

Inapproximability of the Independent Set Polynomial Below the Shearer Threshold^{*†‡}

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Abstract

We study the problem of approximately evaluating the independent set polynomial of bounded-degree graphs at a point λ . Equivalently, this problem can be reformulated as the problem of approximating the partition function of the hard-core model with activity λ on graphs G of maximum degree Δ . For $\lambda > 0$, breakthrough results of Weitz and Sly established a computational transition from easy to hard at $\lambda_c(\Delta) = (\Delta - 1)^{(\Delta-1)}/(\Delta - 2)^\Delta$, which coincides with the tree uniqueness phase transition from statistical physics.

For $\lambda < 0$, the evaluation of the independent set polynomial is connected to the problem of checking the conditions of the Lovász Local lemma (LLL) and applying its algorithmic consequences. Shearer described the optimal conditions for the LLL and identified the threshold $\lambda^*(\Delta) = (\Delta - 1)^{\Delta-1}/\Delta^\Delta$ as the maximum value p such that every family of events with failure probability at most p and whose dependency graph has maximum degree Δ has nonempty intersection. Very recently, Patel and Regts, and Harvey et al. have independently designed FPTASes for approximately computing the partition function whenever $|\lambda| < \lambda^*(\Delta)$.

Our main result establishes for the first time a computational transition at the Shearer threshold. Namely, we show that for all $\Delta \geq 3$, for all $\lambda < -\lambda^*(\Delta)$, it is NP-hard to approximate the partition function on graphs of maximum degree Δ , even within an exponential factor. Thus, our result, combined with the algorithmic results for $\lambda > -\lambda^*(\Delta)$, establishes a phase transition for negative activities. In fact, we now have a complete picture for the complexity of approximating the partition function for all $\lambda \in \mathbb{R}$ and all $\Delta \geq 3$, apart from the critical values.

1. For $-\lambda^*(\Delta) < \lambda < \lambda_c(\Delta)$, there exists an FPTAS for approximating the partition function with activity λ on graphs G of maximum degree Δ .
2. For $\lambda < -\lambda^*(\Delta)$ or $\lambda > \lambda_c(\Delta)$, it is NP-hard to approximate the partition function with activity λ on graphs G of maximum degree Δ , even within an exponential factor.

Rather than the tree uniqueness threshold of the positive case, the phase transition for negative activities corresponds to the existence of zeros for the partition function of the tree below $-\lambda^*(\Delta)$.

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1 Introduction

The independent set polynomial is a fundamental object in computer science which has been studied with various motivations. From an algorithmic viewpoint, the evaluation of this polynomial is crucial for determining the applicability of the Lovász Local Lemma and thus obtaining efficient algorithms for both finding [14] and approximately counting [6, 12] combinatorial objects with specific properties.

The independent set polynomial also arises in statistical physics, where it is called the hard-core partition function. Given a graph G , the value of the independent set polynomial of G at a point λ is equal to the value of the partition function of the hard-core model where the so-called “activity parameter” is equal to λ . We use the following notation. Given a graph G , let \mathcal{I}_G denote the set of independent sets in G . The weight of an independent set $I \in \mathcal{I}_G$ is given by $\lambda^{|I|}$. The hard-core partition function with parameter λ is defined as $Z_G(\lambda) := \sum_{I \in \mathcal{I}_G} \lambda^{|I|}$.

The hard-core model has attracted significant interest in computer science during recent years, due to the pioneering results by Weitz and Sly which established that the computational complexity of approximating the partition function undergoes a transition that coincides with the uniqueness phase transition in statistical physics. Namely, for $\Delta \geq 3$, let $\lambda_c(\Delta) := (\Delta - 1)^{\Delta-1}/(\Delta - 2)^\Delta$. Weitz [22] designed an FPTAS for approximating the partition function on graphs G of maximum degree Δ when the activity parameter λ is in the range $0 < \lambda < \lambda_c(\Delta)$. On the other hand, Sly [19] showed that approximating the partition function for $\lambda > \lambda_c(\Delta)$ is NP-hard (see [20] for the refinement stated here). The threshold $\lambda_c(\Delta)$ coincides with the uniqueness threshold of the infinite Δ -regular tree and it captures whether root-to-leaf correlations persist, or decay exponentially, as the height of the tree goes to infinity. This beautiful connection between computational complexity and phase transitions has led to a classification of the complexity of approximating the partition function of general antiferromagnetic 2-spin systems on graphs of maximum degree Δ (see [11, 18] for the algorithmic side and [20, 3] for the hardness side).

Our goal in this paper is to determine whether a computational transition takes place for negative activities as well, i.e., when $\lambda < 0$. Interestingly, the evaluation of the independent set polynomial for $\lambda < 0$ has significant algorithmic interest due to its connection with the Lovász Local Lemma (LLL) and, more precisely, to the problem of checking when the LLL applies. We will review this well-known connection shortly; prior to that, we introduce the Shearer threshold, which is relevant for our work.

Shearer, as part of his work [17] on the LLL, implicitly established that for every $\Delta \geq 2$, there is a threshold $\lambda^*(\Delta)$, given by $\lambda^*(\Delta) = (\Delta - 1)^{\Delta-1}/\Delta^\Delta$, such that

1. for all $\lambda \geq -\lambda^*(\Delta)$, for all graphs G of maximum degree Δ , it holds that $Z_G(\lambda) > 0$.
2. for all $\lambda < -\lambda^*(\Delta)$, there exists a graph G of maximum degree Δ such that $Z_G(\lambda) \leq 0$.

We refer to the point $-\lambda^*(\Delta)$ as the *Shearer threshold*. Similarly to the positive case, the Δ -regular tree plays a role in determining the location of the Shearer threshold, in the sense that for all $\lambda < -\lambda^*(\Delta)$, the truncation of the tree at an appropriate height yields a (finite) tree T of maximum degree Δ such that $Z_T(\lambda) \leq 0$. Scott and Sokal [16] were the first to realise the relevance of Shearer’s work to the phase transitions of the hard-core model, and to make explicit Shearer’s contribution in this context. They further developed these ideas to study the analyticity of the logarithm of the partition function in the complex plane.

From an algorithmic viewpoint, the Shearer threshold is tacitly present in most, if not all, applications of the (symmetric) LLL. In particular, Shearer [17] proved that $\lambda^*(\Delta)$ is the maximum value p such that every family of events, with failure probability at most p and

with a dependency graph of maximum degree Δ , has nonempty intersection. This simple characterisation is a corollary of far more elaborate conditions formulated in the same work that determine whether a dependency graph falls into the scope of the LLL. To date, no polynomial-time algorithm has been presented that, given as input a dependency graph G of maximum degree Δ , decides whether Shearer's conditions are satisfied when the failure probabilities of some events exceed the threshold $\lambda^*(\Delta)$ and it is very plausible that none exists (see for example [8, Section 4] for results in this direction).

