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Uniqueness of the Gibbs Measure for the Anti-ferromagnetic Potts Model on the Infinite Δ-Regular Tree for Large Δ

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Abstract
In this paper we prove that for any integer $q \geq 5$, the anti-ferromagnetic q-state Potts model on the infinite Δ-regular tree has a unique Gibbs measure for all edge interaction parameters $w \in [1 - q/\Delta, 1)$, provided Δ is large enough. This confirms a longstanding folklore conjecture.

Keywords Gibbs measure · Anti-ferromagnetic Potts model · Infinite regular tree

1 Introduction

The Potts model is a statistical model, originally invented to study ferromagnetism [32]; it also plays a central role in probability theory, combinatorics and computer science, see e.g. [35] for background.

Let $G = (V, E)$ be a finite graph. The anti-ferromagnetic Potts model on the graph G has two parameters, a number of *states, or colors,* $q \in \mathbb{Z}_{\geq 2}$ and an edge interaction parameter $w = e^{kJ/T}$, with $J < 0$ being a coupling constant, k the Boltzmann constant and T the temperature. The case $q = 2$ is also known as the zero-field Ising model. A *configuration* is a map $\sigma : V \to [q] := \{1, \ldots, q\}$. Associated with such a configuration is the *weight*

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$w^{m(\sigma)}$, where $m(\sigma)$ is the number of edges $e = \{u, v\} \in E$ for which $\sigma(u) = \sigma(v)$. There is a natural probability measure, the *Gibbs measure* $\Pr_{G;q,w}[\cdot]$, on the collection of configurations $\Omega = \{\sigma : V \to [q]\}$ in which a configuration is sampled proportionally to its weight. Formally, for a given configuration $\phi : V \to [q]$ the probability that a random configuration $\mathbf{\Phi}$[1] is equal to ϕ, is given by

$$\Pr_{G;q,w}[\mathbf{\Phi} = \phi] = \frac{w^{m(\phi)}}{\sum_{\sigma:V\to[q]} w^{m(\sigma)}}, \tag{1}$$

here the denominator is called *partition function* of the model and we denote it by $Z(G; q, w)$ (or just $Z(G)$ if q and w are clear form the context).

In statistical physics the Potts model is most frequently studied on infinite lattices, such as $\mathbb{Z}^2$. At the cost of introducing some measure theory, the notion of a Gibbs measure can be extended to such infinite graphs, see e.g. [10, 11, 16]. While at any temperature the Gibbs measure on a finite graph is unique, this is no longer the case for all infinite lattices. The transition from having a unique Gibbs measure to multiple Gibbs measures in terms of the temperature is referred to as a *phase transition* in statistical physics [16, 17] and it is an important problem to determine the exact temperature, the *critical temperature, T_c*, at which this happens. There exist predictions for the critical temperature on several lattices in the physics literature by Baxter [2, 3] (see also [36] for more details and further references), but it turns out to be hard to prove these rigorously cf. [36].

In the present paper we consider the anti-ferromagnetic Potts model on the infinite Δ-regular tree, $\mathbb{T}_\Delta = (V, E)$, also known as the *Bethe lattice*, or *Cayley tree*. We briefly recall the formal definition of a Gibbs measure in this situation following [10, 11]. See [34] for a survey on this topic in general.

The sigma algebra is generated by sets of the form $U_\sigma := \{\phi : V \to [q] \mid \phi\restriction_U = \sigma\}$, where $U \subset V$ is a finite set and $\sigma : U \to [q]$. Let $w \in (0, 1)$. A probability measure μ on this sigma algebra is then called a Gibbs measure for the q-state anti-ferromagnetic Potts model on $\mathbb{T}_\Delta$ at w, if for all finite $U \subset V$ and μ-a.e. $\phi : V \to [q]$ the following holds

$$\Pr_\mu[\mathbf{\Phi}\restriction_{U^\circ} = \phi\restriction_{U^\circ} \mid \mathbf{\Phi}\restriction_{V\setminus U^\circ} = \phi\restriction_{V\setminus U^\circ}] = \Pr_{\mathbb{T}_\Delta[U];q,w}[\mathbf{\Phi}\restriction_{U^\circ} = \phi|_{U^\circ} \mid \mathbf{\Phi}\restriction_{\partial U} = \phi|_{\partial U}],$$

where ∂U denotes the collection of vertices in U that have a neighbor in $V \setminus U$ and $U^\circ := U \setminus \partial U$. We note that the probability in the right-hand side of this equation is determined in the finite graph induced by U, $\mathbb{T}_\Delta[U]$. Moreover, we note that for any $w \in (0, 1)$ there exists at least one such Gibbs measure.

For a number of states $q \geq 2$ define

$$w_c := \max\left\{0, 1 - \frac{q}{\Delta}\right\}.$$

It is a longstanding folklore conjecture (cf. [7, page 746]) that the Gibbs measure is unique if and only if $w \geq w_c$ (where the inequality should be read as strict if $q = \Delta$.) We note that using the well known Dobrushin uniqueness theorem, one obtains uniqueness of the Gibbs measure provided $w > 1 - \frac{q}{2\Delta}$ cf. [5, 36], which is still far way from the conjectured threshold. The conjecture was confirmed by Jonasson for the case $w = 0$ [24], by Srivastava, Sinclair and Thurley [38] for $q = 2$ (see also [17]; in this case one can map the model to a ferromagnetic model since the tree is bipartite, which is much better understood), by Galanis, Goldberg and Yang for $q = 3$ [18] and by three of the authors of the present paper for $q = 4$ and $\Delta \geq 5$ [13]. Our main result is a confirmation of this conjecture for all $q \geq 5$ provided the degree of the tree is large enough.

[1] We use the convention to denote random variables with capitals in boldface.

Main Theorem *For each integer $q \geq 5$ there exists $\Delta_0 \in \mathbb{N}$ such that for each $\Delta \geq \Delta_0$ and each $w \in [w_c, 1)$ the q-state anti-ferromagnetic Potts model with edge interaction parameter w has a unique Gibbs measure on the infinite Δ-regular tree $\mathbb{T}_\Delta$.*

It has long been known that there are multiple Gibbs measures when $w < w_c$ [30, 31], see also [22]) and [8, 21, 25, 26]. We will briefly indicate below Lemma 2.2 how one can deduce this. Our main results therefore pinpoints the critical temperature for the anti-ferromagnetic Potts model on the infinite regular tree for large enough degree. For later reference we will refer to w_c as the *uniqueness threshold*.

In Theorem 2.1 below, we will reformulate our main theorem in terms of the conditional distribution of the color of the root vertex of $\mathbb{T}_\Delta$ conditioned on a fixed coloring of the vertices at a certain distance from the root, showing that this distribution converges to the uniform distribution as the distance tends to infinity. We in fact show that this convergence is exponentially fast for subcritical w (i.e. $w > w_c$).

1.1 Motivation from Computer Science

There is a surprising connection between phase transitions on the infinite regular tree and transitions in the computational complexity of approximately computing partition function of 2-state models (not necessarily the Potts model) on bounded degree graphs. For parameters inside the uniqueness region there is an efficient algorithm for this task [27, 38, 39], while for parameters for which there are multiple Gibbs measures on the infinite regular tree, the problem is NP-hard [23, 37]. It is conjectured that a similar phenomenon holds for a larger number of states.

While the picture for q-state models for $q \geq 3$ is far from clear, some progress has been made on this problem for the anti-ferromagnetic Potts model. On the hardness side, Galanis, Štefankvovič and Vigoda [22] showed that for even numbers $\Delta \geq 4$ and any integer $q \geq 3$, approximating the partition function of the Potts model $Z(G; q, w)$ is NP-hard on the family of graphs of maximum degree Δ for any $0 \leq w < 1 - q/\Delta = w_c$, which we now know to be the uniqueness threshold (for Δ large enough). On the other side, much less is known about the existence of efficient algorithms for approximating $Z(G; q, w)$ or sampling from the measure $\Pr_{G;q,w}$ for the class of bounded degree graphs when $w > w_c$. Implicit in [6] there is an efficient algorithm for this problem whenever $1 - \alpha q/\Delta < w \leq 1$, with $\alpha = 1/e$, which has been improved to $\alpha = 1/2$ in [28].

For random regular graphs of large enough degree, our main result implies an efficient randomized algorithm to approximately sample from the Gibbs measure $\Pr_{G;q,w}$ for any $w_c < w \leq 1$ by a result of Blanca, Galanis, Goldberg, Štefankovič, Vigoda and Yang [7, Theorem 2.7]. See also [12] for a very recent improvement. In [14], Efthymiou proved a similar result for Erdős-Rényi random graphs without the assumption that w_c is equal to the uniqueness threshold on the tree. At the very least this indicates that the uniqueness threshold on the infinite regular tree plays an important role in the study of the complexity of approximating the partition function of and sampling from the Potts model on bounded degree graphs.

1.2 Approach

Our approach to prove the main theorem is based on the approach from [13] for the cases $q = 3, 4$. As is well known, to prove uniqueness it suffices to show that for a given root vertex, say v, the probability that v receives a color $i \in [q]$, conditioned on the event that the vertices at distance n from v receive a fixed coloring, converges to $1/q$ as $n \to \infty$ regardless of the fixed coloring of the vertices at distance n. Instead of looking at these probabilities, we look at ratios of these probabilities. It then suffices to show that these converge to 1. The ratios at the root vertex v can be expressed as a rational function of the ratios at the neighbors of v. See Lemma 2.2 below. This function is rather difficult to analyze directly and as in [13] we analyze a simpler function coupled with a geometric approach. A key new ingredient of our approach is to take the limit of Δ, the degree of the tree, to infinity and analyze the resulting function. This function turns out be even simpler and behaves much better in a geometric sense. With some work we translate the results for the limit case back to the finite case and therefore obtain results for Δ large enough. This is inspired by a recent paper [4] in which this idea was used to give a precise description of the location of the zeros of the independence polynomial for bounded degree graphs of large degree.

Organization

In the next section we give a more technical overview of our approach. In particular we recall some results from [13] that we will use and set up some terminology. We also gather two results that will be used to prove our main theorem, leaving the proofs of these results to Sect. 3 and Sect. 4 respectively. Assuming these results, the main theorem will be proved in Subsect 2.4.

2 Preliminaries, Setup and Proof Outline

2.1 Reformulation of the Main Result

We will reformulate our main theorem here in terms of the conditional distribution of the color of the root vertex of $\mathbb{T}_\Delta$ conditioned on a fixed coloring of the vertices at a certain distance from the root.

Let $\Delta \geq 2$ be an integer. In what follows it will be convenient to write $d = \Delta - 1$. For a positive integer n we denote by $\mathbb{T}^n_{d+1}$ the finite tree obtained from $\mathbb{T}_{d+1}$ by fixing a root vertex r, deleting all vertices at distance more than n from the root, deleting one of the neighbors of r and keeping the connected component containing r. We denote the set of leaves of $\mathbb{T}^n_{d+1}$ by Λ_n, except when $n = 0$, in which case we let $\Lambda_0 = \{r\}$. For a positive integer q we call a map $\tau : \Lambda_n \to [q]$ a *boundary condition at level n*.

The following theorem may be seen as a more precise form of our main result.

