Upper Bounds on the 2-Colorability Threshold of Random d-Regular k-Uniform Hypergraphs for $k \geq 3$

Evan Chang
Massachusetts Institute of Technology, USA

Neel Kolhe
University of California, Berkeley, USA

Youngtak Sohn
Department of Mathematics, Massachusetts Institute of Technology, USA

Abstract

For a large class of random constraint satisfaction problems (CSP), deep but non-rigorous theory from statistical physics predict the location of the sharp satisfiability transition. The works of Ding, Sly, Sun (2014, 2016) and Coja-Oghlan, Panagiotou (2014) established the satisfiability threshold for random regular k-NAE-SAT, random k-SAT, and random regular k-SAT for large enough $k \geq k_0$ where k_0 is a large non-explicit constant. Establishing the same for small values of $k \geq 3$ remains an important open problem in the study of random CSPs.

In this work, we study two closely related models of random CSPs, namely the 2-coloring on random d-regular k-uniform hypergraphs and the random d-regular k-NAE-SAT model. For every $k \geq 3$, we prove that there is an explicit $d_\star(k)$ which gives a satisfiability upper bound for both of the models. Our upper bound $d_\star(k)$ for $k \geq 3$ matches the prediction from statistical physics for the hypergraph 2-coloring by Dall'Asta, Ramezanpour, Zecchina (2008), thus conjectured to be sharp. Moreover, $d_\star(k)$ coincides with the satisfiability threshold of random regular k-NAE-SAT for large enough $k \geq k_0$ by Ding, Sly, Sun (2014).

2012 ACM Subject Classification Theory of computation → Randomness, geometry and discrete structures; Mathematics of computing → Random graphs

Keywords and phrases Random constraint satisfaction problem, replica symmetry breaking, interpolation bound

Digital Object Identifier 10.4230/LIPIcs.APPROX/RANDOM.2024.47

Category RANDOM

Related Version *Full Version*: `https://arxiv.org/abs/2308.02075` [14]

Funding *Youngtak Sohn*: Supported by Simons-NSF Collaboration on Deep Learning NSF DMS-2031883 and Elchanan Mossel's Vannevar Bush Faculty Fellowship award ONR-N00014-20-1-2826.

Acknowledgements We thank the MIT PRIMES program and its organizers Pavel Etingof, Slava Gerovitch, and Tanya Khovanova for making this possible. Y.S. thanks Elchanan Mossel, Allan Sly, and Nike Sun for encouraging feedbacks.

1 Introduction

In this work, we study the 2-coloring on random d-regular k-uniform hypergraphs and the random d-regular k-NAE-SAT model for $k \geq 3$. We establish an explicit well-defined upper bound on the satisfiability/colorability threshold that holds for every $k \geq 3$, which is conjectured to be sharp in statistical physics [25] for hypergraph 2-coloring, and matches the previous rigorous results for random regular k-NAE-SAT model for k large enough [28].

Given a k-uniform hypergraph with n nodes and m hyperedges, where every edge consists of k nodes, a hypergraph 2-coloring is an assignment of colors from $\{\mathsf{red}, \mathsf{blue}\} \equiv \{0, 1\}$ to the nodes such that there is no monochromatic hyperedge. If there is such a 2-coloring, the hypergraph is said to be colorable or satisfiable. It is a typical example of a constraint satisfaction problem (CSP) that has been studied extensively in combinatorics and computer science literature [54, 7, 2, 24, 34, 38, 39].

A k-NAE-SAT problem is another closely related CSP studied in computer science [19, 28, 57, 50, 56], which can be viewed as a variant of the infamous k-SAT problem [41]. A k-SAT formula is a boolean CNF formula with n variables formed by taking the AND of m clauses, which is the OR of k variables or their negations. Then, a NAE-SAT solution $\underline{x} \in \{0, 1\}^n$ is an assignment such that $\underline{x}$ and its negation $\neg\underline{x}$ evaluates true in the formula. Thus, denoting each clause as a hyperedge, if no variable is negated in every clause, then a NAE-SAT solution is equivalent to a hypergraph 2-coloring.

A significant direction of research on satisfiability has involved examining the large-system limit of randomly generated problem instances. The study of random constraint satisfaction problems (CSPs) aims to discern typical behaviors and phase transitions in these systems as the number of variables n and the number of constraints m tends to infinity with a fixed ratio $\alpha \equiv \frac{m}{n}$. In this sparse regime, there has been considerable effort into identifying the satisfiability transition, or the critical density, denoted by α_{sat}, beyond which solutions cease to exist [6, 5, 3, 23].

Many of the sparse CSPs belong to a broad universality class called the one-step-replica-symmetry-breaking (1RSB) class from statistical physics [43] (see Chapter 19 of [47] for a survey) - including 2-coloring on random regular k-uniform hypergraphs, random regular k-NAE-SAT, and random k-SAT for $k \geq 3$. The 1RSB class refers to CSPs which are predicted to possess a single layer of hierarchy of well-separated clusters, where a cluster roughly refers to a dense region of the solution space. A shared characteristic of these problems is that in a non-trivial regime below $\alpha_{\mathsf{sat}} \equiv \alpha_{\mathsf{sat}}(k)$, the number of solutions fails to concentrate about its mean due to the clustering effect. This effect thus prevents standard first and second moment methods from locating the exact transition, presenting a significant mathematical challenge.

Despite such difficulties, breakthroughs were made to successfully locate the satisfiability threshold of the random regular k-NAE-SAT [31], the random k-SAT [32], and random regular k-SAT [21] for large enough $k \geq k_0$, where k_0 is a non-explicit large absolute constant. These works carried out a demanding second moment method to the number of clusters instead of the number of solutions based on intuitions from statistical physics [46] and previous mathematical works [6, 20, 21]. See Section 1.1 for further literature.

However, for small values of $k \geq 3$, locating the satisfiability threshold for CSPs in the 1RSB class remains an important open problem. Indeed, for all the aforementioned models in 1RSB class, the physicists conjecture an explicit value $\alpha_\star(k)$ for $\alpha_{\mathsf{sat}}(k)$, the 1RSB threshold, which is expected to be correct for all $k \geq 3$ [45, 46, 25]. The methods of [31, 32, 21] crucially uses the fact that k is large enough for their second moment method to succeed.

In this work, we consider 2-coloring on random d-regular k-uniform hypergraphs, where the random hypergraph is generated uniformly at random from the set of k-uniform hypergraphs such that every variable participates in exactly d hyperedges. We also consider random d-regular NAE-SAT, where k-SAT formula is generated uniformly at random with the condition that every variable participates in exactly d clauses. We establish an upper bound $d_\star(k)$ on the satisfiability thresholds for these problems for every $k \geq 3$, which is sharp [28] for random regular k-NAE-SAT for large $k \geq k_0$ and conjectured to be sharp [25] for $k \geq 3$ for hypergraph 2-coloring.

▶ **Theorem 1.1.** *For $k \geq 3$ and $d_{\text{lbd}}(k) \leq d \leq d_{\text{ubd}}(k)$, where $d_{\text{lbd}}(k), d_{\text{ubd}}(k)$ are defined in* (1.4) *below, there exists a unique solution $x_\star \equiv x_\star(k,d)$ to the equation*

$$d = 1 + \left(\log \frac{1-2x}{1-x}\right) / \log\left(\frac{1-2x^{k-1}}{1-x^{k-1}}\right) \quad \text{on the interval} \quad \frac{1}{2} - \frac{1}{2^k} \leq x \leq \frac{1}{2}. \tag{1.1}$$

Define $d_\star(k)$ by the largest zero of the explicit function

$$^\star\mathbf{\Phi}(d) := -\log(1-x) - d(1-k^{-1}-d^{-1})\log(1-2x^k) + (d-1)\log(1-x^{k-1}), \tag{1.2}$$

where the existence of the root of $^\star\mathbf{\Phi}(d)$ is guaranteed in the interval $[d_{\text{lbd}}(k), d_{\text{ubd}}(k)]$.

Then, for $k \geq 3$, and $d > d_\star(k)$, the random d-regular k-uniform hypergraph is not 2-colorable with probability tending to one as the graph size $n \to \infty$. Similarly for $k \geq 3$ and $d > d_\star(k)$, then the random d-regular k-NAE-SAT instance is not satisfiable with probability tending to one as $n \to \infty$.

A matching lower bound was obtained in [28] for large enough $k \geq k_0$ in random d-regular NAE-SAT by a demanding second moment method. Our proof is based on an interpolation method from statistical physics [35, 37, 52]. We give a proof outline in Section 1.2.

We emphasize that for any $k \geq 3$, determining the colorability threshold for 2-coloring on random d-regular k-uniform hypergraphs was previously open, thus Theorem 1.1 for 2-coloring is novel even for large k. Although it is expected that the colorability threshold for the model matches the satisfiability threshold for random regular k-NAE-SAT, it is highly non-trivial to modify the proof techniques for random regular NAE-SAT [31] to the 2-coloring model since many of the arguments in [31] crucially take advantage of the randomness of clauses. For example, any $\underline{x} \in \{0,1\}^n$ has the same probability of being a NAE-SAT solution by the randomness of the clauses while this is obviously not true for the 2-coloring model. As we see below, even the calculation of the first moment of the solutions is substantially more involved for the 2-coloring model. Let Z_{NAE} be the number of solutions of random d-regular k-NAE-SAT, then it is trivial to calculate $\mathbb{E}Z_{\text{NAE}}$ exactly by taking advantage of the randomness of the clauses:

$$\mathbb{E}Z_{\text{NAE}} = 2^n(1-2^{-k+1})^m = \exp\Big(n\Big(\log 2 + \alpha \log\left(1-2^{-k+1}\right)\Big)\Big) =: \exp\left(n\Phi_k(\alpha)\right). \tag{1.3}$$

On the other hand, if we denote Z_{COL} by the number of 2-colorings on random d-regular k-uniform graphs, then estimating $\mathbb{E}Z_{\text{COL}}$ is more delicate: we appeal to the idea of exponential tilting from large deviations theory [26] and local central limit theorem [13] to prove that $\mathbb{E}Z_{\text{COL}}$ is of the same order as $\exp\left(n\Phi_k(\alpha)\right)$ in Lemma 1.7 below. Using the interpolation bound which is simpler than moment calculations, we clarify a simple mechanism (cf. Lemma 2.2) behind the identical satisfiability upper bounds for both models.

The solution $x_\star(k,d)$ to the equation (1.1) has a mathematical interpretation. Namely, $2x_\star(k,d)$ is the fraction of the so-called *frozen* variables in the *cluster* model. The solution $x_\star(k,d)$ is called the *Belief Propagation* (BP) fixed point for the cluster model in statistical physics. We emphasize that addressing the uniqueness of the BP fixed point is a well-known major obstacle for many combinatorial optimization and statistical inference problems that exhibit sharp phase transitions (e.g. for spherical perceptron model [55]; see [59, Chapter 3] for a further discussion). We establish the uniqueness of the BP fixed point by showing that the *Belief Propagation recursion* (cf. (1.12)) is a contraction for $k \geq 3$ and $[d_{\text{lbd}}(k), d_{\text{ubd}}(k)]$, which might be also useful in obtaining a matching lower bound to Theorem 1.1.

Table 1 A comparison with the upper bound $d_\star(k)$ in Theorem 1.1 with the first moment threshold $d_1(k) := \frac{k\log 2}{-\log\left(1-2^{-k+1}\right)}$ for small values of k. For $3 \le k \le 10$, the values also appear in Table 1 of [25].

k	3	4	5	6	7	8	9	10	11	12	13	14	15
$\lceil d_\star(k)\rceil$	7	20	53	130	307	705	1592	3543	7802	17028	36902	79488	170340
$\lceil d_1(k)\rceil$	8	21	54	131	309	708	1594	3546	7804	17031	36905	79491	170343

Since $\mathbb{E}Z_{\text{NAE}}$ and $\mathbb{E}Z_{\text{COL}}$ are given by $\exp\left(n\Phi_k(\alpha)\right)$ up to a constant (cf. (1.3) and Lemma 1.7), the first moment thresholds for both of the models are given by $d_1(k) := \frac{k\log 2}{-\log(1-2^{-k+1})}$. In Table 1, we report $\lceil d_\star(k)\rceil$ and $\lceil d_1(k)\rceil$ for $3 \le k \le 15$. For every $3 \le k \le 15$, the upper bound $\lceil d_\star(k)\rceil$ in Theorem 1.1 improves over the first moment threshold. For large values of k, $d_\star(k)$ improves over $d_1(k)$ by $\Omega(k)$ (see (1.5) below). The quantities $d_{\text{lbd}}(k)$, and $d_{\text{ubd}}(k)$ are defined by

$$d_{\text{lbd}}(k) = \begin{cases} 6.74 & k=3\,, \\ 16.7 & k=4\,, \\ (2^{k-1}-2)k\log 2 & k\ge 5\,. \end{cases} \qquad d_{\text{ubd}}(k) = \begin{cases} 7.5 & k=3\,, \\ 2^{k-1}k\log 2 & k \ge 4\,. \end{cases} \tag{1.4}$$

▶ Remark 1.1. For $d \le d_{\text{lbd}}(k)$ and large $k \ge k_0$, the second moment method applied to Z_{NAE} succeeds in showing the satisfiability for the random d-regular k-NAE-SAT model (see [28, Section 2.1]). For $k \in \{3,4\}$, $d_{\text{lbd}}(k)$ must be adjusted to be higher to guarantee that ${}^\star\boldsymbol{\Phi}(d)$ is well-defined, i.e. there exists a unique solution to (1.1). The value $d_{\text{ubd}}(k) \equiv 2^{k-1}k\log 2 > d_1(k)$ for $k \ge 4$ is a convenient upper bound for satisfiability. For $k=3$, we take $d_{\text{ubd}}(3)$ to be $7.5 > \frac{3\log 2}{-\log(3/4)} = d_1(3)$, which does not change $d_\star(3)$, but is more convenient for the proof.

Finally, we note that the large k asymptotics of $d_\star(k)$ was proven in [58, Appendix B]:

$$\alpha_\star(k) \equiv \frac{d_\star(k)}{k} = \left(2^{k-1} - \frac{1}{2} - \frac{1}{4\log 2}\right)\log 2 + o_k(1)\,, \tag{1.5}$$

where $o_k(1)$ denotes an error tending to zero as $k \to \infty$. Since $d_1(k) = (2^{k-1}-1/2)k\log 2 + o_k(1)$, we have that $d_\star(k) \le d_1(k) - \Omega(k)$.

