Improved Inapproximability Results for Counting Independent Sets in the Hard-Core Model

Andreas Galanis[1], Qi Ge[2], Daniel Štefankovič[2], Eric Vigoda[1], and Linji Yang[1]

[1] School of Computer Science, Georgia Institute of Technology, Atlanta GA 30332
{agalanis,vigoda,ljyang}@cc.gatech.edu
[2] Department of Computer Science, University of Rochester, Rochester, NY 14627
{qge,stefanko}@cs.rochester.edu

Abstract. We study the computational complexity of approximately counting the number of independent sets of a graph with maximum degree Δ. More generally, for an input graph $G = (V, E)$ and an activity $\lambda > 0$, we are interested in the quantity $Z_G(\lambda)$ defined as the sum over independent sets I weighted as $w(I) = \lambda^{|I|}$. In statistical physics, $Z_G(\lambda)$ is the partition function for the hard-core model, which is an idealized model of a gas where the particles have non-negibile size. Recently, an interesting phase transition was shown to occur for the complexity of approximating the partition function. Weitz showed an FPAS for the partition function for any graph of maximum degree Δ when Δ is constant and $\lambda < \lambda_c(\mathbb{T}_\Delta) := (\Delta-1)^{\Delta-1}/(\Delta-2)^{\Delta}$. The quantity $\lambda_c(\mathbb{T}_\Delta)$ is the critical point for the so-called uniqueness threshold on the infinite, regular tree of degree Δ. On the other side, Sly proved that there does not exist efficient (randomized) approximation algorithms for $\lambda_c(\mathbb{T}_\Delta) < \lambda < \lambda_c(\mathbb{T}_\Delta) + \varepsilon(\Delta)$, unless NP=RP, for some function $\varepsilon(\Delta) > 0$. We remove the upper bound in the assumptions of Sly's result for $\Delta \neq 4, 5$, that is, we show that there does not exist efficient randomized approximation algorithms for all $\lambda > \lambda_c(\mathbb{T}_\Delta)$ for $\Delta = 3$ and $\Delta \geq 6$. Sly's inapproximability result uses a clever reduction, combined with a second-moment analysis of Mossel, Weitz and Wormald which prove torpid mixing of the Glauber dynamics for sampling from the associated Gibbs distribution on almost every regular graph of degree Δ for the same range of λ as in Sly's result. We extend Sly's result by improving upon the technical work of Mossel et al., via a more detailed analysis of independent sets in random regular graphs.

1 Introduction

For a graph $G = (V, E)$ and activity $\lambda > 0$, the hard-core model is defined on the set $\mathcal{I}(G)$ of independent sets of G where set $I \in \mathcal{I}(G)$ has weight $w(I) := \lambda^{|I|}$. The so-called partition function for the model is defined as:

$$Z_G(\lambda) := \sum_{I \in \mathcal{I}(G)} w(I) = \sum_{I \in \mathcal{I}(G)} \lambda^{|I|}.$$

The Gibbs distribution μ is over the set $\mathcal{I}(G)$ where $\mu(I) = w(I)/Z_G(\lambda)$. The case $\lambda = 1$ is especially interesting from a combinatorial perspective, since the partition function is the number of independent sets in G and the Gibbs distribution is uniformly distributed over the set of independent sets.

The hard-core model has received considerable attention in several fields. In statistical physics, it is studied as an idealized model of a gas where the gas particles have non-negligibile size so neighboring sites cannot simultaneously be occupied [4,1]. The activity λ corresponds to the fugacity of the gas. The model also arose in operations research in the study of communication networks [7].

We study the computational complexity of approximating the partition function. Valiant [15] proved that exactly computing the number of independent sets of an input graph $G = (V, E)$ is #P-complete. Greenhill [5] proved that even when the input is restricted to graphs with maximum degree 3, it is still #P-complete. Hence, our focus is on approximating the partition function.

Weitz [16] gave an FPAS (fully polynomial-time approximation scheme) for the partition function of graphs with maximum degree Δ when Δ is constant and $\lambda < \lambda_c(\mathbb{T}_\Delta) := (\Delta - 1)^{\Delta-1}/(\Delta - 2)^{\Delta}$. The activity $\lambda_c(\mathbb{T}_\Delta)$ is the critical activity for the threshold of uniqueness/non-uniqueness of the infinite-volume Gibbs measures on the infinite Δ-regular tree [7]. Recently, Sly [11] proved that, unless $NP = RP$, for every $\Delta \geq 3$, there exists a function $\varepsilon(\Delta) > 0$ such that for graphs with maximum degree Δ there does not exist an FPRAS (fully-polynomial time randomized approximation scheme) for the partition function at activity λ satisfying:

$$\lambda_c(\mathbb{T}_\Delta) < \lambda < \lambda_c(\mathbb{T}_\Delta) + \varepsilon(\Delta). \qquad (\star)$$

It was conjectured in Sly [11] and Mossel et al. [10] that the inapproximability result holds for all $\lambda > \lambda_c(\mathbb{T}_\Delta)$. We almost resolve this conjecture, that is we prove the conjecture for all Δ with the exception of $\Delta \in \{4, 5\}$.

Theorem 1. *Unless NP=RP, there does not exist an FPRAS for the partition function of the hard-core model for graphs of maximum degree at most Δ at activity λ when:*

- *$\Delta = 3$ and $\lambda > \lambda_c(\mathbb{T}_3) = 4$; or*
- *$\Delta \geq 6$ and $\lambda > \lambda_c(\mathbb{T}_\Delta)$; or*
- *$\Delta = 4$ and $\lambda \in (\lambda_c(\mathbb{T}_4) = 1.6875, 2.01538] \cup (4, +\infty)$; or*
- *$\Delta = 5$ and $\lambda \in (\lambda_c(\mathbb{T}_5) = 256/243, 1.45641] \cup (1.6875, 2.01538] \cup (4, +\infty)$.*

Sly's work utilizes earlier work of Mossel et al. [10] which studied the Glauber dynamics. The Glauber dynamics is a simple Markov chain (X_t) that is used to sample from the Gibbs distribution (and hence to approximate the partition function via now standard techniques, see [6,12]). For an input graph $G = (V, E)$ and activity $\lambda > 0$, the state space of the chain is $\mathcal{I}(G)$. From a state $X_t \in \mathcal{I}(G)$, the transitions $X_t \to X_{t+1}$ are defined by the following stochastic process:

– Choose a vertex v uniformly at random from V.
– Let

$$X' = \begin{cases} X_t \cup \{v\} & \text{with probability } \lambda/(1+\lambda) \\ X_t \setminus \{v\} & \text{with probability } 1/(1+\lambda). \end{cases}$$

– If $X' \in \mathcal{I}(G)$, then set $X_{t+1} = X'$, otherwise set $X_{t+1} = X_t$.

