Lemma 7.17, we can in fact conclude that $R_1 = R_2$ and $C_1 = C_2$. It follows that $\overline{\Phi}(\mathbf{q}^*) = \overline{\Phi}(q, 0, 0)$ and hence $MAX = \overline{\Phi}(q, 0, 0)$, contradicting Item 2.
- (4) If \mathbf{q}^* has exactly two nonzero entries, then $\mathbf{q}^* = (q/2, q/2, 0)$. We have that \mathbf{q}^* is good (by Item 1) and \mathbf{q}^* is 2-maximal (by Item 3). By the second part of Lemma 7.15, we obtain that $\mathbf{q}^* = (q/2, q/2, 0)$.
- (5) If all the entries of q* are positive, then q* is not 3-maximal. Since q* is good (by Item (1)), this follows by the first part of Lemma 7.15.
- (6) If all the entries of **q**^{*} are positive, then Φ(**q**^{*}) = Φ(q/2, q/2, 0). To see this, note that **q**^{*} is good (by Item 1) and not 3-maximal (by Item (5)). Consider a maximizer **r**^{*}, **c**^{*} of Φ^S(**q**^{*}, **r**, **c**). By the argument used in Item (3), we can conclude that there exist distinct indices *i*, *j* such that *R_i* = *R_j* and *C_i* = *C_j*. Let *k* be the remaining index, that is, *k* ∈ {1, 2, 3} with *k* ≠ *i*, *j*. Let **q**' := (*q_i* + *q_j*, *q_k*, 0), **r**' := (*R_i*, *R_k*, 0) and **c**' := (*C_i*, *C_k*, 0). We have that Φ(**q**^{*}) = Φ^S(**q**^{*}, **r**^{*}, **c**^{*}) = Φ^S(**q**', **r**', **c**') ≤ Φ(**q**') for some **q**' which has exactly two nonzero entries. Since **q**^{*} is a maximizer of Φ, we have that **q**' is also a maximizer of Φ. It follows by Item (4) that **q**' = (*q*/2, *q*/2, 0) and hence Φ(**q**^{*}) = Φ(*q*/2, *q*/2, 0).
- (7) $\overline{\Phi}(\mathbf{q}^*) = MAX = \overline{\Phi}(q/2, q/2, 0)$. This follows by combining Items (2), (4), and (6).

By Item (7), we have that the triple $\widehat{\mathbf{q}} = (q/2, q/2, 0)$ maximizes $\overline{\Phi}$ and thus all Items (1)–(7) apply for $\mathbf{q}^* = \widehat{\mathbf{q}}$. In particular, by Items (1) and (3), we obtain that (q/2, q/2, 0) is good and 2-maximal. This proves (112), thus finishing the proof of Lemma 7.8. \Box

For the proofs of Lemmas 7.15 and 7.16, we will often perturb the values of q_i 's. The following lemma, proved in Section 7.5, will be very helpful (holds for any triple **q**).

LEMMA 7.18. Let $\mathbf{q} = (q_1, q_2, q_3)$ and $I = \{i | q_i > 0\}$. Suppose that \mathbf{r}, \mathbf{c} achieve the maximum in (109). Then, for $i \in I$ it holds that

$$\frac{\partial \overline{\Phi^S}}{\partial q_i}(\mathbf{q}, \mathbf{r}, \mathbf{c}) = \frac{R_i \sum_j q_j C_j + C_i \sum_j q_j R_j + (d-1)(1-B)R_i C_i}{\sum_j q_j R_j \sum_j q_j C_j + (B-1)\sum_j q_j R_j C_j}.$$
(113)

Moreover, if there exist $i, j \in I$ such that $\frac{\partial \overline{\Phi^S}}{\partial q_i} - \frac{\partial \overline{\Phi^S}}{\partial q_j} \neq 0$, the maximum of $\overline{\Phi}$ is not achieved at the triple **q**.

7.3. Good Triples: Proof of Lemma 7.15

We first prove the statement of the lemma for 3-maximal good triples $\mathbf{q} = (q_1, q_2, q_3)$, the proof for 2-maximal good triples will be easily inferred by appropriately modifying the arguments in the special case $q_2 = 0$.

Let $\mathbf{q} = (q_1, q_2, q_3)$ be a 3-maximal good triple. Since \mathbf{q} is 3-maximal all of the q_i 's are positive. Moreover, \mathbf{q} is good, and hence the maximum in (109) for \mathbf{q} is attained at positive R_i 's and C_j 's. Thus, the R_i 's and C_j 's satisfy $\partial \overline{\Phi^S} / \partial R_i = \partial \overline{\Phi^S} / \partial C_j = 0$

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which give

$$R_i^{1/d} \propto q_1 C_1 + q_2 C_2 + q_3 C_3 + (B-1)C_i, \quad C_j^{1/d} \propto q_1 R_1 + q_2 R_2 + q_3 R_3 + (B-1)R_j.$$
(114)

Since **q** is 3-maximal, we may choose **r**, **c** such that $R_i \neq R_j$ and $C_i \neq C_j$ for all $i \neq j$. Thus, we may assume a strict ordering of the R_i 's, which by (114) implies the reverse ordering of the C_j 's. Without loss of generality, we will use the following ordering:

$$R_1 > R_2 > R_3 > 0$$
 and $0 < C_1 < C_2 < C_3$. (115)

The following lemma, together with the second part of Lemma 7.18, establishes that the maximum of $\overline{\Phi}$ cannot occur at a 3-maximal triple.

LEMMA 7.19. Suppose that R_i 's and C_j 's satisfy (114) and (115). If $R_1/R_3 \neq C_3/C_1$, then $\frac{\partial \overline{\Phi^S}}{\partial q_1} - \frac{\partial \overline{\Phi^S}}{\partial q_3} \neq 0$. If $R_1/R_3 = C_3/C_1$, then $\frac{\partial \overline{\Phi^S}}{\partial q_1} - \frac{\partial \overline{\Phi^S}}{\partial q_2} \neq 0$.

We next give the proof of Lemma 7.19. We will utilize Lemma 7.18 by specifying a particular scaling of the R_i 's and C_j 's which will be beneficial. To do this, set

$$r_1^d = R_1/R_3, r_2^d = R_2/R_3, c_2^d = C_2/C_1, c_3^d = C_3/C_1.$$
 (116)

The R_i 's and C_j 's may be recovered from r_i 's, c_j 's using

$$R_1 \propto r_1^d, \ R_2 \propto r_2^d, \ R_3 \propto 1, \quad \text{and} \quad C_1 \propto 1, \ C_2 \propto c_2^d, \ C_3 \propto c_3^d.$$
 (117)

Translating (115) into r_1, r_2, c_2, c_3 gives

$$r_1 > r_2 > 1 \text{ and } c_3 > c_2 > 1.$$
 (118)

Moreover, dividing appropriate pairs of (114), we also obtain

$$r_{1} = \frac{B + q_{1} - 1 + q_{2}c_{2}^{d} + q_{3}c_{3}^{d}}{q_{1} + q_{2}c_{2}^{d} + (B + q_{3} - 1)c_{3}^{d}}, c_{3} = \frac{B + q_{3} - 1 + q_{2}r_{2}^{d} + q_{1}r_{1}^{d}}{q_{3} + q_{2}r_{2}^{d} + (B + q_{1} - 1)r_{1}^{d}},$$

$$r_{2} = \frac{q_{1} + (B + q_{2} - 1)c_{2}^{d} + q_{3}c_{3}^{d}}{q_{1} + q_{2}c_{2}^{d} + (B + q_{3} - 1)c_{3}^{d}}, c_{2} = \frac{q_{3} + (B + q_{2} - 1)r_{2}^{d} + q_{1}r_{1}^{d}}{q_{3} + q_{2}r_{2}^{d} + (B + q_{1} - 1)r_{1}^{d}}.$$
(119)