1.1 Related work

Many of the earlier mathematical works on CSPs focused on determining their satisfiability thresholds and verifying the sharpness of SAT-UNSAT transitions. For models that are known not to exhibit RSB, such goals were established. These models include random 2-SAT [15, 12], random 1-IN-k-SAT [1], k-XOR-SAT [33, 27, 53], and random linear equations [8]. On the other hand, for the models which are predicted to belong to 1RSB class, intensive studies have been conducted to estimate their satisfiability threshold, as shown in [42, 6, 21] (random k-SAT), [3, 24, 19] (random k-NAE-SAT), and [4, 16, 23, 17] (random graph coloring).

More recently, the satisfiability thresholds for rCSPs that exhibits RSB have been rigorously determined for several models, namely the random regular k-NAE-SAT [31], maximum independent set on d-regular graphs [30], random regular k-SAT [21] and random k-SAT [32] for large k and d. Although determining the location of q-colorability threshold for the sparse Erdős Rényi graph is left open, the *condensation threshold* α_{cond} for random graph coloring, where the *free energy* becomes non-analytic, was settled in [11]. They carried out a technically challenging analysis based on a clever "planting" technique, where the results were further generalized to other models in [18]. Similarly, [10] identified the condensation threshold for random regular k-SAT, where each variable appears $d/2$-times positive and $d/2$-times negative. Further, in the condensation regime $\alpha \in (\alpha_{\mathsf{cond}}, \alpha_{\mathsf{sat}})$, many quantities of interest were established for random regular k-NAE-SAT with large enough k, matching the statistical physics prediction. Namely, the number of solutions at exponential scale (free energy) [58], the concentration of the *overlap* [49, 51], and the local weak limit [56] were established. Establishing the same quantities for other models in the condensation regime is still open.

The closest result to ours in the literature is by Ayre, Coja-Oghlan, and Greenhill [9], where they lower bound the chromatic number (or equivalently, upper bound the colorability threshold) of the random regular graph of any degree, which is conjectured to be tight. [9] also considers the sparse Erdős-Rényi graph, which is more complicated since the conjectured chromatic number is defined in terms of a distributional (rather than real-valued) optimization due to the randomness of the local neighborhoods. In this work, we do not consider Erdős-Rényi type problems, but we additionally address the question of the uniqueness of the BP fixed point for any $k \geq 3$ (unique solution to the equation (1.1)). As in [9], we use an interpolation bound, which gives an upper bound of the satisfiability threshold also for the (non-regular) random k-NAE-SAT model. It would be interesting to address the uniqueness of the BP fixed point for random k-NAE-SAT and random k-sat for small $k \geq 3$. We refer to [55, 48, 60, 36] which addresses the uniqueness of BP fixed point for various models.

1.2 Proof methods

We aim to rigorously establish the upper bound for the satisfiability threshold predicted by the so-called "1RSB cavity method" from statistical physics [25]. To do so, instead of using moment methods, we use a theorem derived from the so called "interpolation method" from the theory of spin glasses developed by [35, 37, 52]. The interpolation method has been successful in upperbounding the satisfiability threshold for random k-SAT [29] for large k, the free energy for random regular k-NAE-SAT [57], and the colorability threshold for random graphs [9].

We first introduce the notations and mathematical framework that we use throughout the paper. For both the d-regular k-uniform hypergraphs and the k-NAE-SAT formula, we can represent them as (labelled) (d, k)-regular bipartite graph. Let $V = \{v_1, \ldots, v_n\}$ be the set of variables or nodes and $F = \{a_1, \ldots, a_m\}$ be the set of clauses or hyperedges. An edge is formed if the variable or node v_i is included in the clause or hyperedge a_j. For an edge e, we denote $v(e)$ (resp. $a(e)$) by the variable (resp. clause) adjacent to it.

Denote $G = (V, F, E)$ by the resulting bipartite graph. Each variable $v \in V$ has incident half-edges δv, while each clause $a \in F$ has incident half-edges δa. Throughout, we denote $\alpha \equiv \frac{m}{n} = \frac{d}{k}$. For the NAE-SAT formula, there is an extra label for each edge $e \in E$, namely the *literal* $\mathtt{L}_e \in \{0, 1\}$, which specifies how the variable $v(e)$ participates in the clause $a(e)$. Then, the labelled graph $\mathcal{G} = (V, F, E, \underline{\mathtt{L}}) \equiv (V, F, E, (\mathtt{L}_e)_{e \in E})$ represents a NAE-SAT instance.

▶ **Definition 1.2.** Given a NAE-SAT instance $\mathcal{G} = (V, F, E, \underline{\mathtt{L}})$, $\underline{x} \in \{0, 1\}^V$ is a (NAE-SAT) **solution** if

$$\prod_{a \in F} \varphi((x_{v(e)} \oplus \mathtt{L}_e)_{e \in \delta a}) = 1\,,$$

where for $\underline{z} = (z_i)_{i \leq k} \in \{0, 1\}^k$, $\varphi(\underline{z}) \equiv \mathbb{1}(z_1 = \ldots = z_k)$, and $\oplus$ denotes addition mod 2. Given a graph $G = (V, F, E)$, $\underline{x} \in \{0, 1\}^V$ is a (hypergraph 2-) **coloring** if $\underline{x}$ is a NAE-SAT solution on G with literals identically zero $(G, \underline{0})$.

The configuration model can be described as follows. Add d (resp. k) half-edges adjacent to each variable (resp. each clause) so that there are total $nd = mk$ number of half-edges adjacent to variables (resp. clauses). Thus, E can be regarded as a perfect matching between to the set of half-edges adjacent to variables to those adjacent to clauses, and hence a permutation in S_{nd}. Then, the configuration model $\boldsymbol{G} = (V, F, \boldsymbol{E})$ is defined by taking $\boldsymbol{E} \sim \text{Unif}(S_{nd})$. For a random d-regular k-NAE-SAT instance $\boldsymbol{\mathcal{G}} = (\boldsymbol{G}, \underline{\mathbf{L}})$, we take the literals $\underline{\mathbf{L}} \equiv (\mathbf{L}_e)_{e\in E} \stackrel{i.i.d.}{\sim} \text{Unif}(\{0,1\})$.

Note that the configuration model $\boldsymbol{G}$ may induce multi-edges. However, if we denote $\mathscr{S}$ to be the event that $\boldsymbol{G}$ is simple, then it is well-known that $\mathbb{P}(\boldsymbol{G} \in \mathscr{S}) = \Omega(1)$ (see e.g. Chapter 9 of [40]). Thus, the configuration model is mutually contiguous with respect to the uniform distribution among all (d, k)-regular graphs, so to prove Theorem 1.1, it suffices to work with the configuration model.

In order to use the interpolation method, we consider the *positive temperature* analogs of the 2-coloring or the NAE-SAT model, which have more desirable properties due to the softness of the constraints - e.g. the concentration of the free energy as seen in Lemma 1.3 below. We introduce notations that allow us to set up the positive temperature models. Let S be a finite set and $\underline{b} \equiv (b_s)_{s\in S}$ be a vector with $b_s \geq 0$. Also, let $\mathcal{X}$ be a finite set encoding the spins and denote $\mathfrak{F}(\mathcal{X})$ by the set of functions $\mathcal{X} \to \mathbb{R}_{\geq 0}$. Let $f : S \to \mathfrak{F}(\mathcal{X})$ be a random function which may be chosen randomly according to any distribution, i.e. $f(\cdot; s) \in \mathfrak{F}(\mathcal{X})$ is random for $s \in S$, and $f_1, \ldots, f_k$ be i.i.d. copies of f. Then, define the random function $\theta : \mathcal{X}^k \to \mathbb{R}$ as follows. For $\underline{x} = (x_1, \ldots, x_k) \in \mathcal{X}^k$, let

$$\theta(\underline{x}) = \sum_{s\in S} b_s \prod_{i=1}^{k} f_i(x_i; s)\,. \tag{1.6}$$

We will consider $S = \mathcal{X} = \{0, 1\}$ in Definition 1.4 below, but one may also consider the case $S \neq \mathcal{X}$ in general. We assume that there exists a constant $\varepsilon \in (0, 1)$ such that for any $\underline{x} \in \mathcal{X}^k$,

$$\varepsilon \leq 1 - \theta(\underline{x}) \leq \varepsilon^{-1} \quad \text{almost surely.} \tag{1.7}$$

On a (d, k)-regular bipartite graph $G = (V, F, E)$, let $(\theta_a)_{a\in F}$ be i.i.d. copies of the random function θ, and define the (random) Gibbs measure on $\mathcal{X}^V$ by

$$\mu_G(\underline{x}) \equiv \frac{1}{Z(G)} \prod_{a\in F} \Big(1 - \theta_a(\underline{x}_{\delta a})\Big)\,,$$

where $Z(G)$ is the normalizing constant explicitly given by

$$Z(G) \equiv \sum_{\underline{x}\in\mathcal{X}^V} \prod_{a\in F} \Big(1 - \theta_a(\underline{x}_{\delta a})\Big)\,. \tag{1.8}$$

We note that the condition (1.7) on θ guarantees that the Gibbs measure μ_G is "finite temperature". In particular, if we define the free energy

$$F_n \equiv \frac{1}{n}\mathbb{E} \log Z(\boldsymbol{G})\,, \tag{1.9}$$

where $\boldsymbol{G}$ is drawn from the configuration model and $\mathbb{E}$ above is over the randomness of $\boldsymbol{G}$ and randomness of $(\theta_a)_{a\in F}$, we have the following concentration of the free energy.

▶ **Lemma 1.3.** *Assume that θ satisfies* (1.7) *with some constant $\varepsilon \in (0,1)$. Then, for any $\delta > 0$, there exists a constant which only depends on $\varepsilon, \delta > 0$ such that*

$$\mathbb{P}\left(\left|\frac{1}{n}\log Z(\boldsymbol{G}) - F_n\right| \geq \delta\right) \leq e^{-cn}.$$

The concentration of free energy in Lemma 1.3 is standard in literature [11, 22, 9], and we provide the proof in Section 2 for completeness.

▶ **Definition 1.4.** (Positive temperature models) For $\beta > 0$, called the inverse temperature, the positive temperature NAE-SAT model $\theta_{\text{NAE}}(\cdot) \equiv \theta_{\text{NAE}}(\cdot\,;\beta)$ is defined as follows. Let $\underline{\mathtt{L}} \equiv (\mathtt{L}_i)_{i\leq k} \stackrel{i.i.d.}{\sim} \text{Unif}(\{0,1\})$ be a sequence of i.i.d. Bernoulli(1/2) random variables. Then for $\underline{x} = (x_i)_{i\leq k} \in \{0,1\}^k$, define

$$\theta_{\text{NAE}}(\underline{x}) \equiv \theta_{\text{NAE}}(\underline{x};\beta) \equiv (1-e^{-\beta})\cdot\left(\prod_{i=1}^{k}(\mathtt{L}_i \oplus x_i) + \prod_{i=1}^{k}(\mathtt{L}_i \oplus x_i \oplus 1)\right). \tag{1.10}$$

That is, in the general form (1.6), we take $S = \mathcal{X} = \{0,1\}$, $b_i \equiv 1 - e^{-\beta}$, and $f(x;0) \equiv 1 - f(x;1) \equiv \mathbb{1}(x \oplus \mathtt{L})$ for $\mathtt{L} \sim \text{Unif}(\{0,1\})$. Moreover, the positive temperature hypergraph 2-coloring model $\theta_{\text{COL}}(\cdot) \equiv \theta_{\text{COL}}(\cdot\,;\beta)$ is defined by taking $\mathtt{L}_i \equiv 0$ above:

$$\theta_{\text{COL}}(\underline{x}) \equiv \theta_{\text{COL}}(\underline{x};\beta) \equiv (1-e^{-\beta})\cdot\sum_{s\in\{0,1\}}\prod_{i=1}^{k}\mathbb{1}(x_i = s), \tag{1.11}$$

which is taking $f(x;s) = \mathbb{1}(x = s)$ in (1.6).

We note that formally taking $\beta = \infty$ and $\theta = \theta_{\text{COL}}(\underline{x};\beta)$, the corresponding partition function $Z(G)$ equals the number of 2-coloring on G. A similar statement holds for the NAE-SAT model.

By constructing a certain sequential coupling of the given factor graph $(\boldsymbol{G}, (\theta)_{a\in F})$ to a set of disjoint trees so that the free energy is monotone at every step, the interpolation method [35, 37, 52] gives an upper bound on the free energy F_n as follows: for $\zeta \in \mathscr{P}\big(\mathscr{P}(\mathscr{P}(\mathcal{X}))\big)$, where $\mathscr{P}(A)$ denotes the set of probability measures on A, and $\lambda \in (0,1)$, there exists an explicit functional $\mathcal{P}(\zeta,\lambda) \equiv \mathcal{P}_{d,k,\theta}(\zeta,\lambda)$ such that we have $F_n \leq \inf_{\zeta,\lambda}\mathcal{P}(\zeta,\lambda) + o_n(1)$. By taking advantage of the interpolation method applied to positive temperature models in Definition 1.4 and the concentration of the free energy in Lemma 1.3, we prove the proposition below in Section 2.

▶ **Proposition 1.5.** *For a given $k \geq 3$ and d, suppose that there is a solution $x \in [1/2 - 1/2^k, 1/2]$ to the* BP *equation* (1.1)*. Further, suppose that ${}^\star\boldsymbol{\Phi}(d)$ in* (1.2) *defined with such x satisfies ${}^\star\boldsymbol{\Phi}(d) < 0$. Then, with probability tending to one, no* NAE-SAT *solution exists on $\boldsymbol{\mathcal{G}}$. Also, with probability tending to one, no 2-coloring exists on $\boldsymbol{G}$.*

Moreover, we show that $d_\star(k)$ in Theorem 1.1 is well-defined and that the assumptions of Proposition 1.5 are meaningful. Note that the BP equation (1.1) is equivalent to $\Psi_d(x) = x$, where $\Psi_d \equiv \Psi_{k,d} : [0,1] \to [0,1]$ is defined by $\Psi_d \equiv \dot{\Psi} \circ \hat{\Psi}$ with

$$\dot{\Psi}(x) \equiv \dot{\Psi}_d(x) \equiv \frac{1 - x^{d-1}}{2 - x^{d-1}}, \qquad \hat{\Psi}(x) \equiv \hat{\Psi}_k(x) \equiv \frac{1 - 2x^{k-1}}{1 - x^{k-1}}. \tag{1.12}$$

The function $\dot{\Psi}(\cdot)$ is *variable* BP *recursion* and $\hat{\Psi}(\cdot)$ is *clause* BP *recursion* (see [31, Section 3.1] for the motivation).

