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ON THE UNIQUENESS OF GIBBS MEASURE IN THE POTTS MODEL ON A CAYLEY TREE WITH EXTERNAL FIELD

LEONID V. BOGACHEV AND UTKIR A. ROZIKOV

To the memory of H.-O. Georgii

ABSTRACT. The paper concerns the q -state Potts model (i.e., with spin values in $\{1, \dots, q\}$) on a Cayley tree \mathbb{T}^k of degree $k \geq 2$ (i.e., with $k + 1$ edges emanating from each vertex) in an external (possibly random) field. We construct the so-called *splitting Gibbs measures* (SGM) using generalized boundary conditions on a sequence of expanding balls, subject to a suitable compatibility criterion. Hence, the problem of existence/uniqueness of SGM is reduced to solvability of the corresponding functional equation on the tree. In particular, we introduce the notion of translation-invariant SGMs and prove a novel criterion of translation invariance. Assuming a ferromagnetic nearest-neighbour spin-spin interaction, we obtain various sufficient conditions for uniqueness. For a model with constant external field, we provide in-depth analysis of uniqueness vs. non-uniqueness in the subclass of completely homogeneous SGMs by identifying the phase diagrams on the “temperature–field” plane for different values of the parameters q and k . In a few particular cases (e.g., $q = 2$ or $k = 2$), the maximal number of completely homogeneous SGMs in this model is shown to be $2^q - 1$, and we make a conjecture (supported by computer calculations) that this bound is valid for all $q \geq 2$ and $k \geq 2$.

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1. INTRODUCTION

1.1. Background and motivation. The *Potts model* was introduced by R. B. Potts [43] as a lattice system with $q \geq 2$ spin states and nearest-neighbour interaction, aiming to generalize the Kramers–Wannier duality [28] of the Ising model ($q = 2$). Since then, it has become the darling of statistical mechanics, both for physicists and mathematicians [4, 64], as one of few “exactly soluble” (or at least tractable) models demonstrating a phase transition [11, 15, 16, 27, 31, 35]. Due to its intuitive appeal to describe *multistate* systems, combined with a rich structure of inner symmetries, the Potts model has been quickly picked up by a host of research in diverse areas, such as probability [25], algebra [33], graph theory [5], conformally invariant scaling limits [46, 54], computer science [18], statistics [23, 39], biology [24], medicine [58, 59], sociology [53, 55], financial engineering [45, 60], computational algorithms [10, 17], technological processes [52, 62], and many more.

Much of this modelling has involved interacting spin system on *graphs*. In this context, tree-like graphs are especially attractive for the analysis due to their recursive structure and the lack of circuits. In particular, regular trees (known as *Cayley trees* or *Bethe lattices* [6]) have become a standard trial template for various models of statistical physics (see, e.g., [1, 2, 3, 34, 37, 61, 63]), which are interesting in their own right but also provide useful insights into (harder) models in more realistic spaces

(such as lattices \mathbb{Z}^d) as their “infinite-dimensional” approximation [4, Chapter 4]. On the other hand, the use of Cayley trees is often motivated by the applications, such as information flows [38] and reconstruction algorithms on networks [15, 36], DNA strands and Holliday junctions [48], evolution of genetic data and phylogenetics [14], bacterial growth and fire forest models [12], or computational complexity on graphs [18]. Crucially, the criticality in such models is governed by phase transitions in the underlying spin systems.

It should be stressed, however, that the Cayley tree is distinctly different from finite-dimensional lattices, in that the ratio of the number of boundary vertices to the number of interior vertices in a large finite subset of the tree does not vanish in the thermodynamic limit.¹ For example, if $k \geq 2$ is the degree of the tree (i.e., each vertex has $k + 1$ neighbours), V_n is a “ball” of radius n (centred at some point x_o) and $\partial V_n = V_{n+1} \setminus V_n$ is the boundary “sphere”, then

$$\frac{|\partial V_n|}{|V_n|} = \frac{(k+1)k^n}{1 + (k+1)(k^n - 1)/(k-1)} \rightarrow k - 1 \geq 1, \quad n \rightarrow \infty.$$

Therefore, the remote boundary may be expected to have a very strong influence on spins located deep inside the graph, which in turn pinpoints a rich and complex picture of phase transitions, including the number of possible pure phases of the system as a function of temperature.

Mathematical foundations of random fields on Cayley trees were laid by Preston [44] and Spitzer [57], followed by an extensive analysis of Gibbs measures and phase transitions (see Georgii [22, Chapter 12] and Rozikov [47], including historical remarks and further bibliography). The Ising model on a Cayley tree has been studied in most detail (see [47, Chapter 2] for a review). In particular, Bleher et al. [8] described the phase diagram of a ferromagnetic Ising model in the presence of an external random field.² Using physical argumentation, Peruggi et al. [41, 42] considered the Potts model on a Cayley tree (both ferromagnetic and antiferromagnetic) with a (constant) external field, and discussed the “order/disorder” transitions (cf. [15, 18]).

In the present paper, we consider a similar (ferromagnetic) model but we are primarily concerned with more general “uniqueness/non-uniqueness” transitions. We choose to work with the so-called *splitting Gibbs measures* (SGM), which are conveniently defined in the thermodynamic limit using generalized boundary conditions (GBC). To be consistent, permissible GBC fields must satisfy a certain functional equation, which can then be used as a tool to identify the number of solutions. In this approach, it is crucial that any extremal Gibbs measure is SGM, and so the problem of uniqueness is reduced to that in the SGM class.

Külske et al. [30] described the full set of completely homogeneous SGMs for the q -state Potts model on a Cayley tree with zero external field; in particular, it was shown that, at sufficiently low temperatures, their number is $2^q - 1$. Recently, Külske and Rozikov [29] found some regions for the temperature parameter ensuring that a given completely homogeneous SGM is extreme/non-extreme; in particular, there exists a temperature interval in which there are at least $2^{q-1} + q$ extreme SGMs. In contrast, in the antiferromagnetic Potts model on a tree, a completely homogeneous SGM is unique at all temperatures and for any field (see [47, Section 5.2.1]).

¹This is the common feature of *nonamenable graphs* (see [7]).

²Note that perturbation caused by the field breaks all symmetries of the model, which renders standard arguments inapplicable (cf. [9, Chapter 6]).

1.2. Set-up. We start by summarizing the basic concepts for Gibbs measures on a Cayley tree, and also fix some notation.

1.2.1. Cayley tree. Let \mathbb{T}^k be a (homogeneous) Cayley tree of degree $k \geq 2$, that is, an infinite connected cycle-free (undirected) regular graph with each vertex incident to $k + 1$ edges.³ For example, $\mathbb{T}^1 = \mathbb{Z}$. Denote by $V = \{x\}$ the set of the vertices of the tree and by $E = \{\langle x, y \rangle\}$ the set of its (non-oriented) edges connecting pairs of neighbouring vertices. The natural distance $d(x, y)$ on \mathbb{T}^k is defined as the number of edges on the unique path connecting vertices $x, y \in V$. In particular, $\langle x, y \rangle \in E$ whenever $d(x, y) = 1$. A (non-empty) set $\Lambda \subset V$ is called *connected* if for any $x, y \in \Lambda$ the path connecting x and y lies in Λ . We denote the complement of Λ by $\Lambda^c := V \setminus \Lambda$ and its *boundary* by $\partial\Lambda := \{x \in \Lambda^c : \exists y \in \Lambda, d(x, y) = 1\}$, and we write $\bar{\Lambda} = \Lambda \cup \partial\Lambda$. The subset of edges in Λ is denoted $E_\Lambda := \{\langle x, y \rangle \in E : x, y \in \Lambda\}$.

Fix a vertex $x_\circ \in V$, interpreted as the *root* of the tree. We say that $y \in V$ is a *direct successor* of $x \in V$ if x is the penultimate vertex on the unique path leading from the root x_\circ to the vertex y ; that is, $d(x_\circ, y) = d(x_\circ, x) + 1$ and $d(x, y) = 1$. The set of all direct successors of $x \in V$ is denoted $S(x)$. It is convenient to work with the family of the radial subsets centred at x_\circ , defined for $n \in \mathbb{N}_0 := \{0\} \cup \mathbb{N}$ by

$$V_n := \{x \in V : d(x_\circ, x) \leq n\}, \quad W_n := \{x \in V : d(x_\circ, x) = n\},$$

interpreted as the “ball” and “sphere”, respectively, of radius n centred at the root x_\circ . Clearly, $\partial V_n = W_{n+1}$. Note that if $x \in W_n$ then $S(x) = \{y \in W_{n+1} : d(x, y) = 1\}$. In the special case $x = x_\circ$ we have $S(x_\circ) = W_1$. For short, we set $E_n := E_{V_n}$.

Remark 1.1. Note that the sequence of balls (V_n) ($n \in \mathbb{N}_0$) is *cofinal* (see [22, Section 1.2, page 17]), that is, any finite subset $\Lambda \subset V$ is contained in some V_n .

1.2.2. The Potts model and Gibbs measures. In the q -state Potts model, the spin at each vertex $x \in V$ can take values in the set $\Phi := \{1, \dots, q\}$. Thus, the spin configuration on V is a function $\sigma : V \rightarrow \Phi$ and the set of all configurations is Φ^V . For a subset $\Lambda \subset V$, we denote by $\sigma_\Lambda : \Lambda \rightarrow \Phi$ the restriction of configuration σ to Λ ,

$$\sigma_\Lambda(x) := \sigma(x), \quad x \in \Lambda.$$

The Potts model with a *nearest-neighbour interaction kernel* $\{J_{xy}\}_{x, y \in V}$ (i.e., such that $J_{xy} = J_{yx}$ and $J_{xy} = 0$ if $d(x, y) \neq 1$) is defined by the formal Hamiltonian

$$H(\sigma) = - \sum_{\langle x, y \rangle \in E} J_{xy} \delta_{\sigma(x), \sigma(y)} - \sum_{x \in V} \xi_{\sigma(x)}(x), \quad \sigma \in \Phi^V, \quad (1.1)$$

where δ_{ij} is the Kronecker delta symbol (i.e., $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ otherwise), and $\boldsymbol{\xi}(x) = (\xi_1(x), \dots, \xi_q(x)) \in \mathbb{R}^q$ is the external (possibly random) field. According to (1.1), the spin-spin interaction is activated only when the neighbouring spins are equal, whereas the additive contribution of the external field is provided, at each vertex $x \in V$, by the component of the vector $\boldsymbol{\xi}(x)$ corresponding to the spin value $\sigma(x)$.

For each finite subset $\Lambda \subset V$ ($\Lambda \neq \emptyset$) and any fixed subconfiguration $\eta \in \Phi^{\Lambda^c}$ (called the *configurational boundary condition*), the *Gibbs distribution* γ_Λ^η is a probability measure in Φ^Λ defined by the formula

$$\gamma_\Lambda^\eta(\varsigma) = \frac{1}{Z_\Lambda^\eta(\beta)} \exp \left\{ -\beta H_\Lambda(\varsigma) + \beta \sum_{x \in \Lambda} \sum_{y \in \Lambda^c} J_{xy} \delta_{\varsigma(x), \eta(y)} \right\}, \quad \varsigma \in \Phi^\Lambda, \quad (1.2)$$

³In the physics literature, an infinite Cayley tree is often referred to as the *Bethe lattice*, whereas the term “Cayley tree” is reserved for rooted trees truncated at a finite height [13, 40].

where $\beta \in (0, \infty)$ is a parameter (having the meaning of *inverse temperature*), H_Λ is the restriction of the Hamiltonian (1.1) to subconfigurations in Λ ,

$$H_\Lambda(\varsigma) = - \sum_{\langle x, y \rangle \in E_\Lambda} J_{xy} \delta_{\varsigma(x), \varsigma(y)} - \sum_{x \in \Lambda} \xi_{\varsigma(x)}(x), \quad \varsigma \in \Phi^\Lambda, \quad (1.3)$$

and $Z_\Lambda^\eta(\beta)$ is the normalizing constant (often called the *canonical partition function*),

$$Z_\Lambda^\eta(\beta) = \sum_{\varsigma \in \Phi^\Lambda} \exp \left\{ -\beta H_\Lambda(\varsigma) + \beta \sum_{x \in \Lambda} \sum_{y \in \Lambda^c} J_{xy} \delta_{\varsigma(x), \eta(y)} \right\}.$$

Due to the nearest-neighbour interaction, formula (1.2) can be rewritten as⁴

$$\gamma_\Lambda^\eta(\varsigma) = \frac{1}{Z_\Lambda^\eta(\beta)} \exp \left\{ -\beta H_\Lambda(\varsigma) + \beta \sum_{x \in \Lambda} \sum_{y \in \partial \Lambda} J_{xy} \delta_{\varsigma(x), \eta(y)} \right\}, \quad \varsigma \in \Phi^\Lambda. \quad (1.4)$$

Finally, a measure $\mu = \mu_{\beta, \xi}$ on Φ^V is called a *Gibbs measure* if, for any non-empty finite set $\Lambda \subset V$ and any $\eta \in \Phi^{\Lambda^c}$,

$$\mu(\sigma_\Lambda = \varsigma \mid \sigma_{\Lambda^c} = \eta) \equiv \gamma_\Lambda^\eta(\varsigma), \quad \varsigma \in \Phi^\Lambda. \quad (1.5)$$

1.2.3. SGM construction. It is convenient to construct Gibbs measures on the Cayley tree \mathbb{T}^k using a version of Gibbs distributions on the balls (V_n) defined via auxiliary fields encapsulating the interaction with the exterior of the balls. More precisely, for a vector field $V \ni x \mapsto \mathbf{h}(x) = (h_1(x), \dots, h_q(x)) \in \mathbb{R}^q$ and each $n \in \mathbb{N}_0$, define a probability measure in V_n by the formula

$$\mu_n^h(\sigma_n) = \frac{1}{Z_n} \exp \left\{ -\beta H_n(\sigma_n) + \beta \sum_{x \in W_n} h_{\sigma_n(x)}(x) \right\}, \quad \sigma_n \in \Phi^{V_n}, \quad (1.6)$$

where $Z_n = Z_n(\beta, \mathbf{h})$ is the normalizing factor and $H_n := H_{V_n}$, that is (see (1.3)),

$$H_n(\sigma_n) = - \sum_{\langle x, y \rangle \in E_n} J_{xy} \delta_{\sigma_n(x), \sigma_n(y)} - \sum_{x \in V_n} \xi_{\sigma_n(x)}(x), \quad \sigma_n \in \Phi^{V_n}. \quad (1.7)$$

The vector field $\{\mathbf{h}(x)\}_{x \in V}$ in (1.6) is called *generalized boundary conditions (GBC)*.

We say that the probability distributions (1.6) are *compatible* (and the intrinsic GBC $\{\mathbf{h}(x)\}$ are *permissible*) if for each $n \in \mathbb{N}_0$ the following identity holds,

$$\sum_{\omega \in \Phi^{W_{n+1}}} \mu_{n+1}^h(\sigma_n \vee \omega) \equiv \mu_n^h(\sigma_n), \quad \sigma_n \in \Phi^{V_n}, \quad (1.8)$$

where the symbol \vee stands for concatenation of subconfigurations. A criterion for permissibility of GBC is provided by Theorem 2.1 (see Section 2.1 below). By Kolmogorov's extension theorem (see, e.g., [56, Chapter II, §3, Theorem 4, page 167]), the compatibility condition (1.8) ensures that there exists a unique measure $\mu^h = \mu_{\beta, \xi}^h$ on Φ^V such that, for all $n \in \mathbb{N}_0$,

$$\mu^h(\sigma_{V_n} = \sigma_n) \equiv \mu_n^h(\sigma_n), \quad \sigma_n \in \Phi^{V_n}, \quad (1.9)$$

or more explicitly (substituting (1.6)),

$$\mu^h(\sigma_{V_n} = \sigma_n) = \frac{1}{Z_n} \exp \left\{ -\beta H_n(\sigma_n) + \beta \sum_{x \in W_n} h_{\sigma_n(x)}(x) \right\}, \quad \sigma_n \in \Phi^{V_n}. \quad (1.10)$$

⁴It is also tacitly assumed in (1.4) that $\langle x, y \rangle \in E$, that is, $d(x, y) = 1$.

It is easy to show that μ^h so defined is a *Gibbs measure* (see (1.5)); since the family (V_n) is cofinal (see Remark 1.1), according to a standard result [22, Remark (1.24), page 17] it suffices to check that, for each $n \in \mathbb{N}_0$ and any $\eta \in \Phi^{V_n^c}$,

$$\mu^h(\sigma_{V_n} = \sigma_n | \sigma_{V_n^c} = \eta) \equiv \gamma_n^\eta(\sigma_n), \quad \sigma_n \in \Phi^{V_n}, \quad (1.11)$$

where γ_n^η is the Gibbs distribution in V_n with configurational boundary condition η (cf. (1.2)). Indeed, denote $\omega := \eta_{W_{n+1}} \in \Phi^{W_{n+1}}$, then, due to the nearest-neighbour interaction in the Hamiltonian (1.1) and according to (1.9), we have

$$\begin{aligned} \mu^h(\sigma_{V_n} = \sigma_n | \sigma_{V_n^c} = \eta) &= \mu^h(\sigma_{V_n} = \sigma_n | \sigma_{W_{n+1}} = \omega) \\ &= \frac{\mu^h(\sigma_{W_{n+1}} = \sigma_n \vee \omega)}{\mu^h(\sigma_{W_{n+1}} = \omega)} \\ &= \frac{\mu_{n+1}^h(\sigma_n \vee \omega)}{\mu_{n+1}^h(\omega)}. \end{aligned}$$

Furthermore, recalling the definitions (1.4) and (1.6), and using the proportionality symbol \propto to indicate omission of factors not depending on σ_n , we obtain

$$\begin{aligned} \mu^h(\sigma_{V_n} = \sigma_n | \sigma_{V_n^c} = \eta) &\propto \mu_{n+1}^h(\sigma_n \vee \omega) \\ &\propto \exp \left\{ -\beta H_{n+1}(\sigma_n \vee \omega) + \beta \sum_{x \in W_{n+1}} h_{\omega(x)}(x) \right\} \\ &\propto \exp \left\{ -\beta H_n(\sigma_n) + \beta \sum_{x \in W_n} \sum_{y \in S(x)} J_{xy} \delta_{\sigma_n(x), \omega(y)} \right\} \\ &\propto \gamma_{V_n}^\eta(\sigma_n), \end{aligned} \quad (1.12)$$

and since both the left- and the right-hand sides of (1.12) are probability measures on Φ^{V_n} , the relation (1.11) follows.

Definition 1.1. Measure μ^h satisfying (1.9) is called a *splitting Gibbs measure (SGM)*.

The term *splitting* was coined by Rozikov and Suhov [50] to emphasize that, in addition to the Markov property (see [22, Section 12.1] and also Remark 1.4 below), such measures enjoy the following factorization property: conditioned on a fixed subconfiguration $\sigma_n \in \Phi^{V_n}$, the values $\{\sigma(x)\}_{x \in W_{n+1}}$ are independent under the law μ^h . Indeed, using (1.6) and (1.9), it is easy to see that, for each $n \in \mathbb{N}_0$ and any $\omega \in \Phi^{W_{n+1}}$,

$$\begin{aligned} \mu^h(\sigma_{W_{n+1}} = \omega | \sigma_{V_n} = \sigma_n) &\propto \prod_{x \in W_{n+1}} \exp \left\{ \beta J_{x'x} \delta_{\sigma_n(x'), \omega(x)} + \beta \xi_{\omega(x)}(x) + \beta h_{\omega(x)}(x) \right\} \\ &\propto \prod_{x \in W_{n+1}} \mu^h(\sigma(x) = \omega(x) | \sigma_{V_n} = \sigma_n), \end{aligned}$$

where the proportionality symbol \propto indicates omission of factors not depending on ω , and $x' = x'(x) \in W_n$ is the unique vertex such that $x \in S(x')$.

Remark 1.2. Note that adding a constant $c = c(x)$ to all coordinates $h_i(x)$ of the vector $\mathbf{h}(x)$ does not change the probability measure (1.6) due to the normalization Z_n . The

same is true for the external field $\boldsymbol{\xi}(x)$ in the Hamiltonian (1.7). Therefore, without loss of generality we can consider *reduced GBC* $\check{\mathbf{h}}(x)$, for example defined as

$$\check{h}_i(x) = h_i(x) - h_q(x), \quad i = 1, \dots, q-1.$$

The same remark also applies to the external field $\boldsymbol{\xi}$ and its reduced version $\check{\boldsymbol{\xi}}(x)$, defined by

$$\check{\xi}_i(x) := \xi_i(x) - \xi_q(x), \quad i = 1, \dots, q-1.$$

Of course, such a reduction can equally be done by subtracting any other coordinate,

$${}_\ell\check{h}_i(x) := h_i(x) - h_\ell(x), \quad {}_\ell\check{\xi}_i(x) := \xi_i(x) - \xi_\ell(x) \quad (i \neq \ell).$$

Remark 1.3. For $q = 2$, the Potts model is equivalent to the Ising model with redefined spins

$$\tilde{\sigma}(x) := 2\sigma(x) - 3 \in \{-1, 1\}, \quad x \in V,$$

whereby the Hamiltonians in the two models are linked through the relations

$$\delta_{\sigma(x), \sigma(y)} = \frac{\tilde{\sigma}(x)\tilde{\sigma}(y) + 1}{2}, \quad \xi_{\sigma(x)}(x) = \frac{\xi_2(x) - \xi_1(x)}{2} \tilde{\sigma}(x) + \frac{\xi_1(x) + \xi_2(x)}{2}.$$

In turn, this leads to rescaling of the inverse temperature $\beta = \frac{1}{2}\tilde{\beta}$.

1.2.4. Boundary laws. Let us comment on the link between the SGM construction outlined in Section 1.2.3 and an alternative (classical) approach to defining Gibbs measures on tree-like graphs (including Cayley trees), as presented in the book by Georgii [22, Chapter 12]. As was already mentioned in [29, pages 641–642], the family of permissible GBC $\{\mathbf{h}(x)\}_{x \in V}$ defines a *boundary law* $\{\mathbf{z}(x, y)\}_{\langle x, y \rangle \in E}$ in the sense of [22, Definition (12.10)] (see also [65]); that is, for any $x, y \in V$ such that $\langle x, y \rangle \in E$, and for all $i \in \Phi$ it holds

$$z_i(x, y) = c(x, y) \prod_{v \in \partial\{x\} \setminus \{y\}} \sum_{j \in \Phi} z_j(v, x) \exp\{\beta J_{xv} \delta_{ij} + \beta \xi_i(x) + \beta \xi_j(v)\}, \quad (1.13)$$

where $c(x, y) > 0$ is an arbitrary constant (not depending on $i \in \Phi$).