As we shall display shortly, the system of Eq. (119) (together with (118)) gives

$$q_{1} = \frac{(1-B)f(r_{1},c_{3}) + q_{2}P\left(c_{2}^{d} - c_{3}^{d}r_{2}^{d}\right)}{P\left(r_{1}^{d}c_{3}^{d} - 1\right)}, \ q_{3} = \frac{(1-B)f(c_{3},r_{1}) + q_{2}P\left(r_{2}^{d} - r_{1}^{d}c_{2}^{d}\right)}{P\left(r_{1}^{d}c_{3}^{d} - 1\right)}$$
(120)

$$r_2 = \frac{r_1 c_3^d - 1 - c_2^d (r_1 - 1)}{c_3^d - 1}, \ r_2^d = \frac{r_1^d c_3 - 1 - c_2 (r_1^d - 1)}{c_3 - 1}, \tag{121}$$

$$f(x, y) := x^{d+1}y^{d+1} - x^d y^{d+1} - xy^{d+1} + y^d + y - 1, \ P := (r_1 - 1)(c_3 - 1) > 0.$$

We first show (121). Using the expressions for r_1, r_2 in (119), we obtain $\frac{r_1-1}{r_2-1} = \frac{c_3^d-1}{c_3^d-c_2^d}$ and solving for r_2 gives the first equation in (121). Similarly, using the expressions for c_2, c_3 in (119), we obtain $\frac{c_3-1}{c_2-1} = \frac{r_1^d-1}{r_1^d-r_2^d}$ and solving for r_2^d gives the second equation in (121). For future use, note that the equation $\frac{c_3-1}{c_2-1} = \frac{r_1^d-1}{r_1^d-r_2^d}$ yields also the expression $c_2 = \frac{r_1^dc_3-1-r_2^d(c_3-1)}{r_1^d-1}$. To derive (120), we plug this expression for c_2 as well as the expression

for r_2 in (121) in the last two equations in (119). This yields the following two equations:

$$\frac{r_1c_3^d - 1 - c_2^d(r_1 - 1)}{c_3^d - 1} = \frac{q_1 + (B + q_2 - 1)c_2^d + q_3c_3^d}{q_1 + q_2c_2^d + (B + q_3 - 1)c_3^d},$$
$$\frac{r_1^d c_3 - 1 - r_2^d(c_3 - 1)}{r_1^d - 1} = \frac{q_3 + (B + q_2 - 1)r_2^d + q_1r_1^d}{q_3 + q_2r_2^d + (B + q_1 - 1)r_1^d}.$$

By clearing denominators, this pair of equations yields a linear system in terms of q_1, q_3 . Solving this system, yields the expressions for q_1, q_3 in (120).

Having established (120) and (121), we show the following lemma which will be important for the proof of Lemma 7.19.

LEMMA 7.20. Assume that $q_1, q_2, q_3, r_1, r_2, c_2, c_3$ satisfy (118), (120), and (121). If $r_1 = c_3$, then $r_2 = c_2$ and $q_1 = q_3$.

PROOF OF LEMMA 7.20. We prove that $r_1 = c_3$ implies $r_2 = c_2$. Once this is done, (120) easily gives that $r_1 = c_3$ implies $q_1 = q_3$ as well, thus proving the lemma.

So, suppose that $z = r_1 = c_3$ and for the sake of contradiction assume $r_2 \neq c_2$. From (118), we have that $r_2, c_2 \in (1, z)$. Eliminating r_2 from (121) we obtain that c_2 (and, by a symmetric argument, r_2) satisfies

$$g(s) := \left(\frac{z^{d+1} - 1 - s^d(z-1)}{z^d - 1}\right)^d + \frac{s(z^d - 1) - (z^{d+1} - 1)}{z - 1} = 0$$

In fact, g(1) = g(z) = 0 as well, so that g has at least four distinct roots in [1, z]. It follows that g'(s) = 0 has at least three distinct solutions in [1, z], say s_i for i = 1, 2, 3. As a consequence of $g'(s_i) = 0$, we easily obtain that the s_i 's satisfy $h(s_i) = c$ where $h(s) := (z^{d+1} - 1)s - s^{d+1}(z - 1)$ and c is a constant which depends only on z, d. Thus, h'(s) = 0 has at least two distinct solutions in [1, z] which is clearly absurd. \Box

PROOF OF LEMMA 7.19. Set

$$DIF_{1,3} := \frac{\partial \overline{\Phi^S}}{\partial q_1} - \frac{\partial \overline{\Phi^S}}{\partial q_3}, \qquad DIF_{1,2} := \frac{\partial \overline{\Phi^S}}{\partial q_1} - \frac{\partial \overline{\Phi^S}}{\partial q_2}.$$

Our goal is to check when $DIF_{1,3} = 0$ or $DIF_{1,2} = 0$. To do this, we will write $DIF_{1,3}$ and $DIF_{1,2}$ in terms of the r_i 's and c_j 's. Note that the expressions in (113) for the derivatives $\frac{\partial \overline{\Phi^S}}{\partial q_i}$ are scale-free with respect to R_i 's and C_j 's, so we just need to make the substitutions (117). For $DIF_{1,3}$, we obtain

$$DIF_{1,3} = \frac{1}{S} \Big[(r_1^d - 1) (q_1 + q_2 c_2^d + q_3 c_3^d) - (c_3^d - 1) (q_1 r_1^d + q_2 r_2^d + q_3) + (d - 1)(1 - B) (r_1^d - c_3^d) \Big],$$
(122)

where $S := (q_1r_1^d + q_2r_2^d + q_3)(q_1 + q_2c_2^d + q_3c_3^d) + (B - 1)(q_1r_1^d + q_2r_2^dc_2^d + q_3c_3^d)$. Note that S > 0 because of (110).

To prove the first part of the lemma, we eliminate q_1, q_3 from the expression (122) for $DIF_{1,3}$ using (120) (one does not need to worry about S). This substitution has the beneficial effect of eliminating q_2, r_2, c_2 from the final expression. In particular, we obtain the following:

$$DIF_{1,3} = -\frac{(1-B)g(r_1, c_3)}{S(r_1 - 1)(c_3 - 1)}, \text{ where}$$

$$g(r_1, c_3) := (r_1 - c_3)(r_1^d - 1)(c_3^d - 1) - d(r_1 - 1)(c_3 - 1)(r_1^d - c_3^d).$$
(123)

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Observe that if $r_1 = c_3$, then $g(r_1, c_3) = 0$. If $r_1 \neq c_3$, we have

$$\frac{g(r_1,c_3)}{d^2(r_1-1)(c_3-1)(r_1-c_3)} = \frac{\sum_{i=0}^{d-1} r_1^i}{d} \frac{\sum_{i=0}^{d-1} c_3^{d-i}}{d} - \frac{\sum_{i=0}^{d-1} r_1^i c_3^{d-i}}{d} > 0,$$

where in the last inequality we used Chebyshev's sum inequality: since $r_1 > 1$ and $c_3 > 1$ from (118), the sequence r_1^i (respectively, c_3^{d-i}) is strictly increasing (respectively, decreasing) with *i*. It follows that $g(r_1, c_3) = 0$ iff $r_1 = c_3$ iff $R_1/R_3 = C_3/C_1$, which yields the first part of the lemma.