It is straightforward to verify that the Glauber dynamics is ergodic, and the unique stationary distribution is the Gibbs distribution. The mixing time T_{mix} is the minimum number of steps T from the worst initial state X_0, so that the distribution of X_T is within (total) variation distance $\leq 1/4$ of the stationary distribution. The chain is said to be *rapidly mixing* if the mixing time is polynomial in $n = |V|$, and it is said to be *torpidly mixing* if the mixing time is exponential in n (for the purposes of this paper, that means $T_{\text{mix}} = \exp(\Omega(n))$. We refer the reader to Levin et al. [8] for a more thorough introduction to the Glauber dynamics.

Mossel et al. [10] proved that the Glauber dynamics is torpidly mixing, for all $\Delta \geq 3$, for graphs with maximum degree Δ when λ satisfies $(\star)$. This improved upon earlier work of Dyer et al. [2] which held for larger λ, but not down to the critical activity $\lambda_c(\mathbb{T}_\Delta)$. The torpid mixing result of Mossel et al. [10] follows immediately (via a conductance argument) from their main result that for a random Δ-regular bipartite graph, for λ satisifying $(\star)$, an independent set drawn from the Gibbs distribution is "unbalanced" with high probability.

The proof of Mossel et al. [10] is a technically involved second moment calculation that Sly [11] calls a "technical tour de force". Our main contribution is to improve upon Mossel et al.'s result, most notably, extending it to all $\lambda > \lambda_c(\mathbb{T}_\Delta)$ for $\Delta = 3$. Our improved analysis comes from using a slightly different parameterization of the second moment of the partition function, which brings in symmetry, and allows for simpler proofs.

To formally state our results for independent sets of random regular graphs, we need to partition the set of independent sets as follows. For a bipartite graph $G = (V_1 \cup V_2, E)$ where $|V_1| = |V_2| = n$, for $\delta > 0$, for $i \in \{1, 2\}$, let $\mathcal{I}_i^\delta = \{I \in \mathcal{I}(G) : |I \cap V_i| > |I \cap V_{3-i}| + \delta n\}$ denote the independent sets that are unbalanced and "biased" towards V_i. Let $\mathcal{I}_B^\delta = \{I \in \mathcal{I}(G) : |I \cap V_i| \leq |I \cap V_{3-i}| + \delta n\}$ denote the set of nearly balanced independent sets.

Let $\mathcal{G}(n, \Delta)$ denote the probability distribution over bipartite graphs with $n + n$ vertices formed by taking the union of Δ random perfect matchings. Strictly speaking, this distribution is over multi-graphs. However, for independent sets the multiplicity of an edge does not matter so we can view $\mathcal{G}(n, \Delta)$ as a distribution over simple graphs with maximum degree Δ. Moreover, since our results hold asymptotically almost surely (a.a.s.) over $\mathcal{G}(n, \Delta)$, as noted in [10, Section 2.1], by standard arguments (see the note after the proof of [9, Theorem 4]), our results also hold a.a.s. for the uniform distribution over bipartite Δ-regular graphs.

Theorem 2. *For all $\Delta \geq 3$ there exists $\varepsilon(\Delta) > 0$, for any λ where $\lambda_c(\mathbb{T}_\Delta) < \lambda < \lambda_c(\mathbb{T}_\Delta) + \varepsilon(\Delta)$, there exist $a > 1$ and $\delta > 0$ such that, asymptotically almost surely, for a graph G chosen from $\mathcal{G}(n, \Delta)$, the Gibbs distribution μ satisfies:*

$$\mu(\mathcal{I}_B^\delta) \leq a^{-n} \min\{\mu(\mathcal{I}_1^\delta), \mu(\mathcal{I}_2^\delta)\}. \tag{1}$$

Therefore, the Glauber dynamics is torpidly mixing. The function $\varepsilon(\Delta)$ satisfies: for $\Delta = 4$, $\varepsilon(4) \geq .327887$; for $\Delta = 5$, $\varepsilon(5) \geq .402912$; for $\Delta \geq 6$, $\varepsilon(\Delta) \geq \lambda_c(\mathbb{T}_\Delta) - \lambda_c(\mathbb{T}_{\Delta+1})$; and for $\Delta = 3$, $\varepsilon(3) = \infty$.

This proves Conjecture 2.4 of [10] for the case $\Delta = 3$ and extends the results of Mossel et al. for $\Delta \geq 4$.

In the following section we look at the first and second moments of the partition function. We then state two technical lemmas (Lemma 3 and Lemma 4) from which Theorems 1, 2 easily follow using work of Sly [11] and Mossel et al. [10]. In Section 3 we prove the technical lemmas. Some of our proofs use Mathematica to prove inequalities involving rational functions, this is discussed in Section 2.4.