▶ **Proposition 1.6.** *For $k \geq 3$ and $d \in [d_{\text{lbd}}(k), d_{\text{ubd}}(k)]$, there exists a unique root to $\Psi_d(x) \equiv (\dot{\Psi} \circ \hat{\Psi})(x) = x$ in the interval $x \in [1/2 - 1/2^k, 1/2]$. Thus, ${}^\star\mathbf{\Phi}(d)$ in equation* (1.2) *is well-defined. Furthermore, $d \to {}^\star\mathbf{\Phi}(d)$ is continuous in the interval $d \in [d_{\text{lbd}}(k), d_{\text{ubd}}(k)]$ with ${}^\star\mathbf{\Phi}(d_{\text{lbd}}(k)) > 0$ and ${}^\star\mathbf{\Phi}(d_{\text{ubd}}(k)) < 0$.*

The proof of Proposition 1.6 is given in Section 3 for $k \geq 4$. We refer to the full version [14] for the proof of Proposition 1.6 for $k = 3$, which requires extra numerical estimates. Finally, we show that the first moment $\mathbb{E}Z_{\text{COL}}$ of the number of 2-colorings on random d-regular k-uniform hypergraphs is the same with $\mathbb{E}Z_{\text{NAE}}$ up to a constant.

▶ **Lemma 1.7.** *For $k \geq 3$, there exist constants $C_{k,d,i}$ for $i = 1, 2,$, which only depends on k, d such that $\mathbb{E}Z_{\text{COL}}/\mathbb{E}Z_{\text{NAE}} \in [C_{k,d,1}, C_{k,d,2}]$*

Proof of Theorem 1.1. By Proposition 1.6, the function ${}^\star\mathbf{\Phi}(d)$ is well-defined and has a root in the interval $[d_{\text{lbd}}(k), d_{\text{ubd}}(k)]$. Moreover, since ${}^\star\mathbf{\Phi}(d_{\text{ubd}}(k)) < 0$ holds and ${}^\star\mathbf{\Phi}(\cdot)$ is continuous, we have ${}^\star\mathbf{\Phi}(d) < 0$ for $d \in (d_\star(k), d_{\text{ubd}}(k)]$. Hence, Proposition 1.5 shows that if $d \in (d_\star(k), d_{\text{ubd}}(k)]$, then the 2-coloring of random d-regular k-uniform hypergraph and random d-regular k-NAE-SAT is not satisfiable, both with probability tending to one as $n \to \infty$. Further, since $\mathbb{E}Z_{\text{COL}} \asymp_{k,d} \mathbb{E}Z_{\text{NAE}} = \exp\left(n\big(\log 2 + \alpha \log\left(1 - 2^{-k+1}\right)\big)\right)$ by Lemma 1.7 and $\log 2 + \alpha \log\left(1 - 2^{-k+1}\right) < 0$ holds for $d > d_{\text{ubd}}(k)$, the same is true for $d > d_{\text{ubd}}(k)$ by Markov's inequality. ◀

2 Satisfiability upper bound by interpolation

In this section, we prove Lemma 1.3, Proposition 1.5, and Lemma 1.7. We prove Proposition 1.5 in Section 2.1 based on the interpolation bound from statistical physics [35, 37]. In Section 2.2, we prove Lemma 1.3 based on Azuma Hoeffding's inequality applied to the Doob martingale with respect to clause revealing filtration. In Section 2.3, we prove Lemma 1.7 based on the local central limit theorem.

2.1 Proof of Proposition 1.5

Throughout, we assume that we are given $k \geq 3$ and d such that there is a solution $x \in [1/2 - 1/2^k, 1/2]$ to the equation (1.1). We use the following *one-step-replica-symmetry-breaking bound* proven in [58, Theorem E.3] for random regular graphs (see also [44]), which is the analog of [52, Theorem 3] for Erdős-Rényi graphs.

▶ **Theorem 2.1** (Theorem E.3 in [58])**.** *Let $\mathcal{X}$ and S be finite sets and consider the partition function $Z(G)$ (cf. Eq. (1.8)), where θ in (1.6) satisfies the condition (1.7) for some $\varepsilon > 0$ and $b_s \geq 0$ holds for $s \in S$. Let $\mathcal{M}_0 \equiv \mathscr{P}(\mathcal{X})$ be the space of probability measures over $\mathcal{X}$, $\mathcal{M}_1 \equiv \mathscr{P}(\mathcal{M}_0)$ be the space of probability measures over $\mathcal{M}_0$, and $\mathcal{M}_2 \equiv \mathscr{P}(\mathcal{M}_1)$ be the space of probability measures over $\mathcal{M}_1$. For $\zeta \in \mathcal{M}_2$, let $\underline{\eta} = (\eta_{a,j})_{a \geq 0, j \geq 0}$ be an array of i.i.d. samples from ζ. For each index (a, j) let $\rho_{a,j} \in \mathscr{P}(\mathcal{X})$ be a conditionally independent sample from $\eta_{a,j}$, and denote $\underline{\rho} = (\rho_{a,j})_{a \geq 0, j \geq 0}$. For $x \in \mathcal{X}$ define random variables*

$$u_a(x) \equiv \sum_{\underline{x} \in \mathcal{X}^k} \mathbb{1}\{x_1 = x\}\big(1 - \theta_a(\underline{x})\big) \prod_{j=2}^{k} \rho_{a,j}(x_j)\,, \qquad u_a \equiv \sum_{\underline{x} \in \mathcal{X}^k} \big(1 - \theta_a(\underline{x})\big) \prod_{j=1}^{k} \rho_{a,j}(x_j)\,,$$

where we recall that $(\theta_a)_{a \geq 0}$ are i.i.d. copies of the random function θ. For any $\lambda \in (0, 1)$ and any $\zeta \in \mathcal{M}_2$,

$$F_n \le \mathcal{P}(\zeta, \lambda) + O_\varepsilon(n^{-1/3}), \quad \text{where}$$
$$\mathcal{P}(\zeta,\lambda) \equiv \mathcal{P}_\theta(\zeta,\lambda) := \lambda^{-1}\mathbb{E}\log \mathbb{E}'\left[\Big(\sum_{x\in\mathcal{X}}\prod_{a=1}^{d} u_a(x)\Big)^{\lambda}\right] - (k-1)\alpha\lambda^{-1}\mathbb{E}\log\mathbb{E}'\left[(u_0)^{\lambda}\right]. \tag{2.1}$$

Here, F_n is the free energy for the configuration model defined in (1.9)*, $\mathbb{E}'$ denotes the expectation over $\underline{\rho}$ conditioned on all else, and $\mathbb{E}$ denotes the overall expectation.*

▶ Remark 2.1. [58, Theorem E.3] is stated more general than Theorem 2.1 by considering independent *external field* $\{h_v\}_{v\in V}$ and random $(b_s)_{s\in S}$. For our purposes, it suffices to consider non-random $b_s \ge 0$ and $h_v \equiv 1$.

We use Theorem 2.1 for the positive temperature models in Definition 1.4. Note that $\theta_{\text{NAE}}(\cdot\,;\beta)$ and $\theta_{\text{COL}}(\cdot\,;\beta)$ satisfies the condition (1.7) with $\varepsilon = e^{-\beta}$. Furthermore, in the bound (2.1), we take $\lambda = \beta^{-1/2}$ and $\zeta \equiv \zeta_{k,d,\beta} \in \mathscr{P}\Big(\mathscr{P}\big(\mathscr{P}(\{0,1\})\big)\Big)$ given by a point mass at $\eta_{k,d,\beta}$:

$$\zeta_{k,d,\beta} \equiv \delta_{\eta_{k,d,\beta}}, \tag{2.2}$$

where $\eta_{k,d,\beta} \in \mathscr{P}(\mathscr{P}(\{0,1\}))$ is defined as follows. Identify $\mathscr{P}(\{0,1\})$ with $[0,1]$ by the map

$$\rho \in \mathscr{P}(\{0,1\}) \leftrightarrow \rho(1) \in [0,1].$$

Thus, denoting $\eta \equiv \eta_{k,d,\beta} \in \mathscr{P}([0,1])$, define

$$\eta\left(\frac{e^{\beta}}{e^{\beta}+e^{-\beta}}\right) = \eta\left(\frac{e^{-\beta}}{e^{\beta}+e^{-\beta}}\right) = x, \quad \eta\left(\frac{1}{2}\right) = 1-2x, \tag{2.3}$$

where $x_\star \equiv x_\star(k,d)$ is the BP fixed point, i.e. the solution to the equation (1.1). Such choice of $\zeta_{k,d,\beta}$ is motivated from physics [43] and previous mathematical works [31, Section 3] and [32, Section 4].

Before proceeding further, we show that if ζ is given as in (2.2), (2.3), then $\mathcal{P}(\zeta,\lambda)$ does not depend on literals. More precisely, suppose that $\zeta = \delta_{\eta_0}$, where $\eta_0 \in \mathscr{P}([0,1])$ is such that $\eta_0(\mathrm{d}x) = \eta_0(\mathrm{d}(1-x))$, i.e. $\rho \stackrel{d}{=} 1-\rho$ holds for $\rho \sim \eta_0$. For a fixed $\underline{\mathtt{L}} = (\mathtt{L}_i)_{i\le k} \in \{0,1\}^k$, let

$$\theta_{\underline{\mathtt{L}}}(\underline{x}) = (1-e^{-\beta}) \cdot \left(\prod_{i=1}^{k}(\mathtt{L}_i \oplus x_i) + \prod_{i=1}^{k}(\mathtt{L}_i \oplus x_i \oplus 1)\right).$$

With abuse of notation, for $x \in \{0,1\}$ and independent samples $\rho_{a,j} \in \mathscr{P}(\{0,1\})$ from η_0, let

$$u_{a,\underline{\mathtt{L}}}(x) \equiv \sum_{\underline{x}\in\{0,1\}^k} \mathbb{1}\{x_1 = x\}\big(1-\theta_{\underline{\mathtt{L}}}(\underline{x})\big)\prod_{j=2}^{k}\rho_{a,j}(x_j), \qquad u_{\underline{\mathtt{L}}} \equiv \sum_{\underline{x}\in\{0,1\}^k}\big(1-\theta_{\underline{\mathtt{L}}}(\underline{x})\big)\prod_{j=1}^{k}\rho_{0,j}(x_j),$$

where we consider $\underline{\mathtt{L}} \in \{0,1\}^k$ to be fixed. Then, for a given sequence of literals $\underline{\mathtt{L}}_a \in \{0,1\}^k$ for $0 \le a \le d$, let

$$\mathcal{P}\big(\delta_{\eta_0}, \lambda; (\underline{\mathtt{L}}_a)_{0\le a\le d}\big) := \lambda^{-1}\log\mathbb{E}'\Big(\sum_{x\in\{0,1\}}\prod_{a=1}^{d}u_{a,\underline{\mathtt{L}}_a}(x)\Big)^{\lambda} - (k-1)\alpha\lambda^{-1}\mathbb{E}\log\mathbb{E}'\big(u_{\underline{\mathtt{L}}_0}\big)^{\lambda}, \tag{2.4}$$

where $\mathbb{E}'$ is the expectation with respect to the independent samples $\rho_{a,j} \in \mathscr{P}(\{0,1\})$ from η_0. Note that if $\underline{\mathtt{L}}_a \stackrel{i.i.d}{\sim} \text{Unif}(\{0,1\}^k)$, then $\mathcal{P}_{\theta_{\text{NAE}}}(\delta_{\eta_0},\lambda) = \mathbb{E}_{\underline{\mathtt{L}}}\mathcal{P}\big(\delta_{\eta_0},\lambda;(\underline{\mathtt{L}}_a)_{0\le a\le d}\big)$ holds, and if $\underline{\mathtt{L}}_a \equiv \underline{0}$ for $0 \le a \le d$, then $\mathcal{P}_{\theta_{\text{COL}}}(\delta_{\eta_0},\lambda) = \mathcal{P}\big(\delta_{\eta_0},\lambda;\underline{0}\big)$ holds. The following lemma then clarifies the mechanism behind the identical satisfiability upper bound in Theorem 1.1.

▶ **Lemma 2.2.** *Consider $\zeta = \delta_{\eta_0}$ for some $\eta_0 \in \mathscr{P}([0,1])$ such that $\eta_0(\mathrm{d}x) = \eta_0(\mathrm{d}(1-x))$. Then, for any literals $\underline{\mathtt{L}}_a \in \{0,1\}^k$ for $0 \le a \le d$, the value $\mathcal{P}\big(\delta_{\eta_0}, \lambda; (\underline{\mathtt{L}}_a)_{0\le a\le d}\big)$ does not depend on $(\underline{\mathtt{L}}_a)_{0\le a\le d}$. Thus, $\mathcal{P}_{\theta_{\text{NAE}}}(\delta_{\eta_0}, \lambda) = \mathcal{P}_{\theta_{\text{COL}}}(\delta_{\eta_0}, \lambda)$ holds.*

Proof. For fixed $\underline{\mathtt{L}}_a \in \{0,1\}^k$ for $0 \le a \le d$, note that the vectors $\big(u_{a,\underline{\mathtt{L}}_a}(0), u_{a,\underline{\mathtt{L}}_a}(1)\big)$ are independent for $0 \le a \le d$. Thus, it suffices to show that for given $\underline{\mathtt{L}}, \underline{\mathtt{L}}' \in \{0,1\}^k$ and $1 \le a \le d$,

$$u_{\underline{\mathtt{L}}} \stackrel{d}{=} u_{\underline{\mathtt{L}}'} \quad \text{and} \quad \big(u_{a,\underline{\mathtt{L}}}(0), u_{a,\underline{\mathtt{L}}}(1)\big) \stackrel{d}{=} \big(u_{a,\underline{\mathtt{L}}'}(0), u_{a,\underline{\mathtt{L}}'}(1)\big)\,. \tag{2.5}$$

To this end, let $\underline{\mathtt{L}}' = \underline{0}$ and we first prove that $u_{\underline{\mathtt{L}}} \stackrel{d}{=} u_{\underline{0}}$ holds. Since $\theta_{\underline{\mathtt{L}}}(\underline{x}) = \theta_{\underline{0}}(\underline{x} \oplus \underline{\mathtt{L}})$,

$$u_{\underline{\mathtt{L}}} \equiv \sum_{\underline{x}\in\{0,1\}^k} \big(1 - \theta_{\underline{\mathtt{L}}}(\underline{x})\big) \prod_{j=1}^k \rho_{0,j}(x_j) = \sum_{\underline{x}\in\{0,1\}^k} \big(1 - \theta_{\underline{0}}(\underline{x})\big) \prod_{j=1}^k \rho_{0,j}(x_j \oplus \mathtt{L}_j)\,.$$

Note that since $(\rho_{0,j})_{1\le j\le k}$ are i.i.d. samples from η_0 and $\eta_0(\mathrm{d}x) = \eta_0(\mathrm{d}(1-x))$ holds, the sequence $\big(\rho_{0,j}(\cdot \oplus \mathtt{L}_j)\big)_{1\le j\le k}$ are also i.i.d. from η_0. Hence, the equation above shows that $u_{\underline{\mathtt{L}}} \stackrel{d}{=} u_{\underline{0}}$ holds.