We next prove the second part of the lemma. Since $R_1/R_3 = C_3/C_1$, we have $r_1 = c_3$ and by Lemma 7.20, $r_2 = c_2$ and $q_1 = q_3$. Using these, (120) and (121) simplify to

$$q_1 = \frac{(1-B)(r_1^{d+1}-1) - q_2 r_2^d(r_1-1)}{(r_1-1)(r_1^d+1)}, \ r_2 = \frac{r_1^{d+1}-1 - r_2^d(r_1-1)}{r_1^d-1}.$$
 (124)

Moreover, using the substitutions (117) and $q_1 = q_3$, we obtain

$$DIF_{1,2} = \frac{1}{S} \Big[(q_1 r_1^d + q_2 r_2^d + q_1) (r_1^d - 2r_2^d + 1) + (d - 1)(1 - B)(r_1^d - r_2^{2d}) \Big] \\ = -\frac{(1 - B)}{(r_1 - 1)S} \Big[(d - 1)(r_1 - 1)r_2^{2d} + 2r_2^d (r_1^{d+1} - 1) - (r_1^{2d+1} + dr_1^{d+1} - dr_1^d - 1) \Big],$$

where in the second equality we substituted the value of q_1 from (124). Observe that the numerator is a quadratic polynomial in r_2^d and, by inspection, for $r_1 > 1$, its roots are of opposite sign. Thus, $DIF_{1,2} = 0$ iff $r_2^d = \rho_1$, where

$$\rho_1(r_1) := \frac{\sqrt{D} - (r_1^{d+1} - 1)}{(d-1)(r_1 - 1)} \text{ and } D := \left(dr_1^{d+1} - (d-1)r_1^d - 1\right)\left(r_1^{d+1} + (d-1)r_1 - d\right).$$

For the sake of contradiction, suppose that $r_2^d = \rho_1$. Then, (124) gives that $r_2 = \rho_2$, where

$$\rho_2(r_1) := \frac{d(r_1^{d+1} - 1) - \sqrt{D}}{(d-1)(r_1^d - 1)}.$$

Thus, $\rho_1 = \rho_2^d$. We obtain a contradiction by showing that for every $r_1 > 1$, it holds that $\rho_2^d < \rho_1$ or equivalently $d \ln \rho_2 < \ln \rho_1$. It is easy to see that in the limit $r_1 \downarrow 1$ the inequality is satisfied at equality, thus it suffices to prove that the derivative of the right-hand side with respect to r_1 is greater than the respective derivative of the left-hand side for $r_1 > 1$.

This differentiation is cumbersome but otherwise straightforward. The final result is

$$\frac{1}{\rho_{1}} \frac{\partial \rho_{1}}{\partial r_{1}} - \frac{d}{\rho_{2}} \frac{\partial \rho_{2}}{\partial r_{1}} = \frac{(d+1)g(r_{1})h(r_{1})}{2(r_{1}-1)\left(r_{1}^{d}-1\right)\left(\sqrt{D}-(r_{1}^{d+1}-1)\right)\left(d(r_{1}^{d+1}-1)-\sqrt{D}\right)}, \quad (125)$$

$$g(r_{1}) \coloneqq r_{1}^{2d} - d^{2}r_{1}^{d+1} + 2(d^{2}-1)r_{1}^{d} - d^{2}r_{1}^{d-1} + 1,$$

$$h(r_{1}) \coloneqq (d+1)\left(r_{1}^{d+1}-1\right) - (d-1)\left(r_{1}^{d}-r_{1}\right) - 2\sqrt{D}.$$

Note that the denominator in the right-hand side of (125) is positive for $r_1 > 1$: the terms involving \sqrt{D} are positive since they are the numerators of ρ_1 , ρ_2 . The final part of the proof consists of proving that $g(r_1) > 0$ and $h(r_1) > 0$ for $r_1 > 1$.

The polynomial g has four sign changes and hence, by the Descartes' rule of signs has at most four positive roots. In fact, a tedious calculation shows that $r_1 = 1$ is a

root by multiplicity 4, thus proving that $g(r_1) > 0$ for $r_1 > 1$. To prove that $h(r_1) > 0$ for $r_1 > 1$, note the identity

$$\left[(d+1)(r_1^{d+1}-1) - (d-1)(r_1^d-r_1)\right]^2 - 4D = (d-1)^2(r_1-1)^2(r_1^d-1)^2$$

This completes the proof of Lemma 7.19. \Box

To prove the second part of Lemma 7.15, assume that $\mathbf{q} = (q_1, q_2, q_3)$ is a 2-maximal good triple. Since **q** is 2-maximal, without loss of generality, we may assume that $q_2 = 0$. Note that the values of R_2 , C_2 do not affect the value of the derivatives $\partial \overline{\Phi^S} / \partial q_1$, $\partial \overline{\Phi^S} / \partial q_3$ when $q_2 = 0$. Similarly, (120) continues to hold even when $q_2 = 0$. Thus, the proof of the first part of Lemma 7.19 carries through verbatim. In particular, if $R_1/R_3 \neq C_3/C_1$, then $\partial \overline{\Phi^S} / \partial q_1 - \partial \overline{\Phi^S} / \partial q_3 \neq 0$. By the second part of Lemma 7.18, it follows that $\mathbf{q} = (q_1, 0, q_3)$ cannot be a maximum unless $R_1/R_3 = C_3/C_1$. In this case, (120) gives $q_1 = q_3$. Since $q_1 + q_3 = q$, we obtain that the only 2-maximal good triples where the maximum of $\overline{\Phi}$ may occur are (q/2, q/2, 0) or its permutations, as desired.

This concludes the proof of Lemma 7.15.

7.4. Bad Triples: Proof of Lemma 7.16

To get a handle on bad triples, we first give necessary conditions so that the maximum in (109) happens at the boundary. The proof of the following lemma is given in Section 7.5.

LEMMA 7.21. Let $0 \le B < 1$. For a triple $\mathbf{q} = (q_1, q_2, q_3)$, let \mathbf{r}, \mathbf{c} achieve the maximum in (109). Then, if $q_i > 0$, the following implications hold:

$$R_i = 0 \Rightarrow \sum_j q_j C_j \le (1 - B)C_i, \quad C_i = 0 \Rightarrow \sum_j q_j R_j \le (1 - B)R_i.$$

In particular, if $q_i > 1 - B$, it holds that $R_i, C_i > 0$. Hence, for every $q \ge 3$, there exists $i \in \{1, 2, 3\}$ such that $R_i, C_i > 0$.

We next examine bad triples. Note that a bad triple $\mathbf{q} = (q_1, q_2, q_3)$, by the second part of Lemma 7.21, must have at least two positive entries. We consider cases whether the triple \mathbf{q} has two or three positive entries. We start with the case where exactly two of the q_i 's are positive. We assume throughout the rest of the section that **r**, **c** achieve the maximum in (109).

Let $\mathbf{q} = (q_1, q_2, 0)$ be a bad triple where $q_1, q_2 > 0$. Since \mathbf{q} is bad, we may assume that at least one of R_1, R_2, C_1, C_2 is zero. Without loss of generality, we may assume $C_2 = 0$. By the second part of Lemma 7.21, it follows that $R_1, C_1 > 0$. There are two cases to consider.

(I)
$$R_2 = 0$$
, (II) $R_2 > 0$. (126)

Case (I) is straightforward. By the first part of Lemma 7.18, we trivially have $\frac{\partial \overline{\Phi^S}}{\partial q_1} > 0$ and $\frac{\partial \overline{\Phi^S}}{\partial q_2} = 0$, so that the second part of Lemma 7.18 yields that **q** does not maximize $\overline{\Phi}$.

