S.T. Yau High School Science Award Research Report

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Title of Research Report

Upper bounds on the 2-colorability threshold of random d-regular k-uniform hypergraphs for $k \geq 3$

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Upper bounds on the 2-colorability threshold of random d-regular k-uniform hypergraphs for $k \geq 3$

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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).

Keywords: random constraint satisfaction problem, NAE-SAT model, satisfiability threshold, interpolation, free energy, replica symmetry breaking

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Contents

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 [DRZ08] for hypergraph 2-coloring, and matches the previous rigorous results for random regular k-NAE-SAT model for k large enough [DSS14].

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 [Sey74, AB88, AM02, COZ12, DFG15, HY13, HY18].

A k-NAE-SAT problem is another closely related CSP studied in computer science [COP12, DSS14, SSZ16, NSS22, SS23], which can be viewed as a variant of the infamous k-SAT problem [Kar72]. 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, viewing each clause as an 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 (rCSPs) 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 [AP04, ANP05, AM06, COV13].

Many of the sparse rCSPs belong to a broad universality class called the one-step-replica-symmetry-breaking (1RSB) class from statistical physics [KMRT+07] (see Chapter 19 of [MM09] 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 rCSP which is 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 [DSS16b], the random k-SAT [DSS22], and random regular k-SAT [COP16] 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 [MPZ02] and previous mathematical works [AP04, COP13, COP16]. See Section 1.1 for further literature.

However, for small values of $k \geq 3$, locating the satisfiability threshold for rCSPs 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 $k \geq 3$ [MMZ06, MPZ02, DRZ08]. The methods of [DSS16b, DSS22, COP16] 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 [DSS14] for random regular k-NAE-SAT for large $k \geq k_0$ and conjectured to be sharp [DRZ08] for $k \geq 3$ for hypergraph 2-coloring.

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

Table 1. A comparison with the upper bound $d_\star(k)$ in Theorem 1.1 with the first moment threshold $d_1(k) := \frac{k \log 2}{-\log(1-2^{-k+1})}$ for small values of k. For $3 \le k \le 10$, the values also appear in Table 1 of [DRZ08].

Theorem 1.1. *For $k \ge 3$ and $d_{\rm lbd}(k) \le d \le d_{\rm ubd}(k)$, where $d_{\rm lbd}(k), d_{\rm ubd}(k)$ are defined in (1.4) below, there exists a unique solution $x \equiv x(k,d)$ to the equation*

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

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 $[d_{\rm lbd}(k), d_{\rm ubd}(k)]$.

Then, for $k \ge 3$, 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 $k \ge 3$ 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 [DSS14] for large enough $k \ge k_0$ in random d-regular NAE-SAT by a demanding second moment method. Our proof is based on an interpolation method from statistical physics [FL03, Gue03, PT04]. We give a proof outline in Section 1.2.

We emphasize that for any $k \ge 3$, determining the colorability threshold for 2-coloring on random d-regular k-uniform hyprgraphs 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 [DSS16b] to the 2-coloring model since many of the arguments in [DSS16b] crucially takes 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 $Z_{\rm NAE}$ be the number of solutions of random d-regular k-NAE-SAT, then it is trivial to calculate $\mathbb{E}Z_{\rm NAE}$ exactly by taking advantage of the randomness of the clauses:

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

On the other hand, if we denote $Z_{\rm COL}$ by the number of 2-colorings on random d-regular k-uniform graphs, then estimating $\mathbb{E}Z_{\rm COL}$ is more delicate: we appeal to the idea of exponential tilting from large deviations theory [DZ10] and local central limit theorem [Bor17] to prove that $\mathbb{E}Z_{\rm COL}$ is of the same order as $\exp\big(n\Phi_k(\alpha)\big)$ in Lemma 1.8 below. Using the interpolation bound which is simpler than moment calculations, we clarify a simple mechanism (cf. Lemma 2.3) behind the identical satisfiability upper bounds for both models.

The solution $x(k,d)$ to the equation (1.1) has a mathematical interpretation. Namely, $2x(k,d)$ is the fraction of the so-called *frozen* variables in the *cluster* model. The solution $x(k,d)$ 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 [ST03]; see [Tal10, 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 $k \ge 3$ and $[d_{\rm lbd}(k), d_{\rm ubd}(k)]$, which might be also useful in obtaining a matching lower bound to Theorem 1.1.