Next, we prove that $\big(u_{a,\underline{\mathtt{L}}}(0), u_{a,\underline{\mathtt{L}}}(1)\big) \stackrel{d}{=} \big(u_{a,\underline{0}}(0), u_{a,\underline{0}}(1)\big)$ holds. Without loss of generality, let $a = 1$. Again since $\theta_{\underline{\mathtt{L}}}(\underline{x}) = \theta_{\underline{0}}(\underline{x} \oplus \underline{\mathtt{L}})$,

$$u_{1,\underline{\mathtt{L}}}(x) = \sum_{\underline{x}\in\{0,1\}^k} \mathbb{1}\{x_1 \oplus \mathtt{L}_1 = x\}\big(1 - \theta_{\underline{0}}(\underline{x})\big) \prod_{j=2}^k \rho_{1,j}(x_j \oplus \mathtt{L}_j)$$

Now, observe that $\theta_{\underline{0}}(\cdot)$ is invariant under global flip, i.e. $\theta_{\underline{0}}(x) = \theta_{\underline{0}}(x \oplus 1)$. Thus, it follows that

$$u_{1,\underline{\mathtt{L}}}(x) = \sum_{\underline{x}\in\{0,1\}^k} \mathbb{1}\{x_1 = x\}[1 - \theta_{\underline{0}}(\underline{x})] \prod_{j=2}^k \rho_{1,j}(x_j \oplus \mathtt{L}_1 \oplus \mathtt{L}_j)\,.$$

By the same reasons as above, $\big(\rho_{1,j}(\cdot \oplus \mathtt{L}_1 \oplus \mathtt{L}_j)\big)_{2\le j\le k}$ have the same distribution as $\big(\rho_{1,j}\big)_{2\le j\le k}$, which are i.i.d. from η_0. Thus, we have that $\big(u_{1,\underline{\mathtt{L}}}(0), u_{1,\underline{\mathtt{L}}}(1)\big) \stackrel{d}{=} \big(u_{1,\underline{0}}(0), u_{1,\underline{0}}(1)\big)$. Therefore, (2.5) holds, which concludes the proof. ◀

The following lemma relates $\mathcal{P}_{\theta_{\text{COL}}}(\zeta_{k,d,\beta}, \beta^{-1/2}) = \mathcal{P}_{\theta_{\text{NAE}}}(\zeta_{k,d,\beta}, \beta^{-1/2})$, and ${}^\star\mathbf{\Phi}(d)$, which plays a crucial role in proving Proposition 1.5. Recall the definition of $\zeta_{k,d,\beta}$ in (2.2) and (2.3).

▶ **Lemma 2.3.** *$\mathcal{P}_{\theta_{\text{COL}}}(\zeta_{k,d,\beta}, \beta^{-1/2}) \le C + \beta^{1/2} \times {}^\star\mathbf{\Phi}(d)$ holds for some constant $C \in \mathbb{R}$, which does not depend on $\beta > 0$.*

Proof. Throughout, let $(\rho_{a,j})_{a\ge0,j\ge0}$ denote i.i.d. samples from $\eta_{k,d,\beta}$ defined in (2.3), and let $\mathbb{E}'$ (resp. $\mathbb{P}'$) denote the expectation (resp. probability) with respect to $(\rho_{a,j})_{a\ge0,j\ge0}$. Also, we use the generic notation C by a constant that does not depend on $\beta > 0$. Note that since θ_{COL} and $\eta_{k,d,\beta}$ are non-random, the outer expectation $\mathbb{E}$ in the definition of $\mathcal{P}(\zeta, \lambda)$ in (2.1) is redundant.

First, we bound the second term of the definition of $\mathcal{P}_{\theta_{\text{COL}}}(\zeta_{k,d,\beta}, \beta^{-1/2})$ in (2.1):

$$\begin{aligned}
&(k-1)\alpha\beta^{1/2} \log \mathbb{E}'\Big[\,(u_0)^{\beta^{-1/2}}\,\Big] \\
&= (k-1)\alpha\beta^{1/2} \log \mathbb{E}'\left[\left(1 - (1 - e^{-\beta})\Big(\prod_{j=1}^k \rho_{0,j}(0) + \prod_{j=1}^k \rho_{0,j}(1)\Big)\right)^{\beta^{-1/2}}\right]
\end{aligned}$$

Note that the expectation inside the log in the right hand side above is bounded below by

$$2^{-\beta^{-1/2}} \cdot \mathbb{P}'\left(1-(1-e^{-\beta})\Big(\prod_{j=1}^{k}\rho_{0,j}(0)+\prod_{j=1}^{k}\rho_{0,j}(1)\Big)\geq\frac{1}{2}\right)=2^{-\beta^{-1/2}}(1-2x^k)\,,$$

where x is the solution to the BP equation (1.1) and the equality holds for large enough $\beta \geq \beta_0$ since for large β and $k \geq 3$, $(1-e^{-\beta})\left(\prod_{j=1}^{k}\rho_{0,j}(0)+\prod_{j=1}^{k}\rho_{0,j}(1)\right)\geq\frac{1}{2}$ holds if and only if either $\rho_{0,j}(1)=\frac{e^{\beta}}{e^{\beta}+e^{-\beta}}$ holds for all $1\leq j\leq k$, or $\rho_{0,j}(1)=\frac{e^{-\beta}}{e^{\beta}+e^{-\beta}}$ holds for all $1 \leq j \leq k$. Thus, it follows that

$$-(k-1)\alpha\lambda^{-1}\mathbb{E}\log\mathbb{E}'\left[(u_0)^{\lambda}\right]\leq C-\beta^{1/2}(k-1)\alpha\log\left(1-2x^k\right). \tag{2.6}$$

Next, we estimate the first term of the definition of $\mathcal{P}_{\theta_{\text{COL}}}(\zeta_{k,d,\beta},\beta^{-1/2})$ in (2.1), which equals

$$\begin{aligned}&\beta^{1/2}\log\mathbb{E}'\Big[\Big(\sum_{x\in\{0,1\}}\prod_{a=1}^{d}u_a(x)\Big)^{\beta^{-1/2}}\Big]\\&=\beta^{1/2}\log\mathbb{E}'\left[\left(\prod_{a=1}^{d}\Big(1-(1-e^{-\beta})\prod_{j=2}^{k}\rho_{a,j}(0)\Big)+\prod_{a=1}^{d}\Big(1-(1-e^{-\beta})\prod_{j=2}^{k}\rho_{a,j}(1)\Big)\right)^{\beta^{-1/2}}\right]\end{aligned} \tag{2.7}$$

We upper bound the expectation inside the log in the above expression by

$$2^{\beta^{-1/2}}\cdot\mathbb{P}'(\mathcal{A})+\left(3e^{-\beta}\right)^{\beta^{-1/2}},$$

where

$$\mathcal{A}:=\left\{\prod_{a=1}^{d}\Big(1-(1-e^{-\beta})\prod_{j=2}^{k}\rho_{a,j}(0)\Big)+\prod_{a=1}^{d}\Big(1-(1-e^{-\beta})\prod_{j=2}^{k}\rho_{a,j}(1)\Big)\geq 3e^{-\beta}\right\}.$$

Define the events $\mathcal{E}_0$ and $\mathcal{E}_1$ involving $(\rho_{a,j})_{1\leq a\leq d,2\leq j\leq k}$ as follows.

- $\mathcal{E}_0$ is the event such that for each $1 \leq a \leq d$, we have for some $j \in \{2,\ldots,k\}$ that $\rho_{a,j}(0) \neq \frac{e^{\beta}}{e^{\beta}+e^{-\beta}}$.
- $\mathcal{E}_1$ is the event such that for each $1 \leq a \leq d$, we have for some $j \in \{2,\ldots,k\}$ that $\rho_{a,j}(1) \neq \frac{e^{\beta}}{e^{\beta}+e^{-\beta}}$.

We now claim that for large enough β, the event $\mathcal{A}$ is included in $\mathcal{E}_0 \cup \mathcal{E}_1$. To this end, suppose that the event $(\mathcal{E}_0\cup\mathcal{E}_1)^{\mathsf{c}}=\mathcal{E}_0^{\mathsf{c}}\cap\mathcal{E}_1^{\mathsf{c}}$ holds. Then, for each $x\in\{0,1\}$, for some $a \equiv a(x) \in \{1,\ldots,d\}$ such that $\rho_{a,j}(x)=\frac{e^{\beta}}{e^{\beta}+e^{-\beta}}$ holds for all $2 \leq j \leq k$. Thus, for $x \in \{0,1\}$, we have

$$\prod_{a=1}^{d}\Big(1-(1-e^{-\beta})\prod_{j=2}^{k}\rho_{a,j}(x)\Big)\leq 1-(1-e^{-\beta})\left(\frac{e^{\beta}}{e^{\beta}+e^{-\beta}}\right)^{k-1}\leq e^{-\beta}+ke^{-2\beta}<\frac{3}{2}e^{-\beta},$$

where the last inequality holds for large enough $\beta \geq \beta_k$ and we used $(1-x)^{k-1} \geq 1-(k-1)x$ for $x > 0$ in the second inequality. Hence, summing over $x \in \{0,1\}$ gives that the event $\mathcal{A}$ cannot hold, which proves our claim that $\mathcal{A} \subset \mathcal{E}_0 \cup \mathcal{E}_1$. Consequently, the term (2.7) is bounded above by

$$\beta^{1/2}\log\left(2^{\beta^{-1/2}}\cdot\mathbb{P}'(\mathcal{E}_0\cup\mathcal{E}_1)+(3e^{-\beta})^{\beta^{-1/2}}\right)\leq\beta^{1/2}\log\mathbb{P}'(\mathcal{E}_0\cup\mathcal{E}_1)+C\,.$$

Note that $\mathbb{P}'\big(\mathcal{E}_0 \cup \mathcal{E}_1\big)$ can be calculated explicitly by

$$\mathbb{P}'(\mathcal{E}_0 \cup \mathcal{E}_1) = 2(1-x^{k-1})^d - (1-2x^{k-1})^d = \frac{(1-x^{k-1})^{d-1}(1-2x^k)}{1-x},$$

where in the final equality, we used the fact that x is the solution to the equation (1.1). Therefore, we have proven that

$$\beta^{1/2}\log \mathbb{E}'\Big[\Big(\sum_{x\in\{0,1\}}\prod_{a=1}^{d} u_a(x)\Big)^{\beta^{-1/2}}\Big] \le C + \beta^{1/2}\big(-\log(1-x) + (d-1)\log(1-x^{k-1}) + \log(1-2x^k)\big)\,. \tag{2.8}$$

In conclusion, combining (2.6) and (2.8), and recalling the definition of ${}^\star\mathbf{\Phi}(d)$ in (1.2), we have

$$\mathcal{P}_{\theta_{\text{COL}}}(\zeta_{k,d,\beta}, \beta^{-1/2}) \le C + \beta^{1/2}\,{}^\star\mathbf{\Phi}(d)\,,$$

which concludes the proof. ◀

Proof of Proposition 1.5. Given a NAE-SAT instance $\mathcal{G}$, let $\mathsf{SOL}(\mathcal{G}) \subset \{0,1\}^V$ denotes the set of NAE-SAT solutions. Also, let $Z_{\beta,\text{NAE}}(\mathcal{G})$ denotes the partition function (1.8) for $\theta = \theta_{\text{NAE}}(\cdot\,;\beta)$. Note that if $\underline{x} \in \mathsf{SOL}(\mathcal{G})$, then $\theta_{\text{NAE}}(\underline{x}_{\delta a}) = 0$ for any $a \in F$, thus we have for any $\beta > 0$ that

$$Z_{\beta,\text{NAE}}(\mathcal{G}) \equiv \sum_{\underline{x}\in\{0,1\}^V}\prod_{a\in F}\big(1-\theta_{\text{NAE}}(\underline{x}_{\delta a};\beta)\big) \ge |\mathsf{SOL}(\mathcal{G})|\,. \tag{2.9}$$

On the other hand, since $\theta_{\text{NAE}}(\cdot\,;\beta)$ satisfies the condition (1.7) with $\varepsilon = e^{-\beta}$, we have by Theorem 2.1 that

$$\frac{1}{n}\mathbb{E}\Big[\log Z_{\beta,\text{NAE}}(\mathcal{G})\Big] \le \mathcal{P}_{\theta_{\text{NAE}}}(\zeta_{k,d,\beta},\beta^{-1/2}) + o_n(1) = \mathcal{P}_{\theta_{\text{COL}}}(\zeta_{k,d,\beta},\beta^{-1/2}) + o_n(1)\,,$$

where the last equality is due to Lemma 2.2. By Lemma 2.3, the right hand side is further bounded by

$$\frac{1}{n}\mathbb{E}\Big[\log Z_{\beta,\text{NAE}}(\mathcal{G})\Big] \le \beta^{1/2}\cdot{}^\star\mathbf{\Phi}(d) + C + o_n(1)\,,$$

for some constant C that does not depend on n nor β. If ${}^\star\mathbf{\Phi}(d) < 0$, then for large enough $\beta > 0$, $\beta^{1/2}\cdot{}^\star\mathbf{\Phi}(d) + C < -1$ holds, thus $n^{-1}\mathbb{E}\big[\log Z_{\beta,\text{NAE}}(\mathcal{G})\big] < -1$ holds for large enough n. For such $\beta = \beta_0(k,d) > 0$, we have by (2.9) and Lemma 1.3 that for large enough n,

$$\mathbb{P}\Big(|\mathsf{SOL}(\mathcal{G})| \ge 1\Big) \le \mathbb{P}\bigg(\bigg|\frac{1}{n}\log Z_{\beta_0,\text{NAE}}(\mathcal{G}) - \frac{1}{n}\mathbb{E}\Big[\log Z_{\beta_0,\text{NAE}}(\mathcal{G})\Big]\bigg| \ge 1\bigg) \le e^{-cn}\,,$$

for some constant c that depends only on $\beta_0 > 0$, which finishes the proof for the NAE-SAT model.