Case (II). Since $\overline{\Phi^S}$ is scale-free (see (111)), we may assume that $C_1 = 1$. Since R_1, R_2 are positive, it holds that $\partial \overline{\Phi^S} / \partial R_1 = \partial \overline{\Phi^S} / \partial R_2 = 0$, yielding (analogously to (114))

$$R_1 \propto y^d$$
, $R_2 \propto 1$, where $y = (q_1 + B - 1)/q_1$.

Observe that $q_1y^{d+1} + q_2 = q_2 + (q_1 + B - 1)y^d$. Substituting the values of R_i 's, C_j 's in Φ^S , we obtain the value of $\overline{\Phi}(\mathbf{q})$:

$$\overline{\Phi}(\mathbf{q}) = (d+1)\ln\left((q_1y^d + q_2)q_1 + (B-1)q_1y^d\right) - d\ln\left(q_1y^{d+1} + q_2\right) - d\ln q_1 = \ln\left(q_1(q_2 + (q_1 + B - 1)y^d)\right).$$

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In terms of y, we have that $q_1 = (1 - B)/(1 - y)$ and $q_2 = q - q_1 = q - (1 - B)/(1 - y)$, so we obtain

$$\overline{\Phi}(\mathbf{q}) = \ln h(y)$$
, where $h(y) := \frac{(1-B)(q(1-y)-(1-B)(1-y^{d+1}))}{(1-y)^2}$.

Let *I* be the interval [0, (q+B-1)/q]. Note that for any $y \in I$, there exists a nonnegative $q_1 \in [0, q]$ such that $y = (q_1 + B - 1)/q_1$. Obviously, if **q** maximizes $\overline{\Phi}$, it must be the case that *y* maximizes h(y) in the interval *I*. We compute h'(y).

$$h'(y) = \frac{(1-B)r(y)}{(1-y)^3}$$
, where $r(y) := q(1-y) - (1-B)((d-1)y^{d+1} - (d+1)y^d + 2)$.

It is immediate to see that r(y) is convex for $y \in [0, 1]$. Since r(0) = q - 2(1 - B) > 0 and r(1) = 0, we obtain that either

(i)
$$r(y) > 0$$
 for all $y \in I$, or
(ii) $\exists y_o \in I: r(y_o) = 0, r(y) > 0$ iff $y < y_o$.

In case (i), h(y) is increasing and hence h(y) is maximized at y = (q + B - 1)/q. This value of y corresponds to $q_1 = q$ and thus $\Phi(\mathbf{q}) = \Phi(q, 0, 0)$.

In case (ii), we have $h(y) \leq h(y_0)$. The value of q_1 corresponding to y_0 is $q_0 := (1 - B)/(1 - y_0)$. We will show that the maximum in (109) does not happen at the boundary $C_2 = 0$ when $\mathbf{q} = (q_0, q - q_0, 0)$, implying that $h(y_0)$ does not equal $\overline{\Phi}(\mathbf{q})$ and hence the maximum of $\overline{\Phi}$ as well. To prove the former, we utilize the first part of Lemma 7.21. In particular, we prove that

$$q_o y_o^d + (q - q_o) > (1 - B).$$
(127)

Note that $r(y_o) = 0$ yields $q = (1 - B)((d - 1)y_o^{d+1} - (d + 1)y_o^d + 2)/(1 - y_o)$. Plugging this expression into (127), we only need to show that

$$\frac{(d-1)y_o^{d+1} - dy_o^d + 1}{1 - y_o} > 1 \text{ or } (d-1)y_o^d + 1 > dy_o^{d-1},$$
(128)

which holds by the AM-GM inequality for any positive $y_o \neq 1$.

Let $\mathbf{q} = (q_1, q_2, q_3)$ be a bad triple where all of the q_i 's are positive. Since \mathbf{q} is bad, we may assume that at least one of the R_i 's and C_j 's is zero. Without loss of generality, we may assume $C_2 = 0$. Moreover, by the second part of Lemma 7.21, we may also assume that $R_1, C_1 > 0$. There are four cases to consider.

(I)
$$R_2 = 0$$
, (II) $R_2, R_3 > 0, C_3 = 0$, (III) $R_2, R_3, C_3 > 0$, (IV) $R_2, C_3 > 0, R_3 = 0$.

We omitted the case $R_2 > 0$ and $R_3 = C_3 = 0$, which is identical to Case (I) after renaming the q_i 's.

Case (I) is straightforward. Since $R_2 = C_2 = 0$, (113) gives $\partial \overline{\Phi^S} / \partial q_2 = 0$. Since $R_1, C_1 > 0$, (113) also gives that $\partial \overline{\Phi^S} / \partial q_1 > 0$, so the second part of Lemma 7.18 yields that **q** does not maximize $\overline{\Phi}$.

Case (II). Since $\overline{\Phi^S}$ is scale-free (see (111)), we may substitute $C_1 = 1$. Setting the derivatives of $\partial \overline{\Phi^S} / \partial R_1$, $\partial \overline{\Phi^S} / \partial R_2$, $\partial \overline{\Phi^S} / \partial R_3$ equal to zero, we obtain

$$R_1 \propto (q_1 + B - 1)^d / q_1^d, \ R_2 \propto 1, \ R_3 \propto 1.$$

It follows that $\overline{\Phi}(\mathbf{q}) = \overline{\Phi}(q_1, q_2 + q_3, 0)$ and hence the maximum of $\overline{\Phi}$ does not occur at \mathbf{q} by the argument for Case (II) in (126).

Case (III). The partial derivatives of $\overline{\Phi^S}$ with respect to R_1, R_2, R_3, C_1, C_3 must vanish so we obtain

$$R_{1}^{1/d} \propto q_{1}C_{1} + q_{2}C_{3} - (1-B)C_{1}, \ R_{2}^{1/d} \propto q_{1}C_{1} + q_{3}C_{3}, \ R_{3}^{1/d} \propto q_{1}C_{1} + q_{3}C_{3} - (1-B)C_{3}, \\ C_{1}^{1/d} \propto q_{1}R_{1} + q_{2}R_{2} + q_{3}R_{3} - (1-B)R_{1}, \ C_{3}^{1/d} \propto q_{1}R_{1} + q_{2}R_{2} + q_{3}R_{3} - (1-B)R_{3}.$$
(129)

If $C_1 = C_3$, then $R_1 = R_3$ and thus we obtain $\overline{\Phi}(q_1, q_2, q_3) \leq \overline{\Phi}(q_1 + q_3, q_2, 0)$. For the sake of contradiction, suppose that the maximum of $\overline{\Phi}$ was attained at $\mathbf{q} = (q_1, q_2, q_3)$. Then, it must also be attained by $\mathbf{q}' := (q_1 + q_3, q_2, 0)$, that is, $\overline{\Phi}(\mathbf{q}) = \max \Phi = \overline{\Phi}(\mathbf{q}')$. Note that the same \mathbf{r}, \mathbf{c} which achieve the maximum in (109) for $\mathbf{q} = (q_1, q_2, q_3)$ must also achieve the maximum in (109) for $\mathbf{q}' = (q_1 + q_3, q_2, 0)$ (since $\overline{\Phi^S}(\mathbf{q}', \mathbf{r}, \mathbf{c}) = \overline{\Phi^S}(\mathbf{q}, \mathbf{r}, \mathbf{c}) = \overline{\Phi}(\mathbf{q}) = \max \overline{\Phi} = \overline{\Phi}(\mathbf{q}')$). We can thus apply the argument for Case (II) in (126) to show that the maximum of $\overline{\Phi}$ is not attained at $\mathbf{q}' = (q_1 + q_3, q_2, 0)$ and hence not at $\mathbf{q} = (q_1, q_2, q_3)$ as well.