Since $\mathbb{E}Z_{\rm NAE}$ and $\mathbb{E}Z_{\rm COL}$ are given by $\exp\big(n\Phi_k(\alpha)\big)$ up to a constant (cf. (1.3) and Lemma 1.8), 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

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

Remark 1.2. For $d \leq d_{\text{lbd}}(k)$ and large $k \geq k_0$, the second moment method applied to Z_{NAE} succeeds in showing the satisfiability for the random d-regular k-NAE-SAT model (see [DSS14, Section 2.1]). For $k \in \{3, 4\}$, $d_{\text{lbd}}(k)$ must be adjusted to be higher to guarantee that ${}^\star\mathbf{\Phi}(d)$ 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 $k \geq 4$ 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 [SSZ22, 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 $d_\star(k) \leq d_1(k) - \Omega(k)$.

1.1 Related work

Many of the earlier mathematical works on rCSPs 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 [CR92, BBC⁺01], random 1-IN-k-SAT [ACIM01], k-XOR-SAT [DM02, DGM⁺10, PS16], and random linear equations [ACOGM20]. 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 [KKKS98, AP04, COP16] (random k-SAT), [AM06, COZ12, COP12] (random k-NAE-SAT), and [AN05, CO13, COV13, COEH16] (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 [DSS16b], maximum independent set on d-regular graphs [DSS16a], random regular k-SAT [COP16] and random k-SAT [DSS22] for large k and d. Although determining the location of q-colorability threshold for the sparse Erdos Renyi graph is left open, the *condensation threshold* α_{cond} for random graph coloring, where the *free energy* becomes non-analytic, was settled in [BCOH⁺16]. They carried out a technically challenging analysis based on a clever "planting" technique, where the results were further generalized to other models in [COKPZ18]. Similarly, [BCO16] 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 was 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) [SSZ22], the concentration of the *overlap* [NSS20, NSS21], and the local weak limit [SS23] were established. Establishing the same quantities for other models in the condensation regime is left open.

The closest result to ours in the literature is by Ayre, Coja-Oghlan, and Greenhill [ACOG22], 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. [ACOG22] also considers the sparse Erdos Renyi 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 Erdos Renyi 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 [ACOG22], 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 [ST03, MRSY19, YP22, GP23] which addresses the uniqueness of BP fixed point for various models.

1.2 Proof methods

We aim to rigorously establish the upper bound the satisfiability threshold predicted by the so-called '1RSB cavity method' from statistical physics [DRZ08]. To do so, instead of using moment methods, we use a technique called 'interpolation method' from the theory of spin glasses developed by [FL03, Gue03, PT04]. The interpolation method has been successful in upperbounding the satisfiability threshold for random k-SAT [DSS15] for large k, the free energy for random regular k-NAE-SAT [SSZ16], and the colorability threshold for random graphs [ACOG22].

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. We denote the neighborhood of $v\in V$ (resp. $a\in F$) by $\delta v:=\{a\in F:(av)\in E\}$ (resp. $\delta a:=\{v\in V:(av)\in E\}$). 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 1.3. 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 $\underline{z}=(z_i)_{i\le k}\in\{0,1\}^k$, $\varphi(\underline{z})\equiv\mathbb{1}(z_1=\ldots=z_k)$, 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 the 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 $\boldsymbol{E}\sim\mathrm{Unif}(S_{nd})$. For a random d-regular k-NAE-SAT instance $\boldsymbol{\mathcal{G}}=(\boldsymbol{G},\underline{\mathbf{L}})$, we take the literals $\underline{\mathbf{L}}\equiv(\mathbf{L}_e)_{e\in E}\overset{i.i.d.}{\sim}\mathrm{Unif}(\{0,1\})$.

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 [JLR00]). 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 1.4 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 $b_s\ge 0$. Also, let $\mathcal{X}$ be a finite set encoding the spins and denote $\mathfrak{F}(\mathcal{X})$ by the set of functions $\mathcal{X}\to\mathbb{R}_{\ge 0}$. Let $f:S\to\mathfrak{F}(\mathcal{X})$ be a random function, 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 $\theta:\mathcal{X}^k\to\mathbb{R}$ by letting for $\underline{x}=(x_1,\ldots,x_k)\in\mathcal{X}^k$,

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

We assume that there exists a constant $\varepsilon\in(0,1)$ such that for any $\underline{x}\in\mathcal{X}^k$,

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

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 1.4. *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 1.4 is standard in literature [BCOH+16, COP19, ACOG22], and we provide the proof in Section 2 for completeness.

Definition 1.5. (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 [FL03, Gue03, PT04] 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 1.5 and the concentration of the free energy in Lemma 1.4, we prove the proposition below in Section 2.

Proposition 1.6. *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 1.6 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 [DSS16b, Section 3.1] for the motivation).