Very recently, there have been two independent works that study the Shearer threshold from an approximate counting perspective. In particular, Patel and Regts [15] and Harvey, Srivastava, and Vondrák [8] (see also [21]) designed FPTASes, using different techniques, that approximate $Z_G(\lambda)$ on graphs G of maximum degree Δ when $-\lambda^*(\Delta) < \lambda < 0$ (and also for complex values λ with $|\lambda| < \lambda^*(\Delta)$). Thus, not only is it trivial to decide whether $Z_G(\lambda)$ is positive above the Shearer threshold, but also it is computationally easy to approximate $Z_G(\lambda)$ within an arbitrarily small polynomial relative error (see [8] for extensions to the multivariate partition function). Apart from partial results in [8] which we shall review shortly, these works left open the regime $\lambda < -\lambda^*(\Delta)$. In light of their results, it is natural to ask whether the Shearer threshold has a computational complexity significance for the problem of approximating $Z_G(\lambda)$ when $\lambda < 0$, analogous to the role that the tree uniqueness threshold has for $\lambda > 0$.

In this work, we answer this question by showing that, for all $\Delta \geq 3$, for all $\lambda < -\lambda^*(\Delta)$, it is NP-hard to approximate $|Z_G(\lambda)|$, even within an exponential factor. To formally state our result, we define the following problem which has three parameters—the activity λ , a degree bound Δ , and a value $c > 1$ which specifies the desired accuracy of the approximation.

Name #HardCore(λ, Δ, c).

Instance An n -vertex graph G with maximum degree at most Δ .

Output A number \hat{Z} such that $c^{-n}|Z_G(\lambda)| \leq |\hat{Z}| \leq c^n|Z_G(\lambda)|$.

We now formally state our result.

► **Theorem 1.** *Let $\Delta \geq 3$ and $\lambda < -\lambda^*(\Delta)$. Then there exists a constant $c > 1$ such that #HardCore(λ, Δ, c) is NP-hard, i.e., it is NP-hard to approximate $|Z_G(\lambda)|$ on graphs G of maximum degree at most Δ , even within an exponential factor.*

The previous known result for the inapproximability of the partition function for $\lambda < 0$ was given in [8, Theorem 4.4] which applies for $\Delta \geq 62$ and $\lambda < -39/\Delta$. Theorem 1 therefore vastly tightens that result, by showing a strong inapproximability result all the way to the Shearer threshold for all degree bounds $\Delta \geq 3$.

To elucidate the content of Theorem 1, we remark that, combined with the algorithmic results of [8, 15], it establishes for the first time a sharp computational transition at the Shearer threshold for negative activities. In fact, we now have a complete picture for the complexity of approximating $Z_G(\lambda)$ for all $\lambda \in \mathbb{R}$ apart from the critical values $-\lambda^*(\Delta)$ and $\lambda_c(\Delta)$.

1. For $-\lambda^*(\Delta) < \lambda < \lambda_c(\Delta)$, there exists an FPTAS for approximating $Z_G(\lambda)$ on graphs G of maximum degree Δ ; this follows by [8, 15] for $-\lambda^*(\Delta) < \lambda < 0$ and by [22] for $0 < \lambda < \lambda_c(\Delta)$. (The case $\lambda = 0$ is trivial since $Z_G(\lambda) = 1$ for all graphs G .)
2. For $\lambda < -\lambda^*(\Delta)$ or $\lambda > \lambda_c(\Delta)$, it is NP-hard to approximate $|Z_G(\lambda)|$ on graphs G of maximum degree Δ , even within an exponential factor; this follows by Theorem 1 for $\lambda < -\lambda^*(\Delta)$ and by [20] for $\lambda > \lambda_c(\Delta)$.

While both of the thresholds $-\lambda^*(\Delta)$ and $\lambda_c(\Delta)$ come from the infinite Δ -regular tree, they are of different nature: the Shearer threshold marks the point where the partition function of the tree of appropriate height eventually becomes negative, while the uniqueness threshold

marks the point where correlations between the root and the leaves persist, as the height of the tree grows.

The interplay between the zeros of graph polynomials and the complexity of approximating partition functions has appeared before in the approximate counting literature, see for example [4, 5]. However, one of the main differences in our present setting is the constant degree bound Δ , which significantly restricts the power of “thickening”. One might then think that perhaps Sly’s technique for establishing inapproximability above the uniqueness threshold might be relevant; this would entail analysing the partition function of random bipartite Δ -regular graphs for negative activities using moment analysis, which, to say the least, quickly runs into severe problems. Working around these difficulties for degrees as low as $\Delta = 3$ is one of the technical contributions of our work—see Section 1.1 for a high-level outline.

We conclude this introductory section by outlining very briefly the series of works that have established the Shearer threshold as an algorithmic benchmark. Beck [2] gave the first algorithmic application of the LLL, albeit with significantly worse guarantees than the non-constructive version; three decades later, Moser [13] and Moser and Tardos [14] succeeded in giving elegant, constructive analogues of the vanilla LLL; Shearer’s conditions were finally used in full generality to give a constructive proof of the LLL by Kolipaka and Szegedy [10], which yielded as a corollary efficient algorithms up to the Shearer threshold. See also [1, 7, 9] for recent algorithmic extensions of the LLL (and a more thorough overview of the LLL literature) and see [6, 12] for new applications of the LLL in approximate counting.

1.1 Proof outline and organisation

At a very high level, to prove Theorem 1 for an activity $\lambda < -\lambda^*(\Delta)$, our strategy is to transform λ into a “nicer” activity. Our key technical lemma, stated as Lemma 4 in Section 2, shows how to simulate a dense set of activities on the real line using graphs of maximum degree Δ as gadgets. As we shall explain later in detail, this lemma crucially uses the assumption that $\lambda < -\lambda^*(\Delta)$ by utilising trees of appropriate depth and combining them in suitable graph constructions that respect the degree bound Δ . Once Lemma 4 is in place, some extra care is needed to obtain the inapproximability results for $\Delta = 3$. Our approach is to construct binary gadgets and use inapproximability results for antiferromagnetic 2-spin systems on 3-regular graphs.