To see this, for any $y \in V$ and $x \in S(y)$ (so that $d(x_\circ, y) = d(x_\circ, x) - 1$), set

$$z_i(x, y) := \exp\{\beta h_i(x)\}, \quad i \in \Phi, \quad (1.14)$$

which defines the values of the boundary law on ordered edges $\langle x, y \rangle$ *pointing to the root* x_\circ . This definition is consistent, in that the equation (1.13) is satisfied (for such edges) due to the assumed permissibility of the GBC $\{\mathbf{h}(x)\}_{x \in V}$ (see Theorem 2.1).

The values $z_i(x, y)$ on the edges $\langle x, y \rangle$ *pointing away from the root* x_\circ (i.e., such that $d(x_\circ, y) = d(x_\circ, x) + 1$) can be identified inductively (up to proportionality constants) using formula (1.13). The base of induction is set out by choosing $x = x_\circ$ and $y \in \partial\{x_\circ\} = S(x_\circ)$. Then for all $v \in S(x_\circ)$ we have $z_i(v, x_\circ) = \exp\{\beta h_i(v)\}$ (see (1.14)), and equation (1.13) yields

$$z_i(x_\circ, y) = c(x_\circ, y) \prod_{v \in S(x_\circ) \setminus \{y\}} \sum_{j \in \Phi} \exp\{\beta h_j(v) + \beta J_{x_\circ, v} \delta_{ij} + \beta \xi_i(x_\circ) + \beta \xi_j(v)\},$$

which defines $z_i(x_\circ, y)$ ($i \in \Phi$) up to an unimportant constant factor. If $z_i(x, y)$ is already defined for all $x \in V_n$ and $y \in S(x)$, then for $x \in W_{n+1}$ and $y \in S(x)$ we have

$$\partial\{x\} \setminus \{y\} = (S(x) \setminus \{y\}) \cup \{x'\},$$

where $x' \in W_n$ is the unique vertex such that $x \in S(x')$. Noting that the values $z_j(x', x)$ ($j \in \Phi$) are already defined by the induction hypothesis and that $z_j(v, x) =$

$\exp\{\beta h_j(v)\}$ for all $v \in S(x)$, formula (1.13) yields $z_i(x, y)$ (again, up to a proportionality constant), which completes the induction step.

Remark 1.4. As a consequence of the equivalence between (permissible) GBC $\{\mathbf{h}(x)\}_{x \in V}$ and boundary laws $\{\mathbf{z}(x, y)\}_{(x, y) \in E}$, it follows from [22, Theorem (12.12), page 243] that any SGM μ^h determines a unique *Markov chain* μ (see [22, Definition (12.2), page 239]), and vice versa, each Markov chain μ defines a unique SGM μ^h .

Remark 1.5. It is known that for each $\beta > 0$ the Gibbs measures form a non-empty convex compact set \mathcal{G} in the space of all probability measures on Φ^V endowed with the weak topology (see, e.g., [22, Chapter 7]). A measure $\mu \in \mathcal{G}$ is called *extreme* if it cannot be expressed as $\frac{1}{2}\mu_1 + \frac{1}{2}\mu_2$ for some $\mu_1, \mu_2 \in \mathcal{G}$ with $\mu_1 \neq \mu_2$. The set of all extreme measures in \mathcal{G} denoted by $\text{ex}\mathcal{G}$ is a *Choquet simplex*, in the sense that any $\mu \in \mathcal{G}$ can be represented as $\mu = \int_{\text{ex}\mathcal{G}} \nu \rho(d\nu)$, with some probability measure ρ on $\text{ex}\mathcal{G}$. The crucial observation, which will be instrumental throughout the paper, is that, by virtue of combining [22, Theorem (12.6)] with Remark 1.4, *any extreme measure* $\mu \in \text{ex}\mathcal{G}$ *is SGM*; therefore, the question of uniqueness of the Gibbs measure is reduced to that in the SGM class.

Using the boundary law $\{\mathbf{z}(x, y)\}_{(x, y) \in E}$, formula (1.10) can be extended to more general subsets in V . Namely, according to [22, formula (12.13), page 243] (adapted to our notation), for any finite *connected* set $\emptyset \neq \Lambda \subset V$ (and $\bar{\Lambda} = \Lambda \cup \partial\Lambda$),

$$\mu^h(\sigma_{\bar{\Lambda}} = \varsigma) = \frac{1}{Z_{\bar{\Lambda}}} \exp \left\{ -\beta H_{\bar{\Lambda}}(\varsigma) + \beta \sum_{x \in \partial\Lambda} h_{\varsigma(x)}^\dagger(x, x_\Lambda) \right\}, \quad \varsigma \in \Phi^{\bar{\Lambda}}, \quad (1.15)$$

where $Z_{\bar{\Lambda}} = Z_{\bar{\Lambda}}(\beta, \mathbf{h})$ is the normalizing factor, x_Λ denotes the unique neighbour of $x \in \partial\Lambda$ belonging to Λ , and

$$h_i^\dagger(x, y) := \beta^{-1} \ln z_i(x, y), \quad i \in \Phi. \quad (1.16)$$

In particular, if $x \in S(y)$ then (combining (1.16) with (1.14))

$$h_i^\dagger(x, y) = h_i(x), \quad i \in \Phi. \quad (1.17)$$

To link the general expression (1.15) with formula (1.10) for balls V_n , consider part of the boundary $\partial\Lambda$ defined as

$$\partial\Lambda^\downarrow := \{x \in \partial\Lambda : S(x) \cap \Lambda = \emptyset\}. \quad (1.18)$$

In other words, $\partial\Lambda^\downarrow$ consists of the points $x \in \partial\Lambda$ such that the corresponding vertex $x_\Lambda \in \Lambda$ is closer to the root x_o than x itself. In view of the definition (1.14), for $x \in \partial\Lambda^\downarrow$ we get $h_i^\dagger(x, x_\Lambda) \equiv h_i(x)$. Clearly, if $x_o \in \Lambda$ then $\partial\Lambda^\downarrow = \partial\Lambda$, but if $x_o \notin \Lambda$ then the set $\partial\Lambda \setminus \partial\Lambda^\downarrow$ is non-empty and, moreover, it contains exactly one vertex, which we denote by \check{x} . Note that $\check{x} \in \partial\Lambda$ is closer to the root x_o than $\check{x}_\Lambda \in \Lambda$, and in this case $h_i^\dagger(\check{x}, \check{x}_\Lambda)$ is only expressible through the GBC $\{\mathbf{h}(x)\}$ via a recursive procedure, as explained above.

Thus, formula (1.15) can be represented more explicitly as follows,

$$\mu^h(\sigma_{\bar{\Lambda}} = \varsigma) = \frac{1}{Z_{\bar{\Lambda}}} \exp \left\{ -\beta H_{\bar{\Lambda}}(\varsigma) + \beta \sum_{x \in \partial\Lambda^\downarrow} h_{\varsigma(x)}(x) + \beta \sum_{x \in \partial\Lambda \setminus \partial\Lambda^\downarrow} h_{\varsigma(x)}^\dagger(x, x_\Lambda) \right\}. \quad (1.19)$$

In fact, the last sum in (1.19) includes at most one term, which corresponds to $x = \check{x}$; more precisely, the latter sum is vacuous whenever $x_o \in \Lambda$, in which case the first sum

in (1.19) is reduced to the sum over all $x \in \partial\Lambda$. In particular, the formula (1.10) is consistent with (1.19) by picking the set $\Lambda = V_{n-1}$ ($n \geq 1$), with boundary $\partial\Lambda = W_n$. For a graphical illustration of the sets involved in formula (1.19), see Figure 1 (for a single-vertex set $\Lambda = \{v\}$ with $v \neq x_\circ$).

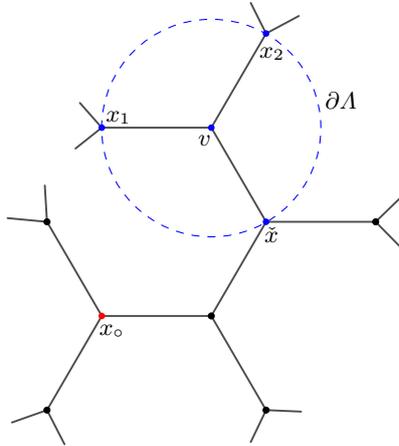


FIGURE 1. Illustration of the sets in formula (1.19) relative to the root x_\circ : $\Lambda = \{v\}$, $\partial\Lambda = \{x_1, x_2, \tilde{x}\}$ (here $\tilde{x}_\Lambda = v$), $\bar{\Lambda} = \{v, x_1, x_2, \tilde{x}\}$, and $\partial\Lambda^\downarrow = \{x_1, x_2\}$ (see (1.18)).

1.2.5. *Layout.* The rest of the paper is organized as follows (cf. the table of contents). We state our main results in Section 2, starting with a general *compatibility criterion* (Theorem 2.1), which reduces the existence of SGM μ^h to the solvability of an infinite system of non-linear equations for permissible GBC $\{\mathbf{h}(x)\}$. This is followed by various sufficient conditions for uniqueness of SGM with *uniform ferromagnetic interaction* (Theorems 2.2, 2.3 and 2.5). As part of our general treatment of the Potts model on the Cayley tree, in Section 2.3.1 we introduce the notion of translation-invariant SGMs (based on a bijection between \mathbb{T}^k and a free group with $k + 1$ generators of period 2 each), and state a novel criterion of translation invariance (Proposition 2.6) in terms of the external field and the GBC.

Non-uniqueness results for a subclass of *completely homogeneous SGMs* (i.e., where the reduced fields $\{\check{\boldsymbol{\xi}}(x)\}$ and $\{\check{\mathbf{h}}(x)\}$ are constant) are summarized in Theorems 2.8, 2.9 and 2.10. The number of such measures is estimated in several special cases by $2^q - 1$ (Theorem 2.11), and we conjecture that this is a universal upper bound. In Section 3, we record some auxiliary lemmas. The proofs of the uniqueness results (Theorems 2.2, 2.3 and 2.5) are presented in Section 4. Section 5 is devoted to the in-depth analysis of completely homogeneous SGMs, culminating in the proof of Theorems 2.8–2.11 (given in Sections 5.2–5.5, respectively). In Section 6, we study some fine properties (such as monotonicity, bounds and zeros) of the critical curves on the temperature–field plane, summarized in Propositions 6.4, 6.5, 6.11–6.14, 6.16 and 6.17. Finally, Appendix A presents the proof of Proposition 2.6, while Appendix B is devoted to the proof of a technical Lemma 5.3 addressing the special case $q = 3$.

2. RESULTS

2.1. **Compatibility criterion.** In view of Remark 1.2, when working with vectors and vector-valued functions and fields it will often be convenient to pass from a generic

vector $\mathbf{u} = (u_1, \dots, u_q) \in \mathbb{R}^q$ to a “reduced vector” $\check{\mathbf{u}} = (\check{u}_1, \dots, \check{u}_{q-1}) \in \mathbb{R}^{q-1}$ by setting $\check{u}_i := u_i - u_q$ ($i = 1, \dots, q-1$).

The following general statement describes a criterion⁵ for the GBC $\{\mathbf{h}(x)\}_{x \in V}$ to guarantee compatibility of the measures $\{\mu_n^h\}_{n \in \mathbb{N}_0}$.

Theorem 2.1. *The probability distributions $\{\mu_n^h\}_{n \in \mathbb{N}_0}$ defined in (1.6) are compatible (and the underlying GBC $\{\mathbf{h}(x)\}_{x \in V}$ are permissible) if and only if the following vector identity holds*

$$\beta \check{\mathbf{h}}(x) = \sum_{y \in S(x)} \mathbf{F}(\beta \check{\mathbf{h}}(y) + \beta \check{\boldsymbol{\xi}}(y); e^{\beta J_{xy}}), \quad x \in V, \quad (2.1)$$

where $\check{\mathbf{h}}(x) = (\check{h}_1(x), \dots, \check{h}_{q-1}(x))$, $\check{\boldsymbol{\xi}}(x) = (\check{\xi}_1(x), \dots, \check{\xi}_{q-1}(x))$,

$$\check{h}_i(x) := h_i(x) - h_q(x), \quad \check{\xi}_i(x) := \xi_i(x) - \xi_q(x), \quad i = 1, \dots, q-1, \quad (2.2)$$

and the map $\mathbf{F}(\mathbf{u}; \theta) = (F_1(\mathbf{u}; \theta), \dots, F_{q-1}(\mathbf{u}; \theta))$ is defined for $\mathbf{u} = (u_1, \dots, u_{q-1}) \in \mathbb{R}^{q-1}$ and $\theta > 0$ by the formulas

$$F_i(\mathbf{u}; \theta) := \ln \frac{(\theta - 1)e^{u_i} + 1 + \sum_{j=1}^{q-1} e^{u_j}}{\theta + \sum_{j=1}^{q-1} e^{u_j}}, \quad i = 1, \dots, q-1. \quad (2.3)$$

Remark 2.1. Likewise, Theorem 2.1 is true for any of the q possible reductions (see Remark 1.2).

Remark 2.2. Note that $\mathbf{F}(\mathbf{0}; \theta) = \mathbf{0}$ for any $\theta > 0$.

Remark 2.3. In view of the link (discussed in Section 1.2.4) between GBC $\{\mathbf{h}(x)\}_{x \in V}$ and boundary laws $\{\mathbf{z}(x, y)\}_{(x, y) \in E}$, the compatibility criterion (2.1) is but a reformulation of the consistency property (1.13) of the boundary law.

By virtue of Theorem 2.1, if the GBC $\{\mathbf{h}(x)\}$ and the external field $\{\boldsymbol{\xi}(x)\}$ satisfy the functional equation (2.1) for some $\beta > 0$ then there is a (unique) SGM $\mu_{\beta, \boldsymbol{\xi}}^h$.

2.2. Uniqueness results. From now on, we confine ourselves to the case of *uniform* (ferromagnetic) nearest-neighbour interaction by setting $J_{xy} = J \geq 0$ if $d(x, y) = 1$ (and $J_{xy} = 0$ otherwise). It will also be convenient to re-parameterize the model by introducing the new parameter $\theta = e^{\beta J} \geq 1$ termed *activity*.

For $\theta \geq 1$, consider the function

$$\varphi(t; \theta) := \frac{(\theta - 1)t}{(\sqrt{\theta(t-1)} + \sqrt{t-\theta})^2}, \quad t \geq \theta, \quad (2.4)$$

which can also be written as

$$\varphi(t; \theta) = \frac{\sqrt{\theta(t-1)} - \sqrt{t-\theta}}{\sqrt{\theta(t-1)} + \sqrt{t-\theta}}, \quad t \geq \theta. \quad (2.5)$$

Noting that

$$\varphi(t; \theta) = \frac{\theta - 1}{\left(\sqrt{\theta - \theta/t} + \sqrt{1 - \theta/t}\right)^2},$$

⁵Earlier versions of this theorem are found in [21, Proposition 1, page 375] or [47, Theorem 5.1, page 106].

it is evident that $t \mapsto \varphi(t; \theta)$ is a decreasing function; in particular, for all $t \geq \theta$

$$1 = \varphi(\theta; \theta) \geq \varphi(t; \theta) \geq \varphi(\infty; \theta) = \frac{\sqrt{\theta} - 1}{\sqrt{\theta} + 1}. \quad (2.6)$$

For brevity, introduce the notation

$$Q(\theta) := (q - 2) \frac{\sqrt{\theta} - 1}{\sqrt{\theta} + 1}, \quad (2.7)$$

and for $k \geq 2$, $q \geq 2$ consider the equation

$$Q(\theta) + \varphi(\theta + 1; \theta) = \frac{1}{k}, \quad \theta \geq 1, \quad (2.8)$$

or more explicitly (noting that $\varphi(\theta + 1; \theta) = (\theta - 1)/(\theta + 1)$),

$$Q(\theta) + \frac{\theta - 1}{\theta + 1} = \frac{1}{k}, \quad \theta \geq 1. \quad (2.9)$$

The left-hand side of (2.9) is a continuous increasing function of $\theta \in [1, \infty)$ ranging from 0 to $q - 1 > k^{-1}$, which implies that there is a unique solution of the equation (2.9), denoted $\theta_0 = \theta_0(k, q)$. In particular, for $q = 2$ we get

$$\theta_0(k, 2) = \frac{k + 1}{k - 1}. \quad (2.10)$$

Let us also consider the equation

$$(q - 1) \frac{\theta - 1}{\theta + 1} = \frac{1}{k}, \quad (2.11)$$

which has the unique root

$$\theta_* = \theta_*(k, q) := \frac{k(q - 1) + 1}{k(q - 1) - 1}. \quad (2.12)$$

Noting from (2.7) that, for any $\theta > 1$,

$$(q - 1) \frac{\sqrt{\theta} - 1}{\sqrt{\theta} + 1} < Q(\theta) + \frac{\theta - 1}{\theta + 1} \leq (q - 1) \frac{\theta - 1}{\theta + 1},$$

and comparing equations (2.9) and (2.11), it follows that

$$\theta_*(k, q) \leq \theta_0(k, q) < (\theta_*(k, q))^2,$$

where the first inequality is in fact strict unless $q = 2$.

Theorem 2.2. *Let $\theta_0 = \theta_0(k, q)$ be the unique solution of the equation (2.9). Then the Gibbs measure $\mu_{\theta, \xi}$ is unique for $\theta \in (1, \theta_0)$ and any external field ξ .*

Remark 2.4. It is known that the Ising model on a Cayley tree with zero external field has a unique Gibbs measure if and only if $\theta \leq \theta_c(k) = \sqrt{1 + \frac{2}{k-1}}$ (see [8]); that is to say, $\theta_c(k)$ is the *critical activity* of the Ising model. Since $\theta_c(k) = \theta_0(k, 2)$, our Theorem 2.2 is sharp in this case. Let $\theta_{\text{cr}}(k, q)$ be the critical activity for the Potts model; its exact value is known only for the binary tree ($k = 2$), namely $\theta_{\text{cr}}(2, q) = 1 + 2\sqrt{q - 1}$ [30]. Note that $\theta_{\text{cr}}(2, 2) = \theta_0(2, 2) (= 3)$ but $\theta_{\text{cr}}(2, q) > \theta_0(2, q)$ for $q \geq 3$, so Theorem 2.2 is not sharp already for $k = 2$, $q \geq 3$.

For $k \geq 2$, $q \geq 2$ and any $\gamma \in \mathbb{R}$, consider the equation (cf. (2.8))

$$Q(\theta) + \varphi(t_\gamma(\theta); \theta) = \frac{1}{k}, \quad \theta \geq 1, \quad (2.13)$$

where $\varphi(t; \theta)$ and $Q(\theta)$ are defined in (2.4) and (2.7), respectively, and

$$t_\gamma(\theta) := \theta + 1 + (q - 2)\theta^\gamma. \quad (2.14)$$

It can be shown (see Lemma 3.5) that equation (2.13) has a unique root, $\theta_\gamma^* = \theta_\gamma^*(k, q)$. More specifically, if $q = 2$ then $t_\gamma(\theta) = \theta + 1$ and equation (2.13) is reduced to equation (2.8) (with $Q(\theta) \equiv 0$), so that $\theta_\gamma^*(k, 2) \equiv \theta_0(k, 2) = (k + 1)/(k - 1)$ (see (2.10)). However, if $q \geq 3$ then the root θ_γ^* is an increasing function of parameter γ with the asymptotic bounds

$$\theta_0(k, q) = \lim_{\gamma \rightarrow -\infty} \theta_\gamma^*(k, q) < \theta_\gamma^*(k, q) < \lim_{\gamma \rightarrow +\infty} \theta_\gamma^*(k, q) = (\theta_*(k, q))^2. \quad (2.15)$$

Definition 2.1. Given the external field $\boldsymbol{\xi}(x) = (\xi_1(x), \dots, \xi_q(x))$ ($x \in V$), define the asymptotic ‘‘gap’’ between its coordinates as follows,

$$\Delta^\xi := \max_{1 \leq \ell \leq q} \liminf_{x \in V} \ell \check{\xi}_{(1)}(x), \quad (2.16)$$

where

$$\ell \check{\xi}_{(1)}(x) := \min_{i \neq \ell} \ell \check{\xi}_i(x) \equiv \min_{i \neq \ell} (\xi_i(x) - \xi_\ell(x)), \quad x \in V. \quad (2.17)$$

Theorem 2.3. *The Gibbs measure $\mu_{\beta, \xi}$ is unique for any $\beta \in (0, \ln \theta_{\Delta^\xi - k}^*)$, where θ_γ^* denotes the unique solution of the equation (2.13).*

Remark 2.5. As already mentioned, if $q = 2$ then $\theta_\gamma^*(k, 2) \equiv \theta_0(k, 2)$ and we recover Theorem 2.2 in this case. But if $q \geq 3$ then $\theta_\gamma^*(k, q) > \theta_0(k, q)$ for any $\gamma \in \mathbb{R}$ (see (2.15)), so that Theorem 2.3 ensures the uniqueness of the SGM $\mu_{\beta, \xi}$ on a wider interval of temperatures as compared to Theorem 2.2, for any Δ^ξ . Moreover, due to the monotonicity of the map $\gamma \mapsto \theta_\gamma^*$ (Lemma 3.5), a larger gap Δ^ξ facilitates uniqueness of SGM; however, the domain of guaranteed uniqueness (in parameter θ) is bounded in all cases (see (2.15)) by $(\theta_*(k, q))^2 \leq (\theta_*(2, 3))^2 = 25/9 \doteq 2.7778$.

Remark 2.6. If the external field $\boldsymbol{\xi}$ is random then the gap (2.16) is a random variable measurable with respect to the ‘‘tail’’ σ -algebra $\mathcal{F}^\infty = \bigcap_{n=0}^\infty \sigma\{\boldsymbol{\xi}(x), x \in V_n^c\}$. Intuitively, this means that Δ^ξ does not depend on the values of the field $\boldsymbol{\xi}(x)$ on any finite set $A \subset V$. If the values of $\boldsymbol{\xi}(x)$ are assumed to be independent (not necessarily identically distributed) for different $x \in V$ then, by Kolmogorov’s zero–one law, $\Delta^\xi = \text{const}$ (and therefore $\theta_{\Delta^\xi - k}^* = \text{const}$) almost surely (a.s.).

Example 2.1. Let us compute the asymptotic gap Δ^ξ in a few examples.