Proposition 1.7. *For $k \geq 3$ and $d \in [d_{\rm lbd}(k), d_{\rm ubd}(k)]$, 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 $d \in [d_{\rm lbd}(k), d_{\rm ubd}(k)]$ with ${}^\star\mathbf{\Phi}(d_{\rm lbd}(k)) > 0$ and ${}^\star\mathbf{\Phi}(d_{\rm ubd}(k)) < 0$.*

The proof of Proposition 1.7 is given in Section 3 for $k \geq 4$ and in Section 4 for $k = 3$, which requires extra numerical estimates. Finally, we show that the first moment $\mathbb{E}Z_{\rm COL}$ of the number of 2-colorings on random d-regular k-uniform hypergraphs is the same with $\mathbb{E}Z_{\rm NAE}$ up to a constant.

Lemma 1.8. *For $k \geq 3$, there exist constants $C_{k,d,i}$ for $i = 1, 2,$, which only depends on k, d such that $\mathbb{E}Z_{\rm COL}/\mathbb{E}Z_{\rm NAE} \in [C_{k,d,1}, C_{k,d,2}]$*

Proof of Theorem 1.1. By Proposition 1.7, the function ${}^\star\mathbf{\Phi}(d)$ is well-defined and has a root in the interval $[d_{\rm lbd}(k), d_{\rm ubd}(k)]$. Moreover, since ${}^\star\mathbf{\Phi}(d_{\rm ubd}(k)) < 0$ holds and ${}^\star\mathbf{\Phi}(\cdot)$ is continuous, we have ${}^\star\mathbf{\Phi}(d) < 0$ for $d \in (d_\star(k), d_{\rm ubd}(k)]$. Hence, Proposition 1.6 shows that if $d \in (d_\star(k), d_{\rm ubd}(k)]$, 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 $\mathbb{E}Z_{\rm COL} \asymp_{k,d} \mathbb{E}Z_{\rm NAE} = \exp\big(n\big(\log 2 + \alpha \log\big(1 - 2^{-k+1}\big)\big)\big)$ by Lemma 1.8 and $\log 2 + \alpha \log\big(1 - 2^{-k+1}\big) < 0$ holds for $d > d_{\rm ubd}(k)$, the same is true for $d > d_{\rm ubd}(k)$ by Markov's inequality. ∎

2 Satisfiability upper bound by interpolation

In this section, we prove Lemma 1.4, Proposition 1.6, and Lemma 1.8. We prove Proposition 1.6 in Section 2.1 based on the interpolation bound from statistical physics [FL03, Gue03]. In Section 2.2, we prove Lemma 1.4 based on Azuma Hoeffding's inequality applied to the Doob martingale with respect to clause revealing filtration. In Section 2.3, we prove Lemma 1.8 based on the local central limit theorem.

2.1 Proof of Proposition 1.6

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 [SSZ22, Theorem E.3] for random regular graphs, which is the analog of [PT04, Theorem 3] for Erdos Renyi graphs.

Theorem 2.1. *(Theorem E.3 in [SSZ22]) 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 $\zeta \in \mathcal{M}_2$,

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

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 2.2. [SSZ22, 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 $b_s \geq 0$ and $h_v \equiv 1$.

We use Theorem 2.1 for the positive temperature models in Definition 1.5. 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, viewing $\eta \equiv \eta_{k,d,\beta} \in \mathscr{P}([0,1])$, 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 $x \equiv x(k,d)$ is the BP fixed point, i.e. the solution to the equation (1.1). Such choice $\zeta_{k,d,\beta}$ is motivated from physics [KMRT+07] and previous mathematical works [DSS16b, Section 3] and [DSS22, 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. $\rho \overset{d}{=} 1-\rho$ 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

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

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

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

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 $\underline{\mathtt{L}}_a \overset{i.i.d}{\sim} \mathrm{Unif}(\{0,1\}^k)$, 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 2.3. *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 $1 \le a \le d$,

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

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

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

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 1.6. Recall the definition of $\zeta_{k,d,\beta}$ in (2.2) and (2.3).