The paper is organised in two parts. In the first part, which is in Section 2, we state our key Lemma 4 and then show how to use it to conclude the inapproximability results of Theorem 1. In the second part, which is in Section 3, we present an overview of the proof of Lemma 4 and then give, in more detail, the proofs of some indicative lemmas.

2 Proof of Theorem 1

To give some rough intuition for our main proof technique of Theorem 1, suppose that we are given a degree bound $\Delta \geq 3$ and an activity $\lambda < -\lambda^*(\Delta)$. We will pursue the freedom to “change” the activity λ to a “nicer” activity λ' by using a suitable graph of maximum degree Δ . We will refer to this construction as *implementing* the activity λ' (cf. Definition 3 for the formal notion that is used throughout the paper). Our reduction for the proof of Theorem 1 is designed so that we need to implement just two well-chosen values of λ' . Using these two activities carefully so that we do not increase the degree Δ , we will construct binary gadgets (i.e., gadgets acting on edges) that will allow us to get our NP-hardness results by reducing from an appropriate (antiferromagnetic) 2-spin model on 3-regular graphs.

To illustrate more precisely the relevant ideas, we will need a few quick definitions. Let $\lambda \in \mathbb{R}$ and $G = (V, E)$ be an arbitrary graph. For a vertex $v \in V$, we will denote

$$Z_{G,v}^{\text{in}}(\lambda) := \sum_{I \in \mathcal{I}_G; v \in I} \lambda^{|I|}, \quad Z_{G,v}^{\text{out}}(\lambda) := \sum_{I \in \mathcal{I}_G; v \notin I} \lambda^{|I|}.$$

Thus, $Z_{G,v}^{\text{in}}(\lambda)$ is the contribution to the partition function $Z_G(\lambda)$ from those independent sets $I \in \mathcal{I}_G$ such that $v \in I$; similarly, $Z_{G,v}^{\text{out}}(\lambda)$ is the contribution to $Z_G(\lambda)$ from those $I \in \mathcal{I}_G$ such that $v \notin I$. We can now formalise the notion of implementation.

► **Definition 2.** Let $\lambda \in \mathbb{R}_{\neq 0}$. We say that the graph G implements the activity $\lambda' \in \mathbb{R}$ with accuracy $\epsilon > 0$ if there is a vertex v in G such that $Z_{G,v}^{\text{out}}(\lambda) \neq 0$ and

1. the degree of vertex v in G is 1,
2. it holds that $\left| \frac{Z_{G,v}^{\text{in}}(\lambda)}{Z_{G,v}^{\text{out}}(\lambda)} - \lambda' \right| \leq \epsilon$.

We will refer to the vertex v as the terminal of G . When Item 2 holds with $\epsilon = 0$, then we will just say that G implements the activity λ' .

► **Definition 3.** Let $\Delta \geq 2$ be an integer and $\lambda \in \mathbb{R}_{\neq 0}$. We say that (Δ, λ) implements the activity $\lambda' \in \mathbb{R}$ if there is a graph G of maximum degree at most Δ which implements the activity λ' .

More generally, we say that (Δ, λ) implements a set of activities $S \subseteq \mathbb{R}$, if for every $\lambda' \in S$ it holds that (Δ, λ) implements λ' .

Our main lemma to prove Theorem 1 is the following, whose proof is given in Section 3 (there, we also give an overview of the proof).

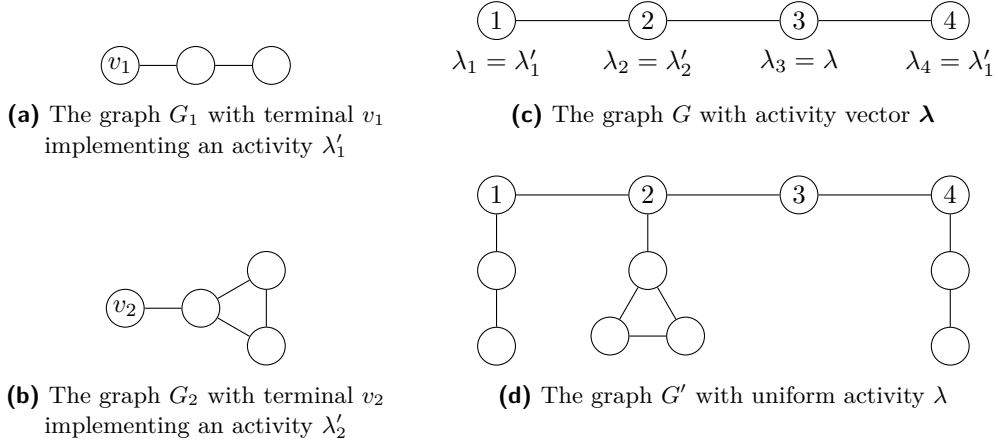
► **Lemma 4.** Let $\Delta \geq 3$ and $\lambda < -\lambda^*(\Delta)$. Then, for every $\lambda' \in \mathbb{R}$, for every $\epsilon > 0$, there exists a graph G of maximum degree at most Δ that implements λ' with accuracy ϵ . In other words, (Δ, λ) implements a set of activities S which is dense in \mathbb{R} .

We remark here that Lemma 4 fails for $\lambda > -\lambda^*(\Delta)$. For example, for $\lambda \geq 0$, it is not hard to see that $0 \leq Z_{G,v}^{\text{in}}(\lambda)/Z_{G,v}^{\text{out}}(\lambda) \leq \lambda$ for all graphs G and all vertices v in G . Moreover, in the regime $\lambda > -\lambda^*(\Delta)$, Scott and Sokal [16] have shown that $Z_{G,v}^{\text{in}}(\lambda)/Z_{G,v}^{\text{out}}(\lambda) > -1$ for all graphs G of maximum degree Δ (and all vertices v in G). This lower bound (in various forms) was also a key ingredient in the approximation algorithms of [8, 15].

We also remark that Lemma 4 does not give any quantitative guarantees on the dependence of the size of the graph G with respect to $\lambda, \lambda', 1/\epsilon$. This is by design: such estimates will not be important for us since our reduction for Theorem 1 invokes Lemma 4 for just two constant values of λ' with some small constant $\epsilon > 0$ (the particular values depend on λ but not on the input). In particular, for our applications of Lemma 4 in the proof of Theorem 1, the sizes of the relevant graphs G will be bounded by a constant (depending on λ).