- (a) Let the random vectors $\boldsymbol{\xi}(x)$ ($x \in V$) be mutually independent, with independent and identically distributed (i.i.d.) coordinates $\xi_i(x)$ ($i = 1, \dots, q$), each taking the values ± 1 with probabilities $\frac{1}{2}$. Note that $\ell \check{\xi}_{(1)}(x) \in \{0, \pm 2\}$ ($\ell = 1, \dots, q$) and

$$\begin{aligned} \mathbb{P}(\ell \check{\xi}_{(1)}(x) = -2) &= \mathbb{P}\left(\xi_\ell(x) = 1, \min_{i \neq \ell} \xi_i(x) = -1\right) \\ &= \mathbb{P}(\xi_\ell(x) = 1) \cdot (1 - \mathbb{P}(\xi_i(x) = 1, i \neq \ell)) \\ &= \frac{1}{2} \left(1 - \left(\frac{1}{2}\right)^{q-1}\right) > 0. \end{aligned} \quad (2.18)$$

The Borel–Cantelli lemma then implies that $\liminf_{x \in V} \ell \check{\xi}_{(1)}(x) = -2$ a.s. and hence, according to (2.16), $\Delta^\xi = -2$ a.s.

- (b) In the previous example, let us remove the i.i.d. assumption for the coordinates, and instead suppose that each of the random vectors $\boldsymbol{\xi}(x)$ (still mutually independent for different $x \in V$) can take two values, $\pm(1, \dots, 1)$, with probability $\frac{1}{2}$ each. Then it is clear that $\ell \check{\xi}_{(1)}(x) \equiv 0$ ($\ell = 1, \dots, q$), hence $\Delta^\xi = 0$ a.s.
- (c) Extending example (b), suppose that, with some $\alpha \in \mathbb{R}$,

$$\mathbb{P}(\xi_i(x) = \alpha \text{ and } \xi_j(x) = 0 \text{ for all } j \neq i) = q^{-1} \quad (i = 1, \dots, q).$$

Of course, for $\alpha = 0$ we have $\boldsymbol{\xi}(x) \equiv \mathbf{0}$ and hence $\Delta^\xi = 0$; thus, let $\alpha \neq 0$. If $q = 2$ then it is straightforward to see that

$$\mathbb{P}(\ell \check{\xi}_{(1)}(x) = \pm\alpha) = \frac{1}{2}, \quad \ell = 1, 2.$$

For $q \geq 3$, if $\alpha > 0$ then, similarly,

$$\mathbb{P}(\ell \check{\xi}_{(1)}(x) = -\alpha) = q^{-1}, \quad \mathbb{P}(\ell \check{\xi}_{(1)}(x) = 0) = 1 - q^{-1}, \quad (2.19)$$

whereas if $\alpha < 0$ then

$$\mathbb{P}(\ell \check{\xi}_{(1)}(x) = -\alpha) = q^{-1}, \quad \mathbb{P}(\ell \check{\xi}_{(1)}(x) = \alpha) = 1 - q^{-1}. \quad (2.20)$$

Thus, in all cases, the Borel–Cantelli lemma yields that $\Delta^\xi = -|\alpha|$ a.s. (which also includes the case $\alpha = 0$).

- (d) Consider i.i.d. vectors $\boldsymbol{\xi}(x)$ ($x \in V$) with i.i.d. coordinates $\xi_i(x)$ ($i = 1, \dots, q$), each with the uniform distribution on $[0, 1]$. Note that $-1 \leq \ell \check{\xi}_{(1)}(x) \leq 1$ ($\ell = 1, \dots, q$) and, for any $\varepsilon \in (0, 1)$,

$$\begin{aligned} \mathbb{P}(\ell \check{\xi}_{(1)}(x) \leq -1 + 2\varepsilon) &\geq \mathbb{P}\left(\xi_\ell(x) \geq 1 - \varepsilon, \min_{i \neq \ell} \xi_i(x) \leq \varepsilon\right) \\ &= \mathbb{P}(\xi_\ell(x) \geq 1 - \varepsilon) \cdot \left(1 - \mathbb{P}\left\{\min_{i \neq \ell} \xi_i(x) \geq \varepsilon\right\}\right) \\ &= \varepsilon (1 - (1 - \varepsilon)^{q-1}) > 0. \end{aligned}$$

The Borel–Cantelli lemma then implies that $\liminf_{x \in V} \ell \check{\xi}_{(1)}(x) \leq -1 + 2\varepsilon$ a.s., and since $\varepsilon > 0$ is arbitrary, it follows that $\liminf_{x \in V} \ell \check{\xi}_{(1)}(x) = -1$ a.s., for each $\ell = 1, \dots, q$; hence, according to (2.16), $\Delta^\xi = -1$ a.s.

- (e) For a “non-ergodic” type of example leading to a random gap Δ^ξ , suppose that $\boldsymbol{\xi}(x) \equiv \boldsymbol{\xi}(x_\circ)$ ($x \in V$), where the distribution of $\boldsymbol{\xi}(x_\circ)$ is as in example (a). That is to say, the values of the field $\boldsymbol{\xi}(x)$ are obtained by duplicating its (random) value at the root. Then, similarly to (2.18), we compute

$$\mathbb{P}(\Delta^\xi = -2) = \frac{1}{2} - \left(\frac{1}{2}\right)^q, \quad \mathbb{P}(\Delta^\xi = 2) = \left(\frac{1}{2}\right)^q, \quad \mathbb{P}(\Delta^\xi = 0) = \frac{1}{2}.$$

- (f) Finally, the simplest “coordinate-oriented” choice $\boldsymbol{\xi}(x) \equiv (\alpha, 0, \dots, 0)$, $x \in V$, with a fixed $\alpha \in \mathbb{R}$, exemplifies translation-invariant (non-random) external fields, including the case of zero field, $\alpha = 0$. Our results for this model will be stated in Section 2.3; for now, let us calculate the value of the gap Δ^ξ . Again, for $\alpha = 0$ we have $\boldsymbol{\xi}(x) \equiv \mathbf{0}$ and hence $\Delta^\xi = 0$; thus, let $\alpha \neq 0$. If $q = 2$ then $1 \check{\xi}_{(1)}(x) = -\alpha$, $2 \check{\xi}_{(1)}(x) = \alpha$, hence it is easy to see that $\Delta^\xi = \max\{-\alpha, \alpha\} = |\alpha|$. For $q \geq 3$, if $\alpha > 0$ then $1 \check{\xi}_{(1)}(x) = -\alpha$ and $\ell \check{\xi}_{(1)}(x) = 0$ ($\ell \neq 1$), whereas if $\alpha < 0$ then still $1 \check{\xi}_{(1)}(x) = -\alpha$ but $\ell \check{\xi}_{(1)}(x) = \alpha$ ($\ell \neq 1$); as a result, $\Delta^\xi = 0$ for $\alpha \geq 0$ and $\Delta^\xi = |\alpha|$ for $\alpha < 0$.

The following general assertion summarizes Example 2.1. Recall that random variables X_1, \dots, X_q are said to be *exchangeable* if the distribution of the random vector (X_1, \dots, X_q) is invariant with respect to permutations of the coordinates. The *support* $\text{supp } X$ of (the distribution of) a random variable X is defined as the (closed) set comprising all points $u \in \mathbb{R}$ such that for any $\varepsilon > 0$ we have $\mathbb{P}(|X - u| \leq \varepsilon) > 0$.

Proposition 2.4. *Suppose that the random vectors $\{\boldsymbol{\xi}(x)\}_{x \in V}$ are i.i.d., and for each $x \in V$ their coordinates $\xi_1(x), \dots, \xi_q(x)$ are exchangeable. Then*

$$\Delta^\xi = \inf\{\text{supp}(\xi_1(x) - \xi_q(x))\} \quad \text{a.s.}$$

In particular, $\Delta^\xi < 0$ a.s., unless $\xi_1(x) = \dots = \xi_q(x)$ a.s., in which case $\Delta^\xi = 0$ a.s.

Proof. Observe that, by exchangeability of $\{\xi_i(x)\}$, the distribution of $\ell\xi_{(1)}(x)$ does not depend on $\ell = 1, \dots, q$ and, moreover,

$$\text{supp } \ell\check{\xi}_{(1)}(x) = \text{supp}(\xi_1(x) - \xi_q(x)). \quad (2.21)$$

Denote $u_0 := \inf\{\text{supp}(\xi_1(x) - \xi_q(x))\}$. From (2.21), it follows that $\ell\check{\xi}_{(1)}(x) \geq u_0$ a.s., and therefore, according to (2.16), $\Delta^\xi \geq u_0$ a.s. On the other hand, for any $\varepsilon > 0$ we have

$$\mathbb{P}(\ell\check{\xi}_{(1)}(x) \leq u_0 + \varepsilon) = \mathbb{P}(\xi_1(x) - \xi_q(x) \leq u_0 + \varepsilon) > 0,$$

and the Borel–Cantelli lemma implies that $\liminf_{x \in V} \ell\check{\xi}_{(1)}(x) \leq u_0 + \varepsilon$ a.s., so that $\Delta^\xi \leq u_0$ a.s. As a result, $\Delta^\xi = u_0$ a.s., as claimed. \square

Theorem 2.5. *Assume that the random external field $\boldsymbol{\xi} = \{\boldsymbol{\xi}(x)\}_{x \in V}$ is as in Proposition 2.4. Let $\theta^\dagger = \theta^\dagger(k, q)$ be the root of the equation⁶*

$$Q(\theta) + \mathbb{E}\{\varphi(t_{\check{\xi}_{(1)}(x)-k}(\theta); \theta)\} = \frac{1}{k}, \quad \theta \geq 1, \quad (2.22)$$

where $\check{\xi}_{(1)}(x) \equiv {}_q\check{\xi}_{(1)}(x) = \min_{i \neq q}(\xi_i(x) - \xi_q(x))$ (cf. (2.17)) and the notation $t_\gamma(\theta)$ is introduced in (2.14). Then, for each $\theta \in [1, \theta^\dagger)$ and for \mathbb{P} -almost all realizations of the random field $\boldsymbol{\xi}$, there is a unique Gibbs measure $\mu_{\theta, \xi}$.

Remark 2.7. Note that Theorem 2.3 guarantees uniqueness of the Gibbs measure in the interval $1 < \theta < \theta_{\Delta^\xi - k}^*$, where $\theta_{\Delta^\xi - k}^*$ is the solution of the equation

$$Q(\theta) + \varphi(t_{\Delta^\xi - k}(\theta); \theta) = \frac{1}{k}, \quad \theta \geq 1.$$

By Proposition 2.4, we have $\check{\xi}_{(1)}(x) \geq \Delta^\xi$ (a.s.), and moreover, $\check{\xi}_{(1)}(x) > \Delta^\xi$ with positive probability, unless $\xi_1(x) = \dots = \xi_q(x)$ a.s. Thus, excluding the case $q = 2$ where $t_\gamma(\theta) = \theta + 1$, by monotonicity of the function $\gamma \mapsto \varphi(t_\gamma; \theta)$ we conclude that $\theta_{\Delta^\xi - k}^*(k, q) < \theta^\dagger(k, q)$, and therefore the domain of uniqueness in Theorem 2.5 is wider than that in Theorem 2.3.

Example 2.2. Let us illustrate Theorem 2.5 with a simple model described in Example 2.1(c), assuming that $q \geq 3$. Suppose first that $\alpha > 0$. Then, according to the distribution (2.19) and notation (2.14), equation (2.22) specializes to

$$Q(\theta) + \frac{1}{q} \varphi\left(\theta + 1 + \frac{q-2}{\theta^{\alpha+k}}; \theta\right) + \frac{q-1}{q} \varphi\left(\theta + 1 + \frac{q-2}{\theta^k}; \theta\right) = \frac{1}{k}.$$

⁶The left-hand side of (2.22) does not depend on $x \in V$ due to the i.i.d. assumption on $\{\boldsymbol{\xi}(x)\}$.

By monotonicity of the function $t \mapsto \varphi(t; \theta)$, it is clear that the root θ^\dagger of this equation is strictly bigger than the root $\theta_{\Delta^\varepsilon - k}^* = \theta_{-\alpha - k}^*$ of the equation

$$Q(\theta) + \varphi\left(\theta + 1 + \frac{q-2}{\theta^{\alpha+k}}; \theta\right) = \frac{1}{k},$$

in accordance with Remark 2.7. Similarly, if $\alpha < 0$ then the distribution (2.19) is replaced by (2.20) and equation (2.22) takes the form

$$Q(\theta) + \frac{1}{q} \varphi\left(\theta + 1 + \frac{q-2}{\theta^{\alpha+k}}; \theta\right) + \frac{q-1}{q} \varphi\left(\theta + 1 + \frac{q-2}{\theta^{-\alpha+k}}; \theta\right) = \frac{1}{k},$$

and by the monotonicity argument it is evident that its root θ^\dagger is strictly bigger than the root $\theta_{\Delta^\varepsilon - k}^* = \theta_{\alpha - k}^*$ of the equation

$$Q(\theta) + \varphi\left(\theta + 1 + \frac{q-2}{\theta^{-\alpha+k}}; \theta\right) = \frac{1}{k},$$

again confirming the observation of Remark 2.7.

2.3. Translation-invariant SGM and the problem of non-uniqueness.

2.3.1. Translation invariance. To introduce the notion of *translations* on the Cayley tree \mathbb{T}^k , let \mathcal{A}_k be the free group with generators a_1, \dots, a_{k+1} of order 2 each (i.e., $a_i^{-1} = a_i$). It is easy to see (cf. [20] and also [47, Section 2.2]) that the Cayley tree $\mathbb{T}^k = (V, E)$ is in a one-to-one correspondence with the group \mathcal{A}_k . Namely, start by associating the root $x_o \in V$ with the identity element $e \in \mathcal{A}_k$, and identify the elements a_1, \dots, a_{k+1} with the $k+1$ nearest neighbours of x_o (i.e., comprising the set $S(x_o) = W_1$). Proceed inductively by expanding the elements $a \in \mathcal{A}_k$ along the tree via *right*-multiplication by the generators a_i ($i = 1, \dots, k+1$), yielding k new elements⁷ corresponding to the set of direct successors of a (see Figure 2). This establishes a bijection $\mathbf{b}: V \rightarrow \mathcal{A}_k$.

Consider the family of *left* shifts $T_g: \mathcal{A}_k \rightarrow \mathcal{A}_k$ ($g \in \mathcal{A}_k$) defined by

$$T_g(a) := ga, \quad a \in \mathcal{A}_k.$$

By virtue of the bijection \mathbf{b} , this determines conjugate translations on V ,

$$\tilde{T}_z := \mathbf{b}^{-1} \circ T_{\mathbf{b}(z)} \circ \mathbf{b}, \quad z \in V. \quad (2.23)$$

Clearly, \tilde{T}_z is an automorphism of V preserving the nearest-neighbour relation; indeed, if $\langle x, y \rangle \in E$ and $y \in S(x)$ (so that $\mathbf{b}(y) = \mathbf{b}(x)a_j$, with some generator a_j) then, according to (2.23), $x' := \tilde{T}_z(x)$ and $y' := \tilde{T}_z(y) = \mathbf{b}^{-1}(\mathbf{b}(z)\mathbf{b}(y)) = \mathbf{b}^{-1}(\mathbf{b}(x')a_j)$ are nearest neighbours, $\langle x', y' \rangle \in E$ (see Figure 2). For example, if $k = 1$ (whereby the Cayley tree \mathbb{T}^1 is reduced to the integer lattice \mathbb{Z}^1), the action of the shift \tilde{T}_z ($z \in \mathbb{Z}^1$) can be written in closed form,

$$\tilde{T}_z(x) = z + (-1)^z x, \quad x \in \mathbb{Z}^1.$$

In turn, the map (2.23) induces shifts on configurations $\sigma \in \Phi^V$,

$$(\tilde{T}_z \sigma)(x) := \sigma(\tilde{T}_z^{-1} x), \quad x \in V. \quad (2.24)$$

⁷Indeed, if $a = wa_j$ then $aa_j = wa_j^2 = w$, so this particular multiplication returns the element w already obtained at the previous step.

Definition 2.2. We say that SGM $\mu^h = \mu_{\theta, \xi}^h$ is *translation invariant* (with respect to the group of shifts (\tilde{T}_z)) if for each $z \in V$ the measures $\mu^h \circ \tilde{T}_z^{-1}$ and μ^h coincide; that is, for any (finite) $\Lambda \subset V$ and any configuration $\varsigma \in \Phi^\Lambda$

$$\mu^h(\sigma_{\tilde{T}_z(\Lambda)} = \tilde{T}_z(\varsigma)) = \mu^h(\sigma_\Lambda = \varsigma). \quad (2.25)$$

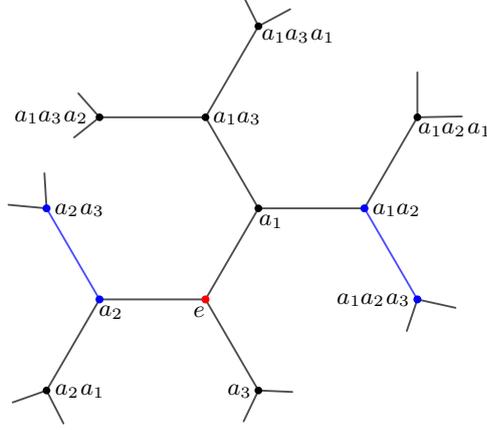


FIGURE 2. A fragment of the Cayley tree \mathbb{T}^2 ($k = 2$), with vertices represented (one-to-one) by elements of the free group \mathcal{A}_2 with generators $\{a_1, a_2, a_3\}$ (of order 2 each). The identity element $e \in \mathcal{A}_2$ designates the root $x_o \in V$. Starting from e , the elements $a \in \mathcal{A}$ are inductively expanded along the tree via right-multiplication by one of the generators. Translations on \mathcal{A}_2 are defined as left shifts, $T_g : a \rightarrow ga$ ($g, a \in \mathcal{A}_2$). For example, under the shift T_{a_1} the edge $\langle a_2, a_2a_3 \rangle$ is mapped to the edge $\langle a_1a_2, a_1a_2a_3 \rangle$.

Recall that the quantities $\check{h}_i^\dagger(x, y)$ ($\langle x, y \rangle \in E$) defining the boundary law were introduced in Section 1.2.4.

Proposition 2.6. *An SGM $\mu^h = \mu_{\theta, \xi}^h$ is translation invariant under the group of shifts $(\tilde{T}_z)_{z \in V}$ if and only if the following conditions are satisfied.*

- (i) *The reduced field $\{\check{\xi}(x)\}$ is constant over the tree,*

$$\check{\xi}(x) = \check{\xi}(x_o), \quad x \in V. \quad (2.26)$$

- (ii) *The reduced field $\{\check{h}^\dagger(x, y)\}$ is symmetric,*

$$\check{h}^\dagger(x, y) = \check{h}^\dagger(y, x), \quad \langle x, y \rangle \in E. \quad (2.27)$$

- (iii) *For any $z \in V$,*

$$\check{h}^\dagger(x, y) = \check{h}^\dagger(\tilde{T}_z(x), \tilde{T}_z(y)), \quad \langle x, y \rangle \in E. \quad (2.28)$$

This result will be proved in Appendix A.

For $x \neq x_o$, denote by x' the unique vertex such that $x \in S(x')$. Then, according to (1.17) and (2.28),

$$\check{h}^\dagger(x, x') = \check{h}(x) = \check{h}(\tilde{T}_{x'}^{-1}(x)). \quad (2.29)$$

Note that $\tilde{T}_{x'}^{-1}(x) \in \partial\{x_o\} = W_1$. Thus, there are $k+1$ (vector) values $\check{h}(x_j)$ ($x_j \in W_1$) that determine a translation-invariant SGM μ^h . By translations (2.29), these values

(which can be pictured as $k + 1$ “colours”) are propagated to all vertices $x \in V$ in a periodic “chessboard” tiling, except the root $x = x_o$ where the value $\check{\mathbf{h}}(x_o)$ is calculated separately, according to the compatibility formula (2.1).

The criterion of translation invariance given by Proposition 2.6 appears to be new. In Georgii [22, Corollary (12.17)], a version of this result is established (in the language of boundary laws) for *completely homogeneous* SGM, that is, assuming the invariance under the group of *all automorphisms* of the tree \mathbb{T}^k .⁸ Namely, we have the following

Corollary 2.7. *An SGM $\mu^h = \mu_{\theta, \xi}^h$ is completely homogeneous if and only if $\check{\xi}(x) \equiv \check{\xi}^0$ for all $x \in V$ and $\check{\mathbf{h}}(x) \equiv \check{\mathbf{h}}^0$ for all $x \neq x_o$.*

Remark 2.8. In the existing studies of Gibbs measures on trees (see, e.g., [19, 30]), it is common to use the term “translation invariant” (and the abbreviation TISGM) having in mind just completely homogeneous SGM. We prefer to keep the terminological distinction between “single-coloured” completely homogeneous GBC $\check{\mathbf{h}}(x) \equiv \check{\mathbf{h}}^0$ and “multi-coloured” translation-invariant GBC as characterized by Proposition 2.6. The latter case is very interesting (especially with regard to uniqueness) but technically more challenging, so it is not addressed here in full generality. However, as we will see below, the subclass of completely homogeneous SGM in the Potts model is very rich in its own right.

2.3.2. Analysis of uniqueness. For the rest of Section 2.3, we deal with *completely homogeneous SGM* $\mu^h = \mu_{\theta, \xi}^h$, that is, with the external field $\{\xi(x)\}_{x \in V}$ and GBC $\{\mathbf{h}(x)\}_{x \in V}$ satisfying the homogeneity conditions of Corollary 2.7. For simplicity, we confine ourselves to the case where all coordinates of the (reduced) vector $\check{\xi}^0$ are zero except one; due to permutational symmetry, we may assume, without loss of generality, that $\check{\xi}_1^0 = \alpha \in \mathbb{R}$ and $\check{\xi}_2^0 = \dots = \check{\xi}_{q-1}^0 = 0$,

$$\check{\xi}^0 = (\alpha, 0, \dots, 0) \in \mathbb{R}^{q-1}. \quad (2.30)$$

We also write

$$\check{\mathbf{h}}^0 = (\check{h}_1^0, \dots, \check{h}_{q-1}^0) \in \mathbb{R}^{q-1}.$$

Then, denoting $z_i := \theta^{\check{h}_i^0/k}$ ($i = 1, \dots, q - 1$), the compatibility equations (2.1) are equivalently rewritten in the form

$$\begin{cases} z_1 = 1 + \frac{(\theta - 1)(\theta^\alpha z_1^k - 1)}{\theta + \theta^\alpha z_1^k + \sum_{j=2}^{q-1} z_j^k}, \\ z_i = 1 + \frac{(\theta - 1)(z_i^k - 1)}{\theta + \theta^\alpha z_1^k + \sum_{j=2}^{q-1} z_j^k}, \quad i = 2, \dots, q - 1. \end{cases} \quad (2.31)$$

Solvability of the system (2.31) can be analysed in some detail; in particular, we are able to characterize the uniqueness of its solution, which in turn gives a criterion of the uniqueness of completely homogeneous SGM in the Potts model.