Thus, we may assume that $C_1 \neq C_3$ and, without loss of generality, we may further assume that $C_1 < C_3$. By (129), this yields

$$R_2 > R_1 > R_3, \ C_1 < C_3. \tag{130}$$

We have the following analogue of Lemma 7.19, which proves that the maximum cannot occur at \mathbf{q} by the second part in Lemma 7.18.

LEMMA 7.22. Suppose that R_i 's and C_j 's satisfy (129) and (130). If $R_1/R_3 \neq C_3/C_1$, then $\frac{\partial \overline{\Phi^S}}{\partial q_1} - \frac{\partial \overline{\Phi^S}}{\partial q_3} \neq 0$. If $R_1/R_3 = C_3/C_1$, then $\frac{\partial \overline{\Phi^S}}{\partial q_1} - \frac{\partial \overline{\Phi^S}}{\partial q_2} \neq 0$.

PROOF OF LEMMA 7.22. The proof is analogous to the proof of Lemma 7.19, we highlight the main differences. Let $r_1^d = R_1/R_3$, $r_2^d = R_2/R_3$, $c_3^d = C_3/C_1$. The R_i 's and C_j 's may be recovered by the r_i 's and c_j 's by

$$R_1 \propto r_1^d, R_2 \propto r_2^d, R_3 \propto 1, \text{ and } C_1 \propto 1, C_3 \propto c_3^d.$$

$$(131)$$

By (130), we have

$$r_2 > r_1 > 1$$
 and $c_3 > 1$.

The expressions for r_1, r_2, c_3 in (119) are exactly the same after substituting $c_2 = 0$. The same is true for (120) and (121) (our derivation for r_2 in (121) holds as is; for (120), one needs to view the expressions for r_1, c_3 in (119) as a system of q_1, q_3 and solve it). It follows that the proof for the first part of Lemma 7.19 holds verbatim in this case as well (note that the ordering of r_1, r_2 is different here but that part of the argument does not use the ordering).

While the proof for the second part of Lemma 7.19 does not carry through as simply, the changes are minor. We assume that $r_1 = c_3$ and set $DIF_{1,2} := \frac{\partial \overline{\Phi^S}}{\partial q_1} - \frac{\partial \overline{\Phi^S}}{\partial q_2}$. Plugging $r_1 = c_3$ and $c_2 = 0$ in (120) and (121) (recall that only the expression for r_2 in (121) is valid) yields, with $T := (r_1^d - 1)(r_1^{d+1} - 1)$,

$$q_1 = \frac{(1-B)T - q_2(r_1-1)r_1^d r_2^d}{(r_1-1)\left(r_1^{2d}-1\right)}, \quad q_3 = \frac{(1-B)T + q_2(r_1-1)r_2^d}{(r_1-1)\left(r_1^{2d}-1\right)}, \quad r_2 = \frac{r_1^{d+1}-1}{r_1^d-1}.$$
 (132)

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We then use the expressions for $\frac{\partial \overline{\Phi^S}}{\partial q_1}$, $\frac{\partial \overline{\Phi^S}}{\partial q_2}$ given in Lemma 7.18 together with the substitutions for R_i 's and C_j 's in (131) (and $C_2 = 0$). We obtain

$$\begin{aligned} DIF_{1,2} &= \frac{1}{S} \Big[\big(r_1^d - r_2^d \big) \big(q_1 + q_3 c_3^d \big) - \big(q_1 r_1^d + q_2 r_2^d + q_3 \big) + (d-1)(1-B) r_1^d \Big] \\ &= \frac{(1-B) h(r_1)}{S(r_1-1)}, \text{ where } h(r_1) \coloneqq \big(r_1^{2d+1} + dr_1^{d+1} - dr_1^d - 1 \big) - \frac{\big(r_1^{d+1} - 1 \big)^{d+1}}{\big(r_1^d - 1 \big)^d}, \end{aligned}$$

where $S := (q_1r_1^d + q_2r_2^d + q_3)(q_1 + q_3c_3^d) + (B - 1)(q_1r_1^d + q_3c_3^d)$ (recall that S > 0 because of (110)). To obtain the second equality, one first substitutes the values of q_1, q_3 from (132) and $c_3 = r_1$; this results in q_2 being eliminated, and then it remains to substitute the value of r_2 given in (132).

By a first derivative argument, the function

$$g(r_1) := \log \bigg(rac{\left(r_1^{d+1}-1
ight)^{d+1}}{\left(r_1^d-1
ight)^d \left(r_1^{2d+1}+dr_1^{d+1}-dr_1^d-1
ight)} \bigg),$$

is strictly increasing for $r_1 > 1$. Indeed, by a direct differentiation, we obtain

$$g'(r_1) = \frac{(d+1)r_1^d \left(r_1^{2d} - d^2 r_1^{d+1} + 2(d^2 - 1)r_1^d - d^2 r_1^{d-1} + 1\right)}{(r_1^d - 1)(r_1^{d+1} - 1)(r_1^{2d+1} + dr_1^{d+1} - dr_1^d - 1)}$$

The denominator of this last expression is positive for $r_1 > 1$. To prove that the numerator is also positive for $r_1 > 1$, it suffices to show that $r_1^{2d} - d^2r_1^{d+1} + 2(d^2-1)r_1^d - d^2r_1^{d-1} + 1 > 0$ for $r_1 > 1$. This has been proved earlier, see (125) and the argument thereafter. Hence, we can conclude that g is an increasing function of r_1 in the interval $[1, +\infty)$. It follows that $g(r_1) < g(+\infty) = 0$, so that $h(r_1) > 0$ for all $r_1 > 1$. This proves that $DIF_{1,2} \neq 0$, as desired. \Box

Case (IV). The partial derivatives of $\overline{\Phi^S}$ with respect to R_1 , R_2 , C_1 , C_3 must vanish so we obtain

$$R_1^{1/d} \propto q_1 C_1 + q_3 C_3 - (1 - B)C_1, \quad R_2^{1/d} \propto q_1 C_1 + q_3 C_3, C_1^{1/d} \propto q_1 R_1 + q_2 R_2 - (1 - B)R_1, \quad C_3^{1/d} \propto q_1 R_1 + q_2 R_2.$$
(133)

Note that we have $R_1 < R_2$ and $C_1 < C_3$.

LEMMA 7.23. If $R_2/R_1 \neq C_3/C_1$, then either $\frac{\partial \overline{\Phi^S}}{\partial q_2} - \frac{\partial \overline{\Phi^S}}{\partial q_3} \neq 0$ or $\frac{\partial \overline{\Phi^S}}{\partial q_1} - \frac{\partial \overline{\Phi^S}}{\partial q_2} \neq 0$. If $R_2/R_1 = C_3/C_1$ and $\frac{\partial \overline{\Phi^S}}{\partial q_1} - \frac{\partial \overline{\Phi^S}}{\partial q_2} = 0$, then the maximum in (109) does not happen at the boundary $C_2 = 0$.