2 Technical Overview

2.1 Phase Transition Revisited

Recall, for the infinite Δ-regular tree $\mathbb{T}_\Delta$, Kelly [7] showed that there is a phase transition at $\lambda_c(\mathbb{T}_\Delta) = (\Delta - 1)^{\Delta-1}/(\Delta - 2)^\Delta$. Formally, this phase transition can be defined in the following manner. Let T_ℓ denote the complete tree of degree Δ and containing ℓ levels. Let p_ℓ denote the marginal probability that the root is occupied in the Gibbs distribution on T_ℓ. Note, for even ℓ the root is in the maximum independent set, whereas for odd ℓ the root is not in the maximum independent set. Our interest is in comparing the marginal probability for the root in even versus odd sized trees. Hence, let $p^+ = \lim_{\ell\to\infty} p_{2\ell}$ and $p^- = \lim_{\ell\to\infty} p_{2\ell+1}$. One can prove these limits exist by analyzing appropriate recurrences. The phase transition on the tree $\mathbb{T}_\Delta$ captures whether p^+ equals (or not) p^-. For all $\lambda \leq \lambda_c(\mathbb{T}_\Delta)$, we have $p^+ = p^-$, and let $p^* := p^+ = p^-$. On the other side, for all $\lambda > \lambda_c(\mathbb{T}_\Delta)$, we have $p^+ > p^-$. Mossel et al. [10] exhibited the critical role these quantities p^+ and p^- play in the analysis of the Gibbs distribution on random graphs $\mathcal{G}(n, \Delta)$.

2.2 First Moment of the Partition Function

Proceeding as in [10], roughly speaking, to prove Theorem 2 we need to prove that there exist graphs G whose partition function is close to the expected value (where the expectation is over a random G). To do that we use the second moment method. We first investigate the first moment of the partition function.

For $\alpha, \beta > 0$, let $\mathcal{I}_G^{\alpha,\beta} = \{I \in \mathcal{I}_G \,|\, |I \cap V_1| = \alpha n, |I \cap V_2| = \beta n\}$, that is, α is the fraction of the vertices in V_1 that are in the independent set and β is the fraction of the vertices in V_2 that are in the independent set.

Let $Z_G^{\alpha,\beta} = \sum_{I \in \mathcal{I}_G^{\alpha,\beta}} \lambda^{(\alpha+\beta)n}$. The first moment of $Z_G^{\alpha,\beta}$ is

$$\mathbb{E}_{\mathcal{G}}[Z_G^{\alpha,\beta}] = \lambda^{(\alpha+\beta)n} \binom{n}{\alpha n} \binom{n}{\beta n} \left(\frac{\binom{(1-\beta)n}{\alpha n}}{\binom{n}{\alpha n}} \right)^{\Delta} \approx \exp(n\Phi_1(\alpha,\beta)),$$

where $\Phi_1(\alpha,\beta) = (\alpha+\beta)\ln(\lambda) + H(\alpha) + H(\beta) + \Delta(1-\beta)H(\frac{\alpha}{1-\beta}) - \Delta H(\alpha)$, and $H(x) = -x\ln x - (1-x)\ln(1-x)$ is the entropy function.

For every $\Delta \geq 2$, we define the region $\mathcal{T}_\Delta = \{(\alpha,\beta) \mid \alpha,\beta > 0 \text{ and } \alpha + \beta + \Delta(\Delta-2)\alpha\beta \leq 1\}$. The following lemma shows that the local maxima of Φ_1 lie in $\mathcal{T}_\Delta$. Note that for $\Delta \geq 2$, we have $\mathcal{T}_{\Delta+1} \subset \mathcal{T}_\Delta$. Hence, the local maxima for all $\Delta \geq 2$ lie in $\mathcal{T}_2$. The first moment was analyzed in the work of Dyer et al. [2]. We use the following lemma from Mossel et al. [10] that relates the properties of the first moment to p^*, p^+ and p^-.

Lemma 1 (Lemma 3.2 and Proposition 4.1 of Mossel et al. [10]). *The following holds:*

1. *the stationary point (α,β) of Φ_1 over $\mathcal{T}_2$ is the solution to $\beta = \phi(\alpha)$ and $\alpha = \phi(\beta)$, where*

$$\phi(x) = (1-x)\left(1 - \left(\frac{x}{\lambda(1-x)}\right)^{1/\Delta}\right), \tag{2}$$

   and the solutions are exactly (p^+,p^-), (p^-,p^+), and (p^*,p^*) when $\lambda > \lambda_c(\mathbb{T}_\Delta)$, and the unique solution is (p^*,p^*) when $\lambda \leq \lambda_c(\mathbb{T}_\Delta)$;
2. *when $\lambda \leq \lambda_c(\mathbb{T}_\Delta)$, (p^*,p^*) is the unique maximum of Φ_1 over $\mathcal{T}_2$, and when $\lambda > \lambda_c(\mathbb{T}_\Delta)$, (p^+,p^-) and (p^-,p^+) are the maxima of Φ_1 over $\mathcal{T}_2$, and (p^*,p^*) is not a local maximum;*
3. *all local maxima of Φ_1 satisfy $\alpha + \beta + \Delta(\Delta-2)\alpha\beta \leq 1$;*
4. *p^+, p^-, p^* satisfy $p^- < p^* < p^+$ and when $\lambda \to \lambda_c(\mathbb{T}_\Delta)$ from above, we have $p^*, p^-, p^+ \to 1/\Delta$.*

2.3 Second Moment of the Partition Function

The second moment of $Z_G^{\alpha,\beta}$ is $\mathbb{E}_{\mathcal{G}}[(Z_G^{\alpha,\beta})^2] \approx \exp(n \cdot \max_{\gamma,\delta,\varepsilon} \Phi_2(\alpha,\beta,\gamma,\delta,\varepsilon))$, where

$$\begin{aligned}\Phi_2(\alpha,\beta,\gamma,\delta,\varepsilon) &= 2(\alpha+\beta)\ln(\lambda) + H(\alpha) + H_1(\gamma,\alpha) + H_1(\alpha-\gamma,1-\alpha)\\ &+H(\beta) + H_1(\delta,\beta) + H_1(\beta-\delta,1-\beta) + \Delta\Big(H_1(\gamma,1-2\beta+\delta) - H(\gamma)\\ &+H_1(\varepsilon,1-2\beta+\delta-\gamma) + H_1(\alpha-\gamma-\varepsilon,\beta-\delta) - H_1(\alpha-\gamma,1-\gamma)\\ &+H_1(\alpha-\gamma,1-\beta-\gamma-\varepsilon) - H_1(\alpha-\gamma,1-\alpha)\Big),\end{aligned} \tag{3}$$

where $H(x) = -x\ln(x) - (1-x)\ln(1-x)$ and $H_1(x,y) = -x(\ln(x) - \ln(y)) + (x-y)(\ln(y-x) - \ln(y))$.