The case $\theta = 1$ is trivial, as the system (2.31) will then have the unique solution $z_1 = \dots = z_{q-1} = 1$. The case $\theta > 1$ and $\alpha = 0$ has been studied in [29]; these results can be reproduced directly by the methods developed in the present work similarly to a more general (and difficult) case $\alpha \neq 0$, and are also obtainable in the limit as $\alpha \rightarrow 0$ (see Lemma 5.1(b) and Remark 5.1).

⁸It is worth pointing out that the latter group is generated by the group of (left) shifts (\tilde{T}_z) and pairwise inversions between vertices $x_j, x_\ell \in \partial\{x_o\}$ [32, §3.5].

Thus, let us focus on the new case $\alpha \neq 0$. By Lemma 5.1(c), the system (2.31) with $\theta > 1$ is reduced either to a single equation

$$u = 1 + \frac{(\theta - 1)(\theta^\alpha u^k - 1)}{\theta + \theta^\alpha u^k + q - 2} \quad (2.32)$$

or to the system of equations (indexed by $m = 1, \dots, q - 2$)

$$\begin{cases} u = 1 + \frac{(\theta - 1)(\theta^\alpha u^k - 1)}{\theta + \theta^\alpha u^k + mv^k + q - 2 - m}, \\ 1 = \frac{(\theta - 1)(1 + v + \dots + v^{k-1})}{\theta + \theta^\alpha u^k + mv^k + q - 2 - m}, \end{cases} \quad (2.33)$$

subject to the condition

$$v \neq 1. \quad (2.34)$$

Let us first address the solvability of the equation (2.32). Denote

$$\theta_c = \theta_c(k, q) := \frac{1}{2} \left(\sqrt{(q-2)^2 + 4(q-1) \left(\frac{k+1}{k-1} \right)^2} - (q-2) \right). \quad (2.35)$$

In particular, if $q = 2$ then $\theta_c(k, 2) = \frac{k+1}{k-1} \equiv \theta_0(k, 2)$ (cf. (2.10)). Let us also set

$$b = b(\theta) := \frac{\theta(\theta + q - 2)}{q - 1}. \quad (2.36)$$

Clearly, $b(1) = 1$ and $b(\theta) > 1$ for $\theta > 1$. Furthermore, comparing (2.35) and (2.36) observe that $b(\theta_c) = \left(\frac{k+1}{k-1} \right)^2$ and $b(\theta) > \left(\frac{k+1}{k-1} \right)^2$ for $\theta > \theta_c$. For $\theta \geq \theta_c$, denote by $x_\pm = x_\pm(\theta)$ the roots of the quadratic equation

$$(b + x)(1 + x) = k(b - 1)x \quad (2.37)$$

with discriminant

$$D = D(\theta) := (k(b - 1) - (b + 1))^2 - 4b = (b - 1)(k - 1)^2 \left(b - \left(\frac{k + 1}{k - 1} \right)^2 \right), \quad (2.38)$$

that is,⁹

$$x_\pm = x_\pm(\theta) := \frac{(b - 1)(k - 1) - 2 \pm \sqrt{D}}{2}. \quad (2.39)$$

Furthermore, introduce the notation

$$a_\pm = a_\pm(\theta) := \frac{1}{x_\pm} \left(\frac{1 + x_\pm}{b + x_\pm} \right)^k, \quad \theta \geq \theta_c. \quad (2.40)$$

Of course, $a_-(\theta_c) = a_+(\theta_c)$, and one can also show that $a_-(\theta) < a_+(\theta)$ for all $\theta > \theta_c$ (see the proof of Theorem 2.8 in Section 5.2). Finally, denote

$$\alpha_\pm = \alpha_\pm(\theta) := -(k + 1) + \frac{1}{\ln \theta} \ln \frac{q - 1}{a_\mp}, \quad \theta \geq \theta_c, \quad (2.41)$$

so that $\alpha_-(\theta_c) = \alpha_+(\theta_c)$ and $\alpha_-(\theta) < \alpha_+(\theta)$ for $\theta > \theta_c$.

⁹Here and in what follows, formulas involving the symbols \pm and/or \mp combine the two cases corresponding to the choice of either the upper or lower sign throughout.

Theorem 2.8. *Let $\nu_0(\theta, \alpha)$ denote the number of solutions $u > 0$ of the equation (2.32). Then*

$$\nu_0(\theta, \alpha) = \begin{cases} 1 & \text{if } \theta \leq \theta_c \text{ or } \theta > \theta_c \text{ and } \alpha \notin [\alpha_-, \alpha_+], \\ 2 & \text{if } \theta > \theta_c \text{ and } \alpha \in \{\alpha_-, \alpha_+\}, \\ 3 & \text{if } \theta > \theta_c \text{ and } \alpha \in (\alpha_-, \alpha_+), \end{cases}$$

where θ_c is given in (2.35) and $\alpha_{\pm} = \alpha_{\pm}(\theta)$ are defined by (2.41).

Let us now state our results on the solvability of the set of equations (2.33). For each $m \in \{1, \dots, q-2\}$, consider the functions

$$L_m(v; \theta) := (\theta - 1)(v^{k-1} + \dots + v) - mv^k - (q - 1 - m), \quad (2.42)$$

$$K_m(v; \theta) := \frac{(v^{k-1} + \dots + v + 1)^k L_m(v; \theta)}{(v^{k-1} + \dots + v + L_m(v; \theta))^k}. \quad (2.43)$$

It can be checked (see Lemma 5.2) that for any $\theta > 1$ there is a unique value $v_m = v_m(\theta) > 0$ such that

$$L_m^*(\theta) := L_m(v_m; \theta) = \max_{v>0} L_m(v; \theta),$$

and moreover, the function $\theta \mapsto L_m^*(\theta)$ is strictly increasing. Denote by θ_m the (unique) value of $\theta > 1$ such that

$$L_m^*(\theta_m) = 0. \quad (2.44)$$

Thus, for any $\theta > \theta_m$ the range of the functions $v \mapsto L_m(v; \theta)$ and $v \mapsto K_m(v; \theta)$ includes positive values,

$$\mathcal{V}_m^+(\theta) := \{v > 0: L_m(v; \theta) > 0\} \equiv \{v > 0: K_m(v; \theta) > 0\} \neq \emptyset, \quad (2.45)$$

and, therefore, the function

$$\alpha_m(\theta) := \frac{1}{\ln \theta} \max_{v \in \mathcal{V}_m^+(\theta)} \ln K_m(v; \theta) = \frac{\ln K_m^*(\theta)}{\ln \theta}, \quad \theta > \theta_m, \quad (2.46)$$

is well defined, where

$$K_m^*(\theta) := \max_{v \in \mathcal{V}_m^+(\theta)} K_m(v; \theta).$$

Example 2.3. In the case $k = 2$, from (2.42) and (2.44) we obtain explicitly

$$\theta_m = 1 + 2\sqrt{m(q - m - 1)}, \quad m = 1, \dots, q - 2. \quad (2.47)$$

In particular, $\theta_1 = 1$ for $q = 2$, and $\theta_1 \geq 3$ whenever $q \geq 3$. Comparing (2.35) and (2.47), we also find that $\theta_c \leq \theta_1$ if and only if $q \geq 6$. For example, for $q = 5$ we have $\theta_1 = 1 + 2\sqrt{3} \doteq 4.4641$, $\theta_2 = 5$, $\theta_c = \frac{1}{2}(\sqrt{153} - 3) \doteq 4.6847$, that is, $\theta_1 < \theta_c < \theta_2$, whereas for $q = 6$ and $q = 7$ we compute $\theta_1 = \theta_c = 5$ and $\theta_1 = 1 + 2\sqrt{5} \doteq 5.4721 > \theta_c = \frac{1}{2}(\sqrt{241} - 5) \doteq 5.2621$, respectively. Another simple case is $q = 3$ (with $m = 1$ and any $k \geq 2$); indeed, it is easy to see that the condition (2.44) is satisfied with $v_1^* = v_1(\theta_1) = 1$ (cf. Lemma 5.2(c)), whence we readily find $\theta_1 = 1 + \frac{2}{k-1}$.

Theorem 2.9. *For each $m \in \{1, \dots, q-2\}$, let $\nu_m(\theta, \alpha)$ denote the number of positive solutions (u, v) of the system (2.33). Then $\nu_m(\theta, \alpha) \geq 1$ if and only if $\theta > \theta_m$ and $\alpha \leq \alpha_m(\theta)$.*

As will be shown in Proposition 6.16(b), $\alpha_+(\theta)$ has a unique zero given by $\theta_0^+ = 1 + \frac{q}{k-1}$, whereas $\alpha_-(\theta)$ has a unique zero θ_0^- , which coincides with the zero θ_1^0 of $\alpha_1(\theta)$. It also holds that $\alpha_1(\theta)$ is a majorant of the family of functions $\{\alpha_m(\theta)\}$ (see Propositions 6.11 and 6.12).

2.3.3. Uniqueness of completely homogeneous SGM. In the case $q = 3$, there appears to be an additional critical value (see Lemma 5.3)

$$\tilde{\theta}_1 = \tilde{\theta}_1(k) := \frac{5 - k + \sqrt{49k^2 + 62k + 49}}{6(k-1)}. \quad (2.48)$$

For example,

$$\tilde{\theta}_1(k) = \begin{cases} \frac{1 + \sqrt{41}}{2} \doteq 3.7016, & k = 2, \\ \frac{7}{3} \doteq 2.3333, & k = 3, \\ \frac{1 + \sqrt{1081}}{18} \doteq 1.8821, & k = 4. \end{cases} \quad (2.49)$$

For $q \geq 2$, consider the following subsets of the half-plane $\{\theta \geq 1\} = \{(\theta, \alpha) : \theta \geq 1, \alpha \in \mathbb{R}\}$,

$$A_q := \{\theta > \theta_c, \alpha_-(\theta) \leq \alpha \leq \alpha_+(\theta)\},$$

$$B_q := \begin{cases} \emptyset & \text{if } q = 2, \\ \{\theta > \theta_1, \alpha < \alpha_1(\theta)\} \cup \{\theta > \tilde{\theta}_1, \alpha = \alpha_1(\theta)\} & \text{if } q = 3, \\ \{\theta > \theta_1, \alpha \leq \alpha_1(\theta)\} & \text{if } q \geq 4. \end{cases} \quad (2.50)$$

Denote the total number of positive solutions $\mathbf{z} = (z_1, \dots, z_{q-1})$ of the system of equations (2.31) by $\nu(\theta, \alpha)$ ($\theta \geq 1, \alpha \in \mathbb{R}$); of course, this number also depends on k and q . Theorems 2.8 and 2.9 can now be summarized as follows.

Theorem 2.10 (Non-uniqueness).

- (a) If $q = 2$ then $\nu(\theta, \alpha) \geq 2$ if and only if $(\theta, \alpha) \in A_2 \cup B_2 = A_2$.
- (b) If $q = 3$ then $\nu(\theta, \alpha) \geq 2$ if $(\theta, \alpha) \in A_3 \cup B_3$. The “only if” statement holds true at least for $k = 2, 3, 4$.
- (c) If $q \geq 4$ then $\nu(\theta, \alpha) \geq 2$ if and only if $(\theta, \alpha) \in A_q \cup B_q$.

Remark 2.9. The special case $q = 3$ in the definition (2.50) and in Theorem 2.10 emerges because for $\theta \leq \tilde{\theta}_1$ and $\alpha = \alpha_1(\theta)$, there is a (hypothetically unique) solution $(u, v) = (\theta - \frac{\theta+2}{k}, 1)$ of the system (2.33), which is, however, not admissible due to the constraint (2.34) and, therefore, does not destroy the uniqueness of solution to (2.31). This hypothesis is conjectured below; if it is true then “if” in Theorem 2.10(b) (i.e., $q = 3$) can be enhanced to “if and only if” for all $k \geq 2$.

Conjecture 2.1. If $q = 3, \theta \leq \tilde{\theta}_1$ and $\alpha = \alpha_1(\theta)$ then $(u, v) = (\theta - \frac{\theta+2}{k}, 1)$ is the sole solution of the system (2.33).

Remark 2.10. Regardless of Conjecture 2.1, the inclusion of a proper part of the curve $\alpha = \alpha_1(\theta)$ in the uniqueness region in the case $q = 3$ is indeed necessary. Namely, it can be proved (see Proposition 5.4) that if $\varepsilon > 0$ is small enough then $\nu(\theta, \alpha_1(\theta)) = 1$ for $\theta_1 < \theta < \theta_1 + \varepsilon$ but $\nu(\theta, \alpha_1(\theta)) \geq 2$ for $\theta > \theta_1^0 - \varepsilon$, where θ_1^0 is the zero of $\alpha_1(\theta)$.

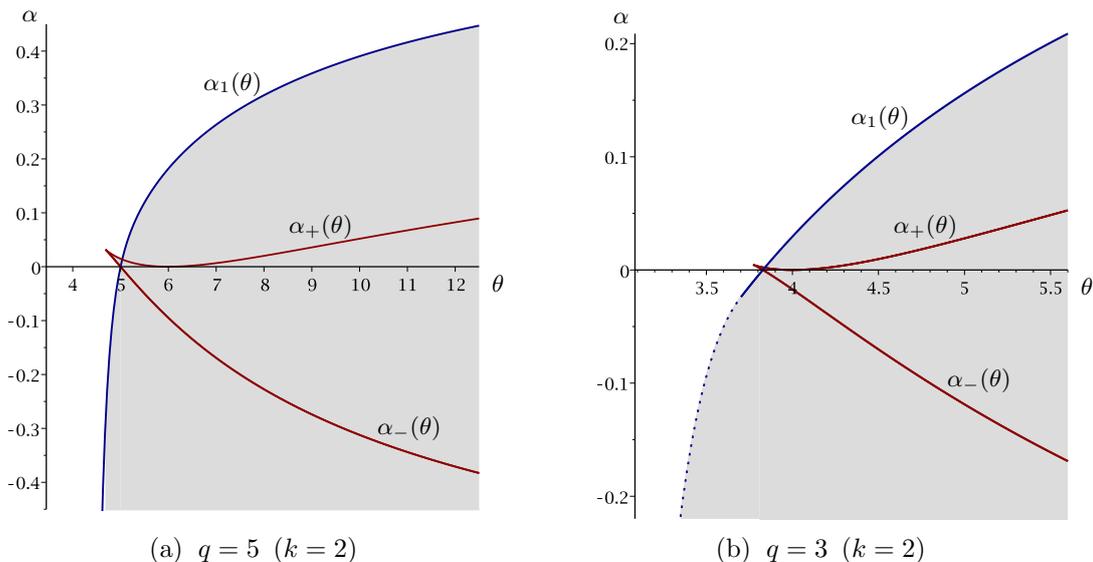


FIGURE 3. The phase diagram for the Potts model (2.30) showing the non-uniqueness region (shaded in grey) according to Theorem 2.10: (a) regular case $q \geq 4$ (shown here for $q = 5$); (b) special case $q = 3$, both with $k = 2$. The critical boundaries are determined by (parts of) the graphs of the functions $\alpha_{\pm}(\theta)$ and $\alpha_1(\theta)$ defined in (2.41) and (2.46), respectively. The dotted part of the boundary on panel (b), given by $\alpha = \alpha_1(\theta)$, $\theta \in (\theta_1, \tilde{\theta}_1]$ (see formula (2.50) with $q = 3$), is excluded from the shaded region (see Theorem 2.10(b) and Conjecture 2.1, proved for $2 \leq k \leq 4$); here, $\theta_1 = 3$ and $\tilde{\theta}_1 = \frac{1}{2}(1 + \sqrt{41}) \doteq 3.7016$.

Theorem 2.10 provides a sufficient and (almost) necessary condition for the uniqueness of solution of (2.31), illustrated in Figure 3 for $q = 5$ and $q = 3$, both with $k = 2$.

To conclude this subsection, the following result describes a few cases where it is possible to estimate the maximal number of solutions of the system (2.31).

Theorem 2.11.

- (a) If $q = 2$ then $\nu(\theta, \alpha) \leq 3$; moreover, $\nu(\theta, \alpha) = 3$ for all $\theta \geq 1$ large enough.
- (b) Let $\alpha = 0$ and $k \geq 2$. Then $\nu(\theta, 0) \leq 2^q - 1$ for all $\theta \geq 1$; moreover, $\nu(\theta, 0) = 2^q - 1$ for all θ large enough.
- (c) If $k = 2$ then $\nu(\theta, \alpha) \leq 2^q - 1$ for all $\theta \geq 1$ and $\alpha \in \mathbb{R}$.

Conjecture 2.2. The upper bound $2^q - 1$ in Theorem 2.11 appears to be universal. There is empirical evidence from exploration of many specific cases (using the computing package¹⁰ Maple) to conjecture that Theorem 2.11(c) holds true for all $k \geq 2$.

2.3.4. *Some comments on earlier work.* For $q = 2$, when the Potts model is reduced to the Ising model, the result of Theorem 2.11(a) is well known (see [22, Section 12.2] or [47, Chapter 2]). The case $\alpha = 0$ (i.e., with zero field) is also well studied (see, e.g., [47, Section 5.2.2.2, Proposition 5.4, pages 114–115] and [30, Theorem 1, page 192]), the result of Theorem 2.11(b) can be considered as a corollary of [30, Theorem 1,

¹⁰Throughout this paper, we used Maple 18 (Build ID 922027) licensed to the University of Leeds.

page 192]); in particular, it is known that there are $\lfloor \frac{1}{2}(q+1) \rfloor$ critical values of θ , including $\theta_0^- = \theta_1^0$ and $\theta_0^+ = 1 + q/(k-1)$.

The general case $q \geq 3$ with $\alpha \in \mathbb{R}$ was first addressed by Peruggi et al. [41] (and continued in [42]) using physical argumentation. In particular, they correctly identified the critical point θ_c [42, equation (22), page 160] (cf. (2.35)) and also suggested an explicit critical boundary in the phase diagram for $\alpha \geq 0$, defined by the expression [42, equation (21), page 160] (adapted to our notation)

$$\tilde{\alpha}_-(\theta) = \frac{(k+1)\ln(1+(q-2)/\theta) - (k-1)\ln(q-1)}{2\ln\theta}.$$

Note that this function enjoys a correct value at $\theta = \theta_c$ (i.e., $\tilde{\alpha}_-(\theta_c) = \alpha_{\pm}(\theta_c)$, see formula (6.4) below), but $\tilde{\alpha}_-(\theta) > \alpha_-(\theta)$ for all $\theta > \theta_c$. The corresponding critical value of activity θ , emerging as zero of $\tilde{\alpha}_-(\theta)$, is reported in [42, equation (20), page 158] as

$$\theta_{\text{cr}} = \theta_{\text{cr}}(k, q) := \frac{q-2}{(q-1)^{(k-1)/(k+1)} - 1}.$$

In particular, θ_{cr} is bigger than the exact critical value $\theta_0^- = \theta_1^0$, where the uniqueness breaks down at $\alpha = 0$ (see Proposition 6.16). For example, the corresponding numerical values (for $k = 5$ and $q = 3$ or $q = 8$) are given by (cf. [42, figure 1, page 159])

$$\theta_{\text{cr}} \doteq \begin{cases} 1.7024, & q = 3, \\ 2.2562, & q = 8, \end{cases} \quad \theta_0^- \doteq \begin{cases} 1.6966, & q = 3, \\ 2.1803, & q = 8. \end{cases}$$

The critical boundary in the phase diagram for $\alpha \leq 0$ was described in [42, page 160] only heuristically, as a line “joining” the points $\theta = \theta_{\text{cr}}(k, q)$, $\alpha = 0$ and $\theta = \theta_{\text{cr}}(k, q-1)$, $\alpha = -\infty$, and illustrated by a sketch graph in the vicinity of $\theta_{\text{cr}}(k, q)$ (for $k = 5$ and $q = 3$ or $q = 8$).

It should be stressed that the phase transition occurring at these critical boundaries is not of type “uniqueness/non-uniqueness”, with which we are primarily concerned in the present paper, but in fact the so-called “order/disorder” phase transition. The latter was studied rigorously in a recent paper by Galanis et al. [18] in connection with the computational complexity of approximating the partition function of the Potts model. The useful classification of critical points deployed in [18] is based on the notion of *dominant phase*; in particular, the critical point $\theta_0^+ = 1 + q/(k-1)$ (conjectured earlier by Häggström [26] in a more general context of random cluster measures on trees) can be explained from this point of view as a threshold beyond which only ordered phases are dominant. Note that the paper [18] studies the Potts model primarily with zero external field ($\alpha = 0$); the authors claim that their methods should also work in a more general ferromagnetic framework including a non-zero field, but no details are spelled out clearly.

In the present paper, we do not investigate the thermodynamical nature of phase transitions, instead focussing on the number of completely homogeneous SGMs, especially on the uniqueness issue. In particular, the order/disorder critical point θ_{cr} is not immediately detectable by our methods. It would be interesting to look into these issues for the Potts model with external field, thus extending the results of [18]. More specifically, our analysis (see Proposition 6.16) shows that the critical point θ_0^+ is the signature of the upper critical function $\alpha_+(\theta)$ at $\alpha = 0$, which has a minimum at $\theta = \theta_0^+$. Therefore, it is reasonable to *conjecture* that the $\alpha > 0$ analogue of the interval of activities θ between the critical points θ_0^- and θ_{cr} is the interval $[\theta_{\alpha}^-, \theta_{\alpha}^+]$,

where θ_α^- is the (sole) root of the equation $\alpha_-(\theta) = \alpha$ and θ_α^+ is the smaller root of the similar equation $\alpha_+(\theta) = \alpha$. However, it is not clear as to what happens in the interval *between* the roots of the latter equation. The counterpart of this picture for $\alpha < 0$ is likely to be simpler, as only the equation $\alpha_-(\theta) = \alpha$ is involved. We intend to address these issues in our forthcoming work.

3. AUXILIARY LEMMAS

In this section, we collect a few technical results that will be instrumental in the proofs of the main theorems. We start with an elementary lemma.