Theorem 2.1 *Let $q \geq 3$ be a positive integer. There exist constants $C > 0$ and $d_0 > 0$ such that for all integers $d \geq d_0$ and all $\alpha \in (0, 1)$ the following holds for any $i \in \{1, \ldots, q\}$:*

$$\lim_{n\to\infty} \max_{\tau:\Lambda_n\to[q]} \left| Pr_{\mathbb{T}^n_{d+1},q,w_c}[\boldsymbol{\Phi}(r) = i \mid \boldsymbol{\Phi}\restriction_{\Lambda_n} = \tau] - \frac{1}{q} \right| = 0, \tag{2}$$

for any boundary condition τ at level n and edge interaction $w(\alpha) = 1 - \frac{\alpha q}{d+1}$,

$$\left| Pr_{\mathbb{T}^n_{d+1},q,w(\alpha)}[\boldsymbol{\Phi}(r) = i \mid \boldsymbol{\Phi}\restriction_{\Lambda_n} = \tau] - \frac{1}{q} \right| \leq C\alpha^{n/2}. \tag{3}$$

Remark 1 We can in fact strengthen (3) in two ways. First of all, for any $\alpha < \hat{\alpha} < 1$ there exists a constant $C_{\hat{\alpha}} > 0$ such that the right-hand side of (3) can be replaced by $C_{\hat{\alpha}}\hat{\alpha}^n$.

Secondly, for any fixed $d \geq d_0$ there exist a constant $C_d > 0$ such that the right-hand side of (3) can be replaced by $C_d \alpha^n$.

As is well known (see e.g. [13, Lemma 1.3].[2]) Theorem 2.1 directly implies our main theorem. Therefore the remainder of the paper is devoted to proving Theorem 2.1.

We now outline how we do this.

2.2 Log-Ratios of Probabilities

Theorem 2.1 is formulated in terms of certain conditional probabilities. For our purposes it turns out to be convenient to reformulate this into *log-ratios* of these probabilities. To introduce these, we recall some relevant definitions from [13]. Throughout we fix an integer $q \geq 3$.

Given a (finite) graph $G = (V, E)$ and a subset $U \subseteq V$ of vertices, we call $\tau : U \to [q]$ a *boundary condition* on G. We say vertices in U are *fixed* and vertices in $V \setminus U$ are *free*. The *partition function restricted to* τ is defined as

$$Z_{U,\tau}(G; q, w) = \sum_{\substack{\sigma : V \to [q] \\ \sigma \restriction_U = \tau}} w^{m(\sigma)}.$$

We just write $Z(G)$ if U, τ and q, w are clear from the context. Given a boundary condition $\tau : U \to [q]$, a free vertex $v \in V \setminus U$ and a state $i \in [q]$ we define $\tau_{v,i}$ as the unique boundary condition on $U \cup \{v\}$ that extends τ and associates i to v. When U and τ are clear from the context, we will denote $Z_{U \cup \{v\}, \tau_{v,i}}(G)$ as $Z_i^v(G)$. Let $\tau : U \to [q]$ be a boundary condition and $v \in V$ be a free vertex. For any $i \in [q]$ we define the *log-ratio* $\tilde{R}_{G,v,i}$ as

$$\tilde{R}_{G,v,i} := \log(Z_i^v(G)) - \log(Z_q^v(G)),$$

where log denotes the natural logarithm. Note that $\tilde{R}_{G,v,q} = 0$. We moreover remark that $\tilde{R}_{G,v,i}$ can be interpreted as the logarithm of the ratio of the probabilities that the root gets color i (resp. q) conditioned on the event that U is colored according to τ.

For trees the log-ratios at the root vertex can be recursively computed from the log-ratios of its neighbors. To describe this compactly we introduce some notation that will be used extensively throughout the paper. Fix $d \in \mathbb{R}_{>1}$ and let $\alpha \in (0, 1]$. Define the maps $G_{d,\alpha;i}, F_{d,\alpha;i} : \mathbb{R}^{q-1} \to \mathbb{R}$ for $i \in \{1, \ldots, q-1\}$ as

$$G_{d,\alpha;i}(x_1, \ldots, x_{q-1}) = \frac{1 - x_i}{\sum_{j=1}^{q-1} x_j + 1 - \frac{\alpha \cdot q}{d+1}} \tag{4}$$

and

$$F_{d,\alpha;i}(x_1, \ldots, x_q) = d \log\left(1 + \frac{\alpha \cdot q}{d+1} \cdot G_{d,\alpha;i}(\exp(x_1), \ldots, \exp(x_{q-1}))\right). \tag{5}$$

Define the map $F_{d,\alpha} : \mathbb{R}^{q-1} \to \mathbb{R}^{q-1}$ whose ith coordinate function is given by $F_{d,\alpha;i}(x_1, \ldots, x_{q-1})$ and define $G_{d,\alpha}$ similarly. To suppress notation we write $F_d = F_{d,1}$ and $G_d = G_{d,1}$. We also define $\exp(x_1, \ldots, x_{q-1}) = (\exp(x_1), \ldots, \exp(x_{q-1}))$ and $\log(x_1, \ldots, x_{q-1}) = (\log(x_1), \ldots, \log(x_{q-1}))$. We note that $G_{d,\alpha}$ and $F_{d,\alpha}$ are analytic

[2] The proof of that lemma in the published version of that paper contains an error; this is corrected in a more recent arXiv version: arXiv:2011.05638v3.

in $1/d$ near 0 when viewing d as a variable. We will now use the map $F_{d,\alpha}$ to give a compact description of the tree recurrence for log-ratios.

Lemma 2.2 *Let $T = (V, E)$ be a tree, $\tau : U \to [q]$ a boundary condition on $U \subsetneq V$. Let v be a free vertex of degree $d \geq 1$ with neighbors $v_1, \dots, v_d$. Denote T_i for the tree that is the connected component of $T - v$ containing v_i. Restrict τ to each T_i in the natural way. Write $\tilde{R}_{i,j}$ for the log-ratio $\tilde{R}_{T_i,v_i,j}$. Then for α such that $w = 1 - \frac{\alpha \cdot q}{d+1}$,*

$$(\tilde{R}_{T,v,1}, \dots, \tilde{R}_{T,v,q-1}) = \sum_{i=1}^{d} \frac{1}{d} F_{d,\alpha}(\tilde{R}_{i,1}, \dots, \tilde{R}_{i,q-1}), \tag{6}$$

a convex combination of the images of the map $F_{d,\alpha}$.

Proof By focusing on the jth entry of the left-hand side and substituting $R_{T,v,j} := \exp(\tilde{R}_{T,v,j})$, we see that (6) follows from the well known recursion for ratios

$$R_{T,v,i} = \prod_{s=1}^{d} \frac{\sum_{l \in [q-1]\setminus\{i\}} R_{T_s,v_s,l} + w R_{T_s,v_s,i} + 1}{\sum_{l \in [q-1]} R_{T_s,v_s,l} + w}. \tag{7}$$

See e.g. [13] for a proof of this. □

We note that if the boundary condition τ is constant on the leaves of the tree $\mathbb{T}^n_{d+1}$, then the log-ratios at the root can be obtained by iterating the univariate function f given by $f(x) = F_{d,\alpha}(x, \dots, x)$ at $w = w(\alpha)$. The point $x = 0$ is a fixed point of f; it satisfies $|f'(0)| \leq 1$ if and only if $w \geq w_c$. From this it is not difficult to extract that there exist multiple Gibbs measures when $w < w_c$.

Denote $\mathbf{0}$ for the zero vector in $\mathbb{R}^{q-1}$. (Throughout we will denote vectors in boldface.) We define for any $n \geq 1$ the set of possible log-ratio vectors

$$\mathcal{R}_n := \{(\tilde{R}_{\mathbb{T}^n_{d+1},r,1}, \dots, \tilde{R}_{\mathbb{T}^n_{d+1},r,q-1}) \in \mathbb{R}^{q-1} | \tau : \Lambda_n \to [q]\}.$$

Here the ratios $\tilde{R}_{\mathbb{T}^n_{d+1},r,1}$ depend on τ but this is not visible in the notation. The following lemma shows how the recursion from Lemma 2.2 will be used.

Lemma 2.3 *Let $q \geq 3$ and $d \geq 2$ be integers. If there exists a sequence $\{\mathcal{T}_n\}_{n\geq 1}$ of convex subsets of $\mathbb{R}^{q-1}$ with the following properties:*

1. *$\mathcal{R}_1 \subseteq \mathcal{T}_1$,*
2. *for every $n \geq 1$, $F_d(\mathcal{T}_n) \subseteq \mathcal{T}_{n+1}$,*
3. *for every $\epsilon > 0$ there is an $N \geq 1$ such that for all $n \geq N$, $\sup_{\mathbf{r} \in \mathcal{T}_\mathbf{n}} \|\mathbf{r}\|_1 \leq \varepsilon$,*

then

$$\lim_{n\to\infty} \max_{\tau:\Lambda_{n,d+1}\to[q]} \left| Pr_{\mathbb{T}^n_d,q,w_c}[\mathbf{\Phi}(r) = i \mid \mathbf{\Phi}\restriction_{\Lambda_{n,d}} = \tau] - \frac{1}{q} \right| = 0. \tag{8}$$

Proof The proof is straightforward and analogous to the proof of Lemma 2.3 in [13] and we therefore omit it. □

We note that the lemma is only stated for $\alpha = 1$. An analogues statement for $\alpha \in (0, 1)$ and F_d replaced by $F_{d,\alpha}$ with a more accurate dependence of N on ε follows from a certain monotonicity of $F_{d,\alpha}$, as will be explained in the proof of Theorem 2.1 below.

In the next section we construct a family of convex sets that allows us to form a sequence $\{\mathcal{T}_n\}_{n\geq 1}$ with the properties required by the lemma.

2.3 Construction of Suitable Convex Sets

We need the standard $q-2$-simplex, which we denote as

$$\Delta = \left\{ (t_1, \ldots, t_{q-2}, 1 - \sum_{i=1}^{q-2} t_i) \mid t_i \geq 0 \text{ for all } i, \sum_{i=1}^{q-2} t_i \leq 1 \right\}.$$

The symmetric group S_q acts on $\mathbb{R}^q$ by permuting entries of vectors. Consider $\mathbb{R}^{q-1} \subset \mathbb{R}^q$ as the subspace spanned by $\{\mathbf{e}_1 - \mathbf{e}_q, \ldots, \mathbf{e}_{q-1} - \mathbf{e}_q\}$, where $\mathbf{e}_i$ denotes the ith standard base vector in $\mathbb{R}^q$. This induces a linear action of S_q on $\mathbb{R}^{q-1}$, also known as the the standard representation of S_q and denoted by $\mathbf{x} \mapsto \pi \cdot \mathbf{x}$ for $\mathbf{x} \in \mathbb{R}^{q-1}$ and $\pi \in S_q$. The following lemma shows that the map $F_{d,\alpha}$ is S_q-equivariant for any $\alpha \in (0, 1]$, essentially because the action permutes the q colors of the Potts model and no color plays a special role.