Lemma 2.4. *$\mathcal{P}_{\theta_{\text{COL}}}(\zeta_{k,d,\beta},\beta^{-1/2}) \le C + \beta^{1/2}\cdot {}^{\star}\mathbf{\Phi}(d)$ holds for some constant $C\in\mathbb{R}$, which does not depend on $\beta>0$.*

Proof. Throughout, let $(\rho_{a,j})_{a\ge 0, j\ge 0}$ 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 $(\rho_{a,j})_{a\ge 0,j\ge 0}$. 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):

$$(k-1)\alpha\beta^{1/2}\log\mathbb{E}'\Big[(u_0)^{\beta^{-1/2}}\Big] = (k-1)\alpha\beta^{1/2}\log\mathbb{E}'\Bigg[\bigg(1-(1-e^{-\beta})\Big(\prod_{j=1}^k\rho_{0,j}(0)+\prod_{j=1}^k\rho_{0,j}(1)\Big)\bigg)^{\beta^{-1/2}}\Bigg]$$

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

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

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

$$-(k-1)\alpha\lambda^{-1}\mathbb{E}\log\mathbb{E}'\Big[(u_0)^{\lambda}\Big]\le C-\beta^{1/2}(k-1)\alpha\log\big(1-2x^k\big)\,. \tag{2.6}$$

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

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

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

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

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 any $1\leq a\leq d$, there exists $j\in\{2,\dots,k\}$ such that $\rho_{a,j}(0)\neq \frac{e^{\beta}}{e^{\beta}+e^{-\beta}}$.
- $\mathcal{E}_1$ is the event such that for any $1\leq a\leq d$, there exists $j\in\{2,\dots,k\}$ such 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 $a\equiv a(x)\in\{1,\dots,d\}$ 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

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

where the last inequality holds for large enough $\beta\geq\beta_k$. 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

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

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

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

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

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

which concludes the proof. ∎

Proof of Proposition 1.6. 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

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

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

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

where the last equality is due to Lemma 2.3. By Lemma 2.4, 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 1.4 that for large enough n,

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

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 2.4 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 1.4 again concludes the proof. ∎

2.2 Proof of Lemma 1.4

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 $t\in\{1,\dots,k\}$, 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 1.4 follows.

Proof of Lemma 1.4. 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 1.8

The following notations are convenient for the proof of Lemma 1.8. 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 $|\gamma - 1/2| \ge n^{-1/3}$ is negligible:

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

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

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

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

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

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

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

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 2.5. *For large enough n and all γ such that $|\gamma - 1/2| \le n^{-1/3}$, 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 $|\gamma - 1/2| \le n^{-1/3}$.*

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 2.5 in hand, we prove Lemma 1.8 by appealing to the local central limit theorem.

Proof of Lemma 1.8. 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 2.5 in equation (2.15). Then, by the local central limit theorem [Bor17],

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

where $X \sim \mathrm{Binom}(k,\gamma)$ and $\widetilde{X} \sim \nu_{\gamma,\lambda(\gamma)}$. Lemma 2.5 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 2.5. 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, combining with (2.18), we have

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

which concludes the proof. ∎

3 Proof of Proposition 1.7 for $k \geq 4$

In this section, we prove Proposition 1.7 for $k \geq 4$, which 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 1.7 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 $d \in [d_{\text{lbd}}(k), d_{\text{ubd}}(k)]$, $\big|(\Psi_d)'(x)\big| < 1$ 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

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

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:

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

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

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

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 $24\log 2 > 16.7 \equiv d_{\rm lbd}(4)$ 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

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

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 $d_{\rm lbd}(4) \equiv 16.7 > 24\log 2$. 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 $d_{\rm lbd}(4) \equiv 16.7$ 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 $k \ge 4$ 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 $k \ge 4$. We start with the case $k \ge 5$. We have shown in (3.4) that $v_0^{d-2} \le 2^{-k}e^{\varepsilon_k}$, holds, and by an analogous proof, $v_0^{d-1} \le 2^{-k}e^{\beta_k}$ holds, where $\beta_k \equiv \varepsilon_k - \frac{1}{2^{k-1}}\left(1 - \frac{2(k-1)}{2^k}\right)$. 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 $k \ge 5$.

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 $v_0^{15.7} \le \frac{2}{9}$ 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, $\left|(\Psi_d)'(x)\right| < 1$ 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 ${}^\star\mathbf{\Phi}(d) \equiv \Phi\big(d, x(k,d)\big)$, where $x(k,d) \in [\frac{1}{2}-\frac{1}{2^k}, \frac{1}{2}]$ 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 $d = d_{\rm lbd}(k)$ can further lower bounded by

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

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 that 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 $\Phi\big(d_{\rm lbd}(k), x\big) > 0$ 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 $k \geq 4$, $\Phi\big(d_{\rm ubd}(k), x\big) < 0$ 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 $x \to \Phi\big(d_{\rm ubd}(k), x\big)$ is increasing for $x \in [\frac{1}{2}-\frac{1}{2^k}, \frac{1}{2}]$ and $d_{\rm ubd}(k) \equiv 2^{k-1}k\log 2$. A direct calculation shows that