Lemma 3.1. *For $a, b, c, d > 0$, consider the function*

$$f(t) := \ln \frac{ae^t + b}{ce^t + d}, \quad t \in \mathbb{R}. \quad (3.1)$$

(a) *If $ad > bc$ then $f(t)$ is monotone increasing on \mathbb{R} and*

$$\ln \frac{b}{d} \leq f(t) \leq \ln \frac{a}{c}, \quad t \in \mathbb{R}. \quad (3.2)$$

Similarly, if $ad < bc$ then $f(t)$ is monotone decreasing on \mathbb{R} and

$$\ln \frac{a}{c} \leq f(t) \leq \ln \frac{b}{d}, \quad t \in \mathbb{R}.$$

(b) *Furthermore,*

$$|f'(t)| \leq \frac{|ad - bc|}{(\sqrt{ad} + \sqrt{bc})^2}, \quad t \in \mathbb{R}. \quad (3.3)$$

Proof. (a) Differentiating equation (3.1), we get

$$f'(t) = \frac{ae^t}{ae^t + b} - \frac{ce^t}{ce^t + d} = \frac{ad - bc}{ace^t + bde^{-t} + ad + bc}. \quad (3.4)$$

If $ad > bc$ then, according to (3.4), the function $f(t)$ is monotone increasing, and the bounds (3.2) follow by taking the limit as $t \rightarrow \pm\infty$. The case $ad < bc$ is similar.

(b) By the inequality between the arithmetic and geometric means, the denominator on the right-hand side of (3.4) is bounded below by

$$2\sqrt{abcd} + ad + bc = (\sqrt{ad} + \sqrt{bc})^2,$$

and the result (3.3) follows. \square

Let us define two norms for vector $u = (u_1, \dots, u_{q-1}) \in \mathbb{R}^{q-1}$,

$$\|u\|_\infty := \max_{1 \leq i \leq q-1} |u_i|, \quad \|u\|_1 := \sum_{i=1}^{q-1} |u_i|. \quad (3.5)$$

The next two lemmas give useful estimates for the function $\mathbf{F} = (F_1, \dots, F_{q-1})$ defined in (2.3) and for its partial derivatives.

Lemma 3.2. *For any $\theta \geq 1$, the following uniform estimate holds,*

$$\sup_{u \in \mathbb{R}^{q-1}} \|\mathbf{F}(u; \theta)\|_\infty \leq \ln \theta. \quad (3.6)$$

Proof. Note that F_i , as a function of u_i , may be represented by formula (3.1) with the coefficients

$$a = \theta, \quad b = 1 + s, \quad c = 1, \quad d = \theta + s, \quad s := \sum_{j \neq i} e^{u_j} \geq 0, \quad (3.7)$$

where

$$ad - bc = \theta(\theta + s) - (1 + s) = (\theta - 1)(\theta + 1 + s) > 0.$$

Therefore, by the estimates (3.2) we have

$$\ln \frac{1 + s}{\theta + s} \leq F_i(u; \theta) \leq \ln \theta. \quad (3.8)$$

Furthermore, noting that $(1 + s)/(\theta + s) \geq 1/\theta$, the two-sided bound (3.8) implies the inequality $|F_i(u; \theta)| \leq \ln \theta$, and the bound (3.6) follows by taking the maximum over $i = 1, \dots, q$. \square

Recall that the function $\varphi(t; \theta)$ is defined by (2.4). Denote by ∇F_i the gradient of the map $\mathbf{u} \mapsto F_i(\mathbf{u}; \theta)$,

$$\nabla F_i(\mathbf{u}; \theta) := \left(\frac{\partial F_i(\mathbf{u}; \theta)}{\partial u_1}, \dots, \frac{\partial F_i(\mathbf{u}; \theta)}{\partial u_{q-1}} \right), \quad \mathbf{u} \in \mathbb{R}^{q-1}.$$

Recall that the norm $\|\cdot\|_1$ is defined in (3.5).

Lemma 3.3. *For $\gamma \in \mathbb{R}$ and any $\mathbf{u} = (u_1, \dots, u_{q-1}) \in \mathbb{R}^{q-1}$ such that $\min_{1 \leq i \leq q-1} u_i \geq \gamma \ln \theta$, it holds*

$$\max_{1 \leq i \leq q-1} \|\nabla F_i(\mathbf{u}; \theta)\|_1 \leq Q(\theta) + \varphi(t_\gamma(\theta); \theta), \quad (3.9)$$

where $Q(\theta)$ is defined in (2.7) and $t_\gamma(\theta) = \theta + 1 + (q - 2)\theta^\gamma$ (see (2.14)). Moreover, the following uniform estimate holds,

$$\max_{1 \leq i \leq q-1} \sup_{\mathbf{u} \in \mathbb{R}^{q-1}} \|\nabla F_i(\mathbf{u}; \theta)\|_1 \leq Q(\theta) + \frac{\theta - 1}{\theta + 1}. \quad (3.10)$$

Proof. Like in the proof of Lemma 3.2, let us represent $F_i(\mathbf{u}; \theta)$ by formula (3.1) with the coefficients (3.7). Then by Lemma 3.1

$$\left| \frac{\partial F_i(\mathbf{u}; \theta)}{\partial u_i} \right| \leq \frac{(\theta - 1)(\theta + 1 + s)}{(\sqrt{\theta(\theta + s)} + \sqrt{1 + s})^2} = \varphi(\theta + 1 + s; \theta), \quad (3.11)$$

where $s = \sum_{j \neq i} e^{u_j} \geq (q - 2)\theta^\gamma = t_\gamma(\theta) - \theta - 1$. Hence, by monotonicity of the map $t \mapsto \varphi(t; \theta)$, from (3.11) it follows that

$$\left| \frac{\partial F_i(\mathbf{u}; \theta)}{\partial u_i} \right| \leq \varphi(t_\gamma(\theta); \theta). \quad (3.12)$$

On the other hand, expressing $F_i(\mathbf{u}; \theta)$ by formula (3.1) with

$$a = 1, \quad b = \theta e^{u_i} + 1 + s', \quad c = 1, \quad d = \theta + e^{u_i} + s', \quad s' := \sum_{\ell \neq i, j} e^{u_\ell} \geq 0,$$

by Lemma 3.1 we obtain

$$\left| \frac{\partial F_i(\mathbf{u}; \theta)}{\partial u_j} \right| \leq \frac{(\theta - 1)|e^{u_i} - 1|}{(\sqrt{\theta + e^{u_i} + s'} + \sqrt{\theta e^{u_i} + 1 + s'})^2}. \quad (3.13)$$

If $u_i > 0$ then the estimate (3.13) specializes to

$$\begin{aligned} \left| \frac{\partial F_i(\mathbf{u}; \theta)}{\partial u_j} \right| &\leq \frac{(\theta - 1)(e^{u_i} - 1)}{(\sqrt{\theta + e^{u_i} + s'} + \sqrt{\theta e^{u_i} + 1 + s'})^2} \\ &\leq \frac{\theta - 1}{(\sqrt{1 + (\theta + 1)/(e^{u_i} - 1)} + \sqrt{\theta + (\theta + 1)/(e^{u_i} - 1)})^2} \\ &\leq \frac{\theta - 1}{(\sqrt{1} + \sqrt{\theta})^2} = \frac{\sqrt{\theta} - 1}{\sqrt{\theta} + 1}. \end{aligned} \quad (3.14)$$

Similarly, if $u_i \leq 0$ then $1 \geq e^{u_i} > 0$ and from (3.13) we obtain

$$\begin{aligned} \left| \frac{\partial F_i(\mathbf{u}; \theta)}{\partial u_j} \right| &\leq \frac{(\theta - 1)(1 - e^{u_i})}{(\sqrt{\theta + e^{u_i} + s'} + \sqrt{\theta e^{u_i} + 1 + s'})^2} \\ &\leq \frac{\theta - 1}{(\sqrt{\theta} + \sqrt{1})^2} = \frac{\sqrt{\theta} - 1}{\sqrt{\theta} + 1}. \end{aligned} \quad (3.15)$$

Thus, combining (3.14) and (3.15), we have

$$\left| \frac{\partial F_i(\mathbf{u}; \theta)}{\partial u_j} \right| \leq \frac{\sqrt{\theta} - 1}{\sqrt{\theta} + 1}, \quad i \neq j. \quad (3.16)$$

As a result, according to the definition (3.5) of the norm $\|\cdot\|_1$, the bounds (3.12) and (3.16) imply the estimate (3.9).

Finally, since

$$\lim_{\gamma \rightarrow -\infty} \varphi(t_\gamma(\theta); \theta) = \varphi(\theta + 1; \theta) = \frac{\theta - 1}{\theta + 1}, \quad (3.17)$$

from (3.9) we obtain (3.10), and the proof of Lemma 3.3 is complete. \square

Remark 3.1. Estimates similar to (3.9) were proved in [49].

Lemma 3.4. *For integer $q \geq 2$ and any $\gamma \in \mathbb{R}$, the map $[1, \infty) \ni \theta \mapsto \varphi(t_\gamma(\theta); \theta)$ is a continuous, strictly increasing function with the range $[0, 1)$.*

Proof. Denoting $\tilde{q} := q - 2 \in \mathbb{N}_0$, by formula (2.5) we have

$$\begin{aligned} \varphi(t_\gamma(\theta); \theta) &= \varphi(\theta + 1 + \tilde{q}\theta^\gamma; \theta) = \frac{\sqrt{\theta(\theta + \tilde{q}\theta^\gamma)} - \sqrt{1 + \tilde{q}\theta^\gamma}}{\sqrt{\theta(\theta + \tilde{q}\theta^\gamma)} + \sqrt{1 + \tilde{q}\theta^\gamma}} \\ &= 1 - 2 \left(1 + \sqrt{\frac{\theta^2 + \tilde{q}\theta^{\gamma+1}}{1 + \tilde{q}\theta^\gamma}} \right)^{-1}. \end{aligned} \quad (3.18)$$

Clearly, the function (3.18) is continuous, so we only need to show that

$$A(\theta) := \frac{\theta^2 + \tilde{q}\theta^{\gamma+1}}{1 + \tilde{q}\theta^\gamma}, \quad \theta \geq 1, \quad (3.19)$$

is an increasing function.

First of all, if $\tilde{q} = 0$ then (3.19) is reduced to $A(\theta) = \theta^2$, so there is nothing to prove. Suppose that $\tilde{q} \geq 1$. Differentiating (3.19), it is easy to see that

$$A'(\theta) = \frac{2\theta + \tilde{q}\theta^\gamma [\theta + 2 + \tilde{q}\theta^\gamma + (1 - \gamma)(\theta - 1)]}{(1 + \tilde{q}\theta^\gamma)^2}, \quad (3.20)$$

and it is evident that the right-hand side of (3.20) is positive for all $\theta \geq 1$ as long as $\gamma \leq 1$. On the other hand, for $\gamma \geq 1$ by Bernoulli's inequality we have

$$\tilde{q}\theta^\gamma \geq \theta^\gamma = (1 + (\theta - 1))^\gamma \geq 1 + \gamma(\theta - 1),$$

and the expression in square brackets in (3.20) is estimated from below by $(\theta + 2) + 1 + (\theta - 1) = 2\theta + 2 > 0$. Thus, in all cases $A'(\theta) > 0$ for $\theta \geq 1$, as required.

Finally, from (3.19) we see that $A(1) = 1$ and $\lim_{\theta \rightarrow \infty} A(\theta) = \infty$, and it follows that the range of the function (3.18) is $[0, 1)$, which completes the proof of the lemma. \square

Lemma 3.5. *For $k \geq 2$, $q \geq 2$ and any $\gamma \in \mathbb{R}$, the equation (2.13) has a unique root $\theta_\gamma^* = \theta_\gamma^*(k, q)$. If $q = 2$ then $\theta_\gamma^*(k, 2) \equiv \theta_0(k, 2) = (k + 1)/(k - 1)$, where $\theta_0(k, q)$ is the root of the equation (2.9). For $q \geq 3$, the root θ_γ^* is a continuous monotone increasing function of γ , such that*

$$\lim_{\gamma \rightarrow -\infty} \theta_\gamma^*(k, q) = \theta_0(k, q), \quad \lim_{\gamma \rightarrow +\infty} \theta_\gamma^*(k, q) = (\theta_*(k, q))^2, \quad (3.21)$$

where $\theta_*(k, q)$ is the root of the equation (2.12); in particular,

$$\theta_0(k, q) < \theta_\gamma^*(k, q) < (\theta_*(k, q))^2. \quad (3.22)$$

Proof. The case $q = 2$ is straightforward, so assume that $q \geq 3$. Due to continuity and monotonicity of the function $Q(\theta)$ (see (2.7)) and by virtue of Lemma 3.4, the left-hand side of equation (2.13) is a continuous increasing function of $\theta \in [1, \infty)$, with the range $[0, q - 1)$ because

$$\lim_{\theta \downarrow 1} (Q(\theta) + \varphi(t_\gamma(\theta); \theta)) = 0, \quad \lim_{\theta \rightarrow \infty} (Q(\theta) + \varphi(t_\gamma(\theta); \theta)) = q - 1.$$

Hence, the equation (2.13) always has a unique solution, $\theta_\gamma^* = \theta_\gamma^*(k, q)$. Since $t_\gamma(\theta)$ is a continuous increasing function of γ , while the map $t \mapsto \varphi(t; \theta)$ is continuous and decreasing, it follows that the root θ_γ^* is continuous and increasing in γ .

Finally, observing that (see (2.6) and (3.17))

$$\lim_{\gamma \rightarrow -\infty} \varphi(t_\gamma(\theta); \theta) = \varphi(\theta + 1; \theta) = \frac{\theta - 1}{\theta + 1}, \quad \lim_{\gamma \rightarrow \infty} \varphi(t_\gamma(\theta); \theta) = \varphi(\infty; \theta) = \frac{\sqrt{\theta} - 1}{\sqrt{\theta} + 1},$$

and comparing equation (2.13) with the limiting equations as $\gamma \rightarrow \pm\infty$ (which have the roots θ_0 and θ_*^2 , respectively), we obtain the required limits (3.21), and hence the asymptotic bounds (3.22) for θ_γ^* . \square

4. PROOFS OF THE MAIN RESULTS RELATED TO UNIQUENESS

4.1. Proof of Theorem 2.1 (criterion of compatibility). For shorthand, denote temporarily $\zeta(x) := \mathbf{h}(x) + \boldsymbol{\xi}(x)$. Suppose that the compatibility condition (1.8) holds. On substituting (1.6), it is easy to see that (1.8) simplifies to

$$\prod_{x \in W_n} \prod_{y \in S(x)} \sum_{\omega(y) \in \Phi} \exp\{\beta(J_{xy} \delta_{\sigma_n(x), \omega(y)} + \zeta_{\omega(y)}(y))\} = \frac{Z_{n+1}}{Z_n} \prod_{x \in W_n} \exp\{\beta h_{\sigma_n(x)}(x)\}, \quad (4.1)$$

for any $\sigma_n \in \Phi^{V_n}$. Consider the equality (4.1) on configurations $\sigma_n^1, \sigma_n^2 \in \Phi^{V_n}$ that coincide everywhere in V_n except at vertex $x \in W_n$, where $\sigma_n^1(x) = i \leq q - 1$ and

$\sigma_n^2(x) = q$. Taking the log-ratio of the two resulting relations, we obtain

$$\sum_{y \in S(x)} \ln \frac{\exp\{\beta(J_{xy} + \zeta_i(y))\} + \sum_{j \neq i} \exp\{\beta \zeta_j(y)\}}{\exp\{\beta(J_{xy} + \zeta_q(y))\} + \sum_{j=1}^{q-1} \exp\{\beta \zeta_j(y)\}} = \beta(h_i(x) - h_q(x)),$$

which is readily reduced to (2.1) in view of the notation (2.2) and (2.3).

Conversely, again using (2.2) and (2.3), equation (2.1) can be rewritten in the coordinate form as follows,

$$\prod_{y \in S(x)} \sum_{j=1}^q \exp\{\beta(J_{xy} \delta_{ij} + \zeta_j(y))\} = a(x) \exp\{\beta h_i(x)\}, \quad i = 1, \dots, q-1, \quad (4.2)$$

where (omitting the immaterial dependence on β , \mathbf{h} and $\boldsymbol{\xi}$) we denote

$$a(x) := \exp\{\beta h_q(x)\} \prod_{y \in S(x)} \sum_{j=1}^q \exp\{\beta(J_{xy} \delta_{qj} + \zeta_j(y))\}, \quad x \in V.$$

Hence, using (4.2) and setting $A_n := \prod_{x \in W_n} a(x)$, we get

$$\begin{aligned} \sum_{\omega \in \Phi^{W_{n+1}}} \mu_{n+1}^h(\sigma_n \vee \omega) &= \frac{\exp\{-\beta H_n(\sigma_n)\}}{Z_{n+1}} \prod_{x \in W_n} \prod_{y \in S(x)} \sum_{j=1}^q \exp\{\beta(J_{xy} \delta_{\sigma_n(x), j} + \zeta_j(y))\} \\ &= \frac{A_n}{Z_{n+1}} \exp\left\{-\beta H_n(\sigma_n) + \beta \sum_{x \in W_n} h_{\sigma_n(x)}(x)\right\} = \frac{A_n Z_n}{Z_{n+1}} \mu_n^h(\sigma_n). \end{aligned} \quad (4.3)$$

Finally, observe that

$$\sum_{\sigma_n \in \Phi^{V_n}} \sum_{\omega \in \Phi^{W_{n+1}}} \mu_{n+1}^h(\sigma_n \vee \omega) = \sum_{\sigma_{n+1} \in \Phi^{V_{n+1}}} \mu_{n+1}^h(\sigma_{n+1}) = 1,$$

whereas from the right-hand side of (4.3) the same sum is given by

$$\sum_{\sigma_n \in \Phi^{V_n}} \frac{A_n Z_n}{Z_{n+1}} \mu_n^h(\sigma_n) = \frac{A_n Z_n}{Z_{n+1}}.$$

Hence, $A_n Z_n / Z_{n+1} = 1$ and formula (4.3) yields (1.8), as required. This completes the proof of Theorem 2.1.

4.2. Preparatory results for the uniqueness of SGM. First, let us rewrite the functional equation (2.1) in a form more convenient for iterations. Recall that we assume $J_{xy} \equiv J > 0$ ($d(x, y) = 1$) and use the notation $\theta = e^{\beta J}$.

Lemma 4.1. *Via the substitutions*

$$\mathbf{g}(x) = \mathbf{F}(\beta \check{\mathbf{h}}(x) + \beta \check{\boldsymbol{\xi}}(x); \theta) \in \mathbb{R}^{q-1}, \quad x \in V, \quad (4.4)$$

and

$$\check{\mathbf{h}}(x) = \beta^{-1} \sum_{y \in S(x)} \mathbf{g}(y), \quad x \in V, \quad (4.5)$$

equation (2.1) is equivalent to the fixed-point equation

$$\mathbf{g}(x) = \boldsymbol{\Psi} \mathbf{g}(x), \quad x \in V, \quad (4.6)$$

where the mapping $\Psi: (\mathbb{R}^{q-1})^V \rightarrow (\mathbb{R}^{q-1})^V$ is defined by

$$\Psi \mathbf{g}(x) := \mathbf{F} \left(\beta \check{\xi}(x) + \sum_{y \in S(x)} \mathbf{g}(y); \theta \right), \quad x \in V. \quad (4.7)$$

Proof. By means of (4.4), the recursive equation (2.1) for $\check{\mathbf{h}}$ can be written as (4.5). Substituting this into (4.4) and using the notation (4.7), we see that \mathbf{g} solves the functional equation (4.6). Conversely, if \mathbf{g} satisfies the equation (4.6) then for $\check{\mathbf{h}}$ defined by (4.5) we have, using (4.7),

$$\begin{aligned} \beta \check{\mathbf{h}}(x) &= \sum_{y \in S(x)} \mathbf{g}(y) = \sum_{y \in S(x)} \Psi \mathbf{g}(y) \\ &= \sum_{y \in S(x)} \mathbf{F} \left(\beta \check{\xi}(y) + \sum_{z \in S(y)} \mathbf{g}(z); \theta \right) \\ &= \sum_{y \in S(x)} \mathbf{F}(\beta \check{\xi}(y) + \beta \check{\mathbf{h}}(y); \theta), \end{aligned}$$

so that $\check{\mathbf{h}}$ solves the equation (2.1). Thus, Lemma 4.1 is proved. \square

In particular, Lemma 4.1 implies that for the proof of uniqueness of SGM it suffices to show that the equation (4.6) has a unique solution $\mathbf{g}(x)$ ($x \in V$).

Let us state and prove one general result in the contraction case. On the vector space $(\mathbb{R}^{q-1})^V$ of \mathbb{R}^{q-1} -valued functions on the vertex set V of the Cayley tree \mathbb{T}^k , introduce the sup-norm

$$\|\mathbf{g}\|_V := \sup_{x \in V} \|\mathbf{g}(x)\|_\infty = \sup_{x \in V} \max_{1 \leq i \leq q-1} |g_i(x)|, \quad \mathbf{g}(x) = (g_1(x), \dots, g_{q-1}(x)).$$

Sometimes, we need the similar norm for functions restricted to subsets $\Lambda \subseteq V$,

$$\|\mathbf{g}\|_\Lambda := \sup_{x \in \Lambda} \|\mathbf{g}(x)\|_\infty, \quad \mathbf{g} \in (\mathbb{R}^{q-1})^\Lambda. \quad (4.8)$$

The next lemma and its proof are an adaptation of a standard result for $\ell^\infty(\mathbb{R})$.

Lemma 4.2. *For any subset $\Lambda \subseteq V$, the space $(\mathbb{R}^{q-1})^\Lambda$ is complete with respect to the sup-norm (4.8).*

Proof. Let $\{\mathbf{g}^n\}$ be a Cauchy sequence in $(\mathbb{R}^{q-1})^\Lambda$, that is, for any $\varepsilon > 0$ there is $N \in \mathbb{N}$ such that for any $n, m \geq N$ we have $\|\mathbf{g}^n - \mathbf{g}^m\|_\Lambda < \varepsilon$. In particular, $\{\mathbf{g}^n\}$ is bounded, $\|\mathbf{g}^n\|_\Lambda \leq M < \infty$ for some $M > 0$ and all $n \in \mathbb{N}$. Note that every coordinate sequence $\{g_i^n(x)\}$ ($i = 1, \dots, q-1$, $x \in \Lambda$) is also a Cauchy sequence (in \mathbb{R}) because, according to (3.5), $|g_i^n(x) - g_i^m(x)| \leq \|\mathbf{g}^n - \mathbf{g}^m\|_\Lambda < \varepsilon$; hence, it converges to a limit which we denote $g_i(x)$. Clearly, $|g_i(x)| \leq M$ and $\|\mathbf{g}\|_\Lambda = \sup_{x \in \Lambda} \max_i |g_i(x)| \leq M < \infty$.