2.1 The hard-core model with non-uniform activities

Implementing activities can be thought of as constructing unary gadgets that allow modification of the activity at a particular vertex v . We will use the implemented activities to simulate a more general version of the hard-core model with non-uniform activities. In particular, let $G = (V, E)$ be a graph and $\boldsymbol{\lambda} = \{\lambda_v\}_{v \in V}$ be a real vector; we associate to every vertex $v \in V$ the activity λ_v . The hard-core partition function with activity vector $\boldsymbol{\lambda}$ is defined as $Z_G(\boldsymbol{\lambda}) = \sum_{I \in \mathcal{I}_G} \prod_{v \in I} \lambda_v$. Note that the standard hard-core model with activity λ is obtained from this general version by setting all vertex activities equal to λ . For a vertex



■ **Figure 1** An illustrative depiction of the construction in the statement of Lemma 5. The graphs G_1, G_2 in Figures 1a, 1b implement the activities λ'_1, λ'_2 , respectively, i.e., $\frac{Z_{G_1, v_1}^{\text{in}}(\lambda)}{Z_{G_1, v_1}^{\text{out}}(\lambda)} = \lambda'_1$ and $\frac{Z_{G_2, v_2}^{\text{in}}(\lambda)}{Z_{G_2, v_2}^{\text{out}}(\lambda)} = \lambda'_2$ for some $\lambda'_1, \lambda'_2 \in \mathbb{R}$. In Figure 1c, we have a graph G with non-uniform activities $\{\lambda_i\}_{i \in [4]}$ such that $\lambda_i \in \{\lambda, \lambda'_1, \lambda'_2\}$ for $i \in [4]$. By sticking onto G the graphs G_1, G_2 as in Figure 1d, we obtain the graph G' . Note that the vertex whose activity was equal to λ was not modified.

$v \in V$, we define $Z_G^{\text{in}}(\lambda)$ and $Z_G^{\text{out}}(\lambda)$ for the non-uniform model analogously to $Z_G^{\text{in}}(\lambda)$ and $Z_G^{\text{out}}(\lambda)$ for the uniform model, respectively.

The following lemma connects the partition function $Z_G(\lambda)$ with non-uniform activities to the hard-core partition function with uniform activity λ . Roughly, whenever all the activities in the activity vector λ can be implemented, we can just stick graphs on the vertices of G which implement the corresponding activities in λ (if a vertex activity equals λ , no action is required).

► **Lemma 5.** *Let $\lambda \in \mathbb{R}_{\neq 0}$, let $t \geq 1$ be an arbitrary integer, and let $\lambda'_1, \dots, \lambda'_t \in \mathbb{R}$. Suppose that, for $j \in [t]$, the graph G_j with terminal v_j implements the activity λ'_j , and let $C_j := Z_{G_j, v_j}^{\text{out}}(\lambda)$. Then, the following holds for every graph $G = (V, E)$ and every activity vector $\lambda = \{\lambda_v\}_{v \in V}$ such that $\lambda_v \in \{\lambda, \lambda'_1, \dots, \lambda'_t\}$ for every $v \in V$.*

For $j \in [t]$, let $V_j := \{v \in V \mid \lambda_v = \lambda'_j\}$. Consider the graph G' obtained from G by attaching, for every $j \in [t]$ and every vertex $v \in V_j$, a copy of the graph G_j to the vertex v and identifying the terminal v_j with the vertex v (see Figure 1). Then, for $C := \prod_{j=1}^t C_j^{|V_j|}$, it holds that $Z_{G'}(\lambda) = C \cdot Z_G(\lambda)$.

► **Remark.** Note that, in the construction of Lemma 5, every vertex $v \in G$ with $\lambda_v = \lambda$ maintains its degree in G' (in fact, the neighbourhood of such a vertex v is the same in G and G'). The degree of every other vertex v in G gets increased by one. This observation will ensure in later applications of Lemma 5 that we do not blow up the degree.

2.2 Antiferromagnetic 2-spin systems on Δ -regular graphs

In our setting, where every vertex has degree at most Δ , an implementation consumes one of the Δ slots that a vertex has available to connect to other vertices. This is particularly problematic for the case where $\Delta = 3$. In the following we circumvent this problem by constructing suitable binary gadgets, so that we can use inapproximability results for computing the partition function of antiferromagnetic 2-spin systems on Δ -regular graphs.

Recall, an antiferromagnetic 2-spin system (without external field) is specified by two parameters $\beta, \gamma > 0$ such that $\beta\gamma < 1$. Let $\mathbf{M} = \{M_{ij}\}_{i,j \in \{0,1\}}$ be the matrix $\begin{bmatrix} \beta & 1 \\ 1 & \gamma \end{bmatrix}$. For a graph $H = (V, E)$, configurations of the 2-spin system are assignments $\sigma : V \rightarrow \{0, 1\}$ and the weight of a configuration σ is given by $w_{H,\beta,\gamma}(\sigma) = \prod_{\{u,v\} \in E} M_{\sigma(u),\sigma(v)}$. The partition function of H is then given by

$$Z_{H,\beta,\gamma} = \sum_{\sigma:V \rightarrow \{0,1\}} w_{H,\beta,\gamma}(\sigma) = \sum_{\sigma:V \rightarrow \{0,1\}} \prod_{\{u,v\} \in E} M_{\sigma(u),\sigma(v)}.$$

For positive parameters β, γ and $c > 1$, we consider the following computational problem, where the input is a 3-regular graph H .

Name #2Spin(β, γ, c).

Instance An n -vertex graph H which is 3-regular.

Output A number \hat{Z} such that $c^{-n} Z_{H,\beta,\gamma} \leq \hat{Z} \leq c^n Z_{H,\beta,\gamma}$.

The case $\beta = \gamma < 1$ corresponds to the well-known (antiferromagnetic) Ising model. As a corollary of results of Sly and Sun [20] (see also [3]), it is known that, for $0 < \beta = \gamma < 1/3$, there exists $c > 1$ such that #2Spin(β, β, c) is NP-hard, i.e., approximating the partition function $Z_{G,\beta,\beta}$ of the Ising model on 3-regular graphs H is NP-hard, even within an exponential factor. The following lemma is somewhat less known but follows easily from the results of [20].

► **Lemma 7.** *Let $\Delta = 3$ and β, γ be such that $0 < \beta, \gamma < 1/3$. Then, there exists $c > 1$ such that #2Spin(β, γ, c) is NP-hard.*

The following lemma will be used in the proof of Theorem 1 to specify the activities that we need to implement to utilise the inapproximability result of Lemma 7. It allows us to use the graph in Figure 2 as a binary gadget to simulate a 2-spin system with parameters β, γ .