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

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

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

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, $\frac{\partial \Phi}{\partial x}\big(d_{\text{ubd}}(k), x\big) > 0$ 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 $x \to \Phi_4\big(d_{\text{ubd}}(4), x\big)$ is convex in the interval $x \in [\frac{7}{16}, \frac{1}{2}]$. From the computation of $\frac{\partial \Phi}{\partial x}\big(d_{\text{ubd}}(k), x\big)$ in (3.9), we can calculate the second derivative by

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

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

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

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 $x \to \Phi_4\big(d_{\text{ubd}}(4), x\big)$ is convex in the interval $x \in [\frac{7}{16}, \frac{1}{2}]$.

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

Proof of Lemma 3.2. By definition, ${}^\star\mathbf{\Phi}(d) = \Phi\big(d, x(k,d)\big)$ 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 $d \to x(k,d)$ 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 $x(k,d)$ is defined to be the root of $\psi(d,\cdot)$, this implies that $d \to x(k,d)$ is continuous by the implicit function theorem. As a consequence, we conclude that $d \to {}^\star\mathbf{\Phi}(d)$ is continuous. Since ${}^\star\mathbf{\Phi}(d_{\text{lbd}}(k)) > 0$ holds by Lemma 3.5 and ${}^\star\mathbf{\Phi}(d_{\text{ubd}}(k)) < 0$ holds by Lemma 3.6, we conclude the proof. ■

4 Proof of Proposition 1.7 for $k = 3$

In this section, we prove Proposition 1.7 for $k = 3$. Previous arguments for $k \geq 4$ in Section 3 do not work because ${}^\star\boldsymbol{\Phi}$ is in fact, not well defined for all d in the interval $[6\log 2, 12\log 2]$. To resolve this, we instead restrict our attention to $d \in [d_{\text{lbd}}(3), d_{\text{ubd}}(3)] \equiv [6.74, 7.5] \subset [6\log 2, 12\log 2]$. In Section 4.1 we show the following lemma which guarantees the existence and the uniqueness of the BP fixed point for $k = 3$.

Lemma 4.1. *For $k = 3$, $d \in [d_{\text{lbd}}(3), d_{\text{ubd}}(3)] \equiv [6.74, 7.5]$, there exists a unique solution to $\Psi_d(x) = x$ in the range $x \in [\frac{1}{2} - \frac{1}{2^3}, \frac{1}{2}]$.*

By Lemma 4.1, the function $d \to {}^\star\boldsymbol{\Phi}(d)$ is well-defined. In Section 4.2, we prove Lemma 4.2 which guarantees that $d_\star(3)$ is well-defined.

Lemma 4.2. *For $k = 3$, the function $d \to {}^\star\boldsymbol{\Phi}(d)$ is continuous for $d \in [d_{\text{lbd}}(3), d_{\text{ubd}}(3)] \equiv [6.74, 7.5]$. Further, ${}^\star\boldsymbol{\Phi}(d_{\text{lbd}}(3)) > 0$ and ${}^\star\boldsymbol{\Phi}(d_{\text{ubd}}(3)) < 0$ hold.*

Proof of Proposition 1.7 for $k = 3$. This is immediate from Lemma 4.1 and Lemma 4.2. ∎

4.1 Proof of Lemma 4.1

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 $k = 3$.

Lemma 4.3. *For $d \in [d_{\text{lbd}}(3), d_{\text{ubd}}(3)] \equiv [6.74, 7.5]$, $\big|(\Psi_d)'(x)\big| < 1$ holds uniformly over $x \in [\frac{1}{2} - \frac{1}{2^3}, \frac{1}{2}]$.*

Proof. For $k = 3$, a direct calculation gives

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

Using the inequality $\frac{1-2x^2}{1-x^2} < 1 - x^2$ in the denominator above, to prove our goal $\big|(\Psi_d)'(x)\big| < 1$, it suffices to prove that for $d \in [6.74, 7.5]$ and $x \in [7/8, 1/2]$,

$$2(d-1)\left(\frac{1-2x^2}{1-x^2}\right)^{d-2} x < \left(2 - (1-x^2)^{d-1}\right)^2 \cdot (1-x^2)^2\,,$$

which rearranges to

$$L(d,x) := \frac{(1-x^2)^d\left((1-x^2)^{d-1} - 2\right)^2}{(1-2x^2)^{d-2}} - 2(d-1)x > 0 \quad \text{for} \quad d \in [6.74, 7.5] \ \text{ and } \ x \in [7/8, 1/2]\,. \tag{4.1}$$