Lemma 2.4 *For any $\pi \in S_q$, any $\alpha \in (0, 1]$, any $\mathbf{x} \in \mathbb{R}^{q-1}$ and any d we have*

$$\pi \cdot F_{d,\alpha}(\mathbf{x}) = F_{d,\alpha}(\pi \cdot \mathbf{x}).$$

Proof This follows as in Section 3.1 in [13]. □

Define for $c \geq 0$ the half space

$$H_{\geq -c} := \left\{ \mathbf{x} \in \mathbb{R}^{q-1} \mid \sum_{i=1}^{q-1} x_i \geq -c \right\}. \tag{9}$$

Define the set

$$P_c = \bigcap_{\pi \in S_q} \pi \cdot H_{\geq -c}. \tag{10}$$

Note that for each $c \geq 0$ the set P_c equals the convex polytope

$$\text{conv}\big(\{(-c, 0, \ldots, 0), \ldots (0, \ldots, 0, -c), (c, \ldots, c)\}\big).$$

Denote $D_c := \text{conv}\big(\{(-c, 0, \ldots, 0), \ldots (0, \ldots, 0, -c), (0, \ldots, 0)\}\big)$. Then we have

$$P_c = \bigcup_{\pi \in S_q} \pi \cdot D_c. \tag{11}$$

We refer to D_c as the fundamental domain of the action of S_q on $\mathbb{R}^{q-1}$.

The following two propositions capture the image of P_c under applications of the map F_d.

Proposition 2.5 *Let $q \geq 3$ be an integer. Then there exists $d_1 > 0$ such that for all $d \geq d_1$ and $c \in [0, q+1]$, $F_d(P_c)$ is convex.*

Proposition 2.6 *Let $q \geq 3$ be an integer. There exists $d_2 > 0$ such that for all $d \geq d_2$ the following holds: for any $c \in (0, q+1]$ there exists $0 < c' < c$ such that*

$$F_d^{\circ 2}(P_c) \subseteq P_{c'}.$$

An intuitive explanation for why we need $F_d^{\circ 2}$ and cannot work with F_d directly is that the derivative of F_d at $\mathbf{0}$ is equal to $-\text{Id}$, which reflects the fact that we are dealing with an anti-ferromagnetic model, while the derivative of $F_d^{\circ 2}$ at $\mathbf{0}$ is equal to Id.

We postpone the proofs of the two results above to the subsequent sections. A crucial ingredient in both proofs will be to analyze the limit $\lim_{d\to\infty} F_d$. We first utilize the two propositions to give a proof of Theorem 2.1.

2.4 A Proof of Theorem 2.1

Fix an integer $q \geq 3$. Let d_1, d_2 be the constants from Propositions 2.5 and 2.6 respectively. Let $d_0 \geq \max\{d_1, d_2\}$ large enough to be determined below. Note that the log-ratios at depth 0 are of the form $\infty \cdot \mathbf{e}_i$ and $-\infty \cdot \mathbf{1}$, where $\mathbf{1}$ denotes the all ones vector. This comes from the fact that the probabilities at level 0 are either 1 or 0 and so the ratios are of the form $\mathbf{1} + \infty\mathbf{e}_i$ or $\mathbf{0}$. This implies that the log-ratios at depth 1 are convex combinations of $F_d(\infty \cdot \mathbf{e}_i) = d\log(1 + \frac{-q}{d+1})\mathbf{e}_i$ and $F_d(-\infty \cdot \mathbf{1}) = d\log(1 + \frac{q}{d+1-q})\mathbf{1}$. So for $d \geq d_0$ and d_0 large enough they are certainly contained in P_{q+1}.

We start with the proof of (2). We construct a decreasing sequence $\{c_n\}_{n\in\mathbb{N}}$ and let $\mathcal{T}_{2n-1} = P_{c_n}$. For even $n > 0$ we set $\mathcal{T}_n = F_d(P_{c_{n-1}})$, which is convex by Proposition 2.5. We set $c_1 = q + 1$ and for $n \geq 1$, given c_n, we can choose, by Proposition 2.6, $c_{n+1} < c_n$ so that $F_d^{\circ 2}(P_{c_n}) \subseteq P_{c_{n+1}}$. Choose such a c_{n+1} as small as possible. We claim that the sequence $\{c_n\}_{n\in\mathbb{N}}$ converges to 0. Suppose not then it must have a limit $c > 0$. Choose $c' < c$ such that $F_d^{\circ 2}(P_c) \subseteq P_{c'}$. Then for n large enough we must have $F_d^{\circ 2}(P_{c_n}) \subseteq P_{c/2+c'/2}$, contradicting the choice of c_{n+1}.

Since $\{c_n\}_{n\in\mathbb{N}}$ converges to 0, it follows that the sequence $\mathcal{T}_n$ converges to $\{0\}$. With Lemma 2.3 this implies (2).

To prove the second part let $\alpha \in (0, 1)$. Consider the decreasing sequence $\{c_n\}_{n\in\mathbb{N}}$ with $c_n = (q + 1)\alpha^{n-1}$. Set $\mathcal{T}_{2n-1} = P_{c_n}$ and $\mathcal{T}_{2n} = F_{d,\alpha}(P_{c_{n-1}})$. We use the following observation.

Lemma 2.7 *For any $\alpha \in (0, 1]$, any $\mathbf{x} \in \mathbb{R}^{q-1}$ and any integer d there is $d' \geq d$ such that $F_{d,\alpha}(\mathbf{x}) = \frac{d}{d'} \cdot F_{d'}(\mathbf{x})$. Moreover, $\frac{d}{d'} \leq \alpha$.*

Proof When viewing α and d as variables, $\frac{1}{d} F_{d,\alpha;i}$ only depends on the ratio $\frac{\alpha}{d+1}$. Therefore the first statement of the lemma holds with d' defined by $\frac{\alpha}{d+1} = \frac{1}{d'+1}$. Since $\frac{d}{d'} = \frac{\alpha d}{d+1-\alpha}$, the second statement also holds. □

The lemma above implies that $F_{d,\alpha}(P_{c_n}) = \frac{d}{d'} \cdot F_{d'}(P_{c_n})$ and hence is convex for each c_n. It moreover implies that

$$F_{d,\alpha}^{\circ 2}(P_{c_n}) \subset \alpha F_{d'}(\alpha F_{d'}(P_{c_n})) \subset \alpha P_{c_n} = P_{c_{n+1}}.$$

By basic properties of the logarithm, (3) now quickly follows. This finishes the proof of Theorem 2.1.

The strengthening mentioned in Remark 1 can be derived from the fact that the derivative of $F_{d,\alpha}$ at $\mathbf{0}$ is equal to $\frac{-\alpha d}{d+1-\alpha}\mathrm{Id}$. Note that $\frac{\alpha d}{d+1-\alpha} < \alpha$ for all $\alpha \in (0, 1)$ and d. Therefore on a small enough open ball B around $\mathbf{0}$ the operator norm of the derivative of $F_{d,\alpha}$ can be bounded by $\hat{\alpha}$ for all $d \geq d_0$ (and by α for fixed $d \geq d_0$). Then for any integer $n \geq 0$, $F_{d,\alpha}^{\circ n}(B) \subset \hat{\alpha}^n B$ ($\alpha^n B$ respectively). For n_0 large enough $P_{c_{n_0}}$ is contained in this ball B. For $n > 2n_0$ we then set $\mathcal{T}_n = \hat{\alpha}^{n-2n_0} B$ ($\alpha^{n-2n_0} B$ respectively). The statements in the remark now follow quickly.

2.5 The $d \to \infty$ Limit Map

As mentioned above, an important tool in our approach is to analyze the maps F_d as $d \to \infty$. Since $F_d(\mathbb{R}^{q-1})$ is bounded, it follows that as $d \to \infty$, $F_d(x_1, \ldots, x_{q-1})$ converges uniformly to the limit map

$$F_\infty(x_1, \ldots, x_{q-1}), \tag{12}$$

with coordinate functions

$$F_{\infty;i}(x_1,\dots,x_{q-1}) := q\,\frac{1-e^{x_i}}{\sum_{j=1}^{q-1} e^{x_i}+1}. \tag{13}$$

We write $G_{\infty;i}(x_1,\dots,x_{q-1}) = q\,\frac{1-x_i}{\sum_{j=1}^{q-1} x_j+1}$ for the ith coordinate function of the fractional linear map G_∞. Note that $F_\infty = G_\infty \circ \exp$.

By Lemma 2.4 for any $\pi \in S_q$, any $\mathbf{x} \in \mathbb{R}^{q-1}$ and any d we have $\pi \cdot F_d(\mathbf{x}) = F_d(\pi \cdot \mathbf{x})$. As the action of π on $\mathbb{R}^{q-1}$ does not depend on d, we immediately see $\pi \cdot F_\infty(\mathbf{x}) = F_\infty(\pi \cdot \mathbf{x})$ follows.

In the next two sections we will prove Propositions 2.5 and 2.6. The idea is to first prove a variant of these propositions for the map F_∞ and then use that $F_d \to F_\infty$ uniformly to finally prove the actual statements. We use the description of P_c as intersection of half spaces $\pi \cdot H_{\geq -c}$ in Sect. 3 and the description as the union of the $\pi \cdot D_c$ in Sect. 4.

3 Convexity of the Forward Image of P_c

This section is dedicated to proving Proposition 2.5.

Fix an integer $q \geq 3$. For $\mu \in \mathbb{R}$ we define the half space $H_{\geq\mu}$ as in (9). The half space $H_{\leq\mu}$ is defined similarly. We denote by H_μ the affine space which is the boundary of $H_{\leq\mu}$.

In what follows we will often use that the map G_∞ is a fractional linear transformation and thus preserves lines and hence maps convex sets to convex sets, see e.g. [9, Section 2.3].

Lemma 3.1 *For all $c > 0$, the set $\exp(H_{\geq -c}) := \{\exp(\mathbf{x}) \mid \mathbf{x} \in H_{\geq -c}\}$ is strictly convex, consequently*

$$G_\infty(\exp(H_{\geq -c}))$$

is strictly convex.

Proof Since G_∞ is a fractional linear transformation, it preserves convex sets. It therefore suffices to show that $\exp(H_{\geq -c})$ is strictly convex.

To this end take any $\mathbf{x}, \mathbf{y} \in \exp(H_{\geq -c})$ and let $\lambda \in (0, 1)$. We need to show that $\lambda\mathbf{x} + (1-\lambda)\mathbf{y} \in \exp(H_{\geq -c})$. By strict concavity of the logarithm we have

$$\sum_{i=1}^{q-1} \log(\lambda x_i + (1-\lambda)y_i) \geq \sum_{i=1}^{q-1} \lambda \log(x_i) + (1-\lambda)\log(y_i) > -c,$$

we conclude that $\exp(H_{\geq -c})$ is strictly convex. □

In what follows we need the *angle* between the tangent space of $G_\infty(\exp(H_{-c}))$ for $c > 0$ at $G_\infty(\mathbf{x})$ for any $\mathbf{x} \in \exp(H_{-c})$ and the space H_0. This angle is defined as the angle of a normal vector of the tangent space pointing towards the interior of $G_\infty(\exp(H_{\geq -c}))$ and the vector $-\mathbf{1}$ (which is a normal vector of H_0).

Lemma 3.2 *For any $c \in [0, q+1]$ and any $\mathbf{x} \in \exp(H_{-c})$ the angle between the tangent space of $G_\infty(\exp(H_{-c}))$ at $G_\infty(\mathbf{x})$ and H_0 is strictly less than $\pi/2$.*

Proof We will first show that the tangent space cannot be orthogonal to H_0.