To make Φ_2 well defined, the variables have to satisfy $(\alpha, \beta) \in \mathcal{T}_2$ and

$$\begin{aligned} \gamma, \delta, \varepsilon \geq 0, \quad \alpha - \gamma - \varepsilon \geq 0, \quad \beta - \delta \geq 0, \quad 1 - 2\beta + \delta - \gamma - \varepsilon \geq 0, \\ 1 - \alpha - \beta - \varepsilon \geq 0, \quad \beta - \delta + \varepsilon + \gamma - \alpha \geq 0. \end{aligned} \tag{4}$$

Define $\gamma^* = \alpha^2, \quad \delta^* = \beta^2, \quad \varepsilon^* = \alpha(1-\alpha-\beta)$. The following technical condition about the second moment was proposed in [11]. If we prove the condition holds then due to work of Mossel et al. [10] Theorem 2 will follow, and further, due to work of Sly [11] then Theorem 1 will follow.

Condition 1 (Condition 1.2[1] of Sly [11]) *Fix $\lambda > 0$ and let p^+ and p^- be the corresponding probabilities. There exists a constant $\chi > 0$ such that when $|p^+ - \alpha| < \chi$ and $|p^- - \beta| < \chi$ then $g_{\alpha,\beta}(\gamma, \delta, \varepsilon) := \Phi_2(\alpha, \beta, \gamma, \delta, \varepsilon)$ achieves its unique maximum in the region (4) at the point $(\gamma^*, \delta^*, \varepsilon^*)$.*

Two known regions of λ for which Condition 1 holds are the following: 1) $\Delta \geq 3$, and $\lambda_c(\mathbb{T}_\Delta) < \lambda < \lambda_c(\mathbb{T}_\Delta) + \varepsilon(\Delta)$ for some $\varepsilon(\Delta) > 0$, ([10, Lemma 6.10, Lemma 5.1]); 2) $\Delta = 6$ and $\lambda = 1$, ([11, Section 5]).

In this paper, we show that Condition 1 holds for a broad range of λ, and this is how we prove Theorems 1, and 2. Before stating the range when Condition 1 holds we need to define the following quantity. Let $\lambda_{1/2}(\mathbb{T}_\Delta)$ be the smallest value of λ such that $\phi(\phi(1/2)) = 1/2$. Equivalently $\lambda_{1/2}(\mathbb{T}_\Delta)$ is the minimum solution of

$$\left(1 + (1/\lambda)^{1/\Delta}\right)^{1-1/\Delta} \left(1 - (1/\lambda)^{1/\Delta}\right)^{1/\Delta} = 1. \tag{5}$$

Lemma 2. *Condition 1 holds for 1) $\Delta = 3$ and $\lambda > \lambda_c(\mathbb{T}_\Delta)$; and 2) $\Delta > 3$ and $\lambda \in (\lambda_c(\mathbb{T}_\Delta), \lambda_{1/2}(\mathbb{T}_\Delta)]$.*

Proof. When Δ and λ are such that $p^+ \leq 1/2$ then the following lemma implies Condition 1 (the precise condition on λ to have $p^+ \leq 1/2$ is $\lambda \in (\lambda_c(\mathbb{T}_\Delta), \lambda_{1/2}(\mathbb{T}_\Delta)]$ where $\lambda_{1/2}(\mathbb{T}_\Delta)$ is defined by (5)).

Lemma 3. *Let $\Delta \geq 3$ and let $(\alpha, \beta) \in \mathcal{T}_\Delta$, $\alpha, \beta > 0$, and $\alpha, \beta \leq 1/2$. Then $g_{\alpha,\beta}(\gamma, \delta, \varepsilon) := \Phi_2(\alpha, \beta, \gamma, \delta, \varepsilon)$ achieves its unique maximum in the region (4) at the point $(\gamma^*, \delta^*, \varepsilon^*)$.*

For all $\lambda \in (\lambda_c(\mathbb{T}_\Delta), \lambda_{1/2}(\mathbb{T}_\Delta)]$ we have $p^+ \leq 1/2$, this follows from the fact that p^+ is continuous in λ (it also follows in a more obvious way from the fact that p^+ increasing, but that fact requires a short proof), and $p^+ = 1/\Delta$ for $\lambda = \lambda_c(\mathbb{T}_\Delta)$). Thus for $\lambda \in (\lambda_c(\mathbb{T}_\Delta), \lambda_{1/2}(\mathbb{T}_\Delta)]$ we have that Condition 1 is satisfied; this follows from Lemma 3 and the fact that $(\alpha, \beta) = (p^+, p^-)$ is contained in the interior of $\mathcal{T}_\Delta$ (this follows from Lemma 1).

For $\Delta = 3$ the following lemma establishes Condition 1 in the case complementary to Lemma 3, more precisely, it establishes the condition for $\Delta = 3$ and λ such that $p^+ \geq 1/2$.

[3] The numbering in this paper for results from Sly's work [11] refer to the `arXiv` version of his paper.

Lemma 4. *Fix $\Delta = 3$ and $\lambda > \lambda_c(\mathbb{T}_\Delta)$. Let p^+ and p^- be the corresponding probabilities. Assume that $1/2 \leq p^+ < 1$. There exists a constant $\chi > 0$ such that when $|p^+ - \alpha| < \chi$ and $|p^- - \beta| < \chi$ then $g_{\alpha,\beta}(\gamma, \delta, \varepsilon) := \Phi_2(\alpha, \beta, \gamma, \delta, \varepsilon)$ achieves its unique maximum in the region (4) at the point $(\gamma^*, \delta^*, \varepsilon^*)$.*

Assume $\Delta = 3$ and $\lambda > \lambda_c(\mathbb{T}_\Delta)$. Let p^+ and p^- be the corresponding probabilities. If $p^+ \leq 1/2$ then Condition 1 follows from Lemma 3 and the fact that $(\alpha, \beta) = (p^+, p^-)$ is contained in the interior of $\mathcal{T}_\Delta$ (this follows from Lemma 1). If $p^+ \geq 1/2$ then Condition 1 follows from Lemma 4 and the fact that $(\alpha, \beta) = (p^+, p^-)$ is contained in the interior of $\mathcal{T}_\Delta$. □

We defer the proofs of Lemmas 3 and 4 to Section 3.