For the rest of the proof, we aim to show (4.1). We first claim that $x \to L(d,x)$ is increasing in the regime of interest. The following observation is useful to prove our claim: suppose we are given differentiable functions $f(x), g(x)$, such that $f(x) \geq 0$, $g(x) \leq 1$, and $g(\cdot)$ is decreasing, i.e. $g'(x) \leq 0$. Then,

$$\big(f(x)g(x)\big)' = f'(x)g(x) + f(x)g'(x) \leq f'(x)\,. \tag{4.2}$$

That is, if we multiply $f(\cdot)$ by a non-negative function by a decreasing function that is less than 1, denoted by $g(\cdot)$, then $(f \cdot g)' \leq f'$. Using this observation for $f(x) = \frac{(1-x^2)^d\left((1-x^2)^{d-1}-2\right)^2}{(1-2x^2)^{d-2}}$ and $g(x) = \frac{(1-2x^2)^{d-2}}{((1-x^2)^2)^{d-2}}$, which is less than 1 and decreasing, we have that

$$\begin{aligned} \frac{\partial L}{\partial x}(d,x) &\geq \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\left((1-x^2)^{d-1} - 2\right)^2}{(1-x^2)^{d-4}}\right) - 2(d-1) \\ &= x \cdot \left(\frac{8(d-4)}{(1-x^2)^{d-3}} + 24(1-x^2)^2 - 2(d+2)(1-x^2)^{d+1} - \frac{2(d-1)}{x}\right)\,. \end{aligned} \tag{4.3}$$

Abbreviating $d_{\rm lbd} \equiv 6.74, d_{\rm ubd} \equiv 7.5$, and $x_{\rm lbd} \equiv 3/8, x_{\rm ubd} \equiv 1/2$, we crudely bound

$$\begin{aligned}
&\frac{8(d-4)}{(1-x^2)^{d-3}} + 24(1-x^2)^2 - 2(d+2)(1-x^2)^{d+1} - \frac{2(d-1)}{x} \\
&\ge \frac{8(d_{\rm lbd}-4)}{(1-x_{\rm lbd}^2)^{d_{\rm lbd}-3}} + 24(1-x_{\rm ubd}^2)^2 - 2(d_{\rm ubd}+2)(1-x_{\rm lbd}^2)^{d_{\rm lbd}+1} - \frac{2(d_{\rm ubd}-1)}{x_{\rm lbd}}\,.
\end{aligned}$$

The right hand side above is a combination of fractions and powers of the numbers $6.74, 7.5, 3/8, 1/2$, thus can be computed up to arbitrary precision (e.g. by Mathematica), and it can be checked that the right hand side above is greater than 10. Therefore, combining with (4.3), this finishes the proof of our claim that $x \to L(d,x)$ is increasing in the regime of interest.

Since $L(d,\cdot)$ is increasing, to prove our goal (4.1), it remains to prove that $L(d,3/8) > 0$ for $d \in [6.74, 7.5]$. By a direct calculation, we have

$$L\Big(d\,,\,\frac{3}{8}\Big) = \frac{(55/64)^{3d-2}}{(23/32)^{d-2}} - \frac{4\,(55/64)^{2d-1}}{(23/32)^{d-2}} + \frac{4(55/64)^d}{(23/32)^{d-2}} - \frac{3(d-1)}{4}\,. \tag{4.4}$$

We next claim that the $d \to L(d,3/8)$ is convex for any $d > 0$. Recalling that $\frac{\mathrm{d}^2\gamma^d}{\mathrm{d}d^2} = \gamma^d(\log\gamma)^2$ for $\gamma > 0$, we can lower bound the second derivative by neglecting the first term in the right hand side:

$$\frac{\mathrm{d}^2 L}{\mathrm{d}d^2}\Big(d\,,\,\frac{3}{8}\Big) \ge 4\left(\frac{32}{23}\right)^2 \left(\frac{(55/64)^d}{(23/32)^d}\left(\log\left(\frac{55/64}{23/32}\right)\right)^2 - \frac{(55/64)^{2d}}{(23/32)^d}\left(\log\left(\frac{(55/64)^2}{23/32}\right)\right)^2 \cdot \frac{64}{55}\right)$$

It can be numerically verified (e.g. by Mathematica) that $\left(\log\left(\frac{55/64}{23/32}\right)\right)^2 > 0.01 > \left(\log\left(\frac{(55/64)^2}{23/32}\right)\right)^2 \cdot \frac{64}{55}$. Further, we have $\frac{(55/64)^d}{(23/32)^d} > \frac{(55/64)^{2d}}{(23/32)^d}$. Thus, the inequality above proves our claim that $d \to L(d,3/8)$ is convex for any $d > 0$.