The map G_∞ is invertible (when restricted to $\mathbb{R}^{q-1}_{>0}$) with inverse G_∞^{-1} whose coordinate functions are given by

$$G^{-1}_{\infty,i}(y_1,\dots,y_{q-1}) = \frac{-q y_i}{\sum_{i=1}^{q-1} y_i + q} + 1.$$

Define $g : \mathbb{R}^{q-1} \setminus H_{-q} \to \mathbb{R}$ by $g(\mathbf{y}) = \prod_{i=1}^{q-1} G^{-1}_{\infty,i}(\mathbf{y})$. Then the image of $\exp(H_{-c})$ under G_∞ is contained in the hypersurface $\{\mathbf{y} \in \mathbb{R}^{q-1} \mid g(\mathbf{y}) = \exp(-c)\}$. Therefore a normal vector of the tangent space of $G_\infty(\exp(H_{-c}))$ at $\mathbf{y} = G_\infty(\mathbf{x})$ is given by the gradient of the function g. Thus to show that this tangent space is not orthogonal to H_0, we need to show that

$$\sum_{i=1}^{q-1} \tfrac{\partial}{\partial y_i} g(\mathbf{y}) \neq 0. \tag{14}$$

We have

$$\begin{aligned}
\sum_{i=1}^{q-1} \tfrac{\partial}{\partial y_i} g(\mathbf{y}) &= \sum_{i=1}^{q-1}\sum_{j=1}^{q-1} \frac{\prod_{k=1}^{q-1} G^{-1}_{\infty,k}(\mathbf{y})}{G^{-1}_{\infty,j}(\mathbf{y})} \tfrac{\partial}{\partial y_i} G^{-1}_{\infty,j}(\mathbf{y}) \\
&= \sum_{j=1}^{q-1} \frac{\prod_{k=1}^{q-1} G^{-1}_{\infty,k}(\mathbf{y})}{G^{-1}_{\infty,j}(\mathbf{y})} \sum_{i=1}^{q-1} \tfrac{\partial}{\partial y_i} G^{-1}_{\infty,j}(\mathbf{y}) \\
&= \sum_{j=1}^{q-1} \frac{\prod_{k=1}^{q-1} G^{-1}_{\infty,k}(\mathbf{y})}{G^{-1}_{\infty,j}(\mathbf{y})} \cdot \frac{-q(\sum_{i=1}^{q-1} y_i + q) + q(q-1)y_j}{(\sum_{i=1}^{q-1} y_i + q)^2} \\
&= \sum_{j=1}^{q-1} \frac{\prod_{k=1}^{q-1} G^{-1}_{\infty,k}(\mathbf{y})}{G^{-1}_{\infty,j}(\mathbf{y})} \cdot \frac{-(q-1)G^{-1}_{\infty,j}(\mathbf{y}) - 1}{\sum_{i=1}^{q-1} y_i + q}.
\end{aligned}$$

Since $G^{-1}_{\infty,k}(\mathbf{y}) > 0$ for each k, all terms in the final sum are nonzero and have the same sign. This proves (14).

Since the angle between the tangent space of $G_\infty(\exp(H_{-c}))$ at $G_\infty(\mathbf{x})$ and H_0 depends continuously on $\mathbf{x}$ this angle should either be always less than $\pi/2$ or always be bigger. Since by the previous lemma the set $G_\infty(\exp(H_{\geq -c}))$ is convex, it is the former. □

We next continue with the finite case. We will need the following definition. The *hypograph* of a function $f : D \to \mathbb{R}$ is the region $\{(x, y) \mid x \in D, y \leq f(x)\}$. Below we will consider a hypersurface contained in $\mathbb{R}^{q-1}$ that we view as the graph of a function with domain contained in H_0. In this context the hypograph of such a function is again contained in $\mathbb{R}^{q-1}$, but the 'positive y-axis' points in the direction of $\mathbf{1}$ as seen from $\mathbf{0} \in H_0$.

Lemma 3.3 *There exists $y_1 > 0$ such that for all $y \in [0, y_1)$ and $c \in [0, q+1]$ the set $F_y(P_c)$ is contained in the hypograph of a concave function, $h_{y,c}$, with a convex compact domain in H_0.*

Proof We first prove that for any $\mathbf{x} \in H_0$ and $c \in [0, q+1]$ there exists an open neighborhood $W_{c,\mathbf{x}} = Y_{c,\mathbf{x}} \times C_{c,\mathbf{x}} \times X_{c,\mathbf{x}}$ of $(0, c, \mathbf{x}) \in [0, 1] \times [0, q+1] \times \mathbb{R}^{q-1}$ such that the following holds for any $(y', c', \mathbf{x}') \in W_{c,\mathbf{x}}$:

the angle between the tangent space of $F_{1/y'}(H_{-c'})$ at $F_{1/y'}(\mathbf{x}'_{c'})$ and H_0

is strictly less than $\pi/2$, (15)

where we denote $\mathbf{x}_c := \mathbf{x} - \frac{c}{q-1}\mathbf{1} \in H_{-c}$. To see this note that by the previous lemma we have that the tangent space of $F_\infty(H_{-c})$ at $F_\infty(\mathbf{x}_c)$ is not orthogonal to H_0 and in fact makes an angle of less than $\pi/2$ with H_0. Say it has angle $\pi/2 - \gamma$. Since $(y, c, \mathbf{x}) \mapsto F_{1/y}(\mathbf{x}_c)$ is analytic, there exists an open neighborhood W_0 of $(0, c, \mathbf{x})$ such that for any $(y', \mathbf{x}', c') \in W_0$ the angle between the tangent space of $F_{1/y'}(H_{-c'})$ at $F_{1/y'}(\mathbf{x}'_{c'})$ and H_0 is at most $\pi/2 - \gamma/2$. Clearly, W_0 contains an open neighborhood of $(0, c, \mathbf{x})$ of the form $Y \times C \times X$ proving (15).

Next fix $c \in [0, q+1]$ and $\mathbf{x} \in H_0$ and write $W_{c,\mathbf{x}} = Y \times C \times X$. Together with the implicit function theorem, (15) now implies that for each $y' \in Y$ and any $c' \in C$, that locally at $\mathbf{x}_{c'}$, $F_{1/y'}(H_{-c})$ is the graph of an analytic function $f_{y',c',\mathbf{x}}$ on an open domain contained in H_0. Here we use that $F_{1/y}$ is invertible with analytic inverse. By choosing Y and C small enough, we may by continuity assume that we have a common open domain, $D_{c,\mathbf{x}}$, for these functions for all $c' \in C$ and $y' \in Y$, where we may moreover assume that these functions are all defined on the closure of $D_{c,\mathbf{x}}$.

We next claim, provided the neighbourhood $W = Y_{c,\mathbf{x}} \times C_{c,\mathbf{x}}$ is chosen small enough, that for each $y' \in Y$ and $c' \in C$,

the largest eigenvalue of the Hessian $f_{y',c',\mathbf{x}}$ on $D_{c,\mathbf{x}}$ is strictly less than 0. (16)

To see this we note that by the previous lemma we know that $F_\infty(H_{\geq -c})$ is strictly convex. Therefore the Hessian[3] of $f_{0,c,\mathbf{x}}$ on $D_{c,\mathbf{x}}$ is negative definite, say its largest eigenvalue is $\delta < 0$. Similarly as before, there exists an open neighborhood $W' \subseteq W$ of $(0, c)$ of the form $W' = Y' \times C'$ such that for each $y' \in Y'$ and $c' \in C'$, the function $f_{y',c',\mathbf{x}}$ has a negative definite Hessian with largest eigenvalue at most $\delta/2 < 0$ for each $\mathbf{z} \in D_{c,\mathbf{x}}$ (by compactness of the closure of $D_{c,\mathbf{x}}$). We now want to patch all these function to form a global function on a compact and convex domain. We first collect some properties of $F_{1/y}$ that will allow us to define the domain.

First of all note that by compactness there exists $a > 0$ such that for each $c \in [0, q+1]$, $\exp(P_c) \subset H_{\leq a}$ (where the inclusion is strict). We now fix such a value of a. Since G_∞ is S_q-equivariant, we know that $G_\infty(H_{\leq a}) = H_{\geq a'}$ for some $a' \in \mathbb{R}$. We now choose $y^* > 0$ small enough such that the following two inclusions hold for all $y \in [0, y^*]$ and $c \in [0, q+1]$

$$F_{1/y}(P_c) \subset H_{\geq a'}, \tag{17}$$

$$\mathrm{proj}_{H_0}(F_\infty(H_{-c}) \cap H_{\geq a'}) \subset \mathrm{proj}_{H_0}(F_{1/y}(H_{-c})), \tag{18}$$

where proj_{H_0} denotes the orthogonal projection onto the space H_0. The first inclusion holds since $F_{1/y}$ converges uniformly to F_∞ as $y \to 0$. For the second inclusion note that

$$F_\infty(H_{-c}) \cap H_{\geq a'} = G_\infty(\exp(H_{-c}) \cap H_{\leq a}) \subset F_\infty(H_{-c}).$$

Because $\exp(H_{-c}) \cap H_{\leq a}$ is compact, the desired conclusion follows since $F_{1/y} \to F_\infty$ uniformly as $y \to 0$.

Let us now consider for $c \in [0, q+1]$ the projection

$$\mathrm{Dom}_c := \mathrm{proj}_{H_0}(F_\infty(H_{-c}) \cap H_{\geq a'}),$$

see Fig. 1. Since $F_\infty(H_{-c}) \cap H_{\geq a'}$ is convex by Lemma 3.1 and compact, it follows that

[3] Recall that the *Hessian* of a function $f : U \to \mathbb{R}$ for an open set $U \subseteq \mathbb{R}^n$ at a point $u \in U$ is defined as the $n \times n$ matrix $H_f(u)$ with $(H_f(u))_{i,j} = \frac{\partial^2 f}{\partial x_i \partial x_j}(u)$. When these partial derivatives are continuous and the domain U is convex, f is concave if and only if its Hessian is negative definite at each point of the domain U [9].

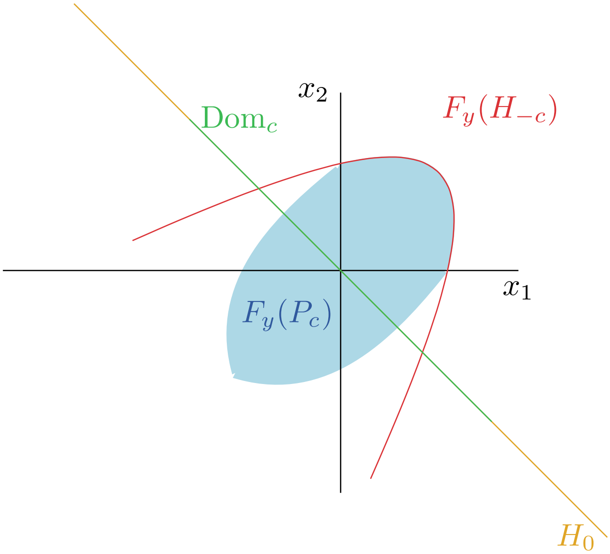

Fig. 1 Depicting the situation in Lemma 3.3, for $q = 3$, $c = 2$ and $y = \frac{1}{20}$. The domain Dom_c of the function $h_{y,c}$ which we define in the proof of Lemma 3.3 is made by choosing $a' = -3$

Dom_c is compact and convex for each $c \in [0, q+1]$. Moreover, we claim that

$$\bigcup_{c\in[0,q+1]} (\{c\} \times \mathrm{Dom}_c) \subseteq [0, q+1] \times H_0 \text{ is compact.} \tag{19}$$

Indeed, it is the continuous image of the compact set $\exp(H_{\geq -q-1}) \cap H_{\leq a}$ under the map

$$\exp(H_{\geq -q-1}) \cap H_{\leq a} \to [0, q+1] \times H_0$$

defined by

$$\mathbf{x} \mapsto \left(\sum_{i=1}^{q-1} x_i, \mathrm{proj}_{H_0}(G_\infty(\mathbf{x})) \right).$$

By (18) Dom_c is contained in $\mathrm{proj}_{H_0}(F_{1/y}(H_{-c}))$ for all $y \in [0, y^*]$ and $c \in [0, q+1]$. It follows that the sets $Y_{c,\mathbf{x}} \times C_{c,\mathbf{x}} \times D_{c,\mathbf{x}}$, where $\mathbf{x}$ ranges over H_0 and c over $[0, q+1]$, form an open cover of $\{0\} \times \cup_{c\in[0,q+1]} (\{c\} \times \mathrm{Dom}_c)$. Since the latter set is compact by (19), we can take a finite sub cover. Therefore there exists $y_1 > 0$ such that for each $y \in [0, y_1)$ and each $c \in [0, q+1]$ we obtain a unique global function $h_{y,c}$ on the union of these finitely many domains, which by (16) has a strictly negative definite Hessian. By construction the union of these domains contains Dom_c for each $c \in [0, q+1]$. Consequently, restricted to Dom_c, $h_{y,c}$ is a concave function for each $y \in [0, y_1)$ and $c \in [0, q+1]$. By (17), it follows that $F_{1/y}(P_c)$ is contained in the hypograph of $h_{y,c}$, as desired. □

We can now finally prove Proposition 2.5, which we restate here for convenience.