► **Lemma 8.** *Let $\lambda < 0$. Then, there exist λ'_1, λ'_2 such that*

$$-1 - \frac{1}{6}|\lambda|^{1/3} < \lambda'_1 < -1, \quad -1 - 2\lambda < \lambda'_2 < -1 - 2\lambda + \frac{\lambda'_1 \lambda}{1 + \lambda'_1 + 3|\lambda|^{1/3}}. \quad (1)$$

For all λ'_1, λ'_2 satisfying (1), the following parameters β, γ (defined in terms of $\lambda, \lambda'_1, \lambda'_2$)

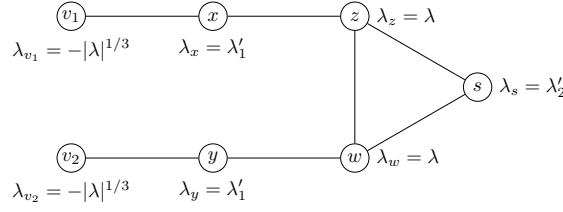
$$\beta = \frac{(1 + \lambda'_1) \left((1 + \lambda'_1)(1 + \lambda'_2 + 2\lambda) - 2\lambda'_1 \lambda \right)}{|\lambda|^{1/3} \left(\lambda'_1 \lambda - (1 + \lambda'_1)(1 + \lambda'_2 + 2\lambda) \right)}, \quad \gamma = \frac{|\lambda|^{1/3} (1 + \lambda'_2 + 2\lambda)}{\lambda'_1 \lambda - (1 + \lambda'_1)(1 + \lambda'_2 + 2\lambda)}. \quad (2)$$

satisfy $0 < \beta, \gamma < 1/3$.

2.3 The reduction & Proof of Theorem 1

The reduction to obtain Theorem 1 uses a binary gadget to simulate an antiferromagnetic 2-spin system on 3-regular graphs, i.e., we will replace every edge of a 3-regular graph H with a suitable graph B which has two special vertices to encode the edge. The gadget B is given in Figure 2, the two special vertices are v_1, v_2 . Note that the gadget B has nonuniform activities but this will be compensated for later by invoking Lemma 5. We thus obtain the following lemma (whose proof is in the full version).

► **Lemma 9.** *Let $\lambda < 0$ and $\lambda'_1, \lambda'_2 \in \mathbb{R}$ satisfy (1). Then, for β, γ as in (2), the following holds. For every 3-regular graph $H = (V_H, E_H)$ we can construct in linear time a graph $G = (V_G, E_G)$ of maximum degree 3 and specify an activity vector $\lambda = \{\lambda_v\}_{v \in V}$ on G such that*



■ **Figure 2** The binary gadget $B = (U, F)$ used in Lemma 9 to simulate an antiferromagnetic 2-spin system on 3-regular graphs. The gadget B is used to encode the edges of a 3-regular graph H . In particular, every edge $e = \{h_1, h_2\}$ of H gets replaced by a distinct copy of B , with the vertices v_1, v_2 of B getting identified with the vertices h_1, h_2 of H , respectively.

1. $Z_{H, \beta, \gamma} = Z_G(\boldsymbol{\lambda}) / C^{|E_H|}$, where $C := |\lambda|^{1/3} (\lambda'_1 \lambda - (1 + \lambda'_1)(1 + \lambda'_2 + 2\lambda)) > 0$.
2. For every vertex v of G , it holds that $\lambda_v \in \{\lambda, \lambda'_1, \lambda'_2\}$. Moreover, if $\lambda_v \neq \lambda$, then v has degree two in G .

Now, we are ready to prove Theorem 1.

Proof of Theorem 1 (Sketch). By Lemma 4, there are graphs G_1, G_2 of max degree Δ with terminals v_1, v_2 which implement activities λ'_1, λ'_2 satisfying the condition (1) of Lemma 8. For later use, set $C_1 := Z_{G_1, v_1}^{\text{out}}(\lambda)$, $C_2 := Z_{G_2, v_2}^{\text{out}}(\lambda)$ and note that C_1, C_2 are explicitly computable constants. Let β, γ be the parameters given by (2). By Lemma 8, it holds that $0 < \beta, \gamma < 1/3$. Thus, by Lemma 7, there exists $c > 1$ such that $\#2\text{Spin}(\beta, \gamma, c)$ is NP-hard. We will use Lemmas 5 and 9 to reduce $\#2\text{Spin}(\beta, \gamma, c)$ to $\#\text{HardCore}(\lambda, \Delta, c')$ for some constant $c' > 1$.

Let H be a 3-regular graph which is an input graph to the problem $\#2\text{Spin}(\beta, \gamma, c)$. By Lemma 9, we can construct in linear time a graph G of maximum degree 3 and specify an activity vector $\boldsymbol{\lambda} = \{\lambda_v\}_{v \in V}$ on G such that

1. $Z_{H, \beta, \gamma} = Z_G(\boldsymbol{\lambda}) / C^{|E_H|}$, where $C := |\lambda|^{1/3} (\lambda'_1 \lambda - (1 + \lambda'_1)(1 + \lambda'_2 + 2\lambda)) > 0$.
2. For every vertex v of G , $\lambda_v \in \{\lambda, \lambda'_1, \lambda'_2\}$. Also, if $\lambda_v \neq \lambda$, then v has degree two in G .

Using the graphs G_1, G_2 that implement λ'_1, λ'_2 respectively, we obtain from Lemma 5 that we can construct in linear time a graph $G' = (V_{G'}, E_{G'})$ of maximum degree at most Δ such that $Z_{G'}(\lambda) = C_1^{n_1} C_2^{n_2} \cdot Z_G(\boldsymbol{\lambda})$, where n_1, n_2 are the number of vertices in G whose activity equals λ'_1, λ'_2 , respectively. Note, the fact that the maximum degree of G' is at most Δ follows from the construction of Lemma 5 and Item 2 (cf. the Remark after Lemma 5).

It follows that $Z_{H, \beta, \gamma} = Z_{G'}(\lambda) / (C^{|E_H|} C_1^{n_1} C_2^{n_2})$. Since the size of G' exceeds the size of H only by a constant factor, there is a constant $c' > 1$ (depending only on λ) such that an approximation to $|Z_{G'}(\lambda)|$ within a factor $(c')^{|V_{G'}|}$ yields an estimate to $|Z_{H, \beta, \gamma}| = Z_{H, \beta, \gamma}$ within a factor $c^{|V_H|}$. It follows that $\#\text{HardCore}(\lambda, \Delta, c')$ is NP-hard. ◀

3 Proof of Lemma 4

In this final section, we give a proof overview of Lemma 4, which is the last missing ingredient used in the proof of Theorem 1. Let us fix a degree bound $\Delta \geq 3$. Our goal is to show that for any fixed $\lambda < -\lambda^*(\Delta)$, we can implement a dense set of activities using graphs of maximum degree Δ . At a very rough level, the proof of Lemma 4 splits into two regimes:

1. when $\lambda < -\lambda^*(2) = -1/4$,
2. when $-1/4 \leq \lambda < -\lambda^*(\Delta)$.