Now, since $L(d,3/8)$ in (4.4) can be computed to arbitrary precision (e.g. by Mathematica), it can be numerically verified that $L(6.74,3/8) > 0.001 > 0$ while $L(6,3/8) < -0.2 < 0$ holds. Therefore, $L(d,3/8) > 0$ holds for $d > 6.74$ since $L(\cdot,3/8)$ is convex. Since we have shown that $L(d,\cdot)$ is increasing, this concludes the proof our goal (4.1). ∎

Lemma 4.4. *For $k = 3$ and $d \in [d_{\rm lbd}(3), d_{\rm ubd}(3)] \equiv [6.74, 7.5]$, $\Psi_d(\frac{1}{2} - \frac{1}{2^3}) > \frac{1}{2} - \frac{1}{2^3}$ holds.*

Proof. By a direct calculation, we have $\Psi_d(3/8) = \big(1-(46/55)^{d-1}\big)/\big(2-(46/55)^{d-1}\big)$, thus $\Psi_d(3/8) > 3/8$ is equivalent to $\left(\frac{55}{46}\right)^{d-1} > \frac{5}{2}$. Since $d \to \left(\frac{55}{46}\right)^{d-1}$ is increasing, it suffices to check this for $d = 6.74$. It can be checked numerically (e.g. by Mathematica) that $\left(\frac{55}{46}\right)^{5.74} > 2.7$, thus $\Psi_d(3/8) > 3/8$ holds for any $d \in [6.74, 7.5]$. ∎

Proof of Lemma 4.1. By Lemma 4.4, $\Psi_d(\frac{1}{2} - \frac{1}{2^3}) > \frac{1}{2} - \frac{1}{2^3}$ holds. Note that $\Psi_d(1/2) < 1/2$ holds since $\dot{\Psi}(x) < 1/2$ holds for any $x \ge 0$. 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 $x \in [\frac{1}{2} - \frac{1}{2^3}, \frac{1}{2}]$. Moreover, $\big|(\Psi_d)'(x)\big| < 1$ holds uniformly over $x \in [\frac{1}{2} - \frac{1}{2^3}, \frac{1}{2}]$ by Lemma 4.3, thus mean value theorem guarantees the uniqueness of the solution to $\Psi_d(x) = x$ for $x \in [\frac{1}{2} - \frac{1}{2^3}, \frac{1}{2}]$. ∎

4.2 Proof of Lemma 4.2

For $k \ge 4$, we have proven ${}^\star\boldsymbol{\Phi}\big(d_{\rm lbd}(k)\big) > 0$ by showing that $\Phi\big(d_{\rm lbd}(k), x\big)$, defined in (3.6), is uniformly positive for $x \in [\frac{1}{2} - \frac{1}{2^k}, \frac{1}{2}]$ in Lemma 3.4. Unfortunately, the same does not hold for $k = 3$. That is, it is not true for $k = 3$ that $\Phi(d_{\rm lbd}(3), x)$ is uniformly positive for $x \in [\frac{1}{2} - \frac{1}{2^3}, \frac{1}{2}]$. Instead, we prove ${}^\star\boldsymbol{\Phi}(6.74) > 0$ by proving a refined estimates for $x \equiv x(3, 6.74)$, the solution to (1.1).

Lemma 4.5. *For $k = 3$, we have ${}^\star\boldsymbol{\Phi}(6.74) > 0$.*

Proof. By Lemma 4.1, there exists a unique solution $x_\circ = x(3, 6.74)$ to $\Psi_d(x) = x$ for $k = 3$ and $d = 6.74$. By the uniqueness guaranteed by Lemma 4.3, if there exists $a, b \in [3/8, 1/2], a < b$ such that $\Psi_d(a) > a$ and $\Psi_d(b) < b$, then $x_\circ \in [a, b]$ holds. By taking $a = 0.4464$ and $b = 0.45$, it can be numerically verified that $\Psi_{6.74}(0.4464) > 0.44645$ and $\Psi_{6.74}(0.45) < 0.449$ holds, thus we have $x_\circ \in [0.4464, 0.45]$.