Now, passing to the limit as $m \rightarrow \infty$ in each inequality $|g_i^n(x) - g_i^m(x)| < \varepsilon$, we obtain $|g_i^n(x) - g_i(x)| \leq \varepsilon$, which implies that $\|\mathbf{g}^n - \mathbf{g}\|_\Lambda \leq \varepsilon$, for all $n \geq N$. Since $\varepsilon > 0$ is arbitrary, we conclude that $\|\mathbf{g}^n - \mathbf{g}\|_\Lambda \rightarrow 0$ as $n \rightarrow \infty$, and the lemma is proved. \square

We also require the following simple estimate.

Lemma 4.3. *Let $f(\mathbf{u}): \mathbb{R}^{q-1} \rightarrow \mathbb{R}$ be a C^1 -function and $\nabla f(\mathbf{u}) = (\frac{\partial f(\mathbf{u})}{\partial u_1}, \dots, \frac{\partial f(\mathbf{u})}{\partial u_{q-1}})$ its gradient. Then, for any $\mathbf{v}, \mathbf{w} \in \mathbb{R}^{q-1}$,*

$$|f(\mathbf{w}) - f(\mathbf{v})| \leq \|\mathbf{w} - \mathbf{v}\|_\infty \sup_{\mathbf{u} \in \mathbb{R}^{q-1}} \|\nabla f(\mathbf{u})\|_1. \quad (4.9)$$

Proof. Define the function $\psi(t) := f(\mathbf{v} + t(\mathbf{w} - \mathbf{v}))$, $t \in [0, 1]$, then

$$f(\mathbf{w}) - f(\mathbf{v}) = \psi(1) - \psi(0) = \int_0^1 \psi'(t) dt = \int_0^1 \sum_{i=1}^{q-1} \frac{\partial f(\mathbf{v} + t(\mathbf{w} - \mathbf{v}))}{\partial u_i} (w_i - v_i) dt,$$

whence the estimate (4.9) readily follows. \square

Theorem 4.4. *Suppose that, for some $\theta > 1$,*

$$\lambda(\theta) := k \max_{1 \leq i \leq q-1} \sup_{\mathbf{u} \in \mathbb{R}^{q-1}} \|\nabla F_i(\mathbf{u}; \theta)\|_1 < 1. \quad (4.10)$$

Then, for every realization of the field $\check{\xi} = \{\check{\xi}(x)\}_{x \in V}$, the equation (4.6) has a unique solution.

Proof. Consider a mapping $\Psi = (\Psi_1, \dots, \Psi_{q-1})$ of the space $(\mathbb{R}^{q-1})^V$ to itself defined by formula (4.7). Solving the functional equation (4.6) is then equivalent to finding a fixed point of Ψ , that is, $\Psi \mathbf{g}^* = \mathbf{g}^*$. The lemma's hypothesis implies that Ψ is a *contraction* on $(\mathbb{R}^{q-1})^{V_0^c}$; indeed, for any functions $\mathbf{g}, \bar{\mathbf{g}} \in (\mathbb{R}^{q-1})^V$ and each $i = 1, \dots, q-1$, we obtain, using (4.7) and Lemma 4.3,

$$|\Psi_i \mathbf{g}(x) - \Psi_i \bar{\mathbf{g}}(x)| \leq \sup_{\mathbf{u} \in \mathbb{R}^{q-1}} \|\nabla F_i(\mathbf{u}; \theta)\|_1 \sum_{y \in S(x)} \|\mathbf{g}(y) - \bar{\mathbf{g}}(y)\|_\infty.$$

Noting that for $x \neq x_0$ the set $S(x)$ contains exactly k vertices, and recalling condition (4.10) with $\lambda(\theta) \in [0, 1)$, it follows that

$$\begin{aligned} \|\Psi \mathbf{g} - \Psi \bar{\mathbf{g}}\|_{V_0^c} &= \sup_{x \in V_0^c} \|\Psi \mathbf{g}(x) - \Psi \bar{\mathbf{g}}(x)\|_\infty \\ &\leq \max_{1 \leq i \leq q-1} \sup_{\mathbf{u} \in \mathbb{R}^{q-1}} \|\nabla F_i(\mathbf{u}; \theta)\|_1 \cdot k \|\mathbf{g} - \bar{\mathbf{g}}\|_{V_0^c} = \lambda(\theta) \|\mathbf{g} - \bar{\mathbf{g}}\|_{V_0^c}. \end{aligned}$$

Thus, because $(\mathbb{R}^{q-1})^{V_0^c}$ is a Banach space (Lemma 4.2), the well-known Banach contraction principle (e.g., [51, Theorem 9.23, page 220]) implies that $\|\mathbf{g} - \bar{\mathbf{g}}\|_{V_0^c} = 0$, that is, $\mathbf{g}(x) = \bar{\mathbf{g}}(x)$ for all $x \in V_0^c$. It remains to notice that the value of the solution $\mathbf{g}(x)$ at $x = x_0$ is uniquely determined from formulas (4.6) and (4.7) using the (unique) values outside $V_0 = \{x_0\}$. This completes the proof of Theorem 4.4. \square

Remark 4.1. The unique solution \mathbf{g}^* can be obtained by iterations [51]; for example, put $\mathbf{g}^0 \equiv \mathbf{0}$ and define $\mathbf{g}^n := \Psi \mathbf{g}^{n-1}$ ($n \in \mathbb{N}$), then $\mathbf{g}^n \rightarrow \mathbf{g}^*$ as $n \rightarrow \infty$ (i.e., $\lim_{n \rightarrow \infty} \|\mathbf{g}^n - \mathbf{g}^*\|_V = 0$).

Remark 4.2. It is straightforward to generalize Theorem 4.4 to the case where the vector $\beta \check{\xi}(x) + \sum_{y \in S(x)} \mathbf{g}(y)$ (see (4.7)) is guaranteed to be in a convex domain $B(x) \subseteq \mathbb{R}^{q-1}$ for any function $\mathbf{g}: V \rightarrow \mathbb{R}^{q-1}$ from a suitable subspace $\mathcal{D} \subseteq (\mathbb{R}^{q-1})^V$, such that \mathcal{D} is closed with respect to the norm $\|\cdot\|_V$ and $\Psi(\mathcal{D}) \subseteq \mathcal{D}$. In that case, the supremum in (4.10) should be taken over all $\mathbf{u} \in B(x)$,

$$\lambda(\theta) := k \sup_{x \in V} \max_{1 \leq i \leq q-1} \sup_{\mathbf{u} \in B(x)} \|\nabla F_i(\mathbf{u}; \theta)\|_1 < 1,$$

and the unique solution \mathbf{g}^* automatically belongs to \mathcal{D} . For our purposes, it will suffice to consider the balls $B(x) = \{\mathbf{u} \in \mathbb{R}^{q-1} : \|\mathbf{u} - \beta \check{\xi}(x)\|_\infty \leq k \ln \theta\}$ and the corresponding subspace $\mathcal{D} = \{\mathbf{g} \in (\mathbb{R}^{q-1})^V : \|\mathbf{g}\|_V \leq \ln \theta\}$ (see Lemma 3.2).

4.3. Proofs of Theorems 2.2, 2.3 and 2.5 (uniqueness). By virtue of Remark 1.5, for the uniqueness in the class of all Gibbs measure it suffices to prove it for SGMs.

4.3.1. *Proof of Theorem 2.2.* By virtue of the uniform bound (3.10) of Lemma 3.3, for every $\theta \in [1, \theta_0)$ we have

$$\lambda(\theta) = k \max_{1 \leq i \leq q-1} \sup_{\mathbf{u} \in \mathbb{R}^{q-1}} \|\nabla F_i(\mathbf{u}; \theta)\|_1 \leq k \left(Q(\theta) + \frac{\theta - 1}{\theta + 1} \right) < 1,$$

and the required result follows by Theorem 4.4.

4.3.2. *Proof of Theorem 2.3.* In view of equation (2.13) with $\gamma = \Delta^\xi - k$, we have

$$Q(\theta) + \varphi(t_{\Delta^\xi - k}(\theta); \theta) < \frac{1}{k}, \quad \theta \in [1, \theta_{\Delta^\xi - k}^*]. \quad (4.11)$$

By continuity of the map $\gamma \mapsto \varphi(t_\gamma(\theta); \theta)$, inequality (4.11) extends to

$$Q(\theta) + \varphi(t_{\Delta^\xi - \delta - k}(\theta); \theta) < \frac{1}{k}, \quad (4.12)$$

for some $\delta > 0$ small enough.

According to the definition (2.16), there exists an integer N such that

$$\max_{1 \leq \ell \leq q} \inf_{x \in V_N^c} \ell \check{\xi}_{(1)}(x) \geq \Delta^\xi - \delta. \quad (4.13)$$

For a specific reduction $\ell \check{\xi}(x) \in \ell \check{\mathbb{R}}^q$, with components $\ell \check{\xi}_j(x) = \xi_j(x) - \xi_\ell(x)$ ($j \neq \ell$), denote by $\ell F_i(\mathbf{u}; \theta)$ ($i \neq \ell$) the corresponding functions analogous to $F_i(\mathbf{u}; \theta)$ that were defined in (2.3) under the standard reduction (i.e., with $\ell = q$). Lemma 3.3 (modified to the case of reduction via the ℓ -th coordinate) implies that

$$\max_{i \neq \ell} \sup_{\mathbf{u} \in B_\ell(x)} \|\nabla \ell F_i(\mathbf{u}; \theta)\|_1 \leq Q(\theta) + \varphi(t_{\ell \check{\xi}_{(1)}(x) - k}(\theta); \theta), \quad (4.14)$$

where

$$B_\ell(x) := \left\{ \mathbf{u} \in \ell \check{\mathbb{R}}^q : \min_{j \neq \ell} u_j \geq (\ell \check{\xi}_{(1)}(x) - k) \ln \theta \right\}.$$

Furthermore, exploiting monotonicity and continuity of the function $t \mapsto \varphi(t; \theta)$, we obtain from (4.14)

$$\min_{1 \leq \ell \leq q} \sup_{x \in V_N^c} \max_{i \neq \ell} \sup_{\mathbf{u} \in B_\ell(x)} \|\nabla \ell F_i(\mathbf{u}; \theta)\|_1 \leq Q(\theta) + \varphi(t_N^*(\theta); \theta), \quad (4.15)$$

with

$$t_N^*(\theta) := \max_{1 \leq \ell \leq q} \inf_{x \in V_N^c} t_{\ell \check{\xi}_{(1)}(x) - k}(\theta).$$

Due to the bound (4.13), we have $t_N^*(\theta) \geq t_{\Delta^\xi - \delta - k}(\theta)$, and by monotonicity of $t \mapsto \varphi(t; \theta)$ it follows that

$$Q(\theta) + \varphi(t_N^*(\theta); \theta) \leq Q(\theta) + \varphi(t_{\Delta^\xi - \delta - k}(\theta); \theta) < \frac{1}{k},$$

according to the estimate (4.12). Together with (4.15), this implies that (cf. condition (4.10))

$$\lambda_N(\theta) := k \min_{1 \leq \ell \leq q} \sup_{x \in V_N^c} \max_{i \neq \ell} \sup_{\mathbf{u} \in B_\ell(x)} \|\nabla \ell F_i(\mathbf{u}; \theta)\|_1 < 1.$$

Hence, by an extended version of Theorem 4.4 (see Remark 4.2), it follows that the solution $\mathbf{g}(x)$ to the functional equation (4.6) is unique on the subset $\{x \in V_N^c\}$. Finally, the values of the solution $\mathbf{g}(x)$ for $x \in V_N$ are retrieved uniquely by the ‘‘backward’’ recursion (4.6) using (4.7). Thus, the proof of Theorem 2.3 is complete.

4.3.3. *Proof of Theorem 2.5.* Let $\mu_{\beta,\xi}$ and $\bar{\mu}_{\beta,\xi}$ be two SGMs determined by the functions $\mathbf{g}(x)$ and $\bar{\mathbf{g}}(x)$, respectively, each satisfying the functional equation (4.6). Our aim is to show that, under the theorem's hypotheses, $\mathbf{g}(x) \equiv \bar{\mathbf{g}}(x)$, which would imply that $\mu_{\beta,\xi} = \bar{\mu}_{\beta,\xi}$. The idea of the proof is to obtain a suitable upper bound on the norm $\|\mathbf{g}(x) - \bar{\mathbf{g}}(x)\|_\infty$ for $x \in W_n$ in terms of $\|\mathbf{g}(y) - \bar{\mathbf{g}}(y)\|_\infty$ for $y \in W_{n+1}$, and to propagate this estimate along the tree. To circumvent cumbersome notation arising from the direct iterations, we will use mathematical induction. Consider the filtration $\mathcal{F}_0 \subset \mathcal{F}_1 \subset \dots \mathcal{F}_n \subset \dots$ consisting of the sigma-algebras \mathcal{F}_n generated by the values of the random field $\boldsymbol{\xi}$ in the sequence of expanding balls $V_n = \{x \in V : d(x_\circ, x) \leq n\}$,

$$\mathcal{F}_n := \sigma\{\boldsymbol{\xi}(x) : x \in V_n\}, \quad n \in \mathbb{N}_0.$$

Put

$$\lambda(\theta) := k \left(Q(\theta) + \mathbb{E}[\varphi(t_{\check{\xi}_{(1)}(x)-k}(\theta); \theta)] \right), \quad (4.16)$$

where the expectation does not depend on $x \in V$ due to the i.i.d. assumption on the field $\{\boldsymbol{\xi}(x)\}$. Let us first show that for each $x \in W_n$ ($n \geq 1$) we have the upper bound

$$\mathbb{E}(\|\mathbf{g}(x) - \bar{\mathbf{g}}(x)\|_\infty | \mathcal{F}_{n-1}) \leq 2 \ln \theta (\lambda(\theta))^m, \quad m \in \mathbb{N}_0, \quad (4.17)$$

where $\mathbb{E}(\cdot | \mathcal{F}_{n-1})$ stands for the conditional expectation.

Fix $x \in W_n$. The base of induction ($m = 0$) is obvious, noting that, due to (4.6), (4.7) and Lemma 3.2,

$$\|\mathbf{g}(x) - \bar{\mathbf{g}}(x)\|_\infty \leq \|\mathbf{g}(x)\|_\infty + \|\bar{\mathbf{g}}(x)\|_\infty \leq 2 \ln \theta.$$

Suppose now that the bound (4.17) is true for some $m \in \mathbb{N}_0$, and show that it holds for $m + 1$ as well. By Lemma 4.3 we have

$$\begin{aligned} \|\mathbf{g}(x) - \bar{\mathbf{g}}(x)\|_\infty &= \|\Psi \mathbf{g}(x) - \Psi \bar{\mathbf{g}}(x)\|_\infty \\ &\leq \max_{1 \leq i \leq q-1} \sup_{\mathbf{u} \in B(x)} \|\nabla F_i(\mathbf{u}; \theta)\|_1 \sum_{y \in S(x)} \|\mathbf{g}(y) - \bar{\mathbf{g}}(y)\|_\infty, \end{aligned} \quad (4.18)$$

where $B(x) \subset \mathbb{R}^{q-1}$ is the ball of radius $k \ln \theta$ centred at $\beta \check{\boldsymbol{\xi}}(x)$,

$$B(x) := \{\mathbf{u} \in \mathbb{R}^{q-1} : \|\mathbf{u} - \beta \check{\boldsymbol{\xi}}(x)\|_\infty \leq k \ln \theta\}.$$

Recalling that $\beta = \ln \theta$, observe that if $\mathbf{u} = (u_1, \dots, u_{q-1}) \in B(x)$ then, for each $i = 1, \dots, q-1$,

$$u_i \geq \beta \check{\xi}_i(x) - k \ln \theta = \ln \theta (\check{\xi}_i(x) - k),$$

and hence

$$\min_{1 \leq i \leq q-1} u_i \geq \ln \theta \min_{1 \leq i \leq q-1} (\check{\xi}_i(x) - k) = \ln \theta (\check{\xi}_{(1)}(x) - k),$$

with $\check{\xi}_{(1)}(x) = \min_{1 \leq i \leq q-1} \check{\xi}_i(x)$. Therefore, on applying Lemma 3.3 we have

$$\max_{1 \leq i \leq q-1} \sup_{\mathbf{u} \in B(x)} \|\nabla F_i(\mathbf{u}; \theta)\|_1 \leq Q(\theta) + \varphi(t_{\check{\xi}_{(1)}(x)-k}(\theta); \theta).$$

Thus, returning to (4.18) we get

$$\|\mathbf{g}(x) - \bar{\mathbf{g}}(x)\|_\infty \leq [Q(\theta) + \varphi(t_{\check{\xi}_{(1)}(x)-k}(\theta); \theta)] \sum_{y \in S(x)} \|\mathbf{g}(y) - \bar{\mathbf{g}}(y)\|_\infty. \quad (4.19)$$

Now, take the conditional expectation $\mathbb{E}(\cdot | \mathcal{F}_n)$ on both sides of (4.19), noting that the factor in front of the sum is a random variable measurable with respect to the

sigma-algebra \mathcal{F}_n , so it can be pulled out of the expectation (see [56, Property **K***, page 216]). This yields

$$\begin{aligned} \mathbb{E}[\|\mathbf{g}(x) - \bar{\mathbf{g}}(x)\|_\infty | \mathcal{F}_n] &\leq [Q(\theta) + \varphi(t_{\xi_{(1)}(x)-k}(\theta); \theta)] \sum_{y \in S(x)} \mathbb{E}[\|\mathbf{g}(y) - \bar{\mathbf{g}}(y)\|_\infty | \mathcal{F}_n] \\ &\leq k [Q(\theta) + \varphi(t_{\xi_{(1)}(x)-k}(\theta); \theta)] \cdot 2 \ln \theta (\lambda(\theta))^m, \end{aligned} \quad (4.20)$$

where in the last inequality we used that $\text{card } S(x) = k$ and also applied the induction hypothesis to each $y \in S(x)$ (see (4.17)). In turn, using the tower property of conditional expectation (see [56, Property **H***, page 216]) with $\mathcal{F}_{n-1} \subset \mathcal{F}_n$, from (4.20) we obtain

$$\begin{aligned} \mathbb{E}(\|\mathbf{g}(x) - \bar{\mathbf{g}}(x)\|_\infty | \mathcal{F}_{n-1}) &= \mathbb{E}[\mathbb{E}[\|\mathbf{g}(x) - \bar{\mathbf{g}}(x)\|_\infty | \mathcal{F}_n] | \mathcal{F}_{n-1}] \\ &\leq k \mathbb{E}[Q(\theta) + \varphi(t_{\xi_{(1)}(x)-k}(\theta); \theta) | \mathcal{F}_{n-1}] \cdot 2 \ln \theta (\lambda(\theta))^m \\ &= k \mathbb{E}[Q(\theta) + \varphi(t_{\xi_{(1)}(x)-k}(\theta); \theta)] \cdot 2 \ln \theta (\lambda(\theta))^m \\ &= 2 \ln \theta (\lambda(\theta))^{m+1} \end{aligned}$$

(see (4.16)). Thus, the induction step is completed and, therefore, the claim (4.17) is true for all $m \geq 0$. In particular, again using the tower property of conditional expectation, from (4.17) we readily get

$$\begin{aligned} \mathbb{E}(\|\mathbf{g}(x) - \bar{\mathbf{g}}(x)\|_\infty) &= \mathbb{E}[\mathbb{E}(\|\mathbf{g}(x) - \bar{\mathbf{g}}(x)\|_\infty | \mathcal{F}_{n-1})] \\ &\leq 2 \ln \theta (\lambda(\theta))^m. \end{aligned} \quad (4.21)$$

Now, if $\theta^\dagger > 1$ is the (unique) solution of the equation (2.22), then $\lambda(\theta) < 1$ for all $\theta \in [1, \theta^\dagger)$. Hence, taking the limit of (4.21) as $m \rightarrow \infty$ gives

$$\mathbb{E}(\|\mathbf{g}(x) - \bar{\mathbf{g}}(x)\|_\infty) = 0, \quad x \neq x_\circ,$$

and therefore $\mathbf{g}(x) = \bar{\mathbf{g}}(x)$ (a.s.) for any $x \neq x_\circ$. It remains to notice that this equality extends to $x = x_\circ$ by the recursion (4.6).

5. ANALYSIS OF THE MODEL WITH CONSTANT FIELD

5.1. **Classification of positive solutions to the system (2.31).** Denote

$$p_k(z) := z^{k-1} + \dots + z, \quad (5.1)$$

so that

$$z^k - 1 = (z - 1)(p_k(z) + 1). \quad (5.2)$$

Lemma 5.1. *Let (z_1, \dots, z_{q-1}) be a solution to (2.31), with $z_i > 0$ ($i = 1, \dots, q-1$).*

- (a) *If $\theta = 1$ then $z_1 = \dots = z_{q-1} = 1$ is the unique solution.*
- (b) *If $\theta > 1$ and $\alpha = 0$ then either $z_1 = \dots = z_{q-1} = 1$ or there is a non-empty subset $\mathcal{I}_0 \subseteq \{1, \dots, q-1\}$, with $m := \text{card } \mathcal{I}_0$ ranging from 1 to $q-1$, such that*

$$z_i = \begin{cases} u & \text{if } i \in \mathcal{I}_0, \\ 1 & \text{otherwise,} \end{cases}$$

where $u = u(\theta, m) \neq 1$ satisfies the equation

$$1 = \frac{(\theta - 1)(p_k(u) + 1)}{\theta + mu^k + q - 1 - m}. \quad (5.3)$$

(c) If $\theta > 1$ and $\alpha \neq 0$ then:

(i) either $z_1 = u$ and $z_2 = \cdots = z_{q-1} = 1$, where $u = u(\theta, \alpha)$ satisfies the equation

$$u = 1 + \frac{(\theta - 1)(\theta^\alpha u^k - 1)}{\theta + \theta^\alpha u^k + q - 2} \quad (5.4)$$

and, in particular, $u \neq 1$;

(ii) or, provided that $q \geq 3$, there is a non-empty subset $\mathcal{I}_1 \subseteq \{2, \dots, q-1\}$, with $m := \text{card } \mathcal{I}_1$ ranging from 1 to $q-2$, such that

$$z_i = \begin{cases} u & \text{if } i = 1, \\ v & \text{if } i \in \mathcal{I}_1, \\ 1 & \text{otherwise,} \end{cases}$$

where $u = u(\theta, \alpha, m)$ and $v = v(\theta, \alpha, m) \neq 1$ satisfy the set of equations

$$\begin{cases} u = 1 + \frac{(\theta - 1)(\theta^\alpha u^k - 1)}{\theta + \theta^\alpha u^k + mv^k + q - 2 - m}, \\ 1 = \frac{(\theta - 1)(p_k(v) + 1)}{\theta + \theta^\alpha u^k + mv^k + q - 2 - m}, \end{cases} \quad (5.5)$$

and, in particular, $u \neq 1$ and $u \neq v$.