Given a configuration model $\boldsymbol{G}$, let $Z_{\beta,\text{COL}}(\boldsymbol{G})$ denote the partition function (1.8) for $\theta = \theta_{\text{COL}}(\cdot\,;\beta)$. Then, by the same reasoning, Theorem 2.1 and Lemma 2.3 shows that if ${}^\star\mathbf{\Phi}(d) < 0$ then $\frac{1}{n}\mathbb{E}\big[\log Z_{\beta,\text{COL}}(\boldsymbol{G})\big] < -1$ holds for large enough $\beta = \beta_0(k,d) > 0$ and n large enough. On the event that there exists a 2-coloring on $\boldsymbol{G}$, $Z_{\beta,\text{COL}}(\boldsymbol{G}) \ge 1$ holds, so Lemma 1.3 again concludes the proof. ◀

2.2 Proof of Lemma 1.3

Recall that $\boldsymbol{G} = (V, F, \boldsymbol{E})$ is generated from the configuration model, where the $\boldsymbol{E}$ is drawn uniformly from S_{nd}. Thus, $\boldsymbol{E}$ has the same law as sequentially drawing random clauses $\boldsymbol{a}_1, \dots, \boldsymbol{a}_m$ as follows. At times $t \in \{1, \dots, m\}$ clause $\boldsymbol{a}_t$ is drawn by connecting the k adjacent half-edges to previously unmatched half-edges adjacent to variables. For $1 \le t \le m$, let $\mathscr{F}_t$ be the σ-algebra generated by $\boldsymbol{a}_1, \dots, \boldsymbol{a}_t$, and $\mathscr{F}_0 \equiv \emptyset$. Denote $M_t \equiv \mathbb{E}\big[\log Z(\boldsymbol{G}) \mid \mathscr{F}_t\big]$ by the associated Doob martingale. Note that if $\boldsymbol{G} = (V, F, E)$ and $\boldsymbol{G}' = (V, F, E')$ has the the same set of edges except for those adjacent to two clauses $a_1 \neq a_2 \in F$, then by our assumption of θ in (1.7) and the definition of $Z(G)$ in (1.8), it follows that $\varepsilon^2 \le Z(G)/Z(G') \le \varepsilon^{-2}$ holds. Thus, we have for every $t \in \{0, 1, \dots, m-1\}$ that

$$\Big|M_{t+1} - M_t\Big| \equiv \Big|\mathbb{E}\big[\log Z(\boldsymbol{G}) \mid \mathscr{F}_{t+1}\big] - \mathbb{E}\big[\log Z(\boldsymbol{G}) \mid \mathscr{F}_t\big]\Big| \le 2\log\big(1/\varepsilon\big)\,, \tag{2.10}$$

from which Lemma 1.3 follows.

Proof of Lemma 1.3. Note that $M_m = \log Z(\boldsymbol{G})$ and $M_0 = \mathbb{E}\big[\log Z(\boldsymbol{G})\big]$ holds and $(M_t)_{0 \le t \le m}$ is a martingale with bounded difference by (2.10). Therefore, the conclusion follows from Azuma Hoeffding's inequality. ◀

2.3 Proof of Lemma 1.7

The following notations are convenient for the proof of Lemma 1.7. For non-negative quantities $f = f_{d,k,n}$ and $g = g_{d,k,n}$, we use any of the equivalent notations $f = O_{k,d}(g), g = \Omega_{k,d}(f), f \lesssim_{k,d} g$ and $g \gtrsim_{k,d} f$ to indicate that there exists a constant $C_{k,d}$, which only depends on k, d such that $f \le C_{k,d} \cdot g$. We drop the subscripts d (resp. k, d) if the constant $C_{k,d}$ does not depend on d (resp. k, d). When $f \lesssim_{k,d} g$ and $g \lesssim_{k,d} f$, we write $f \asymp_{k,d} g$. Similarly when $f \lesssim g$ and $g \lesssim f$, we write $f \asymp g$.

Note that $\mathbb{E}Z_{\text{COL}}$ is the sum over $\underline{x} \in \{0,1\}^V$ of the probabilities that $\underline{x}$ is a 2-coloring on $\boldsymbol{G}$. By symmetry, the probability of $\underline{x} \in \{0,1\}^V$ being a 2-coloring depends only on the number $n\gamma$ of nodes having color 1, which we denote by $\boldsymbol{p}_\gamma$. Thus, $\mathbb{E}Z_{\text{COL}} = \sum_\gamma \binom{n}{n\gamma}\boldsymbol{p}_\gamma$, where the sum is over $\gamma \in (0,1)$ such that $n\gamma \in \mathbb{Z}$. Moreover, we can express $\boldsymbol{p}_\gamma$ as follows. Let $X_1, \dots, X_m$ be i.i.d. $\text{Binom}(k, \gamma)$ random variables and denote $\mathbb{P}_\gamma$ by the probability with repect to $(X_i)_{i \le m}$. Then, we have

$$\begin{aligned}\boldsymbol{p}_\gamma &= \mathbb{P}_\gamma\Big(X_i \notin \{0,k\} \quad \text{for all } 1 \le i \le m \,\Big|\, \sum_{i=1}^m X_i = km\gamma\Big) \\ &\le \frac{\mathbb{P}_\gamma\big(X_i \notin \{0,k\} \quad \text{for all } 1 \le i \le m\big)}{\mathbb{P}_\gamma\big(\sum_{i=1}^m X_i = km\gamma\big)} \lesssim_k \sqrt{m}(1 - \gamma^k - (1-\gamma)^k)^m\,,\end{aligned} \tag{2.11}$$

where the last inequality is due to a Stirling's approximation. It follows that

$$\begin{aligned}&\mathbb{E}Z_{\text{COL}} \le n^{O(1)} \sum_\gamma \exp\Big(nF_\alpha(\gamma)\Big)\,, \quad \text{where} \\ &F_\alpha(\gamma) := H(\gamma) + \alpha\log\big(1 - \gamma^k - (1-\gamma)^k\big)\,.\end{aligned} \tag{2.12}$$

Here, $H(\gamma) \equiv -\gamma\log\gamma - (1-\gamma)\log(1-\gamma)$ is the entropy of γ. Note that $\gamma \to \gamma^k + (1-\gamma)^k$ is uniquely minimized at $\gamma = 1/2$. Further, the entropy $H(\gamma)$ is strictly concave and is maximized at $\gamma = 1/2$. Thus, $\gamma \to F_\alpha(\gamma)$ is uniquely maximized at $\gamma = 1/2$ with $\frac{\partial^2 F_\alpha}{\partial\gamma^2}(1/2) < 0$. Since $\mathbb{E}Z_{\text{NAE}} = \exp\big(nF_\alpha(1/2)\big)$, it follows from (2.12) that

$$\mathbb{E}Z_{\text{COL}} \le n^{O(1)}\exp\big(nF_\alpha(1/2)\big) = n^{O(1)} \cdot \mathbb{E}Z_{\text{NAE}}\,. \tag{2.13}$$

We now show that the polynomial factor $n^{O(1)}$ can actually be removed with a matching lower bound.

First, by (2.11) and the fact that $\gamma \to F_\alpha(\gamma)$ is uniquely maximized at $\gamma = 1/2$ with strictly negative second derivative, the contribution to $\mathbb{E}Z_{\text{COL}}$ from γ such that $|\gamma - 1/2| \geq n^{-1/3}$ is negligible:

$$\sum_{|\gamma-1/2|\geq n^{-1/3}} \binom{n}{n\gamma} \boldsymbol{p}_\gamma \lesssim_{k,d} \exp\big(-\Omega_{k,d}(n^{1/3})\big) \cdot \mathbb{E}Z_{\text{NAE}}\,. \tag{2.14}$$

Thus, we focus on the regime $|\gamma - 1/2| \leq n^{-1/3}$. Note that we can calculate $\boldsymbol{p}_\gamma$ by summing over the empirical distribution ν of $(X_i)_{i\leq m}$. Consider $\nu \in \mathscr{P}(\{1,\ldots,k-1\})$ and let $p_\gamma(j) := \binom{k}{j}\gamma^j(1-\gamma)^{k-j}$. Then,

$$\boldsymbol{p}_\gamma = \frac{\sum_\nu \mathbb{1}\Big(\sum_j j\nu_j = km\gamma\Big) e^{-km\gamma\lambda}\binom{m}{m\nu}\prod_j (p_\gamma(j)e^{\lambda j})^{m\nu_j}}{\mathbb{P}_\gamma\big(\sum_{i=1}^m X_i = km\gamma\big)}\,,$$

where $\binom{m}{m\nu} \equiv \frac{m!}{\prod_j (m\nu_j)!}$ and we introduced a lagrange parameter $\lambda \in \mathbb{R}$ in the last equality. Let

$$\nu_{\gamma,\lambda}(x) := \frac{p_\gamma(x)e^{\lambda x}}{\sum_{j=1}^{k-1} p_\gamma(j)e^{\lambda j}} \quad \text{for} \quad 1 \leq x \leq k-1\,,$$

and denote $\mathbb{P}_{\gamma,\lambda}$ by the probability with respect to $\widetilde{X}_1,\ldots,\widetilde{X}_m \overset{i.i.d.}{\sim} \nu_{\gamma,\lambda}$. Then, it follows that

$$\boldsymbol{p}_\gamma = \frac{\mathbb{P}_{\gamma,\lambda}\big(\sum_{i=1}^m \widetilde{X}_i = km\gamma\big)}{\mathbb{P}_\gamma\big(\sum_{i=1}^m X_i = km\gamma\big)} \exp\big(-m\cdot\Xi(\gamma,\lambda)\big)\,, \text{ where } \Xi(\gamma,\lambda) := k\gamma\lambda - \log\left(\sum_{j=1}^{k-1} p_\gamma(j)e^{\lambda j}\right). \tag{2.15}$$

In order to use the local central limit theorem, we take $\lambda = \lambda(\gamma)$ such that $\mathbb{E}_{\gamma,\lambda}\widetilde{X} = k\gamma$, where $\widetilde{X} \sim \nu_{\gamma,\lambda}$. The existence of such $\lambda(\gamma)$ is guaranteed by the lemma below.

▶ **Lemma 2.4.** *For large enough n and all γ such that $|\gamma - 1/2| \leq n^{-1/3}$, there exists a unique $\lambda = \lambda(\gamma)$ such that $\mathbb{E}_{\gamma,\lambda}\widetilde{X} = k\gamma$ holds. Furthermore, we have $\lambda(1/2) = 0$ and $\big|\lambda(\gamma)\big| \lesssim_k n^{-1/3}$ holds uniformly over $|\gamma - 1/2| \leq n^{-1/3}$.*

Proof. Note that we have $\frac{\partial\Xi}{\partial\lambda}(\gamma,\lambda) = k\gamma - \mathbb{E}_{\gamma,\lambda}\widetilde{X}$ by definition of $\nu_{\gamma,\lambda}$ and $\Xi(\gamma,\lambda)$. Further, we have that

$$\frac{\partial\Xi}{\partial\lambda}\Big(\frac{1}{2}\,,0\Big) = \frac{k}{2} - \mathbb{E}_{\frac{1}{2},0}\widetilde{X} = \frac{k}{2} - \mathbb{E}_{\frac{1}{2}}\big[X \,\big|\, X \notin \{0,k\}\big] = 0\,,$$

where $\mathbb{E}_{\frac{1}{2}}$ is with respect to $X \sim \text{Binom}(1/2)$. Since $\lambda \to \log\big(\sum_{j=1}^{k-1} p_\gamma(j)e^{\lambda j}\big)$ is strongly convex, we have $\frac{\partial^2\Xi}{\partial\lambda^2}\big(\frac{1}{2},0\big) < 0$. Thus, implicit function theorem shows that for $\gamma \in (1/2-\varepsilon, 1/2+\varepsilon)$, where $\varepsilon = \varepsilon(k) > 0$ depends only on k, there exists $\lambda = \lambda(\gamma)$ such that $\frac{\partial\Xi}{\partial\lambda}\big(\gamma,\lambda(\gamma)\big) = 0$ holds, and that $\gamma \to \lambda(\gamma)$ is continuously differentiable. Therefore, for large enough n and $\gamma \in (1/2 - n^{-1/3}, 1/2 + n^{1/3})$, there exists a unique $\lambda = \lambda(\gamma)$ such that $\mathbb{E}_{\gamma,\lambda(\gamma)}\widetilde{X} = k\gamma$, and $|\lambda(\gamma)| \lesssim_k n^{-1/3}$ holds uniformly over $\gamma \in (1/2 - n^{-1/3}, 1/2 + n^{1/3})$. ◀

Having Lemma 2.4 in hand, we prove Lemma 1.7 by appealing to the local central limit theorem.

Proof of Lemma 1.7. The contribution to $\mathbb{E}Z_{\text{COL}}$ from γ such that $|\gamma - 1/2| \geq n^{-1/3}$ is negligible by (2.14), thus we consider γ such that $|\gamma - 1/2| \leq n^{-1/3}$ holds. To this end, we take $\lambda = \lambda(\gamma)$ from Lemma 2.4 in equation (2.15). Then, by the local central limit theorem [13],

$$\boldsymbol{p}_\gamma \asymp \left(\frac{\mathrm{Var}_\gamma\left(X\right)}{\mathrm{Var}_{\gamma,\lambda(\gamma)}\left(\widetilde{X}\right)}\right)^{1/2} \cdot \exp\Big(-m\cdot \Xi\big(\gamma,\lambda(\gamma)\big)\Big)\,, \tag{2.16}$$

where $X \sim \mathrm{Binom}(k,\gamma)$ and $\widetilde{X} \sim \nu_{\gamma,\lambda(\gamma)}$. Lemma 2.4 further shows that $\big|\lambda(\gamma)\big| \lesssim_k n^{-1/3}$, thus we have

$$\mathrm{Var}_{\gamma,\lambda(\gamma)}\left(\widetilde{X}\right) \asymp_k \mathrm{Var}_\gamma\left(X \,\middle|\, 1 \leq X \leq k-1\right) \asymp_k \mathrm{Var}_\gamma(X)\,, \tag{2.17}$$

where the final estimate holds because $|\gamma - 1/2| \leq n^{-1/3}$. Combining with (2.14), it follows that

$$\mathbb{E}Z_{\text{COL}} = \big(1+o_n(1)\big)\sum_{|\gamma-1/2|\leq n^{-1/3}}\binom{n}{n\gamma}\boldsymbol{p}_\gamma \asymp_{k,d} n^{-1/2}\sum_{|\gamma-1/2|\leq n^{-1/3}}\exp\big(nG_\alpha(\gamma)\big)\,, \tag{2.18}$$

where

$$G_\alpha(\gamma) := H(\gamma) - \alpha\cdot\Xi\big(\gamma,\lambda(\gamma)\big)\,.$$

Note that by comparing (2.16) and (2.17) with (2.11), we have $G_\alpha(\gamma) \leq F_\alpha(\gamma)$ for $|\gamma - 1/2| \leq n^{-1/3}$. Also, note that for $\gamma = 1/2$, $G_\alpha(1/2) = F_\alpha(1/2)$ holds since

$$G_\alpha(1/2) = H(1/2) - \alpha\cdot\Xi(1/2,0) = H(1/2) + \alpha\log\big(1-\gamma^k-(1-\gamma)^k\big)\,,$$

where we used $\lambda(1/2) = 0$ by Lemma 2.4. Recalling that $\gamma \to F_\alpha(\gamma)$ is uniquely maximized at $\gamma = 1/2$ with strictly negative second derivative at the maximizer, it follows that the same holds for $\gamma \to G_\alpha(\gamma)$. Therefore, the sum in the right hand side of (2.18) can be approximated by a Gaussian integration, which shows that

$$\mathbb{E}Z_{\text{COL}} \asymp_{k,d} \exp\big(nG_\alpha(1/2)\big) = \mathbb{E}Z_{\text{NAE}}\,.$$

This concludes the proof. ◀

3 Proof of Proposition 1.6

In this section, we prove Proposition 1.6 for $k \geq 4$. The proof of Proposition 1.6 for $k = 3$ is available in the arXiv version [14]. The proof of Proposition 1.6 for $k \geq 4$ can be split into the following two lemmas. In Section 3.1, we prove Lemma 3.1 which guarantees the existence and the uniqueness of the BP fixed point for $k \geq 4$.