Proposition 2.5 *Let $q \geq 3$ be an integer. Then there exists $d_1 > 0$ such that for all $d \geq d_1$ and $c \in [0, q+1]$, $F_d(P_c)$ is convex.*

Proof By the previous lemma we conclude that for d larger than $1/y_1$, $F_d(P_c)$ is contained in the hypograph of the function $h_{1/d,c}$, denoted by $\text{hypo}(h_{c,1/d})$ and moreover that this hypograph is convex, as the function $h_{1/d,c}$ is concave on a convex domain.

Since P_c is invariant under the S_q-action, it follows that

$$\exp(P_c) = \bigcap_{\pi \in S_q} \pi \cdot (\exp(H_{\geq -c}) \cap H_{\leq a})$$

and therefore by Lemma 2.4,

$$F_d(P_c) = \bigcap_{\pi \in S_q} \pi \cdot (F_d(P_c)) \subseteq \bigcap_{\pi \in S_q} \pi \cdot \text{hypo}(h_{1/d,c}). \tag{20}$$

We now claim that the final inclusion in (20) is in fact an equality. To see the other inclusion, take some $\mathbf{z} \in \cap_{\pi \in S_q} \pi \cdot \text{hypo}(h_{1/d,c})$. By symmetry, we may assume that $\mathbf{z}$ is contained in $\mathbb{R}^{q-1}_{\geq 0}$. Then $\mathbf{z}$ is equal to $F_d(\mathbf{x})$ for some $\mathbf{x} \in H_{\geq -c} \cap \mathbb{R}^{q-1}_{\leq 0}$, implying that $\mathbf{z}$ is indeed contained in $F_d(P_c)$.

This then implies that $F_d(P_c)$ is indeed convex being equal to the intersection of the convex sets $\pi \cdot \text{hypo}(h_{1/d,c})$. $\square$

4 Forward Invariance of P_c in two iterations

This section is dedicated to proving Proposition 2.6. We start with a version of the proposition for $d = \infty$ and after that consider finite d.

4.1 Two Iterations of F_∞

Let $\Phi : \mathbb{R}^{q-1} \to \mathbb{R}^{q-1}$ be defined by

$$\Phi(x_1, \ldots, x_{q-1}) = F_\infty^{\circ 2}(x_1, \ldots, x_{q-1})$$

and its 'restriction' to the half line $\mathbb{R}_{\leq/0} \cdot \mathbf{1}$, $\phi : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$, by

$$\phi(t) = -\langle \Phi(-t/(q-1) \cdot \mathbf{1}), \mathbf{1} \rangle,$$

where we use $\langle \cdot, \cdot \rangle$ to denote the standard inner product on $\mathbb{R}^{q-1}$.

This subsection is devoted to proving the following result.

Proposition 4.1 *For any* $c \geq 0$ *we have*

$$\Phi(P_c) \subseteq P_{\phi(c)} \subsetneq P_c.$$

By the definition of P_c in terms of D_c, (11), and the S_q-equivariance of the map F_∞ and hence of the map Φ, it suffices to prove this for P_c replaced by D_c. This can be derived from the following two statements:

(i) For any $c \geq 0$ the minimum of $\langle \Phi(\mathbf{x}), \mathbf{1} \rangle$ on $-c\Delta$ is attained at $-c/(q-1) \cdot \mathbf{1}$.
(ii) For any $c > 0$ we have $\phi(c) < c$.

Indeed, these statements imply that for any $c > 0$ we have that $\Phi(-c\Delta) \subseteq D_{\phi(c)} \subsetneq D_c$. Clearly this is sufficient, since $D_c = \cup_{0 \leq c' \leq c} - c'\Delta$ and therefore

$$\Phi(D_c) = \cup_{0 \leq c' \leq c} \Phi(-c'\Delta) \subseteq \cup_{0 \leq c' \leq c} D_{\phi(c')} \subseteq D_{\phi(c)} \subsetneq D_c.$$

We next prove both statements, starting with the first one.

4.1.1 Statement (i)

Proposition 4.2 *Let $c \geq 0$. Then for any $\mathbf{x} \in -c\Delta$ we have that*

$$\langle \Phi(\mathbf{x}), \mathbf{1} \rangle \geq \left\langle \Phi\left(\frac{-c}{q-1}\mathbf{1}\right), \mathbf{1} \right\rangle.$$

Moreover, equality happens only at $\mathbf{x} = \frac{-c}{q-1}\mathbf{1}$.

Before giving a proof, let us fix some further notation. By definition we have

$$\langle \Phi(\mathbf{x}), \mathbf{1} \rangle = \sum_{i=1}^{q-1} q \frac{1 - e^{F_{\infty;i}(\mathbf{x})}}{\sum_{j=1}^{q-1} e^{F_{\infty;j}(\mathbf{x})} + 1} = \frac{q^2}{\sum_{j=1}^{q-1} e^{F_{\infty;j}(\mathbf{x})} + 1} - q,$$

where we recall that $F_{\infty;j}$ denotes the jth coordinate function of F_∞. Thus the ith coordinate of the gradient of $\langle \Phi(\mathbf{x}), \mathbf{1} \rangle$ is given by

$$\begin{aligned} \psi_i(\mathbf{x}) &:= \frac{-q^2}{\left(\sum_{j=1}^{q-1} e^{F_{\infty;j}(\mathbf{x})} + 1\right)^2} \left(\sum_{j=1}^{q-1} e^{F_{\infty;j}(\mathbf{x})} \cdot \frac{\partial F_{\infty;j}}{\partial x_i}(\mathbf{x}) \right) \\ &= \frac{q^3 e^{x_i} \left(e^{F_{\infty;i}(\mathbf{x})}(1 + \sum_{j=1}^{q-1} e^{x_j}) + \sum_{j=1}^{q-1} e^{F_{\infty;j}(\mathbf{x})}(1 - e^{x_j}) \right)}{\left(\sum_{j=1}^{q-1} e^{F_{\infty;j}(\mathbf{x})} + 1\right)^2 \left(\sum_{j=1}^{q-1} e^{x_j} + 1\right)^2}. \end{aligned}$$

Let us define the following functions $v_i : \mathbb{R}^{q-1} \to \mathbb{R}$ for $i = 1, \ldots, q-1$ as

$$v_i(\mathbf{x}) := x_i \left(e^{G_i}(1 + \sum_{j=1}^{q-1} x_j) + \sum_{j=1}^{q-1} e^{G_j}(1 - x_j) \right),$$

where we write

$$G_i := G_{\infty;i}(\mathbf{x}) = \frac{q(1 - x_i)}{1 + x_1 + \cdots + x_{q-1}}.$$

Then we see that

$$\psi_i(\mathbf{x}) = \frac{q^3}{\left(\sum_{j=1}^{q-1} e^{F_{\infty;j}(\mathbf{x})} + 1\right)^2 \left(\sum_{j=1}^{q-1} e^{x_j} + 1\right)^2} \cdot v_i(e^{x_1}, \ldots, e^{x_{q-1}}),$$

and $\psi_1(\mathbf{x}) = \cdots = \psi_{q-1}(\mathbf{x})$ if and only if $v_1(\exp(\mathbf{x})) = \cdots = v_{q-1}(\exp(\mathbf{x}))$.

***Proof of Proposition* 4.2** First of all observe that the function $\langle \Phi(\mathbf{x}), \mathbf{1} \rangle$ is invariant under the permutation of the coordinates of $\mathbf{x}$. Thus we can assume that

$$\mathbf{x} \in U := \{\mathbf{y} \in \mathbb{R}^{q-1} \mid 0 \geq y_1 \cdots \geq y_{q-1}\}$$

and not all the coordinates of $\mathbf{x}$ are equal. Now it is enough to show that there exists a vector $\mathbf{0} \neq \mathbf{w} \in \mathbb{R}^{q-1}$ such that in the direction of $\mathbf{w}$ the function is (strictly) decreasing, $\langle \mathbf{w}, \mathbf{1} \rangle = 0$ and $\mathbf{x} + t_0\mathbf{w} \in U$ for some small $t_0 > 0$. Let

$$\ell = \min\{1 \leq i \leq q-2 \mid x_i > x_{i+1}\},$$

which is finite, since not all of the coordinates of $\mathbf{x}$ are equal. We claim that $\mathbf{w} = -\frac{\mathbf{e}_1+\cdots+\mathbf{e}_\ell}{\ell} + \mathbf{e}_{\ell+1}$ satisfies the desired conditions. Clearly, $\mathbf{w}$ is perpendicular to $\mathbf{1}$ and $\mathbf{x} + t\mathbf{w} \in U$ for t small enough. Now let us calculate the derivative of

$$g(t) := \langle \Phi(\mathbf{x} + t\mathbf{w}), \mathbf{1} \rangle.$$

Using the notation defined above, we obtain

$$\begin{aligned} g'(0) &= -\frac{\psi_1(\mathbf{x}) + \cdots + \psi_\ell(\mathbf{x})}{\ell} + \psi_{\ell+1}(\mathbf{x}) \\ &= -\psi_\ell(\mathbf{x}) + \psi_{\ell+1}(\mathbf{x}) \\ &= -C \cdot (v_\ell(\exp(\mathbf{x})) - v_{\ell+1}(\exp(\mathbf{x}))) \\ &= -C \cdot (v_\ell(\mathbf{y}) - v_{\ell+1}(\mathbf{y})), \end{aligned}$$

where $C > 0$ and $\mathbf{y} = \exp(\mathbf{x})$. In particular,

$$1 \geq y_1 = y_2 = \cdots = y_\ell > y_{\ell+1} \geq \cdots \geq y_{q-1} \geq 0.$$

So to conclude that $g'(0) < 0$ and finish the proof, we need to show that

$$v_\ell(\mathbf{y}) - v_{\ell+1}(\mathbf{y}) > 0. \tag{21}$$

Lemma 4.3 shows that we may assume $\mathbf{y}$ satisfies $1 \geq y_1 = y_2 = \ldots = y_\ell > y_{\ell+1} \geq y_{\ell+2} = \ldots = y_{q-1} \geq 0$. Lemma 4.4 below shows that for those vectors $\mathbf{y}$ (21) is indeed true. So by combining Lemma 4.3 and Lemma 4.4 below we obtain (21) and finish the proof. □

Lemma 4.3 *If* $1 \geq y_1 = y_2 \ldots = y_\ell > y_{\ell+1} \geq \ldots \geq y_{q-1} \geq 0$ *for some* $1 \leq \ell \leq q-2$, *then*

$$v_\ell(\mathbf{y}) - v_{\ell+1}(\mathbf{y}) \geq v_\ell(\mathbf{x}) - v_{\ell+1}(\mathbf{x}),$$

where $\mathbf{x} \in \mathbb{R}^{q-1}$ *is defined as*

$$x_j = \begin{cases} y_j & \text{if } j \leq \ell+1 \\ \frac{y_{\ell+2}+\cdots+y_{q-1}}{q-\ell-2} & \text{if } j > \ell+1 \end{cases}$$

for $1 \leq j \leq q-1$.