PROOF OF LEMMA 7.23. The approach for the first part is similar to the proof of Lemma 7.19. Set $r_2^d = R_2/R_1$ and $c_3^d = C_3/C_1$, so that $r_1, c_3 > 1$. Dividing appropriate pairs in (133), we obtain

$$r_2 = \frac{q_1 + q_3 c_3^d}{(q_1 + B - 1) + q_3 c_3^d}, \quad c_3 = \frac{q_1 + q_2 r_2^d}{(q_1 + B - 1) + q_2 r_2^d}.$$
 (134)

It follows that

$$q_2 = \frac{q_1 - (q_1 + B - 1)c_3}{r_2^d(c_3 - 1)}, \quad q_3 = \frac{q_1 - (q_1 + B - 1)r_2}{c_3^d(r_2 - 1)}.$$
(135)

Using these, we obtain

$$\frac{\partial \Phi^{\overline{S}}}{\partial q_2} - \frac{\partial \overline{\Phi^{\overline{S}}}}{\partial q_3} = 0 \Rightarrow f(r_2) = f(c_3), \text{ where } f(x) := \frac{x^{d+1}}{x-1}, \tag{136}$$

$$\frac{\partial \Phi^S}{\partial q_1} - \frac{\partial \Phi^S}{\partial q_2} = 0 \Rightarrow r_2^{d+1}(c_3 - 1) - (d+1)r_2c_3 + d(r_2 + c_3) - (d-1) = 0.$$
(137)

From (137), we obtain

$$c_3 = g(r_2), \text{ where } g(r_2) := \frac{r_2^{d+1} - dr_2 + (d-1)}{r_2^{d+1} - (d+1)r_2 + d}.$$
 (138)

It follows that $r_2 = c_3$ is equivalent to

$$r_2^{d+1} = (d+1)r_2 - (d-1).$$
(139)

A standard first derivative argument shows that (139) has exactly one solution for $r_2 > 1$, say $r_2 = x$. Using the expression for c_3 from (138), (136) gives

$$h(r_2) = 0$$
, where $h(r_2) := r_2^{d+1} - \frac{\left(r_2^{d+1} - dr_2 + (d-1)\right)^{d+1}}{\left(r_2^{d+1} - (d+1)r_2 + d\right)^d}$

Lengthy calculations show that h is strictly increasing for $r_2 > 1$ (and every $d \ge 2$), see Appendix D.3 for the details. Moreover, it holds that h(x) = 0, so that (136) and (137) can only hold simultaneously when $r_2 = c_3$, which yields the first part of the lemma.

For the second part, we have that $r_2 = c_3$ and $\frac{\partial \overline{\Phi^S}}{\partial q_1} - \frac{\partial \overline{\Phi^S}}{\partial q_2} = 0$, and hence from (137), we obtain that r_2 also satisfies (139). To prove that the maximum does not happen at the boundary $C_2 = 0$, we use the first part of Lemma 7.21. It suffices to prove that

$$q_1 + q_2 r_2^d > (1 - B) r_2^d. (140)$$

Since $r_2 = c_3$, Eq. (135) gives $q_2 = q_3 = (q - q_1)/2$ (using also that $q_1 + q_2 + q_3 = q$), so (134) gives

$$q_1 = \frac{q(r_2^{d+1} - r_2^d) - 2r_2(1 - B)}{(r_2 - 1)(r_2^d - 2)}, \quad q_2 = q_3 = \frac{q - r_2(q + B - 1)}{(r_2 - 1)(r_2^d - 2)}.$$
(141)

Since r_2 satisfies (139), we have that $r_2^d > 2$ (otherwise, $r_2^{d+1} \le 2r_2 < (d+1)r_2 - (d-1)$). Plugging (141) into (140) thus yields the equivalent inequality

$$\frac{(1-B)(r_2^d+r_2-r_2^{d+1})}{r_2-1}>0.$$

To see the latter, use (139) to obtain

$$r_2^d + r_2 - r_2^{d+1} = r_2^d + (d-1) - dr_2 > 0$$
, for all $r_2 > 1$ by the AM-GM inequality

This completes the proof. \Box

7.5. Remaining Proofs

PROOF OF LEMMA 7.6. Without loss of generality, we may assume that the scaling factors in (107) are equal to 1. Let $R_i = r_i^d$, $C_i = c_i^d$, $r = \sum_{i=1}^q r_i^d$, and $c = \sum_{i=1}^q c_i^d$. We have

$$r_i = c - (1 - B)c_i^d$$
 and $c_i = r - (1 - B)r_i^d$

It is clear from this equation that $R_i = R_j$ iff $C_i = C_j$ and hence also $t_R = t_C$. We also obtain that for i = 1, ..., q,

$$r_i = c - (1 - B)(r - (1 - B)r_i^d)^d.$$
(142)

Since *r* is the sum of r_i^d and the r_i are positive, we have $(1 - B)r_i^d < r$. Fix the values of *r*, *c* and let *I* be the interval where $(1 - B)x^d < r$. Using (142), we shall prove that $t_R \leq 3$ by arguing that $f(x) = c - (1 - B)(r - (1 - B)x^d)^d - x$ has at most three positive roots in the interval *I*, counted by multiplicities. We have

$$f'(x) = (1-B)^2 d^2 (r - (1-B)x^d)^{d-1} x^{d-1} - 1 = \left(\sum_{i=0}^{d-2} g(x)^i\right) (g(x) - 1),$$

where

$$g(x) = ((1 - B)d)^{2/(d-1)}(r - (1 - B)x^d)x.$$

Note that g(x) > 0 in the interval I and hence all roots of f'(x) in this interval come from g(x) - 1. The polynomial g(x) - 1 has at most two positive roots by Descartes' rule of signs, hence f'(x) has at most two positive roots in I. Thus, f(x) has at most three positive roots in I, all roots counted by their multiplicities. This concludes the proof. \Box

PROOF OF LEMMA 7.9. Let q' = q/2. Recall from Theorem 4.1 that the maxima of Ψ_1 are in one-to-one correspondence with fixpoints of the tree recursions (107). To better align with the results of Section 7.3, let us assume that the fixpoint is of type (q', 0, q') (note, by Lemma 7.8, such a fixpoint corresponds to a maximum of Ψ_1). In Section 7.3, we proved that this can be the case only if $R_1/R_3 = C_3/C_1$ or (in the parameterization of Section 7.3) $r_1 = c_3 =: x$ where x > 1. Equation (119) for $q_2 = 0$, $q_1 = q_3 = q'$ gives that x satisfies

$$x = \frac{B + q' - 1 + q' x^d}{q' + (B + q' - 1)x^d},$$
(143)

where recall that $d = \Delta - 1$. We first prove that (143) has exactly one solution x > 1 for all $0 \le B < \frac{\Delta - q}{\Lambda}$. We can rewrite (143) as

$$p(x) := (B+q'-1)x^{d+1} - q'x^d + q'x - (B+q'-1) = 0.$$

We have p(1) = 0 and p'(1) = (d + 1)(B + q' - 1) - (d - 1)q' < 0, where in the last inequality we used that $B < (\Delta - q)/\Delta$. Thus, p(x) is negative for some x > 1 and since p(x) is positive for large x, we can conclude that a root ρ with $\rho > 1$ exists. Note that $1/\rho$, 1, ρ are three distinct roots of p(x). Applying Descartes' rule of signs, we obtain that these must be the only roots and hence ρ is the only positive root of p(x) greater than 1, as wanted.

The values of R_1, C_1, R_3, C_3 may be recovered by (117), which in the case $q_2 = 0$ give

$$R_1 \propto x^d, R_3 \propto 1 ext{ and } C_1 \propto 1, C_3 \propto x^d.$$

This proves the second part of Lemma 7.9.