Roughly, in regime 1, we will be able to use *paths* to implement a dense set of activities. In regime 2, we will first use a $(\Delta - 1)$ -ary tree to implement an activity $\lambda' < -1/4$. Then,

using the activity λ' , we will be able to use the path construction of the first regime to implement a dense set of activities.

Unfortunately, the actual proof is more intricate, since as it turns out there is a set $\mathcal{B} \subset \mathbb{R}$, dense in $(-\infty, -1/4)$, such that, if $\lambda \in \mathcal{B}$, paths exhibit a periodic behaviour in terms of implementing activities (and thus can only be used to implement a finite set of activities). The following lemma will be important in specifying the set \mathcal{B} and understanding this periodic behaviour. The proof is a manipulation with trigonometric identities and can be found in Section 3.2 of the full version.

► **Lemma 10.** *Let $\lambda < -1/4$ and $\theta \in (0, \pi/2)$ be such that $\lambda = -1/(2 \cos \theta)^2$. Then, the partition function of the path P_n with n vertices is given by*

$$Z_{P_n}(\lambda) = \frac{\sin((n+2)\theta)}{2^n (\cos \theta)^n \sin(2\theta)}.$$

The “bad” set \mathcal{B} of activities (for which paths exhibit a periodic behaviour) can be read off from Lemma 10. To make this precise, let

$$\mathcal{B} := \left\{ \lambda \in \mathbb{R} \mid \lambda = -\frac{1}{4(\cos \theta)^2} \text{ for some } \theta \in (0, \pi/2) \text{ which is a rational multiple of } \pi \right\}. \quad (3)$$

Note, for example, that $-1, -1/2, -1/3 \in \mathcal{B}$ (set $\theta = \pi/3, \pi/4, \pi/6$, respectively). For $\lambda < -1/4$, it is not hard to infer from Lemma 10 that the ratio $\frac{Z_{P_n, v}^{\text{in}}(\lambda)}{Z_{P_n, v}^{\text{out}}(\lambda)}$ is equal to $-\frac{1}{2 \cos \theta} \frac{\sin(n\theta)}{\sin((n+1)\theta)}$. Therefore, when $\lambda \in \mathcal{B}$ or equivalently θ is a rational multiple of π , the ratio is periodic in terms of the number of vertices n in the path. On the other hand, when $\lambda < -1/4$ and $\lambda \notin \mathcal{B}$, then we can show that the ratio is dense in \mathbb{R} as n varies (this follows essentially from the fact that $\{n\theta \bmod 2\pi \mid n \in \mathbb{Z}\}$ is dense on the circle when θ is irrational) and hence we can use paths to implement a dense set of activities. This is the scope of the next lemma, which is proved in Section 3.2 of the full version.

► **Lemma 11.** *Let $\lambda < -1/4$ be such that $\lambda \notin \mathcal{B}$. Let P_n denote a path with n vertices and let v be one of the endpoints of P_n . Then, for every $\lambda' \in \mathbb{R}$, for every $\epsilon > 0$, there exists n such that $\left| \frac{Z_{P_n, v}^{\text{in}}(\lambda)}{Z_{P_n, v}^{\text{out}}(\lambda)} - \lambda' \right| \leq \epsilon$.*

When $\lambda \in \mathcal{B}$, we can no longer use paths to implement a dense set of activities, as we explained earlier, and we need to use a more elaborate argument. A key observation is that, for $\lambda \in \mathcal{B}$, the partition function of a path of appropriate length is equal to 0. In particular, we have the following simple corollary of Lemma 10.

► **Corollary 12.** *Let $\lambda < -1/4$ be such that $\lambda \in \mathcal{B}$. Denote by P_n the path with n vertices. Then, there is an integer $n \geq 1$ such that the partition function of the path P_n is zero, i.e., $Z_{P_n}(\lambda) = 0$.*

Having a path P whose partition function is 0 allows us to implement the activity -1 : indeed, for an endpoint v of the path P , we have that $Z_{P, v}^{\text{in}}(\lambda) + Z_{P, v}^{\text{out}}(\lambda) = Z_P(\lambda) = 0$, and hence P , with terminal v , implements $\frac{Z_{P, v}^{\text{in}}(\lambda)}{Z_{P, v}^{\text{out}}(\lambda)} = -1$ (note, we will later ensure that P is such that $Z_{P, v}^{\text{out}}(\lambda) \neq 0$). A somewhat ad-hoc gadget allows us to also implement the activity $+1$. Using these two implemented activities, -1 and $+1$, we then show how to implement *all* rational numbers using graphs whose structure resembles a caterpillar (the proof is inspired by the “ping-pong” lemma in group theory, used to establish free subgroups). We carry out this scheme in a more general setting where, instead of a path, we have a tree whose partition function is zero (this will also be relevant in the regime $\lambda > -1/4$). More precisely, we have the following lemma, whose proof is given in Section 3.1.

► **Lemma 13.** *Suppose that $\lambda \in \mathbb{R}_{\neq 0}$ and that T is a tree with $Z_T(\lambda) = 0$. Let d be the maximum degree of T and let $\Delta = \max\{d, 3\}$. Then, (Δ, λ) implements a dense set of activities in \mathbb{R} .*

We thus obtain the following throughout the regime 1 ($\lambda < -1/4$).

► **Lemma 14.** *Let $\lambda < -1/4$. For $\Delta = 3$, (Δ, λ) implements a dense set of activities in \mathbb{R} .*

Proof. We may assume that $\lambda \in \mathcal{B}$, otherwise the result follows directly from Lemma 11. For $\lambda \in \mathcal{B}$, we have by Corollary 12 a path P such that $Z_P(\lambda) = 0$. Since P has maximum degree 2, applying Lemma 13 gives the desired conclusion. ◀

Note, Lemma 14 applies only for values of λ which are far from the threshold $-\lambda^*(\Delta)$ for any $\Delta \geq 3$ and thus it should not be surprising that we can implement a dense set of activities using graphs of maximum degree 3. This highlights the next obstacle that we have to address: for general degree bounds $\Delta \geq 3$, to get all the way to the threshold $-\lambda^*(\Delta)$ we need to use graphs with maximum degree Δ (rather than just 3) to have some chance of implementing interesting activities.