▶ **Lemma 3.1.** *For $k \geq 4$ and $d \in [d_{\text{lbd}}(k), d_{\text{ubd}}(k)]$, there exists a unique solution to $\Psi_d(x) = x$ in the range $x \in [\frac{1}{2} - \frac{1}{2^k}, \frac{1}{2}]$.*

By Lemma 3.1, the function $d \to {}^\star\boldsymbol{\Phi}(d)$ is well-defined. In Section 3.2, we prove Lemma 3.2 which guarantees that $d_\star(k)$ is well-defined for $k \geq 4$.

▶ **Lemma 3.2.** *For $k \geq 4$, the function $d \to {}^\star\boldsymbol{\Phi}(d)$ is continuous for $d \in [d_{\text{lbd}}(k), d_{\text{ubd}}(k)]$. Further, ${}^\star\boldsymbol{\Phi}(d_{\text{lbd}}(k)) > 0$ and ${}^\star\boldsymbol{\Phi}(d_{\text{ubd}}(k)) < 0$ hold.*

Proof of Proposition 1.6 for $k \geq 4$. This is immediate from Lemma 3.1 and Lemma 3.2. ◀

3.1 Proof of Lemma 3.1

Recall the variable BP recursion $\dot{\Psi}$ and the clause BP recursion $\hat{\Psi}$ defined in (1.12). To prove the uniqueness of the BP fixed point, we show that the BP recursion $\Psi_d \equiv \dot{\Psi} \circ \hat{\Psi}$ is a contraction for $k \geq 4$.

▶ **Lemma 3.3.** *For $k \geq 4$ and $d \in [d_{\text{lbd}}(k), d_{\text{ubd}}(k)]$, $|(\Psi_d)'(x)| < 1$ holds uniformly over $x \in [\frac{1}{2} - \frac{1}{2^k}, \frac{1}{2}]$.*

Proof. Throughout, we let $x \in [1/2 - 1/2^k, 1/2]$ and denote $v = \hat{\Psi}(x)$. We first consider $k \geq 5$. Observe that the derivative of the clause BP recursion can simply be bounded in absolute value by

$$\left|(\hat{\Psi})'(x)\right| = \frac{(k-1)x^{k-2}}{(1-x^{k-1})^2} \leq \frac{(k-1)\cdot 2^{-k+2}}{(1-2^{-k+1})^2} = \frac{4(k-1)}{2^k(1-2^{-k+1})^2}\,, \tag{3.1}$$

where the inequality holds since $x \to \frac{x^{k-2}}{(1-x^{k-1})^2}$ is increasing. Similarly, we bound the derivative of the variable BP recursion:

$$\left|(\dot{\Psi})'(v)\right| = \frac{(d-1)v^{d-2}}{(2-v^{d-1})^2} \leq \frac{(d-1)v_0^{d-2}}{(2-v_0^{d-1})^2} \leq \frac{(d-1)v_0^{d-2}}{(2-v_0^{d-2})^2}\,, \tag{3.2}$$

where we denoted $v_0 := \hat{\Psi}(x_0)$ for $x_0 = 1/2 - 1/2^k$. The first inequality holds because $x \to \hat{\Psi}(\cdot)$ is decreasing on $[1/2 - 1/2^k, 1/2]$, and the last inequality holds since $v_0 < 1$. To this end, we upper bound v_0^{d-2} by

$$v_0^{d-2} = \left(1 - \frac{x_0^{k-1}}{1-x_0^{k-1}}\right)^{d-2} \leq (1-x_0^{k-1})^{d-2} \leq e^{-(d-2)x_0^{k-1}}\,. \tag{3.3}$$

Note that $x_0^{k-1} = \left(\frac{1}{2}\right)^{k-1}\left(1 - \frac{2}{2^k}\right)^{k-1} \geq \left(\frac{1}{2}\right)^{k-1}\left(1 - \frac{2(k-1)}{2^k}\right)$ and $d \geq (2^{k-1}-2)k\log 2$ hold, thus we can lower bound $(d-2)x_0^{k-1}$ by

$$(d-2)x_0^{k-1} \geq \left(k\log 2 - \frac{4k\log 2 + 4}{2^k}\right)\cdot\left(1 - \frac{2(k-1)}{2^k}\right)\,.$$

Thus, combining with (3.3) shows that

$$v_0^{d-2} \leq 2^{-k}e^{\varepsilon_k}\,, \quad \text{where} \quad \varepsilon_k := \frac{2(k-1)k\log 2}{2^k} + \frac{4k\log 2 + 4}{2^k}\left(1 - \frac{2(k-1)}{2^k}\right)\,. \tag{3.4}$$

Plugging this bound into (3.2), we have

$$|(\dot{\Psi})'(v)| < (d-1)\frac{v_0^{d-2}}{(2-v_0^{d-2})^2} \leq (2^{k-1}k\log 2 - 1)\cdot\frac{2^{-k}\cdot e^{\varepsilon_k}}{(2-2^{-k}e^{\varepsilon_k})^2}\,.$$

Combining with the contraction of clause BP recursion in (3.1), we have

$$|(\Psi_d)'(x)| \leq \alpha_k := \frac{2k(k-1)\log 2}{2^k}\cdot\left(1 - \frac{1}{2^{k-1}k\log 2}\right)\cdot\frac{e^{\varepsilon_k}}{(1-2^{-k+1})^2(2-2^{-k}e^{\varepsilon_k})^2}\,.$$

By comparing ε_k and ε_{k+1} for $k \geq 5$, it can be easily checked that $k \to \varepsilon_k$ is decreasing, and the same holds for $k \to \frac{2k(k-1)\log 2}{2^k}\cdot\left(1 - \frac{1}{2^{k-1}k\log 2}\right)$. Thus, $k \to \alpha_k$ is decreasing for $k \geq 5$. Furthermore, α_5 can be calculated up to arbitrary precision (e.g. by Mathematica), which satisfies $\alpha_5 < 0.99 < 1$. Consequently, $|(\Psi_d)'(x)| < 1$ holds for $k \geq 5$.

The case where $k = 4$ is more delicate, and the previous strategy of bounding the derivative of clause and variable BP recursions separately no longer is successful. To this end, we bound $(\Psi_d)'(x)$ directly. If we denote $v = \hat{\Psi}_k(x)$, then

$$\left|(\Psi_d)'(x)\right| = \left|(\hat{\Psi})'(x)\right| \cdot \left|(\dot{\Psi})'(v)\right| = \frac{(k-1)(d-1)v^{d-2}}{(2-v^{d-1})^2} \cdot \frac{x^{k-1}}{(1-x^{k-1})^2} \cdot \frac{1}{x}\,.$$

Since $v \equiv \hat{\Psi}_k(x) \equiv \frac{1-2x^{k-1}}{1-x^{k-1}}$, rearranging gives $x^{k-1} = \frac{1-v}{2-v}$. Substituting this in for x^{k-1}, we have that

$$\left|(\Psi_d)'(x)\right| = (k-1)(d-1) \cdot \frac{v^{d-2}(2-v)(1-v)}{(2-v^{d-1})^2} \cdot \frac{1}{x}\,. \tag{3.5}$$

We now claim that $v \to \frac{v^{d-2}(2-v)(1-v)}{(2-v^{d-1})^2}$ is increasing for $v \in [\hat{\Psi}_4(1/2), \hat{\Psi}_4(1/2 - 1/2^4)]$ and $d \in [24\log 2, 32\log 2]$ (recall that $24\log 2 > 16.7 \equiv d_{\text{lbd}}(4)$ holds). Since $v \to (2-v^{d-1})^2$ is decreasing, it suffices to show that $v \to v^{d-2}(2-v)(1-v)$ is increasing. Note that

$$\frac{\mathrm{d}}{\mathrm{d}v}\Big(v^{d-2}(2-v)(1-v)\Big) = (dv^2 - 3(d-1)v + 2(d-2))v^{d-3} > 0 \iff d > \frac{4-3v}{(2-v)(1-v)}\,.$$

Note that $v \to \frac{4-3v}{(2-v)(1-v)}$ is increasing since its derivative is given by $\frac{3v^2-8v+6}{(2-v)^2(1-v)^2} > 0$. Thus, to prove our claim, it suffices to check that for $d_0 := 24\log 2$ and $v_0 = \hat{\Psi}_4(1/2 - 1/2^4)$ that $d_0 > \frac{4-3v_0}{(2-v_0)(1-v_0)}$ holds. By a direct calculation, $v_0 = 3410/3753 < 0.91$ and $24\log 2 > 16 > \frac{4-3\cdot 0.91}{(2-0.91)(1-0.91)}$ holds, thus the claim that $v \to \frac{v^{d-2}(2-v)(1-v)}{(2-v^{d-1})^2}$ is increasing is proven for d, v in the regime of interest.

Note that $x \to v = \hat{\Psi}_4(x)$ is decreasing, thus (3.5) and our previous claim shows that for all $x_0 \le x \le 1/2$, where $x_0 = 1/2 - 1/2^4$, we have

$$\left|(\Psi_d)'(x)\right| \le (d-1)(k-1)\frac{v_0^{d-2}(2-v_0)(1-v_0)}{(2-v_0^{d-1})^2} \cdot \frac{1}{x_0}\,,$$

where $v_0 = \hat{\Psi}_4(x_0) = 3410/3753$. We next show that the right hand side as a function of $d \in [24\log 2, 32\log 2]$ is decreasing: since $d \to (2-v_0^{d-1})^2$ is increasing, it suffices to show that $d \to (d-1)v_0^{d-2}$ is decreasing. Note that

$$\frac{\mathrm{d}}{\mathrm{d}d}\Big((d-1)v_0^{d-2}\Big) = v_0^{d-2}\Big(1-(d-1)\log\big(1/v_0\big)\Big) < 0 \iff d > \frac{1}{\log(1/v_0)} + 1\,,$$

and it can be verified that $24\log 2 > 16 > 1/\log(3753/3410) + 1$ holds. Therefore, for $k = 4$, it follows that for $d_0 = 24\log 2$,

$$\left|(\Psi_d)'(x)\right| \le 3(d_0-1)\frac{v_0^{d_0-2}(2-v_0)(1-v_0)}{(2-v_0^{d_0-1})^2} \cdot \frac{1}{x_0}\,.$$

The right hand side can be computed to arbitrary precision (e.g. by Mathematica), it can be verified that $3(d_0-1)\frac{v_0^{d_0-2}(2-v_0)(1-v_0)}{(2-v_0^{d_0-1})^2} \cdot \frac{1}{x_0} < 0.9 < 1$. This concludes the proof for the case $k = 4$. ◀

In the proof of Lemma 3.3, we did not use the adjustment for $d_{\text{lbd}}(4) \equiv 16.7 > 24\log 2$. That is, $\max_{\frac{1}{2}-\frac{1}{2^4} \le x \le \frac{1}{2}} \left|(\Psi_d)'(x)\right| < 1$ holds for $d \in [24\log 2, 32\log 2]$. The adjustment $d_{\text{lbd}}(4) \equiv 16.7$ is needed for the following lemma, which guarantees the existence of the solution to $\Psi_d(x) = x$.

▶ **Lemma 3.4.** $\Psi_d(\frac{1}{2}-\frac{1}{2^k}) > \frac{1}{2}-\frac{1}{2^k}$ *holds for* $k \geq 4$ *for* $d \in [d_{\rm lbd}(k), d_{\rm ubd}(k)]$.

Proof. Let $v_0 \equiv v_0(k) = \hat{\Psi}\left(\frac{1}{2}-\frac{1}{2^k}\right)$ as before. Then, from the definition of $\dot{\Psi}, \hat{\Psi}$ in (1.12), $\Psi_d(\frac{1}{2}-\frac{1}{2^k}) > \frac{1}{2}-\frac{1}{2^k}$ is equivalent to $v_0^{d-1} < \frac{4}{2^k+2}$, which we aim to show for $k \geq 4$. We start with the case $k \geq 5$. We have shown in (3.4) that $v_0^{d-2} \leq 2^{-k}e^{\varepsilon_k}$, holds, and by an analogous proof, $v_0^{d-1} \leq 2^{-k}e^{\beta_k}$ holds, where $\beta_k \equiv \varepsilon_k - \frac{1}{2^{k-1}}\big(1-\frac{2(k-1)}{2^k}\big)$. Thus, it suffices to show that

$$e^{\beta_k}\left(1+\frac{1}{2^{k-1}}\right) < 4\,, \quad \text{where} \quad \beta_k \equiv \frac{2(k-1)k\log 2}{2^k} + \frac{4k\log 2+2}{2^k}\left(1-\frac{2(k-1)}{2^k}\right).$$

For $k=5$, $e^{\beta_5}(1+1/2^4)$ can be computed to arbitrary precision (e.g. by Mathematica), and it can be numerically verified that $e^{\beta_5}(1+1/2^4) < 3.7$. Further, $k \to \beta_k$ is decreasing by comparing β_k and β_{k+1}, thus this concludes the proof for $k \geq 5$.