As a corollary of Lemma 2 we get that Condition 1 holds for the range of λ specified in Theorem 2.

Corollary 1. *Condition 1 holds for:*

1. *For $\Delta = 3$ and $\lambda > \lambda_c(\mathbb{T}_3)$.*
2. *For $\Delta \geq 6$ and $\lambda_c(\mathbb{T}_\Delta) < \lambda \leq \lambda_{1/2}(\mathbb{T}_\Delta)$ and $\lambda_{1/2}(\mathbb{T}_\Delta) > \lambda_c(\mathbb{T}_{\Delta-1})$.*
3. *For $\Delta = 5$ and $\lambda_c(\mathbb{T}_5) < \lambda \leq \lambda_c(\mathbb{T}_5) + .402912$.*
4. *For $\Delta = 4$, $\lambda_c(\mathbb{T}_4) < \lambda \leq \lambda_c(\mathbb{T}_4) + .327887$.*

Theorem 2 follows from Corollary 1 via the second-moment method. That proof closely follows the work of Mossel et al. [10], and hence we omit the details here and refer the interested reader to the full version of this paper [3]. For Theorem 1 for the case of $\Delta = 3$, we use Theorem 2 (or closely related results) combined with the reduction of Sly [11]. That proof closely follows the work of Sly [11], so once again we refer the interested reader to the full version [3]. To extend the inapproximability result for $\Delta = 3$ to $\Delta \geq 6$ we use the following simple combinatorial result.

Lemma 5. *Let G be a graph of maximum degree Δ and let $k > 1$ be an integer. Consider the graph H obtained from G be replacing each vertex by k copies of that vertex and each edge by the complete bipartite graph between the corresponding copies. Then, $Z_G((1+\lambda)^k - 1) = Z_H(\lambda)$.*

2.4 On the Use of Computational Assistance

We are going to use Mathematica to prove inequalities involving rational functions in regions bounded by rational functions. Such inequalities are known to be decidable by Tarski's quantifier elimination [14], the particular version of Collins algebraic decomposition (CAD) used by Mathematica's `Resolve` command is described in [13].

3 Analysis of the Second Moment Function

In this section, we will prove Lemmas 3 and 4. The proofs of the lemmas introduced in this section are deferred to the full version of the paper [3].

The derivatives of Φ_2 with respect to $\gamma, \delta, \varepsilon$ are

$$\exp\left(\frac{\partial \Phi_2}{\partial \gamma}\right) = \frac{(1-2\beta+\delta-\gamma-\varepsilon)^{\Delta}(\alpha-\gamma-\varepsilon)^{\Delta}(1-2\alpha+\gamma)^{\Delta-1}}{(1-\beta-\gamma-\varepsilon)^{\Delta}(\beta-\alpha+\gamma-\delta+\varepsilon)^{\Delta}(\alpha-\gamma)^{\Delta-2}\gamma}, \tag{6}$$

$$\exp\left(\frac{\partial \Phi_2}{\partial \delta}\right) = \frac{(\beta-\alpha-\delta+\gamma+\varepsilon)^{\Delta}(1-2\beta+\delta)^{\Delta-1}}{(1-2\beta+\delta-\gamma-\varepsilon)^{\Delta}(\beta-\delta)^{\Delta-2}\delta}, \tag{7}$$

$$\exp\left(\frac{\partial \Phi_2}{\partial \varepsilon}\right) = \frac{(1-2\beta+\delta-\gamma-\varepsilon)^{\Delta}(\alpha-\gamma-\varepsilon)^{\Delta}(1-\alpha-\beta-\varepsilon)^{\Delta}}{\varepsilon^{\Delta}(\beta-\alpha-\delta+\gamma+\varepsilon)^{\Delta}(1-\beta-\gamma-\varepsilon)^{\Delta}}. \tag{8}$$

We first argue that the maximum of $g_{\alpha,\beta}$ cannot occur on the boundary of the region defined by (4).

Lemma 6. *For every $\Delta \geq 3$ and $(\alpha, \beta) \in \mathcal{T}_\Delta$, $g_{\alpha,\beta}(\gamma, \delta, \varepsilon) := \Phi_2(\alpha, \beta, \gamma, \delta, \varepsilon)$ attains its maximum in the interior of (4).*

Fix $\Delta, \alpha, \beta, \gamma, \delta$ and view Φ_2 as a function of ε. We follow [10] who solved $\frac{\partial \Phi_2}{\partial \varepsilon} = 0$ (which is equivalent to (8) $= 1$) for ε, and showed that there is a unique solution in the interior of (4):

$$\hat{\varepsilon} := \hat{\varepsilon}(\alpha, \beta, \gamma, \delta) = \frac{1}{2}(1+\alpha-\beta-2\gamma-\sqrt{D}), \tag{9}$$

where $D = (1+\alpha-\beta-2\gamma)^2 - 4(\alpha-\gamma)(1-2\beta-\gamma+\delta) = (\alpha+\beta-1)^2 + 4(\alpha-\gamma)(\beta-\delta)$. Note that $\hat{\varepsilon}$ is a maximum of Φ_2, since

$$\frac{\partial \Phi_2}{\partial^2 \varepsilon} = -\frac{\Delta}{1-2\beta+\delta-\gamma-\varepsilon} - \frac{\Delta}{\alpha-\gamma-\varepsilon} - \frac{\Delta}{\varepsilon} - \frac{\Delta}{\beta-\delta-\alpha+\gamma+\varepsilon} - \frac{\Delta}{1-\alpha-\beta-\varepsilon} + \frac{\Delta}{1-\beta-\gamma-\varepsilon} < 0.$$