Proof. As a general remark, observe that $z_i = 1$ solves the i -th equation of the system (2.31) regardless of all other z_j with $j \neq i$.

(a) Obvious.

(b) In this case, the system (2.31) takes the form

$$z_i = 1 + \frac{(\theta - 1)(z_i^k - 1)}{\theta + \sum_{j=1}^{q-1} z_j^k}, \quad i = 1, \dots, q-1. \quad (5.6)$$

Suppose that the set $\mathcal{I}_0 := \{i \geq 1: z_i \neq 1\}$ is non-empty. By virtue of the identity (5.2), for any $i \in \mathcal{I}_0$ equation (5.6) is reduced to

$$(\theta - 1)p_k(z_i) = 1 + \sum_{j=1}^{q-1} z_j^k. \quad (5.7)$$

Because the right-hand side of (5.7) does not depend on $i \in \mathcal{I}_0$ and the function $p_k(z)$ is strictly increasing for $z > 0$, it follows that $z_i =: u = \text{const}$ ($i \in \mathcal{I}_0$). Specifically, if $\text{card } \mathcal{I}_0 = m \geq 1$ then equation (5.6) specializes to (5.3).

(c) The proof is similar to part (b). First of all, note that $u := z_1 \neq 1$, for otherwise the first equation in (2.31) is not satisfied unless $\theta = 1$ or $\alpha = 0$, either of which is ruled out. Next, if $z_2 = \cdots = z_{q-1} = 1$ then the first equation for $z_1 = u$ in (2.31) specializes to (5.4), as stated.

Suppose now that $\mathcal{I}_1 := \{i \geq 2: z_i \neq 1\} \neq \emptyset$, then similarly as above we show that $z_i = \text{const}$ ($i \in \mathcal{I}_1$), and the system (2.31) specializes to equations (5.5) with $z_1 = u$ and $z_i = v$ ($i \in \mathcal{I}_1$).

Finally, assuming to the contrary that $u = v$ and comparing the equations in (5.5), we would conclude that $\theta^\alpha u^k = u^k$, that is, $\alpha = 0$, which is ruled out. Hence, $u \neq v$ as claimed.

Thus, the proof of Lemma 5.1 is complete. \square

Remark 5.1. It is not hard to check that, in the limit as $\alpha \rightarrow 0$, case (c) of Lemma 5.1 transforms into case (b).

5.2. Proof of Theorem 2.8. By the substitution

$$u^k = \frac{(q-1)x}{\theta^{\alpha+1}}, \quad x > 0, \quad (5.8)$$

equation (2.32) can be represented in the form

$$ax = f(x), \quad f(x) := \left(\frac{1+x}{b+x} \right)^k, \quad (5.9)$$

with the coefficients (cf. (2.36))

$$a = a(\theta) := \frac{q-1}{\theta^{k+1+\alpha}} > 0, \quad b = b(\theta) := \frac{\theta(\theta+q-2)}{q-1} \geq 1. \quad (5.10)$$

Equation (5.9) is well known in the theory of Markov chains on the Cayley tree (see, e.g., [44, Proposition 10.7] or [57, page 389]), and it is easy to analyse the number of its positive solutions. The case $b = 1$ is obvious. Assuming $b > 1$, it is straightforward to check that $f(x)$ is an increasing function, with $f(0) = b^{-k} < 1$ and $\lim_{x \rightarrow \infty} f(x) = 1$; also, it has one inflection point $x_0 = \frac{1}{2}(b(k-1) - (k+1))$, such that $f(x)$ is convex for $x < x_0$ and concave for $x > x_0$ (note that $x_0 > 0$ only when $b > \frac{k+1}{k-1}$). Therefore, the equation (5.9) has at least one and at most three positive solutions. In fact, by fixing $b > 0$ and gradually increasing the slope $a > 0$ of the ray $y = ax$ ($x \geq 0$), it is evident that there are more than one solutions (i.e., intersections with the graph $y = f(x)$) if and only if the equation $xf'(x) = f(x)$ has at least one solution, each such solution $x = x_*$ corresponding to the line $y = ax$, with $a = f'(x_*)$, serving as a tangent to the graph $y = f(x)$ at point $x = x_*$. In turn, from (5.9) we compute

$$f'(x) = k \left(\frac{1+x}{b+x} \right)^{k-1} \frac{b-1}{(b+x)^2} = f(x) \frac{k(b-1)}{(b+x)(1+x)}, \quad (5.11)$$

and it readily follows that the condition $xf'(x) = f(x)$ transcribes as the quadratic equation (2.37), with discriminant D given by (2.38). Thus, if $D > 0$, that is, $b > \left(\frac{k+1}{k-1}\right)^2$, then the equation (2.37) has two distinct roots $0 < x_- < x_+$, corresponding to the ‘‘critical’’ values $a_{\pm} = f(x_{\pm})/x_{\pm}$ (see (2.39) and (2.40)). Furthermore, using (5.11) it is easy to see that the function $x \mapsto f(x)/x$ is increasing on the interval $x \in [x_-, x_+]$; hence, $a_- < a_+$.

To summarize, if $b \leq \left(\frac{k+1}{k-1}\right)^2$ then the equation (5.9) has a unique solution, whereas if $b > \left(\frac{k+1}{k-1}\right)^2$ then there are one, two or three solutions according as $a \notin [a_-, a_+]$, $a \in \{a_-, a_+\}$ or $a \in (a_-, a_+)$, respectively. Adapting these results to equation (2.32), in view of the second formula in (5.10) the condition $b(\theta) > \left(\frac{k+1}{k-1}\right)^2$ is equivalent to $\theta > \theta_c$, with $\theta_c = \theta_c(k, q)$ defined in (2.35). The corresponding critical values α_{\pm} of the field parameter α are determined by the first formula in (5.10), that is,

$$\theta^{k+1+\alpha_{\pm}} = \frac{q-1}{a_{\mp}}, \quad (5.12)$$

leading to formula (2.41). This completes the proof of Theorem 2.8.

5.3. Proof of Theorem 2.9. For $m \in \{1, \dots, q-2\}$, denote by $m' := q-1-m$ the “conjugate” index, $m' \in \{1, \dots, q-2\}$. Recall the notation (2.42),

$$L_m(v; \theta) := (\theta - 1)p_k(v) - mv^k - m', \quad \theta \geq 1, v \geq 0, \quad (5.13)$$

where the polynomial $p_k(v)$ is defined in (5.1).

Lemma 5.2.

- (a) For every $\theta > 1$, there is $v_m = v_m(\theta) > 0$ such that the function $v \mapsto L_m(v; \theta)$ is increasing for $0 < v < v_m$ and decreasing for $v > v_m$, thus attaining its unique maximum value at $v = v_m$,

$$L_m^*(\theta) := L_m(v_m(\theta); \theta) = \max_{v>0} L_m(v; \theta), \quad \theta > 1. \quad (5.14)$$

- (b) For each $m \geq 1$, the function $\theta \mapsto L_m^*(\theta)$ defined in (5.14) is continuous and monotone increasing, with $\lim_{\theta \rightarrow \infty} L_m^*(\theta) = \infty$. Furthermore, $L_m^*(\theta)$ has a unique zero $\theta_m > 1$, that is,

$$L_m^*(\theta_m) = L_m(v_m(\theta_m); \theta_m) = 0. \quad (5.15)$$

- (c) The value $v_m^* := v_m(\theta_m)$ is the unique positive root of the equation

$$m \sum_{i=1}^{k-1} iv^{k-i} - m' \sum_{i=1}^{k-1} iv^{i-k} = 0. \quad (5.16)$$

In particular, $v_m^* = 1$ if $m = \frac{1}{2}(q-1)$ and $v_m^* > 1$ if $m < \frac{1}{2}(q-1)$.

Proof. (a) Differentiating (5.13) with respect to v , we get

$$\begin{aligned} \frac{\partial L_m(v; \theta)}{\partial v} &= (\theta - 1)p'_k(v) - kmv^{k-1} \\ &= v^{k-1} \left((\theta - 1) \sum_{i=1}^{k-1} \frac{k-i}{v^i} - km \right). \end{aligned} \quad (5.17)$$

It is evident that the function in the parentheses in (5.17) is continuous and monotone decreasing in $v > 0$, with the limiting values $+\infty$ as $v \downarrow 0$ and $-km < 0$ as $v \rightarrow \infty$. Hence, there is a unique root $v_m = v_m(\theta)$ of the equation $\partial L_m(v; \theta)/\partial v = 0$, that is,

$$(\theta - 1)p'_k(v_m) - kmv_m^{k-1} = 0, \quad (5.18)$$

and, moreover, $\partial L_m/\partial v > 0$ for $0 < v < v_m$ and $\partial L_m/\partial v < 0$ for $v > v_m$. Thus, claim (a) is proved.

(b) Note that the derivative $v'_m(\theta)$ exists by the inverse function theorem applied to equation (5.17). Differentiating (5.14) and using (5.18), we get

$$\begin{aligned} \frac{dL_m^*(\theta)}{d\theta} &= \left. \frac{\partial L_m(v; \theta)}{\partial v} \right|_{v=v_m(\theta)} \times \frac{dv_m(\theta)}{d\theta} + \left. \frac{\partial L_m(v; \theta)}{\partial \theta} \right|_{v=v_m(\theta)} \\ &= p_k(v_m(\theta)) > 0. \end{aligned}$$

Thus, $L_m^*(\theta)$ is continuously differentiable and (strictly) increasing.¹¹ Observe from (5.14) that

$$\begin{aligned} L_m^*(\theta) &\geq L_m(v; \theta)|_{v=1} \\ &= (\theta - 1)p_k(1) - m - m' \\ &= (\theta - 1)(k - 1) - (q - 1) \rightarrow +\infty, \quad \theta \rightarrow \infty. \end{aligned} \quad (5.19)$$

On the other hand, from (5.17) we see that if $1 < \theta < \frac{k}{k-1}$ then, for all $m \geq 1$,

$$\begin{aligned} \left. \frac{\partial L_m(v; \theta)}{\partial v} \right|_{v=1} &= (\theta - 1) \sum_{i=1}^{k-1} (k - i) - km \\ &= (\theta - 1) \frac{(k - 1)k}{2} - km \\ &< k \left(\frac{1}{2} - m \right) < 0. \end{aligned}$$

Therefore, by part (a), for such θ we have $0 < v_m(\theta) < 1$, hence, for all $m \leq q - 2$,

$$\begin{aligned} L_m^*(\theta) &= (\theta - 1)p_k(v_m) - mv_m^k - m' \\ &< \left(\frac{k}{k-1} - 1 \right) p_k(1) - m' \\ &= 1 - m' \leq 0. \end{aligned} \quad (5.20)$$

Thus, combining (5.19) and (5.20), it follows that there is a unique root $\theta = \theta_m$ of the equation $L_m^*(\theta) = 0$, which proves claim (b).

(c) Elimination of $\theta = \theta_m$ from the system of equations (5.15) and (5.18) gives for $v_m^* = v_m(\theta_m)$ a closed equation,

$$mkv^{k-1}p_k(v) - (mv^k + m')p_k'(v) = 0, \quad (5.21)$$

which can be rearranged to a more symmetric form (5.16). The uniqueness of the root v_m^* is obvious, because the left-hand side of (5.16) is a continuous, increasing function in $v > 0$, with the range from $-\infty$ to $+\infty$. Finally, observe that for $v = 1$ the left-hand side of (5.16) is reduced to $(m - m') \cdot k(k - 1)/2$, which vanishes if $m = m'$ and is negative if $m < m'$, so that, respectively, $v_m^* = 1$ or $v_m^* > 1$, as claimed.

Thus, the proof of Lemma 5.2 is complete. \square

Remark 5.2. The statements of Lemma 5.2 including the identity (5.15) are valid with a *continuous* parameter m .

We can now proceed to the proof of Theorem 2.9. Assume that $\alpha \neq 0$. The second equation in the system (5.5) is reduced to

$$\theta + \theta^\alpha u^k + mv^k + m' - 1 = (\theta - 1)(p_k(v) + 1), \quad (5.22)$$

which can be rewritten, using the notation (5.13), in the form

$$\theta^\alpha u^k = L_m(v; \theta). \quad (5.23)$$

¹¹The monotonicity of $L_m^*(\theta)$ is obvious without proof, because the function $\theta \mapsto L_m(v; \theta)$ is monotone increasing for each $v > 0$, since $\partial L_m / \partial \theta = p_k(v) > 0$.

Furthermore, substituting (5.22) and (5.23) into the denominator and numerator, respectively, of the ratio in the first equation of (5.5), we get

$$u = \frac{p_k(v) + L_m(v; \theta)}{p_k(v) + 1}. \quad (5.24)$$

Finally, substituting (5.24) back into (5.23), we obtain the equation

$$\theta^\alpha = K_m(v; \theta), \quad (5.25)$$

where (cf. (2.43))

$$K_m(v; \theta) := \frac{L_m(v; \theta)(p_k(v) + 1)^k}{(p_k(v) + L_m(v; \theta))^k}. \quad (5.26)$$

Conversely, all steps above are reversible, so equations (5.24) and (5.25) imply the system (5.5).

Note from (5.25) that $v > 0$ must satisfy the condition $K_m(v; \theta) > 0$, that is, $v \in \mathcal{V}_m^+(\theta)$ (see (2.45)); by Lemma 5.2(b), this is possible if and only if $\theta > \theta_m$. Moreover, the equation (5.25) has a solution $v > 0$ if and only if $\alpha \leq \alpha_m(\theta)$, with the critical threshold $\alpha_m(\theta)$ defined in (2.46). This completes the proof of Theorem 2.9.

5.4. Proof of Theorem 2.10. Recall that the critical point $\tilde{\theta}_1$ was defined in (2.48). If $q = 2$ then the only solutions of the compatibility system (2.31) are provided by equation (2.32); therefore, Theorem 2.10(a) readily follows from Theorem 2.8.

More generally (i.e., for $q \geq 3$), in order that $\nu(\theta, \alpha) \geq 2$, either there must be at least two solutions of equation (2.32), that is, $(\theta, \alpha) \in A_q$ (see Theorem 2.8), or, since we always have $\nu_0(\theta, \alpha) \geq 1$, there should exist at least one solution (u, v) of the system (2.33). By Theorem 2.9, such solutions exist if $\alpha \leq \alpha_m(\theta)$ for some m ; since $\alpha_1(\theta)$ is a majorant of the family $\{\alpha_m(\theta)\}$ (see Proposition 6.12), the latter condition is reduced to $\alpha \leq \alpha_1(\theta)$, which leads to the inclusion $(\theta, \alpha) \in B_q$. However, we must ensure that this solution also satisfies the constraint $v \neq 1$ (see (2.34)). By Lemma 6.10, this is certainly true if $m = 1 < \frac{1}{2}(q-1)$, that is, $q > 3$, which proves Theorem 2.10(c).

Finally, Theorem 2.10(b) (for $q = 3$) readily follows by the next lemma about the maximum of the function $v \mapsto K_1(v; \theta)$ over the domain $v \in \mathcal{V}_1^+(\theta)$ (see (2.45)).

Lemma 5.3. *Let $q = 3$ and $k \geq 2$.*

- (a) *For all $\theta > \tilde{\theta}_1$, we have $K_1(v; \theta)|_{v=1} < \max_{v \in \mathcal{V}_1^+(\theta)} K_1(v; \theta)$.*
- (b) *Let $k \in \{2, 3, 4\}$. If $1 < \theta \leq \tilde{\theta}_1$ then the function $v \mapsto K_1(v; \theta)$ has the unique maximum at $v = 1$, that is, $K_1(v; \theta) < K_1(1; \theta)$ for any $v \neq 1$.*

The proof of the lemma is elementary but tedious, so it is deferred to Appendix B.

Remark 5.3. The maximum of the function $v \mapsto K_m(v; \theta)$, as well as the number of solutions $v > 0$ of the equation (5.25) for various values of parameters are illustrated in Figure 4 (for the regular case $q \geq 4$) and in Figure 5 (for the special case $q = 3$).

As mentioned in Remark 2.10, the case $q = 3$ is truly critical with regard to the uniqueness. Recall that $\nu(\theta, \alpha)$ denotes the number of positive solutions of the system (2.31); the function $\alpha_1(\theta)$ is defined in (2.46) and θ_1^0 is its zero. The proof of the next proposition relies on some lemmas that will be proved later, in Sections 6.2 and 6.3.

Proposition 5.4. *Let $q = 3$ and $k \geq 2$. There exists $\varepsilon > 0$ small enough such that*

- (a) *$\nu(\theta, \alpha_1(\theta)) = 1$ if $1 \leq \theta < \theta_1 + \varepsilon$,*
- (b) *$\nu(\theta, \alpha_1(\theta)) \geq 2$ for all $\theta > \theta_1^0 - \varepsilon$.*

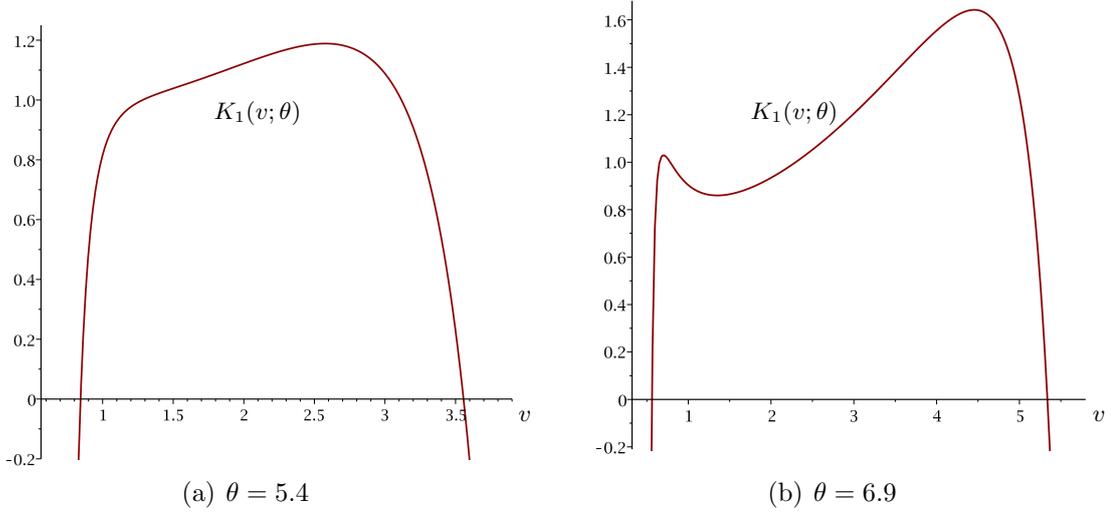


FIGURE 4. The graph of the function $v \mapsto K_1(v; \theta)$ (i.e., with $m = 1$) for $k = 2$, $q = 5$ and various values of $\theta > \theta_1 = 1 + 2\sqrt{3} \doteq 4.4641$, illustrating different possible numbers of solutions $\nu_1 = \nu_1(\theta, \alpha)$ of the equation (5.25): (a) $\theta = 5.4$, $0 \leq \nu_1 \leq 2$; (b) $\theta = 6.9$, $0 \leq \nu_1 \leq 4$.

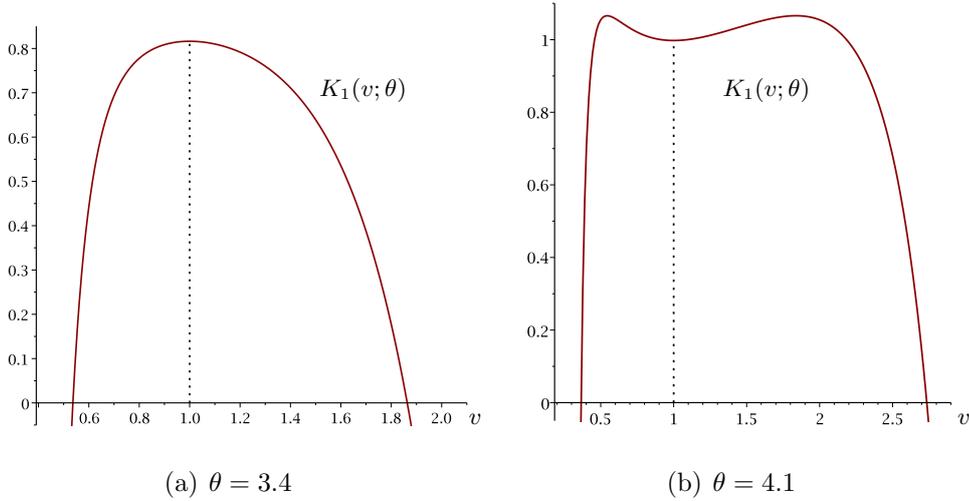


FIGURE 5. The graph of the function $v \mapsto K_1(v; \theta)$ for $q = 3$ and $k = 2$, illustrating the location of its maximum point depending on whether $\theta_c < \theta < \tilde{\theta}_1$ or $\theta > \tilde{\theta}_1$; here, $\theta_c = 3$ and $\tilde{\theta}_1 = \frac{1}{2}(1 + \sqrt{41}) \doteq 3.7016$.

Proof. (a) As shown in the proof of Lemma 5.3 (see Appendix B), $\partial^2 K_1 / \partial v^2|_{v=1} < 0$ for all $\theta \in [\theta_1, \tilde{\theta}_1]$; in particular, $\partial^2 K_1(\theta_1, v) / \partial v^2|_{v=1} < 0$. By Lemma 5.2(c), the set $\mathcal{Y}_1^+(\theta)$ (see (2.45)) is reduced for $\theta = \theta_1$ to the single point $v = 1$, and $K_1^*(\theta_1) = \max_{v \in \mathcal{Y}_1^+(\theta_1)} K_1(v; \theta_1) = K_1(1; \theta_1) = 0$. By continuity, it follows that $\partial^2 K_1(\theta; v) / \partial v^2 < 0$ for each $\theta \in [\theta_1, \theta_1 + \varepsilon)$ and all $v \in \mathcal{Y}_1^+(\theta)$; that is, the function $v \mapsto K_1(v; \theta)$ is concave on $\mathcal{Y}_1^+(\theta)$ and therefore has a unique maximum located at $v = 1$ (remembering that $\partial K_1 / \partial v|_{v=1} = 0$). But the solution (u, v) with $v = 1$ is not admissible (see (2.34)), hence $\nu(\theta, \alpha_1(\theta)) = 1$, with the only solution of (2.31) coming from equation (2.32).