Proof By continuity, it suffices to show

$$v_\ell(\mathbf{y}) - v_{\ell+1}(\mathbf{y}) \geq v_\ell(\mathbf{x}) - v_{\ell+1}(\mathbf{x}), \tag{22}$$

where $\mathbf{x} \in \mathbb{R}^{q-1}$ is defined as

$$x_j = \begin{cases} y_j & \text{if } j \neq i, i+1 \\ \frac{y_i+y_{i+1}}{2} & \text{if } j = i \text{ or } j = i+1 \end{cases}$$

for $1 \leq j \leq q-1$ and any $i \geq \ell+2$.

For $t \in \mathbb{R}$ we define $\mathbf{y}(t)$ by

$$y_j(t) := \begin{cases} y_j & \text{if } j \neq i, i+1 \\ y_i - t & \text{if } j = i \\ y_{i+1} + t & \text{if } j = i+1 \end{cases}$$

for $j = 1, \ldots, q-1$. Note that $\mathbf{y}(0) = \mathbf{y}$ and $\mathbf{y}(y_i/2 - y_{i+1}/2) = \mathbf{x}$. We further define

$$\Delta(t) := v_\ell(\mathbf{y}(t)) - v_{\ell+1}(\mathbf{y}(t)).$$

After a straightforward calculation we can express $\Delta(t)$ as

$$\begin{aligned}\Delta(t) &= y_\ell e^{G_\ell}(1+\sum_{j\geq 1}^{q-1} y_j) - y_{\ell+1}e^{G_{\ell+1}}(1+\sum_{j\geq 1}^{q-1} y_j)\\ &+ y_\ell \sum_{j\neq i,i+1} e^{G_j}(1-y_j) - y_{\ell+1}\sum_{j\neq i,i+1} e^{G_j}(1-y_j)\\ &+ (y_\ell - y_{\ell+1})\left(e^{G_i(t)}(1-y_i+t) + e^{G_{i+1}(t)}(1-y_{i+1}-t)\right),\end{aligned}$$

where we write $G_\ell := G_{\infty;\ell}(\mathbf{y}(t)) = \frac{q(1-y_\ell)}{1+y_1+\cdots+y_{q-1}}$, for $\ell \notin \{i, i+1\}$ and we write $G_\ell(t) = G_{\infty;\ell}(\mathbf{y}(t))$ when $\ell \in \{i, i+1\}$. This notation indicates that G_ℓ is a constant function of t when $\ell \notin \{i, i+1\}$. Now observe that the function appearing in the last row,

$$g(t) := e^{G_i(t)}(1-y_i+t) + e^{G_{i+1}(t)}(1-y_{i+1}-t),$$

is convex on $t \in [0, y_i - y_{i+1}]$, since its second derivative is given by

$$\begin{aligned}g''(t) &= e^{G_i(t)}\frac{(1-y_i+t)q^2}{(1+y_1+\cdots+y_{q-1})^2} + 2e^{G_i(t)}\frac{q}{1+y_1+\cdots+y_{q-1}}\\ &+ e^{G_{i+1}(t)}\frac{(1-y_{i+1}-t)q^2}{(1+y_1+\cdots+y_{q-1})^2} + 2e^{G_{i+1}(t)}\frac{q}{1+y_1+\cdots+y_{q-1}} > 0.\end{aligned}$$

As $g(t) = g(y_i - y_{i+1} - t)$, we obtain that $g(t)$ has a unique minimizer in $[0, y_i - y_{i+1}]$ exactly at t such that $= y_i - y_{i+1} - t$. In other words,

$$t = \frac{y_i - x_{i+1}}{2}$$

is the unique minimizer of $g(t)$ on this interval and thus for $\Delta(t)$. This implies (22) and hence the lemma. □

Lemma 4.4 *Let* $1 \geq x_1 > x_2 \geq x_3 \geq 0$ *and* $q-2 \geq l \geq 1$. *Then*

$$v_l(\underbrace{x_1,\ldots,x_1}_{l}, x_2, \underbrace{x_3,\ldots,x_3}_{q-l-2}) > v_{l+1}(\underbrace{x_1,\ldots,x_1}_{l}, x_2, \underbrace{x_3,\ldots,x_3}_{q-l-2}).$$

Proof The algebraic manipulations that are done in this proof, while elementary, involve quite large expressions. Therefore we have supplied additional Mathematica code in Appendix A that can be used to verify the computations. We define

$$\begin{aligned}\Delta(y_1,y_2,y_3;t) :=& (y_1y_3(t-l-1) + (l+1)y_1 + (l+1)y_1y_2 - ly_2)\, e^{A_1(y_1,y_2,y_3;t)} +\\ & (-y_2y_3(t-l-1) - (l+1)y_1y_2 + y_1 - 2y_2)\, e^{A_2(y_1,y_2,y_3;t)} +\\ & (y_1-y_2)\,(1-y_3)\,(t-l-1)e^{A_3(y_1,y_2,y_3;t)},\end{aligned}$$

where

$$A_i(y_1,y_2,y_3;t) := \frac{(t+1)(1-y_i)}{1+ly_1+y_2+(t-(l+1))y_3}$$

for $i = 1, 2, 3$ (see Listing 1). One can check that

$$\Delta(x_1,x_2,x_3;q-1) = v_l(x_1,\ldots,x_1,x_2,x_3,\ldots,x_3) - v_{l+1}(x_1,\ldots,x_1,x_2,x_3,\ldots,x_3).$$

We will treat t as a variable and vary it while keeping the values that appear in the exponents constant. To that effect let $C_i = A_i(x_1, x_2, x_3; q-1)$ and define

$$y_1(t) = \frac{C_1(l-t-1) + C_3(t-l-1) + C_2 + t + 1}{C_3(t-l-1) + C_1 l + C_2 + t + 1},$$
$$y_2(t) = \frac{C_3(t-l-1) + C_1 l - C_2 t + t + 1}{C_3(t-l-1) + C_1 l + C_2 + t + 1},$$
$$y_3(t) = \frac{C_1 l - C_3(l+2) + C_2 + t + 1}{C_3(t-l-1) + C_1 l + C_2 + t + 1}.$$

These values are chosen such that for $t_0 = q-1$ we have $y_i(t_0) = x_i$ and $A_i(y_1(t), y_2(t), y_3(t); t) = C_i$ independently of t for $i = 1, 2, 3$ (see Listings 2 and 3). Therefore $\Delta(y_1(t), y_2(t), y_3(t); t)$ is a rational function of t and we want to show that it is positive at $t = q-1$. We can explicitly calculate that

$$\Delta(y_1(t), y_2(t), y_3(t); t) = \left(\frac{1+t}{C_3(t-l-1) + C_1 l + C_2 + t + 1}\right)^2 \cdot r(t),$$

where r is a linear function (see Listing 4). It is thus enough to show that $r(q-1) > 0$. We will do this by showing that $r(l+1) > 0$ and that the slope of r is positive. We find that $r(l+1)$ is equal to

$$r(l+1) = u_1 \cdot e^{C_1} + u_2 \cdot e^{C_2},$$

where

$$u_1 = 2 + l + C_2 - 2C_1 + lC_1C_2 - lC_1^2$$
$$u_2 = -\left(2 + l + lC_1 - (l+1)C_2 + C_1C_2 - C_2^2\right).$$

This is part of the output of Listing 5. Note that by construction, since $1 \geq x_1 > x_2 \geq x_3$, we have $0 \leq C_1 < C_2 \leq C_3$. Therefore the sum of the coefficients of e^{C_1} and e^{C_2} satisfies

$$\begin{aligned} u_1 + u_2 &= (l+2)(C_2 - C_1) + (l-1)C_1C_2 - lC_1^2 + C_2^2 \\ &= (l + 2 + C_2 + lC_1)(C_2 - C_1) > 0. \end{aligned}$$

Now we will separate two cases depending on the sign of the coefficient of u_2. If u_2 is non-negative, then

$$r(l+1) = u_1 e^{C_1} + u_2 e^{C_2} \geq u_1 e^{C_1} + u_2 e^{C_1} = (u_1 + u_2)e^{C_1} > 0.$$

If u_2 is negative, then

$$2 + (1 + C_1 - C_2)l > C_2 - C_1C_2 + C_2^2 = (1 + C_2 - C_1)C_2.$$

In particular $2 + (1 + C_1 - C_2)l > 0$. Thus

$$\begin{aligned} r(l+1) &= e^{C_2}(u_1 e^{C_1 - C_2} - u_2) \\ &\geq (1 + C_1 - C_2)u_1 - u_2 = C_1(C_2 - C_1)(2 + (1 + C_1 - C_2)l) > 0. \end{aligned}$$

The slope of r is given by

$$s := (1 + C_3 - C_1)\, e^{C_1} - (1 + C_3 - C_2)e^{C_2} + (C_2 - C_1)C_3 e^{C_3}.$$

This is part of the output of Listing 5. To show that this is positive we show that $s \cdot e^{-C_2}$ is positive. Because both $1 + C_3 - C_1$ and $C_2 - C_1$ are positive we find

$$s \cdot e^{-C_2} = (1 + C_3 - C_1)\, e^{C_1 - C_2} - (1 + C_3 - C_2) + (C_2 - C_1)C_3 e^{C_3 - C_2}$$

$$\begin{aligned}&\geq (1+C_3-C_1)\,(1+C_1-C_2)-(1+C_3-C_2)+(C_2-C_1)C_3(1+C_3-C_2)\\&=(C_2-C_1)(C_1+C_3(C_3-C_2)),\end{aligned}$$

which is positive because $0 \leq C_1 < C_2 \leq C_3$. This concludes the proof. □

We now continue with the second statement.