Analyzing more complicated graphs for $\Delta \geq 3$ and $-1/4 \leq \lambda < -\lambda^*(\Delta)$ might sound daunting given the story for $\lambda < -1/4$, but it turns out that all we need to do is construct a graph G of maximum degree Δ that implements an activity $\lambda' < -1/4$. Then, to show that (Δ, λ) implements a dense set of activities, we only need to consider whether $\lambda' \in \mathcal{B}$. If $\lambda' \notin \mathcal{B}$, we can argue by decorating the paths from Lemma 11 using the graph G . Otherwise, if $\lambda' \in \mathcal{B}$, we can first construct a tree T of maximum degree Δ such that $Z_T(\lambda) = 0$ (by decorating the path from Lemma 12), and then invoke Lemma 13. Thus, we are left with the task of implementing an activity $\lambda' < -1/4$. For that, we combine appropriately $(\Delta - 1)$ -ary trees of appropriate depth, which can be analysed relatively simply using a recursion. (A technical detail here is that, initially, we are not able to implement this boosted activity λ' in the sense of Definition 3 since the terminal of the relevant tree has degree bigger than 1; nevertheless, the degree of the terminal is at most $\Delta - 2$, so it can be combined with the paths without overshooting the degree bound Δ .) Putting together these pieces yields the following lemma (see Section 3.5 of the full version).

► **Lemma 15.** *Let $\Delta \geq 3$ and $-1/4 \leq \lambda < -\lambda^*(\Delta)$. Then, (Δ, λ) implements a dense set of activities in \mathbb{R} .*

Using Lemmas 14 and 15, the proof of Lemma 4 is immediate.

3.1 The case where the partition function of some tree is zero

In this section, we prove Lemma 13 which is an ingredient in both Lemmas 14 and 15.

We start with the following lemma, whose full proof is given in the full version. Roughly, in the proof, the implementation of -1 uses as a gadget the tree T with a leaf as the terminal; the implementation of $+1$ uses an ad-hoc gadget.

► **Lemma 19.** *Let $\lambda \in \mathbb{R}_{\neq 0}$ and $d \geq 2$ be a positive integer. Suppose that there exists a tree T with maximum degree d such that $Z_T(\lambda) = 0$. Then, for $\Delta = \max\{d, 3\}$, we have that (Δ, λ) implements the activities -1 and $+1$.*

The following functions f_+ and f_- will be important in what follows:

$$f_+ : \mathbb{R} \setminus \{-1\} \mapsto \mathbb{R} \setminus \{0\}, \text{ given by } f_+(x) = \frac{1}{1+x} \text{ for all } x \neq -1,$$

$$f_- : \mathbb{R} \setminus \{+1\} \mapsto \mathbb{R} \setminus \{0\}, \text{ given by } f_-(x) = \frac{1}{1-x} \text{ for all } x \neq +1.$$

► **Definition 20.** Let $S \subseteq \mathbb{R}$ be the set of real numbers defined as follows: $z \in S$ iff for some integer $n \geq 0$, there exists a sequence x_0, \dots, x_n such that $x_0 = 0$, $x_n = z$ and for all $i = 0, \dots, n-1$ it holds that either $x_{i+1} = f_+(x_i)$ or $x_{i+1} = f_-(x_i)$.

The set S in Definition 20 is obtained by the following recursive procedure. Set $S_0 = \{0\}$. For $h = 0, 1, \dots$, define S_{h+1} by first letting $S_{h+1}^+ = f_+(S_h)$ and $S_{h+1}^- = f_-(S_h)$ and then setting $S_{h+1} = S_{h+1}^+ \cup S_{h+1}^-$. S can then be recovered by taking the union of the sets S_h , i.e., $S = \bigcup_{h=0}^{\infty} S_h$. Our interest in the set S is due to the following lemma (proof in the full version).

► **Lemma 21.** Let $\Delta \geq 3$ and $\lambda < 0$. Suppose that (Δ, λ) implements the activities -1 and $+1$. Then, (Δ, λ) also implements the set of activities $\{\lambda z \mid z \in S\}$.

It is simple to see that all numbers in the set S of Definition 20 are rationals. Somewhat surprisingly, the following lemma asserts that S is in fact the set \mathbb{Q} of all rational numbers.

► **Lemma 22.** Let $S \subseteq \mathbb{R}$ be the set in Definition 20. Then, $S = \mathbb{Q}$.

Proof. Recall that $S \subseteq \mathbb{Q}$, so we only need to argue that $\mathbb{Q} \subseteq S$. Since $0 \in S$ (by taking $n = 0$ in Definition 20) and $f_+(0) = 1$, we have that $0, 1 \in S$. Note that

$$f_-(f_-(f_+(x))) = -x \text{ for } x \neq -1, 0. \quad (4)$$

It follows that $-1 \in S$. Also, $1/2, 2 \in S$ since $f_+(f_+(0)) = 1/2$ and $f_-(f_+(f_+(0))) = 2$. Let $T := \{-1, 0, 1/2, 1, 2\}$; the arguments above established that $T \subseteq S$. Consider an arbitrary $\rho \in \mathbb{Q}$ such that $\rho \notin T$. To prove the lemma, we need to show that $\rho \in S$.

We will show that, for some integer $n \geq 0$, there is a sequence $\{\rho_i\}_{i=0}^n$ such that

- (i) $\rho_0 = \rho$, $\rho_n = -1$.
- (ii) $\rho_i \notin \{0, 1/2, 1\}$ for $i = 0, \dots, n-1$.
- (iii) $\rho_{i+1} = f_+(\rho_i)$ or $\rho_{i+1} = f_-(\rho_i)$ for $i = 0, \dots, n-1$.

Before proving the existence of such a sequence, we first show how to conclude that $\rho \in S$. To do this, let $x_i := \rho_{n-i}$ for $i = 0, \dots, n$. Properties (i)–(iii) of the sequence $\{\rho_i\}_{i=0}^n$ translate into the following properties of the sequence $\{x_i\}_{i=0}^n$:

- (a) $x_0 = -1$, $x_n = \rho$.
- (b) $x_i \notin \{0, 1/2, 1\}$ for $i = 1, 2, \dots, n$.
- (c) $x_i = f_+^{-1}(x_{i-1})$ or $x_i = f_-^{-1}(x_{i-1})$ for $i = 1, 2, \dots, n$.