Define

$$\hat{\eta} := \hat{\eta}(\alpha, \beta, \gamma, \delta) = \frac{1}{2}(1-\alpha+\beta-2\delta-\sqrt{D}), \tag{10}$$

and note that

$$\begin{aligned} \alpha-\gamma-\hat{\varepsilon} = \beta-\delta-\hat{\eta} &= \frac{1}{2}(-(1-\alpha-\beta)+\sqrt{D}), \\ (\alpha-\gamma-\hat{\varepsilon})(1-\alpha-\beta-\hat{\varepsilon}-\hat{\eta}) &= \hat{\varepsilon}\hat{\eta}. \end{aligned} \tag{11}$$

The new parameter $\hat{\eta}$ (not used in [10]) is symmetric with $\hat{\varepsilon}$ (the constrains and formulas we have are invariant under a symmetry that swaps $\alpha, \gamma, \hat{\varepsilon}$ with $\beta, \delta, \hat{\eta}$) and allows for simpler arguments (using the symmetry).

Equation (9) allows us to eliminate variable ε. Let

$$f(\gamma, \delta) := g_{\alpha,\beta}(\gamma, \delta, \hat{\varepsilon}) = \Phi_2(\alpha, \beta, \gamma, \delta, \hat{\varepsilon}).$$

To prove that $(\gamma^*, \delta^*, \varepsilon^*)$ is the unique global maximum of $g_{\alpha,\beta}$ in the interior of the region defined by (4), it suffices to prove that (γ^*, δ^*) is the unique global

maximum of f for (γ, δ) in the interior of the following region (which contains the (γ, δ)-projection of the region defined by (4)):

$$\begin{aligned} 0 \le \gamma \le \alpha, \quad 0 \le \delta \le \beta, \\ 0 \le 1 - 2\beta + \delta - \gamma, \quad 0 \le 1 - 2\alpha + \gamma - \delta. \end{aligned} \tag{12}$$

Each inequality in (12) is implied by the inequalities in (4) (the only non-trivial case is the last inequality which is the sum of $1 - \alpha - \beta - \varepsilon \ge 0$ and $\beta - \delta + \varepsilon + \gamma - \alpha \ge 0$).

The first derivatives of f with respect to γ, δ are

$$\frac{\partial f}{\partial \gamma}(\gamma, \delta) = \Delta \ln W_{11} + \ln W_{12}, \tag{13}$$

$$\frac{\partial f}{\partial \delta}(\gamma, \delta) = \Delta \ln W_{21} + \ln W_{22}, \tag{14}$$

where

$$W_{11} = \frac{(\alpha - \gamma - \hat{\varepsilon})\hat{\varepsilon}(1 - 2\alpha + \gamma)}{\hat{\eta}(\alpha - \gamma)^2} = \frac{\hat{\varepsilon}(1 - 2\alpha + \gamma)}{(1 - \alpha - \beta - \hat{\varepsilon})(\alpha - \gamma)}, \quad W_{12} = \frac{(\alpha - \gamma)^2}{(1 - 2\alpha + \gamma)\gamma},$$
$$W_{21} = \frac{(\beta - \delta - \hat{\eta})\hat{\eta}(1 - 2\beta + \delta)}{\hat{\varepsilon}(\beta - \delta)^2} = \frac{\hat{\eta}(1 - 2\beta + \delta)}{(1 - \alpha - \beta - \hat{\eta})(\beta - \delta)}, \quad W_{22} = \frac{(\beta - \delta)^2}{(1 - 2\beta + \delta)\delta}.$$

(The equalities in the definition of W_{11} and the definition of W_{21} follow from (10) and (11).)

To determine whether (13) and (14) are zero it will be useful to understand conditions that make $W_{11}, W_{12}, W_{21}, W_{22}$ greater or equal to 1. The following lemma gives such conditions.

Lemma 7. *For every $(\alpha, \beta) \in \mathcal{T}_2$, and (γ, δ) in the interior of (12),*

$$W_{11} \ge 1 \iff (1 - \alpha)^2\delta + \beta^2(2\alpha - 1 - \gamma) \ge 0, \quad W_{12} \ge 1 \iff \gamma \le \alpha^2,$$
$$W_{21} \ge 1 \iff (1 - \beta)^2\gamma + \alpha^2(2\beta - 1 - \delta) \ge 0, \quad W_{22} \ge 1 \iff \delta \le \beta^2.$$

For every $\Delta \ge 3$, and $(\alpha, \beta) \in \mathcal{T}_\Delta$, we have (γ^*, δ^*) is a stationary point of f (this follows from the fact that for $\gamma = \alpha^2$ and $\delta = \beta^2$ the inequalities on the right-hand sides in Lemma 7 become equalities, and from (13), (14) we have that the derivatives of f vanish). By considering the sign of (13) and (14) and Lemma 7, we have the stationary points of f (and hence of $g_{\alpha,\beta}$) can only be in

$$0 < \gamma \le \alpha^2, \, 0 < \delta \le \beta^2, \tag{15}$$
$$(1 - \alpha)^2\delta + \beta^2(2\alpha - 1 - \gamma) \le 0, \, (1 - \beta)^2\gamma + \alpha^2(2\beta - 1 - \delta) \le 0, \tag{16}$$

or

$$\alpha^2 \le \gamma < \alpha, \, \beta^2 \le \delta < \beta, \tag{17}$$
$$(1 - \alpha)^2\delta + \beta^2(2\alpha - 1 - \gamma) \ge 0, \, (1 - \beta)^2\gamma + \alpha^2(2\beta - 1 - \delta) \ge 0. \tag{18}$$

We are going to prove that (γ^*, δ^*) is the unique maximum of f for every $\Delta \geq 3$, $(\alpha, \beta) \in \mathcal{T}_\Delta$, $\alpha, \beta > 0$ and $\alpha, \beta \leq 1/2$, by showing that the Hessian matrix of f is always negative definite in the region defined by the union of (15) and (17) (and hence the function f is strictly concave).