4.1.2 Statement (ii)

Proposition 4.5 *For any $x > 0$ we have that*

$$\left\langle \Phi\left(\frac{-x}{q-1}\mathbf{1}\right), \mathbf{1}\right\rangle > -x.$$

Proof The statement is equivalent to

$$\phi(x) < x.$$

for $x > 0$. By definition we know that

$$\phi(x) = (q-1)\frac{q(e^{f(x)}-1)}{(q-1)e^{f(x)}+1},$$

where

$$f(x) = -q\frac{e^{-x/(q-1)}-1}{(q-1)e^{-x/(q-1)}+1}.$$

First note that $\phi(\mathbb{R}_{>0}) \subseteq (0, q)$. This means that if $x \geq q$, the statement holds. Thus we can assume that $0 < x < q$. Now, the inequality $\phi(x) < x$ can be written as

$$e^{f(x)} < \frac{x+q(q-1)}{(q-1)(q-x)},$$

because $q - x > 0$. By taking logarithm of both sides, we see that $\phi(x) < x$ is equivalent to

$$-q\frac{e^{-x/(q-1)}-1}{(q-1)e^{-x/(q-1)}+1} < \log\left(\frac{x+q(q-1)}{(q-1)(q-x)}\right).$$

Since $\frac{x+q(q-1)}{(q-1)(q-x)} > \frac{0+q(q-1)}{(q-1)q} \geq 1$, we can use the inequality $\log(b) > 2\frac{b-1}{b+1}$ for $b = \frac{x+q(q-1)}{(q-1)(q-x)}$. Therefore, to show $\phi(x) < x$, it is sufficient to prove that

$$-q\frac{e^{-x/(q-1)}-1}{(q-1)e^{-x/(q-1)}+1} \leq \frac{-2qx}{(q-2)x-2q(q-1)},$$

or, equivalently

$$(2q-2-x) \leq (x+2q-2)e^{-x/(q-1)}.$$

This follows from the fact that $g(t) = (t+2q-2)e^{-t/(q-1)} - (2q-2-t)$ is a convex function on $\mathbb{R}_{\geq 0}$, its derivative satisfies $g'(0) = 0$ and $g(0) = 0$. This concludes the proof. □

4.2 Two Iterations of F_d

As before, we view $y = 1/d$ as a continuous variable. Let us define $\Phi : \mathbb{R}^{q-1} \times [0, \frac{1}{2}] \to \mathbb{R}^{q-1}$ by

$$\Phi(x_1, \dots, x_{q-1}, y) = F_{1/y}^{\circ 2}(x_1, \dots, x_{q-1}).$$

Note that this map is analytic in all its variables. For simplicity, if y^* is fixed, then we use the notation $\Phi_{y^*}(x_1, \dots, x_{q-1})$ for $\Phi(x_1, \dots, x_{q-1}, y)|_{y=y^*}$, and if $y = 0$, then $\Phi(x_1, \dots, x_{q-1}) := \Phi_0(x_1, \dots, x_{q-1})$.

Lemma 4.6 *There exist positive constants $A > 0$ and $c_0 > 0$, such that for any $0 < c \leq c_0$ we have*

$$c - \phi(c) \geq Ac^3.$$

Proof By definition we know that

$$\phi(x) = (g \circ f)(x) = (q-1)\frac{q(e^{f(x)} - 1)}{(q-1)e^{f(x)} + 1},$$

where

$$f(x) = -q\frac{e^{-x/(q-1)} - 1}{(q-1)e^{-x/(q-1)} + 1},$$
$$g(x) = (q-1)q\frac{e^x - 1}{(q-1)e^x + 1}.$$

Let us calculate the Taylor expansion of $f(x)$ and $g(x)$ around 0:

$$f(x) = \frac{1}{q-1}x + \frac{q-2}{2(q-1)^2 q}x^2 + \frac{(q^2 - 6q + 6)}{6(q-1)^3 q^2}x^3 + O(x^4),$$
$$g(x) = (q-1)x - \frac{(q-1)(q-2)}{2q}x^2 + \frac{(q-1)(q^2 - 6q + 6)}{6q^2}x^3 + O(x^4).$$

Thus their composition has the following Taylor expansion around 0:

$$(g \circ f)(x) = x - \frac{1}{6(q-1)^2}x^3 + O(x^4).$$

This implies that there exists $c_0 > 0$ and $A > 0$, such that for any $c_0 \geq x \geq 0$ we have

$$x - \phi(x) \geq Ax^3,$$

as desired. □

The next proposition implies forward invariance of P_c under $F_d^{\circ 2}$ for c small enough and d large enough.

Proposition 4.7 *There exists $c_0 > 0$ and $d_0 > 0$. Such that for all $c \in (0, c_0]$ and integers $d \geq d_0$ there exists $0 < c' < c$ such that*

$$F_d^{\circ 2}(D_c) \subset D_{c'}.$$

Proof By the previous lemma we know that there is a $c_0' > 0$ and an $A > 0$, such that for any $c \leq c_0'$ we have

$$\|\Phi(-c/(q-1)\cdot\mathbf{1}) + c/(q-1)\cdot\mathbf{1}\| \geq Ac^3.$$

Here we denote by $\|\mathbf{x}\| = \left(\sum_{i=1}^{q-1} x_i^2\right)^{1/2}$, the standard 2-norm on $\mathbb{R}^{q-1}$. By Proposition 4.2, we have that for any $\mathbf{x} \in D_c$, $\Phi(\mathbf{x})$ is contained in $D_{\phi(c)}$. Therefore, denoting by $B_r(y)$ the ball of radius r around y,

$$B_{Ac^3/2}(\Phi(\mathbf{x})) \cap (-\infty, 0]^{q-1} \subseteq D_{\phi(c)+Ac^3/2} \subsetneq D_c. \tag{23}$$

Now let us consider the Taylor approximation of $\Phi_y(x_1, \ldots, x_{q-1})$ at $\mathbf{0} = (0, \ldots, 0)$. Since for any $y^* \in [0, 1]$ the map $F_{1/y^*}(x_1, \ldots, x_{q-1})$ has $\mathbf{0}$ as a fixed point of derivative $-\mathrm{Id}$, there exists constants $c_1, C_1 \geq 0$ such that for any $y \in [0, 1]$ and $\mathbf{x} = (x_1, \ldots, x_{q-1}) \in [-c_1, 0]^{q-1}$ we have

$$\|\Phi_y(\mathbf{x}) - \mathrm{Id}(\mathbf{x}) - T_{3,y}(\mathbf{x})\| \leq C_1 \cdot \|\mathbf{x}\|^4,$$

where $\mathrm{Id}(\mathbf{x}) + T_{3,y}(\mathbf{x})$ is the 3rd order Taylor approximation of $\Phi_y(\mathbf{x})$ at $\mathbf{0}$. Note that the second order term is equal to 0 because the derivative of $F_{1/y^*}(x_1, \ldots, x_{q-1})$ at $\mathbf{0}$ equals $-\mathrm{Id}$. In particular, $T_{3,y}(\mathbf{x}) = T_y((\mathbf{x}), (\mathbf{x}), (\mathbf{x}))$ for some multi-linear map $T_y \in \mathrm{Mult}((\mathbb{R}^{q-1})^3, \mathbb{R}^{q-1})$, and as $y \to 0$ the map $T_{3,y}$ converges uniformly on $[-q, 0]^{q-1}$ to $T_{3,0}$. Specifically, for any $\mathbf{x} = (x_1, \ldots, x_{q-1}) \in [-c_1, 0]^{q-1}$

$$\|T_{3,y}(\mathbf{x}) - T_{3,0}(\mathbf{x})\| \leq A_3(y)\|\mathbf{x}\|^3$$

for some function A_3 that satisfies $\lim_{y\to 0} A_3(y) = 0$.

Putting this together and making use of the triangle inequality, we obtain that for any $0 < c \leq \min\{c_1, c_0'\}$ and any $\mathbf{x} = (x_1, \ldots, x_{q-1}) \in D_c$

$$\begin{aligned}
\|\Phi_y(\mathbf{x}) - \Phi(\mathbf{x})\| &\leq \|\Phi_y(\mathbf{x}) - \mathrm{Id}(\mathbf{x}) - T_{3,y}(\mathbf{x})\| \\
&\quad + \|\mathrm{Id}(\mathbf{x}) + T_{3,y}(\mathbf{x}) - \mathrm{Id}(\mathbf{x}) - T_{3,0}(\mathbf{x})\| \\
&\quad + \|\mathrm{Id}(\mathbf{x}) + T_{3,0}(\mathbf{x}) - \Phi(\mathbf{x})\| \\
&\leq 2C_1\|x\|^4 + A_3(y))\|x\|^3 \leq K(2C_1 c + A_3(y))c^3,
\end{aligned}$$

for some constant $K > 0$ (using that the 2-norm and the 1-norm are equivalent on $\mathbb{R}^{q-1}$.) Now let us fix $0 < c_0 \leq \min\{c_1, c_0'\}$ small enough such that $K2C_1c_0 < A/4$ and fix a $y_0 > 0$ such that for any any $0 \leq y \leq y_0$ we have $KA_3(y) \leq A/4$.

Then by (23), for any $0 \leq y \leq y_0$, $0 \leq c \leq c_0$ and $\mathbf{x} = (x_1, \ldots, x_{q-1}) \in D_c$,

$$\Phi_y(D_c) \subseteq B_{Ac^3/2}(\Phi(D_c)) \cap (-\infty, 0]^{q-1} \subseteq D_{\phi(c)+Ac^3/2} \subsetneq D_c.$$

So we can take $c' = \phi(c) + Ac^3/2$. □

4.3 Proof of Proposition 2.6

We are now ready to prove Proposition 2.6, which we restate here for convenience.

Proposition 2.6 *Let $q \geq 3$ be an integer. There exists $d_2 > 0$ such that for all integers $d \geq d_2$ the following holds: for any $c \in (0, q+1]$ there exists $0 < c' < c$ such that*

$$F_d^{\circ 2}(P_c) \subset P_{c'}.$$

Proof We know by Proposition 4.7 there is a $d_0 > 0$ and a $c_0 > 0$ such that for $d \geq d_0$ and $c \in (0, c_0)$ there exist $c' < c$ such that $F_d^{\circ 2}(D_c) \subset D_{c'}$. As $P_c = \cup_{\pi \in S_q} \pi \cdot D_c$, we see by Lemma 2.4 that for $d \geq d_0$ and $c \in (0, c_0)$ we have $F_d^{\circ 2}(P_c) \subset P_{c'}$.

Next we consider $c \in [c_0, q+1]$. By Proposition 4.1 we know $F_\infty^{\circ 2}(P_c) \subset P_{\phi(c)}$ and $\phi(c) < c$ for any $c > 0$. As F_d converges to F_∞ uniformly, we see for each $c \in [c_0, q+1]$ there is a $d_c > 0$ large enough such that for $d \geq d_c$ and $c' = c/2 + \phi(c)/2$ we have $F_d^{\circ 2}(P_{\hat{c}}) \subsetneq P_{c'}$ for all $\hat{c}$ sufficiently close to c. By compactness of $[c_0, q+1]$, we obtain that there is a $d_{\max} > 0$ such that for any $d > d_{\max}$ and any $c \in [c_0, q+1]$ there exists $c' < c$ such that $F_d^{\circ 2}(P_c) \subsetneq P_{c'}$. The proposition now follows by taking $d_2 = \max(d_0, d_{\max})$. □

5 Concluding Remarks

Although we have only proved uniqueness of the Gibbs measure on the infinite regular tree for a sufficiently large degree d, our method could conceivably be extended to smaller values of d. With the aid of a computer we managed to check that for $q = 3$ and $q = 4$ and all $d \geq 2$ the map $F_d^{\circ 2}$ maps P_c into $P_{\phi_d(-c)}$, where ϕ_d is the restriction of $-F_d^{\circ 2}$ to the line $\mathbb{R} \cdot \mathbf{1}$. It seems reasonable to expect that for other small values of q a similar statement could be proved. A general approach is elusive so far. It is moreover also not clear that $F_d(P_c)$ is convex, not even for $q = 3$. In fact, for $q = 3$ and c large enough $F_3(P_c)$ is **not** convex. But for reasonable values of c it does appear to be convex. For larger values of q this is even less clear.