Next, we consider the case $k=4$. Since $d \to v_0^{d-1}$ is maximized at $d = d_{\rm lbd}(4) \equiv 16.7$, it suffices to show that $v_0^{15.7} \leq \frac{2}{9}$ holds, where $v_0 \equiv \hat{\Psi}_4(1/2-1/2^4) = 3410/3753$. Since $v_0^{15.7} = (3410/3753)^{15.7}$ can be computed to arbitrary precision (e.g. by Mathematica), it can be checked that $v_0^{15.7} = (3410/3753)^{15.7} < 0.2221 < \frac{2}{9}$ holds, so this concludes the proof. ◀

Proof of Lemma 3.1. By Lemma 3.4, $\Psi_d(\frac{1}{2}-\frac{1}{2^k}) > \frac{1}{2}-\frac{1}{2^k}$ holds for $k \geq 4$. Note that $\Psi_d(1/2) < 1/2$ holds since $\dot{\Psi}(x) < 1/2$ holds for any $x \geq 0$. Thus, since $x \to \Psi_d(x)$ is continuous and differentiable, intermediate value theorem guarantees the existence of the solution to $\Psi_d(x) = x$ for $x \in [\frac{1}{2}-\frac{1}{2^k}, \frac{1}{2}]$. Moreover, $\big|(\Psi_d)'(x)\big| < 1$ holds uniformly over $x \in [\frac{1}{2}-\frac{1}{2^k}, \frac{1}{2}]$ by Lemma 3.3, thus mean value theorem guarantees the uniqueness of the solution to $\Psi_d(x) = x$ for $x \in [\frac{1}{2}-\frac{1}{2^k}, \frac{1}{2}]$. ◀

3.2 Proof of Lemma 3.2

Recall that ${}^\star\mathbf{\Phi}(d)$ is defined in (1.2) as ${}^\star\mathbf{\Phi}(d) \equiv \Phi\big(d, x_\star(k,d)\big)$, where $x_\star(k,d) \in [\frac{1}{2}-\frac{1}{2^k}, \frac{1}{2}]$ is the solution to $\Psi_d(x) = x$, and we defined the function $\Phi(d,x)$ by

$$\Phi(d,x) \equiv \Phi_k(d,x) := -\log(1-x) - d(1-k^{-1}-d^{-1})\log(1-2x^k) + (d-1)\log(1-x^{k-1})\,. \tag{3.6}$$

To prove ${}^\star\mathbf{\Phi}\big(d_{\rm lbd}(k)\big) > 0$ and ${}^\star\mathbf{\Phi}\big(d_{\rm ubd}(k)\big) < 0$, we show respectively in Lemmas 3.5 and 3.6 that $\Phi\big(d_{\rm lbd}(k), x\big) > 0$ and $\Phi\big(d_{\rm ubd}(k), x\big) < 0$ hold uniformly over $x \in [\frac{1}{2}-\frac{1}{2^k}, \frac{1}{2}]$.

▶ **Lemma 3.5.** *For* $k \geq 4$, $\Phi(d_{\rm lbd}(k), x) > 0$ *holds uniformly over* $x \in [\frac{1}{2}-\frac{1}{2^k}, \frac{1}{2}]$.

Proof. Note that rearranging $\Phi(d,x)$ gives

$$\begin{aligned}\Phi(d,x) &= -\log(1-x) - d\big((1-k^{-1})\log(1-2x^k) - \log(1-x^{k-1})\big) + \log(1-2x^k) - \log(1-x^{k-1}) \\ &\geq -\log(1-x) - d\big((1-k^{-1})\log(1-2x^k) - \log(1-x^{k-1})\big)\,,\end{aligned} \tag{3.7}$$

where the inequality holds since $\log(1-2x^k) \geq \log(1-x^{k-1})$ holds for $x \in [0,1/2]$. Note that the first term in the right hand side $x \to -\log(1-x)$ is convex, so the linear approximation at $x = 1/2$ shows that $-\log(1-x) \geq \log 2 + 2(x-1/2)$ holds. Further, the function $x \to (1-k^{-1})\log(1-2x^k) - \log(1-x^{k-1})$ is increasing since

$$\frac{\mathrm{d}}{\mathrm{d}x}\Big((1-k^{-1})\log(1-2x^k) - \log(1-x^{k-1})\Big) = \frac{(k-1)x^{k-2}(1-2x)}{(1-2x^k)(1-x^{k-1})} \geq 0\,.$$

Thus, the right hand side in (3.7) for $d = d_{\mathrm{lbd}}(k)$ can further be lower bounded by

$$\begin{aligned}\Phi\big(d_{\mathrm{lbd}}(k), x\big) &\geq \log 2 + 2\big(x - 1/2\big) + \frac{d_{\mathrm{lbd}}(k)}{k} \cdot \log\left(1 - 2^{-k+1}\right) \\ &\geq \log 2 - 2^{-k+1} + \frac{d_{\mathrm{lbd}}(k)}{k} \cdot \log\left(1 - 2^{-k+1}\right) =: F(k)\,, \end{aligned} \tag{3.8}$$

where we used $x \geq 1/2 - 1/2^k$ in the last inequality. Using the inequality $\log(1-a) \geq -a - \frac{a^2}{2} - \frac{a^3}{2}$ for $a = 2^{-k+1} \leq \frac{1}{8}$, we have, for $k \geq 5$, that

$$F(k) = \log 2 - 2^{-k+1} + (2^{k-1}-2)\log 2 \cdot \log(1-2^{-k+1}) \geq \frac{1}{2^k}\left(3\log 2 - 2 - \frac{6\log 2}{2^k} + \frac{8\log 2}{2^{2k}}\right).$$

For $k \geq 6$, the right hand side above is positive since $3\log 2 - 2 - \frac{3\log 2}{32} > 0.01$, thus (3.8) shows that $\Phi\big(d_{\mathrm{lbd}}(k), x\big) > 0$ holds for $k \geq 6$ and $x \in [\frac{1}{2} - \frac{1}{2^k}, \frac{1}{2}]$. For $k \in \{4, 5\}$, we can explicitly calculate $F(k)$ by $F(4) \equiv \log 2 - 1/8 + (16.7/4)\log(7/8) > 0.01 > 0$, and $F(5) \equiv \log 2 - 1/16 + 14\log 2 \cdot \log(15/16) > 0.004 > 0$, thus (3.8) again concludes the proof for $k \in \{4, 5\}$. ◀

▶ **Lemma 3.6.** *For $k \geq 4$, $\Phi\big(d_{\mathrm{ubd}}(k), x\big) < 0$ holds uniformly over $x \in [\frac{1}{2} - \frac{1}{2^k}, \frac{1}{2}]$.*

Proof. We first claim that for $k \geq 5$, the function $x \to \Phi\big(d_{\mathrm{ubd}}(k), x\big)$ is increasing for $x \in [\frac{1}{2} - \frac{1}{2^k}, \frac{1}{2}]$ and $d_{\mathrm{ubd}}(k) \equiv 2^{k-1}k\log 2$. A direct calculation shows that

$$\begin{aligned}\frac{\partial\Phi}{\partial x}\big(d_{\mathrm{ubd}}(k), x\big) &= \frac{1}{1-x} - (2^{k-1}k\log 2 - 1)(k-1) \cdot \frac{x^{k-2}(1-2x)}{(1-x^{k-1})(1-2x^k)} - \frac{2x^{k-1}}{1-2x^k} \\ &\geq \frac{1}{\frac{1}{2} + \frac{1}{2^k}} - (2^{k-1}k\log 2 - 1)(k-1) \cdot \frac{x^{k-2}(1-2x)}{(1-x^{k-1})(1-2x^k)} - \frac{4}{2^k - 2}\,, \end{aligned} \tag{3.9}$$

where the inequality holds since $x \to (1-x)^{-1}$ increasing, so it is minimized at $x = 1/2 + 1/2^k$, and $x \to 2x^{k-1}/(1-2x^k)$ is increasing, so it is maximized at $x = 1/2$. Further, it is straightforward to check that $x \to x^{k-2}(1-2x)$ is decreasing for $x \in [\frac{1}{2} - \frac{1}{2^k}, \frac{1}{2}]$, thus it is maximized at $x = 1/2 - 1/2^k$. Also, $x \to (1-x^{k-1})(1-2x^k)$ is minimized at $x = 1/2$. Thus, by plugging in these bounds, we can further bound

$$\begin{aligned}\frac{\partial\Phi}{\partial x}\big(d_{\mathrm{ubd}}(k), x\big) &\geq 2 - \left(\frac{2}{2^{k-1}+1} + \frac{4}{2^k - 2} + \frac{(2^{k-1}k\log 2 - 1)(k-1)}{2^{2k-3}} \cdot \left(1 - \frac{1}{2^{k-1}}\right)^{k-4}\right) \\ &\geq 2 - \left(\frac{2}{2^{k-1}+1} + \frac{4}{2^k - 2} + \frac{(2^{k-1}k\log 2 - 1)(k-1)}{2^{2k-3}}\right) =: 2 - G(k)\,. \end{aligned} \tag{3.10}$$

Note that the function $k \to G(k)$ is increasing for $k \geq 5$. Furthermore, using the bound $\log 2 < 0.7$, we can bound $G(5) = \frac{2}{17} + \frac{2}{15} + \frac{80\log 2 - 1}{32} < 1.97 < 2$. Therefore, $\frac{\partial\Phi}{\partial x}\big(d_{\mathrm{ubd}}(k), x\big) > 0$ holds for $k \geq 5$ and $x \in [\frac{1}{2} - \frac{1}{2^k}, \frac{1}{2}]$, which proves our first claim.

Consequently, for the case $k \geq 5$, it suffices to show that $\Phi(2^{k-1}k\log 2, x) < 0$ holds for $x = 1/2$. A direct calculation gives

$$\Phi\left(2^{k-1}k\log 2, \frac{1}{2}\right) = \log 2 + 2^{k-1}\log 2 \cdot \log\left(1 - \frac{1}{2^{k-1}}\right) < 0\,, \tag{3.11}$$

where the inequality holds since $\log(1-a) < -a$ holds for $a \in (0,1)$. This concludes the proof for $k \geq 5$.

It remains to consider the case $k = 4$. For $k = 4$, we claim that $x \to \Phi_4\big(d_{\mathrm{ubd}}(4), x\big)$ is convex in the interval $x \in [\frac{7}{16}, \frac{1}{2}]$. From the computation of $\frac{\partial \Phi}{\partial x}\big(d_{\mathrm{ubd}}(k), x\big)$ in (3.9), we can calculate the second derivative by

$$\frac{\partial^2 \Phi}{\partial x^2}\big(d_{\mathrm{ubd}}(4), x\big) = \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{1-x} - \frac{2x^3}{1-2x^4}\right) + 3(32\log 2 - 1)\cdot \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{x^2(2x-1)}{(1-x^3)(1-2x^4)}\right). \quad (3.12)$$

The first term in the right hand side can be bounded by

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{1-x} - \frac{2x^3}{1-2x^4}\right) = \frac{1}{(1-x)^2} - \frac{6x^2+4x^6}{(1-2x^4)^2} > \frac{1}{(1-\frac{7}{16})^2} - \frac{6\left(\frac{1}{2}\right)^2 + 4\left(\frac{1}{2}\right)^6}{(1-2\left(\frac{1}{2}\right)^4)^2} > 0, \quad (3.13)$$

where the final inequality is equivalent to $\frac{256}{81} - \frac{100}{49} > 0$. The second term can be calculated as

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{x^2(2x-1)}{(1-x^3)(1-2x^4)}\right) = \frac{x(-16x^8 + 10x^7 + 4x^5 - 4x^4 - x^3 + 6x - 2)}{(1-x^3)^2(1-2x^4)^2}.$$

Note that by neglecting the terms $10x^7 + 4x^5$ above, we can lower bound

$$-16x^8 + 10x^7 + 4x^5 - 4x^4 - x^3 + 6x - 2 > 6 \cdot \frac{7}{16} - 2 - \left(\frac{1}{2}\right)^3 - 4\left(\frac{1}{2}\right)^4 - 16\left(\frac{1}{2}\right)^8 > 0,$$

thus $\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{x^2(2x-1)}{(1-x^3)(1-2x^4)}\right) > 0$ holds for $x \in [\frac{7}{16}, \frac{1}{2}]$ as well. Therefore, combining with (3.12) and (3.13) finishes the proof of our claim that $x \to \Phi_4\big(d_{\mathrm{ubd}}(4), x\big)$ is convex in the interval $x \in [\frac{7}{16}, \frac{1}{2}]$.

Thus, by convexity, $x \to \Phi_4\big(d_{\mathrm{ubd}}(4), x\big)$ is maximized at the end points $x \in \{7/16, 1/2\}$, and it suffices to show that $\Phi_4\big(d_{\mathrm{ubd}}(4), 7/16\big) < 0$ and $\Phi_4\big(d_{\mathrm{ubd}}(4), 1/2\big) < 0$. For $x = 7/16$, $\Phi_4\big(d_{\mathrm{ubd}}(4), 7/16\big)$ can be computed to arbitrary precision (e.g. by Mathematica), and it can be checked that $\Phi_4\big(d_{\mathrm{ubd}}(4), 7/16\big) < -0.08 < 0$. For $x = 1/2$, (3.11) shows that $\Phi_4\big(d_{\mathrm{ubd}}(4), 1/2\big) < 0$ holds. This concludes the proof for the case $k = 4$. ◀

Proof of Lemma 3.2. By definition, ${}^\star\mathbf{\Phi}(d) = \Phi\big(d, x_\star(k,d)\big)$ holds, and $(d, x) \to \Phi(d, x)$ is clearly continuous. Thus, in order to show the continuity of ${}^\star\mathbf{\Phi}(\cdot)$, it suffices to show that $d \to x_\star(k,d)$ is continuous for any fixed $k \geq 4$. To that end, note that the function $\psi(d,x) := \Psi_d(x) - x$ satisfies $\frac{\partial \psi}{\partial x} < 0$ by Lemma 3.3. Since $x_\star(k,d)$ is defined to be the root of $\psi(d,\cdot)$, this implies that $d \to x_\star(k,d)$ is continuous by the implicit function theorem. As a consequence, we conclude that $d \to {}^\star\mathbf{\Phi}(d)$ is continuous. Since ${}^\star\mathbf{\Phi}(d_{\mathrm{lbd}}(k)) > 0$ holds by Lemma 3.5 and ${}^\star\mathbf{\Phi}(d_{\mathrm{ubd}}(k)) < 0$ holds by Lemma 3.6, we conclude the proof. ◀

References

1 Dimitris Achlioptas, Arthur Chtcherba, Gabriel Istrate, and Cristopher Moore. The phase transition in 1-in-k SAT and NAE 3-sat. In *Proceedings of the Twelfth Annual ACM-SIAM Symposium on Discrete Algorithms*, SODA '01, pages 721–722, Philadelphia, PA, USA, 2001. Society for Industrial and Applied Mathematics. URL: `http://dl.acm.org/citation.cfm?id=365411.365760`.