For the first part, to check Jacobian stability of the fixpoint $(R_1, \ldots, R_q, C_1, \ldots, C_q)$ with type (q', q', 0), we proceed as in the proof of Lemma 7.4. Note that a fixpoint of type (q', q', 0) has $R_1 = \cdots = R_{q'}$ and $R_{q'+1} = \cdots = R_{2q'}$ (and similarly for the $C'_j s$). Recall that the condition for Jacobian stability is related to the spectrum of $\mathbf{L} = \begin{bmatrix} 0 & \mathbf{A} \\ \mathbf{A}^{\mathsf{T}} & 0 \end{bmatrix}$ where \mathbf{A} is the $q \times q$ matrix whose (i, j)-entry is given by $B_{ij}R_iC_j/\sqrt{\alpha_i\beta_j}$ and α_i, β_j are given by (29). Moreover, 1 and -1 are eigenvalues of \mathbf{L} and the condition for Jacobian stability is that all the other eigenvalues have absolute value less than $1/(\Delta - 1)$. Finally, recall that the spectrum of \mathbf{L} is symmetric with respect to 0, see footnote 3.

The eigenvalues of the matrix **L** in this case (with the specific matrix **B** and the values of R_i 's and C_j 's) can be computed as follows. Let $i \neq j$ be such that $R_i = R_j$, we then have $C_i = C_j$, $\alpha_i = \alpha_j$ and $\beta_i = \beta_j$ as well. The (2q)-dimensional vector whose nonzero entries are 1's at the positions of R_i , C_i (i.e., the *i*th and (i + q)-th coordinate) and -1's at the positions of R_j , C_j is an eigenvector of **L**; also the vector with 1's at the positions of R_i , C_j and -1's at the positions of R_j , C_i (and zero elsewhere) is an eigenvector of **L**. This gives us the eigenvalues $\pm \lambda_1$ each with multiplicity 2q' - 2 = q - 2, where

$$\lambda_1 := (1-B) \frac{R_1 C_1}{\sqrt{\alpha_1 \beta_1}} = \frac{(1-B) x^{d/2}}{\sqrt{(q' + (B+q'-1) x^d)(B+q'-1+q' x^d)}}$$

Denote by $\pm X$ the remaining eigenvalues of **L**. We can compute X by considering the determinant of **L**. We have $\text{Det}(\mathbf{L}) = (-1)^q (\text{Det}(\mathbf{A}))^2$. Note that $\text{Det}(\mathbf{A}) = \text{Det}(\mathbf{B}) \prod_i \frac{R_i}{\sqrt{\alpha_i}} \prod_j \frac{C_j}{\sqrt{\beta_j}}$, so $\text{Det}(\mathbf{A}) = (-1)^{q-1}(1-B)^{q-1}(B+q-1)(\frac{R_1C_1}{\sqrt{\alpha_1\beta_1}})^q$. We thus obtain

$$X^2(1-B)^{2(q-2)}\left(\frac{R_1C_1}{\sqrt{\alpha_1\beta_1}}\right)^{2(q-2)} = (B+q-1)^2(1-B)^{2(q-1)}\left(\frac{R_1C_1}{\sqrt{\alpha_1\beta_1}}\right)^{2q},$$

and hence the eigenvalues of **L** are given by ± 1 by multiplicity $1, \pm \lambda_1$ by multiplicity q - 2 and $\pm \frac{B+q-1}{1-B}\lambda_1^2$ by multiplicity 1.

To prove that the absolute values of the eigenvalues different from 1 are less than 1/d, it suffices to prove that $\lambda_1 < 1/d$ (since $\frac{B+q-1}{1-B} < d$ for $B < \frac{d+1-q}{d+1}$). Use (143) to solve for q' and plug the value into the expression for λ_1 . This yields that λ_1 is equal to $x^{(d-1)/2}(x-1)/(x^d-1)$, which by the AM-GM inequality is less than 1/d for x > 1. \Box

PROOF OF LEMMA 7.10. For nonnegative $\mathbf{q} = (q_1, q_2, q_3)$ with $q_1 + q_2 + q_3 = q$, consider the function

$$\overline{F}(\mathbf{q}) = \max_{\mathbf{r},\mathbf{c}} F(\mathbf{q},\mathbf{r},\mathbf{c}), \text{ where } F(\mathbf{q},\mathbf{r},\mathbf{c}) := \sum_{i=1}^{3} q_i R_i \sum_{j=1}^{3} q_j C_j + (B-1) \sum_{i=1}^{3} q_i R_i C_i,$$
(144)

and the maximum is over the compact region (by restricting to $R_i = C_i = 0$ whenever $q_i = 0$)

$$\sum_{i=1}^{3} q_i R_i^{(d+1)/d} \le 1, \ \sum_{j=1}^{3} q_j C_j^{(d+1)/d} \le 1,
R_1, R_2, R_3, C_1, C_2, C_3 \ge 0.$$
(145)

Note that $\overline{F}(\mathbf{q}) > 0$, since we can set all of the R_i 's and C_j 's equal to x, where $qx^{(d+1)/d} = 1$. We have that $\overline{\Phi}(\mathbf{q}) \ge (d+1) \ln \overline{F}(\mathbf{q})$ since for the \mathbf{r}, \mathbf{c} which achieve the maximum in (144) we have $\overline{\Phi^S}(\mathbf{q}, \mathbf{r}, \mathbf{c}) \ge (d+1) \ln \overline{F}(\mathbf{q})$. Also, since $\overline{\Phi^S}(\mathbf{q}, \mathbf{r}, \mathbf{c})$ is scale-free with respect to \mathbf{r} and \mathbf{c} (see (111)), we may scale \mathbf{r}, \mathbf{c} to satisfy (145) and hence $\overline{\Phi}(\mathbf{q}) = \sup_{\mathbf{r}, \mathbf{c}} \overline{\Phi^S}(\mathbf{q}, \mathbf{r}, \mathbf{c}) \le (d+1) \ln \overline{F}(\mathbf{q})$, proving that $\overline{\Phi}(\mathbf{q}) = (d+1) \ln \overline{F}(\mathbf{q})$ and consequently the supremum is attained.

To prove that $\sup_{\mathbf{q}} \overline{\Phi}(\mathbf{q})$ is attained, it suffices to prove that $L := \sup_{\mathbf{q}} \overline{F}(\mathbf{q})$ is attained. This can be accomplished by using variants of Berge's Maximum Theorem and showing that the function $\overline{F}(\mathbf{q})$ is upper semicontinuous. We give a more direct argument, which is similar to the proof of Berge's Maximum Theorem and can also easily be adapted to show that $\overline{F}(\mathbf{q})$ is upper semicontinuous.

Note first that $L < \infty$ by a simple application of Hölder's inequality. Let \mathbf{q}_n , n = 1, 2, ... be a sequence such that $\overline{F}(\mathbf{q}_n) \uparrow L$. Since the \mathbf{q}_n lie in a compact region, by

restricting to a subsequence we may assume that $\mathbf{q}_n \to \mathbf{q}$. Let \mathbf{r}_n , \mathbf{c}_n be maximizers for $\overline{F}(\mathbf{q}_n)$ in (144).

Suppose first that **q** has positive entries. Then, for sufficiently large *n*, the maximizers \mathbf{r}_n , \mathbf{c}_n lie in a compact set and hence a standard diagonalisation argument yields a convergent subsequence $(\mathbf{q}_{n_k}, \mathbf{r}_{n_k}, \mathbf{c}_{n_k}) \rightarrow (\mathbf{q}, \mathbf{r}, \mathbf{c})$. By continuity, \mathbf{r}, \mathbf{c} must lie in the region (145) defined by **q** and moreover $\overline{F}(\mathbf{q}_{n_k}) = F(\mathbf{q}_{n_k}, \mathbf{r}_{n_k}, \mathbf{c}_{n_k}) \rightarrow F(\mathbf{q}, \mathbf{r}, \mathbf{c})$. Thus, $L = F(\mathbf{q}, \mathbf{r}, \mathbf{c})$ and the supremum is attained.