We show by induction on i that $x_i \in S$ for all $i = 0, \dots, n$, which for $i = n$ gives that $\rho \in S$ (since by Item (a) we have $x_n = \rho$). For the base case $i = 0$, we have that $x_0 = -1$ by Item (a) and hence $x_0 \in S$. For the induction step, assume that $x_i \in S$ for some integer $0 \leq i \leq n-1$, our goal is to show that $x_{i+1} \in S$. The main observation is that the inverses of the functions f_- and f_+ can be obtained by composing appropriately the functions f_- and f_+ . Namely, we have that

$$f_-^{-1}(x) = \frac{x-1}{x} = f_-(f_-(x)) \text{ for } x \neq 0, 1, \quad (5)$$

$$f_+^{-1}(x) = \frac{1-x}{x} = f_-(f_-(f_+(f_-(f_-(x)))))) \text{ for } x \neq 0, \frac{1}{2}, 1. \quad (6)$$

(5) is proved by just making the substitutions. (6) is obtained from (4) and (5), and checking when $f_-(f_-(x)) = \frac{x-1}{x}$ equals -1 and 0 . Since by Items (a) and (b) we have that $x_j \neq 0, 1/2, 1$ for all $0 \leq j \leq n$ and $x_i \in S$ by the induction hypothesis, it follows by Item (c) and (5), (6) that $x_{i+1} \in S$, as wanted.

It remains to establish the existence of the sequence $\{\rho_i\}_{i=0}^n$ with the properties (i)–(iii). Consider the following set S_ρ , which is defined analogously to the set S with the only

difference that the starting point for S_ρ is the point ρ (instead of 0 that was used in the definition of S). Formally, $z \in S_\rho$ iff for some integer $n \geq 0$, there exists a sequence $\{\rho_i\}_{i=0}^n$ such that $\rho_0 = \rho$, $\rho_n = z$ and for all $i = 0, \dots, n-1$ it holds that either $\rho_{i+1} = f_+(\rho_i)$ or $x_{i+1} = f_-(\rho_i)$. For convenience, we will call such a sequence a certificate that $z \in S_\rho$ and we will refer to n as the length of the certificate. We will show that, for any $\rho \in \mathbb{Q}$ such that $\rho \notin T = \{-1, 0, 1/2, 1, 2\}$, it holds that

$$0, 1 \notin S_\rho, \quad -1 \in S_\rho. \quad (7)$$

By considering a certificate of smallest length that $-1 \in S_\rho$ (existence is guaranteed by (7)), we obtain a sequence $\{\rho_i\}_{i=0}^n$ that has all of the required properties (i), (ii), and (iii), see the full version for the details. Thus, in the following we focus on establishing (7). First, we show that $0, 1 \notin S_\rho$. Observe that $\rho \neq 0, 1$, so any certificate that $0, 1 \in S_\rho$ must have nonzero length. Further, the range of the functions f_+, f_- excludes 0, which implies that $0 \notin S_\rho$. Moreover, the only way that we can have $1 \in S_\rho$ is if for some $x \in S_\rho$ it holds that $f_+(x) = 1$ or $f_-(x) = 1$. Both of these mandate that $x = 0$, but $0 \notin S_\rho$ as we just showed.

The remaining bit of (7), i.e., that $-1 \in S_\rho$, will require more effort to prove. As a starting point, note that from $\rho \in \mathbb{Q}$, we have that $S_\rho \subseteq \mathbb{Q}$. Also, S_ρ is nonempty since $\rho \in S_\rho$. Thus, there exists $z^* \in S_\rho$ such that $z^* = p/q$ where p, q are integers such that $|p| + |q|$ is minimum. Since $|p| + |q|$ is minimum, it must be the case that $\gcd(p, q) = 1$.

We first prove that $z^* \in T$; note, we already know that $z^* \neq 0, 1$ since $0, 1 \notin S_\rho$ and $z^* \in S_\rho$, but keeping the values 0, 1 into consideration will be convenient for the upcoming argument. Namely, for the sake of contradiction, assume that $z^* \notin T$, which implies in particular that $z^* \neq 0, -1$. Since $z^* \in S_\rho$, by (4), we obtain that $-z^* \in S_\rho$ as well. By switching to $-z^*$ if necessary, we may thus assume that z^* is positive and hence that $p, q > 0$, i.e., that both p, q are positive integers. Since $z^* \neq 1$ (from $z^* \notin T$), we have that $p \neq q$. For each of the cases $p > q$ and $p < q$, we obtain a contradiction to the minimality of $p + q$ by constructing $z' = p'/q' \in S_\rho$ with p', q' positive integers such that $0 < p' + q' < p + q$.

Case 1. $p > q$. Since $z^* \neq 1, 2$ (from $z^* \notin T$), we have that $p/q \neq 1$ and $f_-(p/q) = \frac{q}{q-p} \neq 0, -1$, so by (4) we have that $f_-(f_-(f_+(f_-(p/q)))) = \frac{q}{p-q}$. Thus, letting $p' = q$ and $q' = p - q$ yields $z' = p'/q' \in S_\rho$ with $p' > 0, q' > 0$ and $0 < p' + q' < p + q$.

Case 2. $p < q$. Since $z^* \neq 0, 1/2, 1$ (from $z^* \notin T$), we obtain from (6) that $f_-(f_-(f_+(f_-(f_-(p/q)))))) = \frac{q-p}{p}$. Thus, letting $p' = q - p$ and $q' = p$ yields $z' = p'/q' \in S_\rho$ with $p' > 0, q' > 0$ and $0 < p' + q' < p + q$.

This concludes the proof that $z^* \in T$. In fact, we can now deduce easily that $-1 \in S_\rho$. As noted earlier, we have that $z^* \neq 0, 1$ as a consequence of $0, 1 \notin S_\rho$, so in fact $z^* \in \{-1, 1/2, 2\}$. If $z^* = -1$, then we automatically have that $-1 \in S_\rho$ since z^* was chosen to be in S_ρ . If $z^* = 2$, then we have that $2 \in S_\rho$ and hence $f_-(2) = -1 \in S_\rho$ as well. Finally, if $z^* = 1/2$, we have that $1/2 \in S_\rho$ and hence $f_-(f_-(1/2)) = -1 \in S_\rho$. Thus, it holds that $-1 \in S_\rho$, which completes the proof of (7) and hence the proof of Lemma 22. \blacktriangleleft

Combining Lemmas 19, 21 and 22, we obtain Lemma 13.

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