Let

$$R_1 = \frac{1-\alpha-\beta}{1-\alpha-\beta-\hat{\varepsilon}-\hat{\eta}}, \quad R_2 = \frac{\sqrt{D}}{1-2\alpha+\gamma}, \quad R_3 = \frac{2(\alpha-\gamma-\hat{\varepsilon})}{\alpha-\gamma},$$
$$R_4 = \frac{\sqrt{D}}{\gamma}, \quad R_5 = \frac{2(1-\beta-\gamma-\hat{\varepsilon})}{\alpha-\gamma}, \quad R_6 = \frac{\sqrt{D}}{1-2\beta+\delta},$$
$$R_7 = \frac{2(\alpha-\gamma-\hat{\varepsilon})}{\beta-\delta}, \quad R_8 = \frac{\sqrt{D}}{\delta}, \quad R_9 = \frac{2(1-\beta-\gamma-\hat{\varepsilon})}{\beta-\delta}.$$

Inspecting the R_i we obtain the following observation.

Observation 3 *$R_1, \ldots, R_9$ are positive when $(\alpha, \beta) \in \mathcal{T}_2$ and (γ, δ) in the interior of (12).*

Let

$$M = \begin{pmatrix} \frac{\partial f}{\partial^2 \gamma}(\gamma, \delta) & \frac{\partial f}{\partial \gamma \partial \delta}(\gamma, \delta) \\ \frac{\partial f}{\partial \delta \partial \gamma}(\gamma, \delta) & \frac{\partial f}{\partial^2 \delta}(\gamma, \delta) \end{pmatrix}.$$

In terms of $R_1, \ldots, R_9$ we have $\frac{\partial f}{\partial \gamma \partial \delta}(\gamma, \delta) = \frac{\partial f}{\partial \delta \partial \gamma}(\gamma, \delta) = \frac{\Delta R_1}{\sqrt{D}}$,

$$\frac{\partial f}{\partial^2 \gamma}(\gamma, \delta) = \frac{1}{\sqrt{D}}\Big[(-R_1 + R_2 + R_3)\Delta - R_2 - R_3 - R_4 - R_5\Big], \tag{19}$$

$$\frac{\partial f}{\partial^2 \delta}(\gamma, \delta) = \frac{1}{\sqrt{D}}\Big[(-R_1 + R_6 + R_7)\Delta - R_6 - R_7 - R_8 - R_9\Big]. \tag{20}$$

From the positivity of R_1 (when $(\alpha, \beta) \in \mathcal{T}_2$ and (γ, δ) in the interior of (12)) we immediately obtain the following observation.

Observation 4 *For every $(\alpha, \beta) \in \mathcal{T}_2$, and (γ, δ) in the interior of (12) we have $\frac{\partial f}{\partial \gamma \partial \delta}(\gamma, \delta) = \frac{\partial f}{\partial \delta \partial \gamma}(\gamma, \delta) > 0$.*

We prove the following technical inequality on the R_i.

Lemma 8. *For every $(\alpha, \beta) \in \mathcal{T}_2$, and (γ, δ) in the interior of (12) we have $R_1 > R_2 + R_3$ and $R_1 > R_6 + R_7$.*

Plugging Lemma 8 into (19) and (20) we obtain:

Corollary 2. *For every $(\alpha, \beta) \in \mathcal{T}_2$, and (γ, δ) in the interior of (12) we have $\frac{\partial f}{\partial^2 \gamma}(\gamma, \delta) < 0$ and $\frac{\partial f}{\partial^2 \delta}(\gamma, \delta) < 0$.*

To show that M is negative definite it is enough to show that the determinant of M is positive (Corollary 2 implies that the sum of the eigenvalues of M is negative and if the determinant is positive we can conclude that both eigenvalues are negative). We have

$$\begin{aligned}\det(M) &= \frac{\partial f}{\partial^2\gamma}(\gamma,\delta)\cdot\frac{\partial f}{\partial^2\delta}(\gamma,\delta) - \frac{\partial f}{\partial\gamma\partial\delta}(\gamma,\delta)\cdot\frac{\partial f}{\partial\delta\partial\gamma}(\gamma,\delta)\\ &= \frac{1}{D}\Bigg\{\ (\Delta-1)^2\Big[(-R_1+R_2+R_3)(-R_1+R_6+R_7)-R_1^2\Big]\\ &\qquad +(\Delta-1)\Big[(-R_1+R_2+R_3)(-R_1-R_8-R_9)+\\ &\qquad\qquad +(-R_1+R_6+R_7)(-R_1-R_4-R_5)-2R_1^2\Big]\\ &\qquad +\Big[(-R_1-R_8-R_9)(-R_1-R_4-R_5)-R_1^2\Big]\Bigg\}. \end{aligned}\tag{21}$$

By proving technical inequalities on $R_1,\ldots,R_9$ we will establish the positivity of $\det M$ in the following two cases.

Lemma 9. $\det(M)>0$ *for every* $\Delta\ge 3$, $(\alpha,\beta)\in\mathcal{T}_\Delta$, $\alpha,\beta>0$, (γ,δ) *in the interior of (12) and* (γ,δ) *in (15).*

Lemma 10. $\det(M)>0$ *for every* $\Delta\ge 3$, $(\alpha,\beta)\in\mathcal{T}_\Delta$, $\alpha,\beta\le 1/2$, $\alpha,\beta>0$, (γ,δ) *in the interior of (12) and* (γ,δ) *in (17).*

Assuming the lemmas, the proof of Lemma 3 is immediate.