2 Dimitris Achlioptas and Cristopher Moore. On the 2-colorability of random hypergraphs. In José D. P. Rolim and Salil Vadhan, editors, *Randomization and Approximation Techniques in Computer Science*, pages 78–90, Berlin, Heidelberg, 2002. Springer Berlin Heidelberg.

3 Dimitris Achlioptas and Cristopher Moore. Random k-SAT: two moments suffice to cross a sharp threshold. *SIAM J. Comput.*, 36(3):740–762, 2006. `doi:10.1137/S0097539703434231`.

4 Dimitris Achlioptas and Assaf Naor. The two possible values of the chromatic number of a random graph. *Ann. of Math. (2)*, 162(3):1335–1351, 2005. `doi:10.4007/annals.2005.162.1335`.

5 Dimitris Achlioptas, Assaf Naor, and Yuval Peres. Rigorous location of phase transitions in hard optimization problems. *Nature*, 435(7043):759–764, 2005.

6 Dimitris Achlioptas and Yuval Peres. The threshold for random k-SAT is $2^k \log 2 - O(k)$. *J. Amer. Math. Soc.*, 17(4):947–973, 2004. doi:10.1090/S0894-0347-04-00464-3.

7 N. Alon and Z. Bregman. Every 8-uniform 8-regular hypergraph is 2-colorable. *Graphs and Combinatorics*, 4(1):303–306, 1988. doi:10.1007/BF01864169.

8 Peter Ayre, Amin Coja-Oghlan, Pu Gao, and Noëla Müller. The satisfiability threshold for random linear equations. *Combinatorica*, 40(2):179–235, 2020. doi:10.1007/s00493-019-3897-3.

9 Peter Ayre, Amin Coja-Oghlan, and Catherine Greenhill. Lower bounds on the chromatic number of random graphs. *Combinatorica*, 42(5):617–658, 2022. doi:10.1007/s00493-021-4236-z.

10 Victor Bapst and Amin Coja-Oghlan. The condensation phase transition in the regular k-SAT model. In *Approximation, randomization, and combinatorial optimization. Algorithms and techniques*, volume 60 of *LIPIcs. Leibniz Int. Proc. Inform.*, pages Art. No. 22, 18. Schloss Dagstuhl – Leibniz-Zentrum für Informatik, 2016.

11 Victor Bapst, Amin Coja-Oghlan, Samuel Hetterich, Felicia Raßmann, and Dan Vilenchik. The condensation phase transition in random graph coloring. *Comm. Math. Phys.*, 341(2):543–606, 2016. doi:10.1007/s00220-015-2464-z.

12 Béla Bollobás, Christian Borgs, Jennifer T. Chayes, Jeong Han Kim, and David B. Wilson. The scaling window of the 2-SAT transition. *Random Structures Algorithms*, 18(3):201–256, 2001. doi:10.1002/rsa.1006.

13 A. A. Borovkov. Generalization and refinement of the integro-local stone theorem for sums of random vectors. *Theory of Probability & Its Applications*, 61(4):590–612, 2017. doi:10.1137/S0040585X97T988368.

14 Evan Chang, Neel Kolhe, and Youngtak Sohn. Upper bounds on the 2-colorability threshold of random d-regular k-uniform hypergraphs for $k \geq 3$. *arXiv:2308.02075*, 2023.

15 V. Chvatal and B. Reed. Mick gets some (the odds are on his side) (satisfiability). In *Proceedings of the 33rd Annual Symposium on Foundations of Computer Science*, SFCS '92, pages 620–627, Washington, DC, USA, 1992. IEEE Computer Society. doi:10.1109/SFCS.1992.267789.

16 Amin Coja-Oghlan. Upper-bounding the k-colorability threshold by counting covers. *Electron. J. Combin.*, 20(3):Paper 32, 28, 2013.

17 Amin Coja-Oghlan, Charilaos Efthymiou, and Samuel Hetterich. On the chromatic number of random regular graphs. *J. Combin. Theory Ser. B*, 116:367–439, 2016. doi:10.1016/j.jctb.2015.09.006.

18 Amin Coja-Oghlan, Florent Krząkała, Will Perkins, and Lenka Zdeborová. Information-theoretic thresholds from the cavity method. *Adv. Math.*, 333:694–795, 2018. doi:10.1016/j.aim.2018.05.029.

19 Amin Coja-Oghlan and Konstantinos Panagiotou. Catching the k-NAESAT threshold [extended abstract]. In *STOC'12—Proceedings of the 2012 ACM Symposium on Theory of Computing*, pages 899–907. ACM, New York, 2012. doi:10.1145/2213977.2214058.

20 Amin Coja-Oghlan and Konstantinos Panagiotou. Going after the k-sat threshold. In *Proceedings of the Forty-Fifth Annual ACM Symposium on Theory of Computing*, STOC '13, pages 705–714, New York, NY, USA, 2013. Association for Computing Machinery. doi:10.1145/2488608.2488698.

21 Amin Coja-Oghlan and Konstantinos Panagiotou. The asymptotic k-SAT threshold. *Adv. Math.*, 288:985–1068, 2016. doi:10.1016/j.aim.2015.11.007.

22 Amin Coja-Oghlan and Will Perkins. Spin systems on Bethe lattices. *Communications in Mathematical Physics*, 372(2):441–523, 2019. doi:10.1007/s00220-019-03544-y.

23 Amin Coja-Oghlan and Dan Vilenchik. Chasing the k-colorability threshold. In *2013 IEEE 54th Annual Symposium on Foundations of Computer Science—FOCS '13*, pages 380–389. IEEE Computer Soc., Los Alamitos, CA, 2013. doi:10.1109/FOCS.2013.48.

24 Amin Coja-Oghlan and Lenka Zdeborová. The condensation transition in random hypergraph 2-coloring. In *Proceedings of the Twenty-Third Annual ACM-SIAM Symposium on Discrete Algorithms*, SODA '12, pages 241–250. ACM, New York, 2012.

25 L. Dall'Asta, A. Ramezanpour, and R. Zecchina. Entropy landscape and non-gibbs solutions in constraint satisfaction problems. *Physical Review E*, 77(3), March 2008. `doi:10.1103/physreve.77.031118`.

26 Amir Dembo and Ofer Zeitouni. *Large deviations techniques and applications*, volume 38 of *Stochastic Modelling and Applied Probability*. Springer-Verlag, Berlin, 2010. `doi:10.1007/978-3-642-03311-7`.

27 Martin Dietzfelbinger, Andreas Goerdt, Michael Mitzenmacher, Andrea Montanari, Rasmus Pagh, and Michael Rink. Tight thresholds for cuckoo hashing via XORSAT. In Samson Abramsky, Cyril Gavoille, Claude Kirchner, Friedhelm Meyer auf der Heide, and Paul G. Spirakis, editors, *Automata, Languages and Programming*, pages 213–225, Berlin, Heidelberg, 2010. Springer Berlin Heidelberg.

28 Jian Ding, Allan Sly, and Nike Sun. Satisfiability threshold for random regular nae-sat. In *Proceedings of the Forty-Sixth Annual ACM Symposium on Theory of Computing*, STOC '14, pages 814–822, New York, NY, USA, 2014. Association for Computing Machinery. `doi:10.1145/2591796.2591862`.

29 Jian Ding, Allan Sly, and Nike Sun. Proof of the satisfiability conjecture for large k. In *Proceedings of the Forty-seventh Annual ACM Symposium on Theory of Computing*, STOC '15, pages 59–68, New York, NY, USA, 2015. ACM. `doi:10.1145/2746539.2746619`.

30 Jian Ding, Allan Sly, and Nike Sun. Maximum independent sets on random regular graphs. *Acta Math.*, 217(2):263–340, 2016. `doi:10.1007/s11511-017-0145-9`.

31 Jian Ding, Allan Sly, and Nike Sun. Satisfiability threshold for random regular NAE-SAT. *Commun. Math. Phys.*, 341(2):435–489, 2016.

32 Jian Ding, Allan Sly, and Nike Sun. Proof of the satisfiability conjecture for large k. *Annals of Mathematics*, 196(1):1–388, 2022. `doi:10.4007/annals.2022.196.1.1`.

33 Olivier Dubois and Jacques Mandler. The 3-XORSAT threshold. In *Proceedings of the 43rd Symposium on Foundations of Computer Science*, FOCS '02, pages 769–778, Washington, DC, USA, 2002. IEEE Computer Society. URL: `http://dl.acm.org/citation.cfm?id=645413.652160`.

34 Martin Dyer, Alan Frieze, and Catherine Greenhill. On the chromatic number of a random hypergraph. *Journal of Combinatorial Theory, Series B*, 113:68–122, 2015. `doi:10.1016/j.jctb.2015.01.002`.

35 Silvio Franz and Michele Leone. Replica bounds for optimization problems and diluted spin systems. *Journal of Statistical Physics*, 111(3):535–564, 2003. `doi:10.1023/A:1022885828956`.

36 Yuzhou Gu and Yury Polyanskiy. Uniqueness of bp fixed point for the potts model and applications to community detection. *arXiv preprint, arXiv:2303.14688*, 2023.

37 Francesco Guerra. Broken replica symmetry bounds in the mean field spin glass model. *Communications in Mathematical Physics*, 233(1):1–12, 2003. `doi:10.1007/s00220-002-0773-5`.

38 Michael A. Henning and Anders Yeo. 2-colorings in k-regular k-uniform hypergraphs. *European Journal of Combinatorics*, 34(7):1192–1202, 2013. `doi:10.1016/j.ejc.2013.04.005`.

39 Michael A. Henning and Anders Yeo. Not-all-equal 3-sat and 2-colorings of 4-regular 4-uniform hypergraphs. *Discrete Mathematics*, 341(8):2285–2292, 2018. `doi:10.1016/j.disc.2018.05.002`.

40 Svante Janson, Tomasz Luczak, and Andrzej Rucinski. *Random graphs*. Wiley-Interscience Series in Discrete Mathematics and Optimization. Wiley-Interscience, New York, 2000. `doi:10.1002/9781118032718`.

41 Richard M. Karp. *Reducibility among Combinatorial Problems*, pages 85–103. Springer US, Boston, MA, 1972. `doi:10.1007/978-1-4684-2001-2_9`.

42 Lefteris M. Kirousis, Evangelos Kranakis, Danny Krizanc, and Yannis C. Stamatiou. Approximating the unsatisfiability threshold of random formulas. *Random Structures Algorithms*, 12(3):253–269, 1998. `doi:10.1002/(SICI)1098-2418(199805)12:3<253::AID-RSA3>3.3.CO;2-H`.

43 Florent Krząkała, Andrea Montanari, Federico Ricci-Tersenghi, Guilhem Semerjian, and Lenka Zdeborová. Gibbs states and the set of solutions of random constraint satisfaction problems. *Proceedings of the National Academy of Sciences*, 104(25):10318–10323, 2007. `doi:10.1073/pnas.0703685104`.

44 Marc Lelarge and Mendes Oulamara. Replica bounds by combinatorial interpolation for diluted spin systems. *Journal of Statistical Physics*, 173(3–4):917–940, February 2018. `doi:10.1007/s10955-018-1964-6`.

45 Stephan Mertens, Marc Mézard, and Riccardo Zecchina. Threshold values of random k-sat from the cavity method. *Random Structures & Algorithms*, 28(3):340–373, 2006. `doi:10.1002/rsa.20090`.

46 M. Mézard, G. Parisi, and R. Zecchina. Analytic and algorithmic solution of random satisfiability problems. *Science*, 297(5582):812–815, 2002. `doi:10.1126/science.1073287`.

47 Marc Mézard and Andrea Montanari. *Information, physics, and computation*. Oxford Graduate Texts. Oxford University Press, Oxford, 2009. `doi:10.1093/acprof:oso/9780198570837.001.0001`.

48 Andrea Montanari, Feng Ruan, Youngtak Sohn, and Jun Yan. The generalization error of max-margin linear classifiers: Benign overfitting and high-dimensional asymptotics in the overparametrized regime. *arXiv*, 2019. `arXiv:1911.01544`.

49 Danny Nam, Allan Sly, and Youngtak Sohn. One-step replica symmetry breaking of random regular NAE-SAT I. *arXiv preprint*, 2020. `arXiv:2011.14270`.

50 Danny Nam, Allan Sly, and Youngtak Sohn. One-step replica symmetry breaking of random regular NAE-SAT. In *2021 IEEE 62nd Annual Symposium on Foundations of Computer Science (FOCS)*, pages 310–318, 2022. `doi:10.1109/FOCS52979.2021.00039`.

51 Danny Nam, Allan Sly, and Youngtak Sohn. One-step replica symmetry breaking of random regular NAE-SAT II. *Communications in Mathematical Physics*, 405(3):61, 2024. `doi:10.1007/s00220-023-04868-6`.

52 Dmitry Panchenko and Michel Talagrand. Bounds for diluted mean-fields spin glass models. *Probability Theory and Related Fields*, 130(3):319–336, 2004. `doi:10.1007/s00440-004-0342-2`.

53 Boris Pittel and Gregory B. Sorkin. The satisfiability threshold for k-XORSAT. *Combin. Probab. Comput.*, 25(2):236–268, 2016. `doi:10.1017/S0963548315000097`.

54 P. D. Seymour. On the two-coloring of hypergraphs. *The Quarterly Journal of Mathematics*, 25(1):303–311, January 1974. `doi:10.1093/qmath/25.1.303`.

55 Mariya Shcherbina and Brunello Tirozzi. Rigorous solution of the Gardner problem. *Communications in Mathematical Physics*, 234(3):383–422, 2003.

56 Allan Sly and Youngtak Sohn. Local geometry of NAE-SAT solutions in the condensation regime. *arXiv preprint*, 2023. `arXiv:2305.17334`.

57 Allan Sly, Nike Sun, and Yumeng Zhang. The number of solutions for random regular NAE-SAT. In *Proceedings of the 57th Symposium on Foundations of Computer Science*, FOCS '16, pages 724–731, 2016.

58 Allan Sly, Nike Sun, and Yumeng Zhang. The number of solutions for random regular NAE-SAT. *Probability Theory and Related Fields*, 182(1-2):1–109, 2022. `doi:10.1007/s00440-021-01029-5`.

59 Michel Talagrand. *Mean Field Models for Spin Glasses: Volume I*. Springer-Verlag, Berlin, 2010.

60 Qian Yu and Yury Polyanskiy. Ising model on locally tree-like graphs: Uniqueness of solutions to cavity equations. *arXiv preprint*, 2022. `arXiv:2211.15242`.