We now prove that for $k = 3$ and $d = 6.74$, the function $x \to \Phi(6.74, x)$ is increasing for $x \in [0.44, 0.45]$, where Φ is defined in (3.6). By a direct calculation,

$$\Phi(6.74, x) = -\log(1 - x) - \frac{262}{75}\log(1 - 2x^3) + \frac{287}{50}\log(1 - x^2)\,.$$

Differentiating in x gives that for $x \in [0.44, 0.45]$

$$\begin{aligned}\frac{\partial\Phi}{\partial x}(6.74, x) &= \frac{1}{1-x} + \frac{524}{25}\cdot\frac{x^2}{1-2x^3} - \frac{287}{25}\cdot\frac{x}{1-x^2}\\ &\geq \frac{1}{1-0.44} + \frac{524}{25}\cdot\frac{(0.44)^2}{1-2(0.44)^3} - \frac{287}{25}\cdot\frac{0.45}{1-(0.45)^2} > 0.1\,,\end{aligned}$$

thus $x \to \Phi(6.74, x)$ is increasing for $x \in [0.44, 0.45]$.

As a consequence, it follows that ${}^\star\mathbf{\Phi}(6.74) \geq \inf_{x\in[0.4464,0.45]} \Phi(6.74, x) = \Phi(6.74, 0.4464)$ holds. Further, $\Phi(6.74, 0.4464)$ can be calculated up to arbitrary precision (e.g. by Mathematica), and it can be checked that $\Phi(6.74, 0.4464) > 4 \cdot 10^{-5} > 0$, which concludes the proof. ■

To show that ${}^\star\mathbf{\Phi}(7.5) > 0$ holds for $k = 3$, we use a similar strategy as in the proof of Lemma 4.5.

Lemma 4.6. *For $k = 3$, we have ${}^\star\mathbf{\Phi}(7.5) < 0$ holds.*

Proof. Let $x'_\circ \equiv x(3, 7.5)$ be the unique solution to $\Psi_d(x) = x$ for $k = 3$ and $d = 7.5$ (cf. Lemma 4.1). By taking $a = 0.46$ and $b = 0.48$, it can be numerically verified that $\Psi_{7.5}(a) < a$ and $\Psi_{7.5}(b) > b$ holds, thus by uniqueness, we have $x'_\circ \in [0.46, 0.48]$.

We now prove that for $k = 3$ and $d = 7.5$, the function $x \to \Phi(7.5, x)$ is increasing for $x \in [0.46, 0.48]$. By definition of Φ in (3.6), we have

$${}^\star\mathbf{\Phi}(7.5) = -\log(1 - x) - 4\log(1 - 2x^3) + 6.5\log(1 - x^2)\,.$$

Differentiating in x gives that for $x \in [0.46, 0.48]$

$$\begin{aligned}\frac{\partial\Phi}{\partial x}(6.74, x) &= \frac{1}{1-x} + \frac{24x^2}{1-2x^3} - \frac{13x}{1-x^2} = -\frac{2x^3 - 24x^2 + 12x - 1}{(x-1)(x+1)(2x^3-1)}\\ &\geq \frac{1}{1-0.46} + \frac{24\cdot(0.46)^2}{1-2(0.46)^3} - \frac{13\cdot 0.48}{1-(0.48)^2} > 0.04 > 0\,,\end{aligned}$$

thus $x \to \Phi(7.5, x)$ is increasing for $x \in [0.46, 0.48]$.

Consequently, it follows that ${}^\star\mathbf{\Phi}(7.5) \leq \sup_{x\in[0.46,0.48]} \Phi(7.5, x) = \Phi(7.5, 0.48)$. Further, $\Phi(7.5, 0.48)$ can be calculated up to arbitrary precision (e.g. by Mathematica), and the inequality $\Phi(7.5, 0.48) < -0.04 < 0$ can be checked, which concludes the proof. ■

Proof of Lemma 4.2. By definition, ${}^\star\mathbf{\Phi}(d) = \Phi\big(d, x(3, d)\big)$ holds, where $x(3, d)$ is solution to (1.1). Since $(d, x) \to \Phi(d, x)$ is continuous, to prove the continuity of ${}^\star\mathbf{\Phi}(\cdot)$, it suffices to show that $d \to x(3, d)$ is continuous. Note that the function $\psi(d, x) := \Psi_d(x) - x$ satisfies $\frac{\partial\psi}{\partial x} < 0$ by Lemma 4.3. Since $x(3, d)$ is defined to be the root of $\psi(d, \cdot)$, this implies that $d \to x(3, d)$ is continuous by the implicit function theorem. Hence, we conclude that $d \to {}^\star\mathbf{\Phi}(d)$ is continuous. Since ${}^\star\mathbf{\Phi}(d_{\mathrm{lbd}}(3)) > 0$ holds by Lemma 4.5 and ${}^\star\mathbf{\Phi}(d_{\mathrm{ubd}}(3)) < 0$ holds by Lemma 4.6, we conclude the proof. ■

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