Proof of Lemma 3. Lemma 9 and Lemma 10 imply that f has a unique maximum at (γ^*,δ^*) for every $\Delta\ge 3$, $(\alpha,\beta)\in\mathcal{T}_\Delta$, $\alpha,\beta>0$, $\alpha,\beta\le 1/2$, (γ,δ) in the interior of (12). This follows from the fact that $\det(M)>0$ implies that the Hessian of f is negative definite in the region of interest, i.e., where $g_{\alpha,\beta}$ could possibly have stationary points, which in turn implies that f is strictly concave in the region and hence has a unique maximum. By the definition of f, it follows that $g_{\alpha,\beta}$ has a unique maximum at $(\gamma^*,\delta^*,\varepsilon^*)$. □

When $\Delta=3$, by (2), we have the solution of $\beta=\phi(\alpha)$ and $\alpha=\phi(\beta)$ satisfies $\alpha^2-2\alpha+\alpha\beta+1-2\beta+\beta^2=0$. We define $\mathcal{T}_3'$ to be the set of pairs (α,β) such that $\alpha^2-2\alpha+\alpha\beta+1-2\beta+\beta^2=0$, $1/2\le\alpha<1$ and $0<\beta\le(3-\sqrt{5})/4$. Our goal is to show that $\det(M)>0$ for every $(\alpha,\beta)\in\mathcal{T}_3'$, (γ,δ) in the interior of (12) and (γ,δ) in (17).

We can rewrite $\det(M)$ using the formula in (21) as

$$\det(M)=\frac{1}{D}\Big[3R_1(U_1+U_2)+U_1U_2\Big]=\frac{U_1}{D}\Big[3R_1(1+U_2/U_1)+U_2\Big],\tag{22}$$

where $U_1=R_8+R_9-2R_6-2R_7$ and $U_2=R_4+R_5-2R_2-2R_3$.

By proving technical inequalities on $U_1,U_2,R_1,\ldots,R_9$ we will establish the positivity of $\det M$ in the interior of (12).

Lemma 11. $\det(M)>0$ *for every* $(\alpha,\beta)\in\mathcal{T}_3'$, (γ,δ) *in the interior of (12) and* (γ,δ) *in (17).*

Proof of Lemma 4. By Lemma 11, $g_{\alpha,\beta}(\gamma,\delta,\varepsilon):=\Phi_2(\alpha,\beta,\gamma,\delta,\varepsilon)$ achieves its unique maximum in the region (4) at $(\gamma^*,\delta^*,\varepsilon^*)$, for every $(\alpha,\beta)\in\mathcal{T}_3'$. We next

show that $g_{\alpha,\beta}(\gamma,\delta,\varepsilon) := \Phi_2(\alpha,\beta,\gamma,\delta,\varepsilon)$ also achieves its unique maximum in the region (4) at $(\gamma^*,\delta^*,\varepsilon^*)$ in a small neighborhood of $\mathcal{T}_3'$. First note that Φ_2 is continuous. By Lemma 6, we have for sufficiently small $\chi > 0$, the maximum of $g_{\alpha,\beta}$ cannot be obtained on the boundary of the region (4). Note that the derivatives of Φ_2 are continuous. It follows that for sufficiently small $\chi > 0$, all stationary points of $g_{\alpha,\beta}$ have to be close to the point $(\gamma^*,\delta^*,\varepsilon^*)$. We can choose χ such that $\det(M) > 0$ in the neighborhood of the point $(\gamma^*,\delta^*,\varepsilon^*)$, which implies that $g_{\alpha,\beta}$ has a unique stationary point and it is a maximum. □

References

1. van den Berg, J., Steif, J.E.: Percolation and the hard-core lattice gas model. Stochastic Processes and their Applications 49(2), 179–197 (1994)
2. Dyer, M., Frieze, A.M., Jerrum, M.: On counting independent sets in sparse graphs. SIAM J. Comput. 31(5), 1527–1541 (2002)
3. Galanis, A., Ge, Q., Štefankovič, D., Vigoda, E., Yang, L.: Improved Inapproximability Results for Counting Independent Sets in the Hard-Core Model (2011) Preprint available from the arXiv at, `http://arxiv.org/abs/1105.5131`
4. Gaunt, D.S., Fisher, M.E.: Hard-Sphere Lattice Gases. I. Plane-Square Lattice. Journal of Chemical Physics 43(8), 2840–2863 (1965)
5. Greenhill, C.: The complexity of counting colourings and independent sets in sparse graphs and hypergraphs. Computational Complexity 9(1), 52–72 (2000)
6. Jerrum, M.R., Valiant, L.G., Vazirani, V.V.: Random generation of combinatorial structures from a uniform distribution distribution. Theoretical Computer Science 43(2-3), 169–186 (1986)
7. Kelly, F.P.: Loss Networks. Annals of Applied Probability 1(3), 319–378 (1991)
8. Levin, D.A., Peres, Y., Wilmer, E.L.: Markov Chains and Mixing Times. American Mathematical Society, Providence (2009)
9. Molloy, M., Robalewska, H., Robinson, R.W., Wormald, N.C.: 1-factorizations of random regular graphs. Random Structures and Algorithms 10(3), 305–321 (1997)
10. Mossel, E., Weitz, D., Wormald, N.: On the hardness of sampling independent sets beyond the tree threshold. Probability Theory and Related Fields 143(3-4), 401–439 (2009)
11. Sly, A.: Computational Transition at the Uniqueness Threshold. In: Proceedings of the 51st Annual IEEE Symposium on Foundations of Computer Science (FOCS), pp. 287-296 (2010), Full version available from the arXiv at, `http://arxiv.org/abs/1005.5584`
12. Štefankovič, D., Vempala, S., Vigoda, E.: Adaptive Simulated Annealing: A Near-optimal Connection between Sampling and Counting. Journal of the ACM 56(3), 1–36 (2009)
13. Strzebonski, A.W.: Cylindrical algebraic decomposition using validated numerics. J. Symb. Comput. 41(9), 1021–1038 (2006)
14. Tarski, A.: RAND Corporation, Santa Monica, Calif. RAND Corporation, Santa Monica (1948)
15. Valiant, L.G.: The Complexity of Enumeration and Reliability Problems. SIAM J. Computing 8(3), 410–421 (1979)
16. Weitz, D.: Counting independent sets up to the tree threshold. In: Proceedings of the 38th Annual ACM Symposium on Theory of Computing (STOC), pp. 140–149 (2006)