Knowing that there is a unique Gibbs measure on the infinite regular tree is by itself not sufficient to design efficient algorithms to approximately compute the partition function/sample from the associated distribution on all bounded degree graphs. One needs a stronger notion of decay of correlations, often called *strong spatial mixing* [19, 20, 29, 39] or absence of complex zeros for the partition function near the real interval $[w, 1]$ [1, 6, 28, 33]. It is not clear whether our current approach is capable of proving such statements (these certainly do not follow automatically), but we hope that it may serve as a building block in determining the threshold(s) for strong spatial mixing and absence of complex zeros. We note that even for the case $w = 0$, corresponding to proper colorings, the best known bounds for strong spatial mixing on the infinite tree [15] are still far from the uniqueness threshold. Very recently (after the current article was posted to the arXiv) these bounds have been significantly improved [12].

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A Supplementary Mathematica Code to Lemma 4.4

The functions A_i for $i = 1, 2, 3$ and Δ are defined as follows.

Listing 1 The functions A_i and Δ

```
A1[y1_, y2_, y3_, m_]:= (m+1) (1 −y1)/(1 + l y1 + y2 + (m − (l + 1)) y3)
A2[y1_, y2_, y3_, m_]:= (m+1) (1 −y2)/(1 + l y1 + y2 + (m − (l + 1)) y3)
A3[y1_, y2_, y3_, m_]:= (m+1) (1 −y3)/(1 + l y1 + y2 + (m − (l + 1)) y3)

Delta[y1_, y2_, y3_, m_]:= (y1 y3 (m − l − 1) + (l + 1) y1 + (l + 1) y1 y2 − l y2) Exp[A1[y1,
    y2, y3, m]]
+ (−y2 y3 (m − l − 1) − (l + 1) y1 y2 + y1 − 2 y2) Exp[A2[y1, y2, y3, m]]
+ (y1 − y2) (1 − y3) (m − l − 1) Exp[A3[y1, y2, y3, m]]
```

The functions $y_i(t)$ are defined as follows.

Listing 2 The functions y_i

```
{y1[t_], y2[t_], y3[t_]} = {y1, y2, y3} /. Solve[A1[y1, y2, y3, t] == C1 && A2[y1, y2, y3, t]
    == C2 && A3[y1, y2, y3, t] == C3, {y1, y2, y3 }][[1]]
```

Listing 3 Verification that $y_i(q-1) = x_i$. This expression yields $\{x_1, x_2, x_3\}$

```
Simplify[{y1[q − 1], y2[q − 1], y3[q − 1]} /. {Rule[C1, A1[x1, x2, x3, q − 1]], Rule[C2, A2[x1,
    x2, x3, q − 1]], Rule[C3, A3[x1, x2, x3, q − 1]]}]
```

The function $r(t)$ can subsequently be found with the following code.

Listing 4 The function r

```
r[t_] = Simplify[Delta[y1[t], y2[t], y3[t], t] ((1 + t)/(1 + C2 − C3 + C1 l − C3 l + t + C3 t))
    ^(−2)]
```

It can be observed that r is indeed linear in t. To calculate $r(l+1)$ and the slope of r we use the following piece of code.

Listing 5 The values of $r(l+1)$ and the slope of r

```
Simplify[{r[l + 1], Coefficient[r[t], t]}]
```

References

1. Barvinok, A.: Combinatorics and complexity of partition functions. Algorithms and combinatorics, vol. 30. Springer, Cham (2016)
2. Baxter, R.J.: Critical antiferromagnetic square-lattice Potts model. Proc. Roy. Soc. London Ser. A **383**(1784), 43–54 (1982)
3. Baxter, R.J.: q colourings of the triangular lattice. J. Phys. A **19**(14), 2821–2839 (1986)
4. Bencs, F., Buys, P., Peters, H.: The limit of the zero locus of the independence polynomial for bounded degree graphs. arXiv preprint arXiv:2111.06451, (2021)
5. Borgs, C., Chayes, J., Kahn, J., Lovász, L.: Left and right convergence of graphs with bounded degree. Random Struct. Algorithm. **42**(1), 1–28 (2013)
6. Bencs, F., Davies, E., Patel, V., Regts, G.: On zero-free regions for the anti-ferromagnetic Potts model on bounded-degree graphs. Ann. Inst. Henri Poincaré D **8**(3), 459–489 (2021)
7. Blanca, A., Galanis, A., Goldberg, L.A., Štefankovič, D., Vigoda, E., Yang, K.: Sampling in uniqueness from the Potts and random-cluster models on random regular graphs. SIAM J. Discret. Math. **34**(1), 742–793 (2020)
8. Bogachev, L.V., Rozikov, U.A.: On the uniqueness of Gibbs measure in the Potts model on a Cayley tree with external field. J. Stat. Mech. Theory Exp. **7**, 073205 (2019)
9. Boyd, S., Vandenberghe, L.: Convex optimization. Cambridge University Press, Cambridge (2004)
10. Brightwell, G.R., Winkler, P.: Graph homomorphisms and phase transitions. J. Comb. Theory Ser. B **77**(2), 221–262 (1999)

11. Brightwell, G.R., Winkler, P.: Random colorings of a Cayley tree. In: Bollobas, B. (ed.) Contemporary Combinatorics, vol. 10, pp. 247–276. Springer, Berlin (2002)
12. Chen, Z., Liu, K., Mani, N., Moitra, A.: Strong spatial mixing for colorings on trees and its algorithmic applications. arXiv preprint arXiv:2304.01954, (2023)
13. de Boer, D., Buys, P., Regts, G.: Uniqueness of the Gibbs measure for the 4-state anti-ferromagnetic Potts model on the regular tree. Combinatorics Prob. Comput. **32**(1), 158–182 (2023)
14. Efthymiou, C.: On sampling symmetric Gibbs distributions on sparse random graphs and hypergraphs. In *49th EATCS International Conference on Automata, Languages, and Programming*, volume 229 of *LIPIcs. Leibniz Int. Proc. Inform.*, pages Art. No. 57, 16. Schloss Dagstuhl. Leibniz-Zent. Inform., Wadern, (2022)
15. Efthymiou, C., Galanis, A., Hayes, T. P., Štefankovič, D., Vigoda, E.: Improved strong spatial mixing for colorings on trees. In *Approximation, randomization, and combinatorial optimization. Algorithms and techniques*, volume 145 of *LIPIcs. Leibniz Int. Proc. Inform.*, pages Art. No. 48, 16. Schloss Dagstuhl. Leibniz-Zent. Inform., Wadern, (2019)
16. Friedli, S., Velenik, Y.: Statistical mechanics of lattice systems: a concrete mathematical introduction. Cambridge University Press, Cambridge (2017)
17. Georgii, H.-O.: Gibbs measures and phase transitions. De Gruyter Studies in Mathematics, vol. 9. Walter de Gruyter & Co., Berlin (1988)
18. Galanis, A., Goldberg, L.A., Yang, K.: Uniqueness for the 3-state antiferromagnetic Potts model on the tree. Electron. J. Probab. **23**, 43 (2018)
19. Gamarnik, D., Katz, D.: Correlation decay and deterministic FPTAS for counting colorings of a graph. J. Discrete Algorithms **12**, 29–47 (2012)
20. Gamarnik, D., Katz, D., Misra, S.: Strong spatial mixing of list coloring of graphs. Random Struct. Algorithms **46**(4), 599–613 (2015)
21. Gandolfo, D., Rahmatullaev, M.M., Rozikov, U.A.: Boundary conditions for translation-invariant Gibbs measures of the Potts model on Cayley trees. J. Stat. Phys. **167**(5), 1164–1179 (2017)
22. Galanis, A., Štefankovič, D., Vigoda, E.: Inapproximability for antiferromagnetic spin systems in the tree nonuniqueness region. J. ACM (JACM) **62**(6), 1–60 (2015)
23. Galanis, A., Štefankovič, D., Vigoda, E.: Inapproximability of the partition function for the anti-ferromagnetic Ising and hard-core models. Combinatorics Probability Computing **25**(4), 500–559 (2016)
24. Jonasson, J.: Uniqueness of uniform random colorings of regular trees. Stat. Probab. Lett. **57**(3), 243–248 (2002)
25. Külske, C., Rozikov, U.A.: Fuzzy transformations and extremality of Gibbs measures for the Potts model on a Cayley tree. Random Struct. Algorithms **50**(4), 636–678 (2017)
26. Külske, C., Rozikov, U.A., Khakimov, R.M.: Description of the translation-invariant splitting Gibbs measures for the Potts model on a Cayley tree. J. Stat. Phys. **156**(1), 189–200 (2014)
27. Li, L., Lu, P., Yin, Y.: Correlation decay up to uniqueness in spin systems. In *Proceedings of the twenty-fourth annual ACM-SIAM symposium on Discrete algorithms*, pages 67–84. SIAM, (2013)
28. Liu, J., Sinclair, A., Srivastava, P.: Correlation decay and partition function zeros: algorithms and phase transitions. SIAM J. Comput. (2019). https://doi.org/10.1137/20M1317384
29. Lu, P., Yin, Y.: Improved FPTAS for multi-spin systems. In *Approximation, Randomization, and Combinatorial Optimization. Algorithms and Techniques*, pp. 639–654. Springer, (2013)
30. Peruggi, F., di Liberto, F., Monroy, G.: The Potts model on Bethe lattices. I. Gen. Res. J. Phys. A **16**(4), 811–827 (1983)
31. Peruggi, F., di Liberto, F., Monroy, G.: Phase diagrams of the q-state Potts model on Bethe lattices. Physica A **141**(1), 151–186 (1987)
32. Potts, R.B.: Some generalized order-disorder transformations. Proc. Cambridge Philos. Soc. **48**, 106–109 (1952)
33. Patel, V., Regts, G.: Deterministic polynomial-time approximation algorithms for partition functions and graph polynomials. SIAM J. Comput. **46**(6), 1893–1919 (2017)
34. Rozikov, U.A.: Gibbs measures of Potts model on Cayley trees: a survey and applications. Rev. Math. Phys. **33**(10), 2130007 (2021)
35. Sokal, A.D.: The multivariate Tutte polynomial (alias Potts model) for graphs and matroids. In: Surveys in combinatorics 2005, Volume 327 of London Math. Soc. Lecture Note Ser., pp. 173–226. Cambridge Univ. Press, Cambridge (2005)
36. Salas, J., Sokal, A.D.: Absence of phase transition for antiferromagnetic Potts models via the Dobrushin uniqueness theorem. J. Stat. Phys. **86**(3–4), 551–579 (1997)
37. Sly, A., Sun, N.: Counting in two-spin models on d-regular graphs. Ann. Probab. **42**(6), 2383–2416 (2014)

38. Sinclair, A., Srivastava, P., Thurley, M.: Approximation algorithms for two-state anti-ferromagnetic spin systems on bounded degree graphs. J. Stat. Phys. **155**(4), 666–686 (2014)
39. Weitz, D.: Counting independent sets up to the tree threshold. In: Proceedings of the thirty-eighth annual ACM symposium on Theory of Computing, pp. 140–149 (2006)