Suppose now that \mathbf{q} has an entry equal to zero, say q_1 , so that $q_{1n} \to 0$ (with the natural notation for entries of the subsequences). In this setting, R_{1n} , C_{1n} might escape to infinity, so assume that R_{1n} , $C_{1n} \uparrow \infty$, by restricting to a subsequence if necessary. (145) implies $q_{1n}R_{1n}^{(d+1)/d}$, $q_{1n}C_{1n}^{(d+1)/d} \leq 1$ and hence $q_{1n}R_{1n}$, $q_{1n}C_{1n} \to 0$. Note that $q_{1n}R_{1n}C_{1n} \to 0$ as well; otherwise there exists a subsequence with $q_{1nk}R_{1nk}C_{1nk} \geq \varepsilon > 0$. This contradicts that $\mathbf{r}_{n_k}, \mathbf{c}_{n_k}$ maximize $F(\mathbf{q}_{n_k}, \cdot, \cdot)$, since setting $R_{1,n_k} = C_{1,n_k} = 0$ would maintain feasibility in (145) and achieve a bigger value of F for all sufficiently large k (recall that B < 1). Thus, $q_{1n}R_{1n}, q_{1n}C_{1n}, q_{1n}R_{1n} \to 0$, yielding once again $L = F(\mathbf{q}, \mathbf{r}, \mathbf{c})$.

PROOF OF LEMMAS 7.14, 7.17 AND 7.18. We first prove Lemma 7.18. Recall that $I = \{i \in [3] | q_i > 0\}$. Let $I_R = \{i \in I | R_i > 0\}$ and define analogously I_C (note that it may be that $I_R \neq I_C$). For $i \in I_R$, it must hold that $\partial \overline{\Phi^S} / \partial R_i = 0$. Since $q_i > 0$ for $i \in I$, it follows that

$$R_i^{1/d} \propto \sum_j q_j C_j - (1 - B)C_i \quad \text{for all } i \in I_R,$$
(146)

and hence

$$R_i^{(d+1)/d} \propto R_iig(\sum_j q_j C_j - (1-B)C_iig) ext{ for all } i \in I_i$$

Thus, for $i \in I$, it holds that

$$\frac{R_i^{(d+1)/d}}{\sum_j q_j R_j^{(d+1)/d}} = \frac{R_i \left(\sum_j q_j C_j - (1-B)C_i\right)}{\sum_j q_j R_j \sum_j q_j C_j + (B-1)\sum_j q_j R_j C_j},$$
(147)

and an analogous argument for the C_i 's gives

$$\frac{C_i^{(d+1)/d}}{\sum_j q_j C_j^{(d+1)/d}} = \frac{C_i \left(\sum_j q_j R_j - (1-B)R_i\right)}{\sum_j q_j R_j \sum_j q_j C_j + (B-1)\sum_j q_j R_j C_j}.$$
(148)

Moreover, by a direct calculation we have

$$\frac{\partial \overline{\Phi^{S}}}{\partial q_{i}} = \frac{(d+1) \left(R_{i} \sum_{j} q_{j} C_{j} + C_{i} \sum_{j} q_{j} R_{j} + (B-1) R_{i} C_{i} \right)}{\sum_{j} q_{j} R_{j} \sum_{j} q_{j} C_{j} + (B-1) \sum_{j} q_{j} R_{j} C_{j}} - \frac{d R_{i}^{(d+1)/d}}{\sum_{j} q_{j} R_{j}^{(d+1)/d}} - \frac{d C_{i}^{(d+1)/d}}{\sum_{j} q_{j} C_{i}^{(d+1)/d}}.$$
(149)

Plugging (147) and (148) in (149) proves the first part of Lemma 7.18.

For the second part of Lemma 7.18, assume without loss of generality, that $q_1, q_2 > 0$ and $\frac{\partial \overline{\Phi^S}}{\partial q_1} - \frac{\partial \overline{\Phi^S}}{\partial q_2} > 0$. For $\varepsilon > 0$, consider $\mathbf{q}' = (q_1 + \varepsilon, q_2 - \varepsilon, q_3)$. Since q_1, q_2 are positive, for small enough ε , \mathbf{q}' has positive entries which sum to q. Moreover, for small enough ε the value of $\overline{\Phi^S}$ increases, while still maintaining feasibility in the region (110). Hence, \mathbf{q} does not maximize $\overline{\Phi}$, as desired.

Lemma 7.14 and Lemma 7.17 follow from our earlier considerations. In the setting of Lemma 7.17, we have the extra assumption that **q** is good, which means that for every

maximizer \mathbf{r}, \mathbf{c} it holds that $I = I_R = I_C$. Let i, j be such that $q_i, q_j > 0$, that is, $i, j \in I$. We have that $i, j \in I_R$ and hence the desired equivalence $R_i = R_j$ iff $C_i = C_j$ follows from (146). In the setting of Lemma 7.14, in addition to \mathbf{q} being good, we have that \mathbf{q} is maximal and that the q_i 's are nonnegative integers. By maximality of \mathbf{q} , there exists a maximizer \mathbf{r}, \mathbf{c} such that, for every two distinct indices $i, j \in I$, it holds that $R_i \neq R_j$ and $C_i \neq C_j$. Now just use (146) and the fact that q_1, q_2, q_3 are nonnegative integers to obtain that this maximizer \mathbf{r}, \mathbf{c} specifies a fixpoint of (107) of type (q_1, q_2, q_3) .

PROOF OF LEMMA 7.21. Suppose that $q_i > 0$ and $\sum_j q_j C_j > (1 - B)C_i$. We look at the derivative $\partial \overline{\Phi^S} / \partial R_i$ evaluated at $R_i = 0$:

$$\frac{\partial \Phi^S}{\partial R_i} = \frac{(d+1)q_i(q_1C_1 + q_2C_2 + q_3C_3 - (1-B)C_i)}{\sum_j q_jR_j\sum_j q_jC_j + (B-1)\sum_j q_jR_jC_j} > 0.$$

Thus, increasing the value of R_i by a sufficiently small amount, increases the value of $\overline{\Phi^S}$. Hence, the maximum cannot be obtained at the boundary $R_i = 0$. The second part of the lemma follows easily from the first part. Suppose that $q_i > 0$

The second part of the lemma follows easily from the first part. Suppose that $q_i > 1 - B$. Since the C_j 's are nonnegative, we have that $\sum_j q_j C_j \ge (1 - B)C_i$ with equality only if $q_j C_j = 0$ for all $j \in [3]$. This is excluded from (110). Thus, by the first part of the lemma, we may conclude that $R_i > 0$ and, similarly, $C_i > 0$.

To derive that there always exists an index $i \in [3]$ with $R_i, C_i > 0$ whenever $q \ge 3$, note that $q_1 + q_2 + q_3 = q$ implies that the largest q_i is $\ge q/3 \ge 1 \ge 1 - B$. Equality can only hold when B = 0, q = 3 and $q_1 = q_2 = q_3 = 1$. This (very) special case can be handled as follows. From (110), at least one of the C_j 's has to be positive, say $C_1 > 0$. We may assume that $R_1 = 0$, otherwise we are done. Since $R_1 = 0$ and $q_2 = q_3 = 1 > 0$, by the first part of the lemma, we obtain that $C_2 = C_3 = 0$. By the same token, $C_2 = C_3 = 0$ implies that $R_2 = R_3 = 0$. Thus, $R_1 = R_2 = R_3 = 0$, which is excluded from (110). \Box

ELECTRONIC APPENDIX

The electronic appendix for this article can be accessed in the ACM Digital Library.

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