(b) We have $\alpha_1(\theta_1^0) = 0$, hence $K_1^*(\theta_1^0) = 1$ (see (2.46)) and, by Lemma 6.15(b), also $L_1^*(\theta_1^0) = 1$. If $v_1 = v_1(\theta_1^0)$ is the point where the latter maximum is attained, that is, $L_1(v_1; \theta_1^0) = L_1^*(\theta_1^0) = 1$, then it holds that $v_1 > 1$ (see Lemma 6.7 below). Furthermore, according to Lemma 5.2(a), v_1 is the unique maximum of the function $v \mapsto L_1(v; \theta_1^0)$, and in particular $L_1(1; \theta_1^0) < L_1^*(\theta_1^0) = 1$.

From the definition (5.26), it follows that also $K_1(v_1; \theta_1^0) = 1 = K_1^*(\theta_1^0)$,¹² and since $L_1(1; \theta_1^0) < 1$, Lemma 6.15(a) implies that $K_1(1; \theta_1^0) < 1 = K_1^*(\theta_1^0)$. Thus, the corresponding solution of the system (2.33) satisfies the condition (2.34), and therefore $\nu(\theta_1^0, \alpha_1(\theta_1^0)) \geq 2$.

By continuity of $K_1(1; \theta)$ and $K_1^*(\theta)$, for all $\theta \in (\theta_1^0 - \varepsilon, \theta_1^0]$ (with $\varepsilon > 0$ small enough) we still have that $K_1(1; \theta) < K_1^*(\theta)$, so the maximum is attained outside $v = 1$. Thus, by the same argument as before, the claim follows. \square

5.5. Proof of Theorem 2.11. (a) First, let $q = 2$. According to Lemma 5.1, the system (2.31) is reduced to the single equation (2.32), and by Theorem 2.8 the number of its solutions is not more than $3 = 2^2 - 1$; furthermore, for $\theta > \theta_c = \frac{k+1}{k-1}$ and $\alpha_-(\theta) < \alpha < \alpha_+(\theta)$, there are exactly three solutions, so the upper bound is attained.

(b) Let now $\alpha = 0$ (and $q \geq 3$). Due to Lemma 5.1(b), either $z_i \equiv 1$ or the system (2.32) is reduced to the equation (5.3) indexed by $m = 1, \dots, q-1$, which can be rewritten as $L_m(u; \theta) = 1$ (see (5.13)). By Lemma 5.2(a), the latter equation has no more than two roots. Hence, considering permutations of the values $u \neq 1$ over the $q-1$ places, it is clear that the total number of solutions to (2.32) is bounded by

$$1 + 2 \sum_{m=1}^{q-1} \binom{q-1}{m} = 1 + 2(2^{q-1} - 1) = 2^q - 1. \quad (5.27)$$

Moreover, for $\theta > 1$ large enough, there will be exactly two roots of each of the equations $L_m(u; \theta) = 1$, because $L_m^*(\theta) = \max_{u>0} L_m(u; \theta) \rightarrow \infty$ as $\theta \rightarrow \infty$ (see Lemma 5.2(b)). Therefore, the upper bound (5.27) is attained.

(c) Finally, let $k = 2$ and $\alpha \neq 0$. First of all, up to three solutions of the system (2.32) arising from the equation (5.4) are ensured by Lemma 5.1 (see also Theorem 2.8). Other solutions are determined by the system (5.5) indexed by $m = 1, \dots, q-2$, which in turn depends on the solvability of the equation (5.25). In the case $k = 2$, the latter is a polynomial equation of degree 4, and therefore has at most four roots $v > 0$, for each m . The value $u > 0$ is then determined uniquely by formula (5.24), and it occupies the first place in the vector $\mathbf{z} = (z_1, \dots, z_{q-1})$. As for the root $v > 0$, it occupies m out of the $q-2$ remaining places. Counting the total number of such permutations, we get the upper bound

$$3 + 4 \sum_{m=1}^{q-2} \binom{q-1}{m} = 3 + 4(2^{q-2} - 1) = 2^q - 1,$$

as required. This completes the proof of Theorem 2.11.

6. FURTHER PROPERTIES OF THE CRITICAL CURVES $\alpha_{\pm}(\theta)$ AND $\alpha_m(\theta)$

6.1. Properties of $\alpha_{\pm}(\theta)$.

¹²By the scaling property (6.15), we also have $K_1(v_1^{-1}; \theta_1^0) = K_1(v_1; \theta_1^0) = 1$.

Lemma 6.1. *The quantities a_{\pm} , defined in (2.40) for $b \geq \left(\frac{k+1}{k-1}\right)^2$, satisfy the identity*

$$a_+ \times a_- = b^{-k-1}. \quad (6.1)$$

Proof. Using (2.40) and noting that $x_- = b/x_+$ (see equation (2.37)), we find

$$\begin{aligned} a_- &= \frac{1}{x_-} \left(\frac{1+x_-}{b+x_-} \right)^k \\ &= \frac{x_+}{b} \left(\frac{1+b/x_+}{b+b/x_+} \right)^k \\ &= \frac{x_+}{b^{k+1}} \left(\frac{b+x_+}{1+x_+} \right)^k \\ &= \frac{b^{-k-1}}{a_+}, \end{aligned}$$

and formula (6.1) follows. \square

Lemma 6.2. *Suppose that $b \geq \left(\frac{k+1}{k-1}\right)^2$. Then the following inequalities hold,*

$$a_+ < b^{-1}, \quad a_- > b^{-k}. \quad (6.2)$$

Proof. From (5.11), for all $x \geq 0$ we get the upper bound

$$f'(x) = \left(1 + \frac{b-1}{1+x}\right)^{-k} \frac{k(b-1)}{(b+x)(1+x)} < \frac{1}{b+x} \leq \frac{1}{b},$$

noting that, by Bernoulli's inequality,

$$\left(1 + \frac{b-1}{1+x}\right)^k > \frac{k(b-1)}{1+x}.$$

Hence, $a_+ = f'(x_+) < b^{-1}$, and the first inequality in (6.2) is proved. The second inequality then readily follows from the identity (6.1). \square

Lemma 6.3. *The functions $\alpha_{\pm}(\theta)$ satisfy the following identity,*

$$\alpha_-(\theta) + \alpha_+(\theta) = \frac{2 \ln(q-1) + (k+1)(\ln b(\theta) - 2)}{\ln \theta}, \quad \theta \geq \theta_c, \quad (6.3)$$

where $b(\theta)$ is defined in (2.36). In particular, if $q = 2$ then $\alpha_-(\theta) + \alpha_+(\theta) \equiv 0$ for all $\theta \geq \theta_c = \frac{k+1}{k-1}$.

Proof. Using (5.12), we obtain

$$\theta^{2(k+1)+\alpha_-(\theta)+\alpha_+(\theta)} = \frac{(q-1)^2}{a_-(\theta)a_+(\theta)}, \quad \theta \geq \theta_c,$$

and the identity (6.3) follows upon substituting formula (6.1). \square

Proposition 6.4. *The functions $\alpha_{\pm}(\theta): [\theta_c, \infty) \rightarrow \mathbb{R}$ defined in (2.41) have the following "boundary" values,*

$$\alpha_{\pm}(\theta_c) = -(k+1) + \frac{1}{\ln \theta_c} \left(\ln(q-1) + (k+1) \ln \frac{k+1}{k-1} \right), \quad (6.4)$$

$$\alpha_{\pm}(\theta) \rightarrow \pm(k-1) \quad (\theta \rightarrow \infty). \quad (6.5)$$

In particular, $\alpha_{\pm}(\theta_c) = 0$ if $q = 2$ and $\alpha_{\pm}(\theta_c) > 0$ if $q > 2$.

Proof. Recall from the proof of Theorem 2.8 (see Section 5.2) that the critical value $\theta = \theta_c$ corresponds to $b(\theta_c) = \left(\frac{k+1}{k-1}\right)^2$, whereby the quadratic equation (2.37) has the double root

$$x_{\pm}(\theta_c) = \sqrt{b(\theta_c)} = \frac{k+1}{k-1}.$$

Hence, using (2.40), we find

$$a_{\pm}(\theta_c) = \left(\frac{k-1}{k+1}\right)^{k+1},$$

which, together with (5.12), yields formula (6.4).

If $q = 2$ then formula (2.35) gives $\theta_c = \frac{k+1}{k-1}$, and it readily follows from (6.4) that $\alpha(\theta_c) = 0$. For $q > 2$, using the relation (5.12) observe that the required inequality $\alpha_{\pm}(\theta_c) > 0$ is reduced to

$$\theta_c^{k+1} < \frac{q-1}{a_{\pm}(\theta_c)} = \left(\frac{k+1}{k-1}\right)^{k+1} (q-1),$$

that is,

$$\theta_c < \left(\frac{k+1}{k-1}\right) (q-1)^{1/(k+1)}. \quad (6.6)$$

Denote

$$\rho_k := \frac{k+1}{k-1} > 1, \quad s := (q-1)^{1/(k+1)} > 1,$$

then (6.6) takes the form

$$\theta_c < \rho_k s. \quad (6.7)$$

Furthermore, recalling that $b(\theta_c) = \left(\frac{k+1}{k-1}\right)^2 = \rho_k^2$ and $b(\theta)$ is monotone increasing for $\theta > 1$ (see (2.35) and (2.36)), the inequality (6.7) is equivalent to

$$\rho_k^2 = b(\theta_c) < b(\rho_k s) = \frac{\rho_k s (\rho_k s + s^{k+1} - 1)}{s^{k+1}},$$

that is,

$$s^{k+1} - 1 > \rho_k (s^k - s),$$

which is reduced, upon dividing by $s - 1 > 0$ and substituting $\rho_k - 1 = \frac{2}{k-1}$, to

$$\phi_k(s) := s^k + 1 - \frac{2p_k(s)}{k-1} > 0. \quad (6.8)$$

In fact, it is easy to show that $\phi_k(s) > 0$ for any $s > 1$. Indeed, since $p_k(1) = k - 1$, we have $\phi_k(1) = 0$, while

$$\begin{aligned} \phi'_k(s) &= k s^{k-1} - \frac{2}{k-1} \sum_{i=1}^{k-1} i s^{i-1} \\ &= s^{k-1} \left(k - \frac{2}{k-1} \sum_{i=1}^{k-1} i s^{-(k-i)} \right) \\ &> s^{k-1} \left(k - \frac{2}{k-1} \sum_{i=1}^{k-1} i \right) \\ &= s^{k-1} \left(k - \frac{2}{k-1} \cdot \frac{k(k-1)}{2} \right) = 0. \end{aligned}$$

Thus, inequality (6.8) is verified, which implies that $\alpha(\theta_c) > 0$, as argued above.

Let us now prove (6.5). Using the definition of $b = b(\theta)$ and $D = D(\theta)$ (see (2.36) and (2.38), respectively), we obtain the following asymptotics as $\theta \rightarrow \infty$,

$$b = \frac{\theta^2}{q-1} + O(\theta), \quad \sqrt{D} = \frac{\theta^2(k-1)}{q-1} + O(\theta),$$

and

$$x_+ = \frac{\theta^2(k-1)}{q-1} + O(\theta), \quad x_- = \frac{b}{x_+} = \frac{1}{k-1} + O(\theta^{-1}).$$

Hence,

$$\ln x_{\pm} = (1 \pm 1) \ln \theta + O(1), \quad \ln \frac{b + x_{\pm}}{1 + x_{\pm}} = (1 \mp 1) \ln \theta + O(1).$$

Using formula (2.40), this yields

$$\begin{aligned} -\ln a_{\pm}(\theta) &= \ln x_{\pm} + k \ln \frac{b + x_{\pm}}{1 + x_{\pm}} \\ &= ((k+1) \mp (k-1)) \ln \theta + O(1). \end{aligned}$$

Therefore, from (5.12) we get

$$k+1 + \alpha_{\pm} = -\frac{\ln a_{\mp}(\theta)}{\ln \theta} + o(1) = (k+1) \pm (k-1) + o(1),$$

and the limit (6.5) follows. \square

Proposition 6.5. *The functions $\alpha_{\pm}(\theta)$ satisfy the following bounds,*

$$\alpha_-(\theta) > -(k-1), \quad \theta \geq \theta_c, \quad (6.9)$$

$$\alpha_+(\theta) < k-1, \quad \theta \geq \max\{\theta_c, \bar{\theta}\}, \quad (6.10)$$

where

$$\bar{\theta} = \bar{\theta}(k, q) := \begin{cases} \frac{q-2}{(q-1)^{(k-1)/k} - 1}, & q > 2, \\ 1, & q = 2. \end{cases} \quad (6.11)$$

Proof. Using the relation (5.12), the first inequality in (6.2) and the definition of b in (5.10), we get

$$\begin{aligned} \theta^{k+1+\alpha_-} &= \frac{q-1}{a_+} > (q-1)b \\ &= \theta(\theta + q - 2) \geq \theta^2, \quad q \geq 2, \end{aligned}$$

which proves the bound (6.9).

Similarly, using the second inequality in (6.2) we have

$$\begin{aligned} \theta^{k+1+\alpha_+} &= \frac{q-1}{a_-} < (q-1)b^k \\ &= (q-1)^{1-k} \theta^{2k} \left(1 + \frac{q-2}{\theta}\right)^k. \end{aligned} \quad (6.12)$$

Noting from (6.11) that, for $\theta \geq \bar{\theta}$,

$$1 + \frac{q-2}{\theta} \leq 1 + \frac{q-2}{\bar{\theta}} = (q-1)^{(k-1)/k}, \quad q \geq 2,$$

it is easy to see that the right-hand side of (6.12) is bounded above by θ^{2k} ; hence, the inequality (6.10) follows. \square

Remark 6.1. Note that $\bar{\theta} > 1$ for $q \geq 3$. Of course, if $\theta_c \geq \bar{\theta}$ then the upper bound (6.10) holds for all $\theta \geq \theta_c$; however, the ordering between θ_c and $\bar{\theta}$ depends on k and q . For example, for $k = 2$ and $q = 5$

$$\bar{\theta} = 3 < \theta_c \doteq 4.6847,$$

whereas for $k = 2$ and $q = 50$

$$\bar{\theta} = 8 > \theta_c \doteq 7.8904.$$

In fact, for large q the upper bound (6.10) fails near θ_c ; indeed, using (2.35) we get

$$\theta_c = \frac{q-2}{2} \left(\sqrt{1 + \frac{4(q-1)}{(q-2)^2} \left(\frac{k+1}{k-1} \right)^2} - 1 \right) \sim \left(\frac{k+1}{k-1} \right)^2, \quad q \rightarrow \infty,$$

and, according to (6.4),

$$\alpha_{\pm}(\theta_c) \sim \frac{\ln q}{\ln \theta_c} \rightarrow \infty, \quad q \rightarrow \infty.$$

Conjecture 6.1. The function $\alpha_-(\theta)$ is monotone decreasing for all $\theta \geq \theta_c$, whereas $\alpha_+(\theta)$ is decreasing for $\theta \leq \theta_0^+$ and increasing for $\theta \geq \theta_0^+$, with the unique minimum $\alpha_+(\theta_0^+) = 0$ at the critical point

$$\theta_0^+ = \theta_0^+(k, q) := 1 + \frac{q}{k-1}. \quad (6.13)$$

In the case $q = 2$, we have $\theta_c = \theta_0^+ = \frac{k+1}{k-1}$ and, by Lemma 6.3, $\alpha_+(\theta) \equiv -\alpha_-(\theta)$; hence, the function $\alpha_+(\theta)$ should be monotone increasing for all $\theta \geq \theta_c$.

This conjecture is supported by computer plots (see Figure 6). Towards a proof, we have been able to characterize the unique zero θ_0^- of $\alpha_-(\theta)$ and to show rigorously that $\alpha_+(\theta_0^+) = 0$ and $\alpha'_+(\theta_0^+) = 0$ (see Proposition 6.16(b)), but the monotonicity properties are more cumbersome to verify.

Remark 6.2. Note that the value (6.13) coincides with a known critical point in the case $\alpha = 0$, above which the solution $\mathbf{z} = \mathbf{1}$ is unstable (see [47, Section 5.2.2.2, Proposition 5.4]). Our Proposition 6.16(b-i) explains the emergence of this critical point and its explicit value (6.13).

6.2. Properties of $L_m(v; \theta)$ and $K_m(v; \theta)$. Here and below, we assume that $q \geq 3$. Recall that $v_m = v_m(\theta)$ is the unique maximum of the function $v \mapsto L_m(v; \theta)$ (see Lemma 5.2(a)), and θ_m is defined by the relation (5.15), where $1 \leq m \leq q-2$.

Remark 6.3. All results in this section hold true for a *continuous* parameter m (cf. Remark 5.2), which is evident by inspection of the proofs.

The next lemma describes the useful scaling properties of the functions $L_m(v; \theta)$ and $K_m(v; \theta)$ (see (5.13) and (5.26)) under the conjugation $m \mapsto m'$.

Lemma 6.6. *For each $m = 1, \dots, q-2$ and $m' = q-1-m$, the following identities hold for all $v > 0$ and $\theta > \theta_m$,*

$$L_{m'}(v; \theta) = v^k L_m(v^{-1}; \theta), \quad (6.14)$$

$$K_{m'}(v; \theta) = K_m(v^{-1}; \theta). \quad (6.15)$$

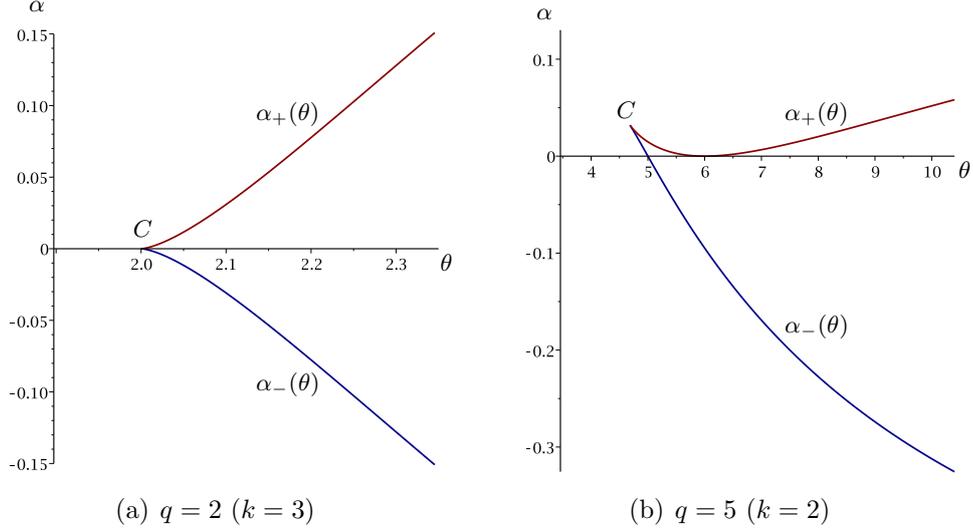


FIGURE 6. The graphs of the functions $\alpha_+(\theta)$ and $\alpha_-(\theta)$ (see (2.41)): (a) $q = 2$, $k = 3$; (b) $q = 5$, $k = 2$. The coordinates of the cusp point C (see (2.35) and (6.4)) are given numerically by: (a) $\theta_c = 2$, $\alpha_{\pm}(\theta_c) = 0$; (b) $\theta_c \doteq 4.6847$, $\alpha_{\pm}(\theta_c) \doteq 0.0319$. The axis $\alpha = 0$ is a tangent line for $\alpha_+(\theta)$ at $\theta_0^+ = 1 + q/(k - 1)$ (see Proposition 6.16(b-i)): (a) $\theta_0^+ = 2$ ($=\theta_c$); (b) $\theta_0^+ = 6$. In panel (b), the function $\alpha_-(\theta)$ has zero at $\theta_0^- = 5$ (see Proposition 6.16(b-ii) and Example 6.1), whereas in panel (a) we have $\theta_0^- = \theta_0^+ = 2$ (see Proposition 6.4). Note that the graphs display the monotone behaviour as predicted by Conjecture 6.1.

Proof. Recalling the notation (5.1), note that

$$p_k(v^{-1}) = v^{-(k-1)} + \dots + v^{-1} = v^{-k} p_k(v), \quad (6.16)$$

and similarly

$$p_k(v^{-1}) + 1 = v^{-(k-1)} + \dots + v^{-1} + 1 = v^{-k+1} (p_k(v) + 1). \quad (6.17)$$

Using (5.13) and (6.16), we can write

$$\begin{aligned} L_m(v^{-1}; \theta) &= (\theta - 1) p_k(v^{-1}) - m v^{-k} - m' \\ &= v^{-k} ((\theta - 1) p_k(v) - m - m' v^k) \\ &= v^{-k} L_{m'}(v; \theta), \end{aligned}$$

and formula (6.14) follows. Furthermore, using (6.14) and substituting (6.16) and (6.17), we obtain

$$\begin{aligned}
 K_m(v^{-1}; \theta) &= \frac{L_m(v^{-1}; \theta)(p_k(v^{-1}) + 1)^k}{(p_k(v^{-1}) + L_m(v^{-1}; \theta))^k} \\
 &= \frac{v^{-k} L_{m'}(v; \theta) \cdot v^{-(k-1)k} (p_k(v) + 1)^k}{(v^{-k} p_k(v) + v^{-k} L_{m'}(v; \theta))^k} \\
 &= \frac{L_{m'}(v; \theta)(p_k(v) + 1)^k}{(p_k(v) + L_{m'}(v; \theta))^k} \\
 &= K_{m'}(v; \theta),
 \end{aligned}$$

which proves formula (6.15). \square

For $\theta > \theta_m$, let $v_m = v_m(\theta)$ be the point where the function $v \mapsto L_m(v; \theta)$ attains its (positive) maximum value, that is, $L_m(v_m; \theta) = \max_{v \in \mathcal{V}_m^+(\theta)} L_m(v; \theta)$ (see Lemma 5.2). The next result provides a strict lower bound for v_m (cf. Lemma 5.2(c) for $\theta = \theta_m$).

Lemma 6.7. *For all m in the range $1 \leq m \leq \frac{1}{2}(q-1)$, we have*

$$v_m(\theta) > 1, \quad \theta > \theta_m. \quad (6.18)$$

Proof. To the contrary, suppose first that $v_m < 1$ for some $\theta > \theta_m$. Then, according to Lemma 6.6, we have

$$L_m(v_m^{-1}; \theta) = v_m^{-k} L_{m'}(v_m; \theta) > L_{m'}(v_m; \theta), \quad (6.19)$$

and furthermore,

$$\begin{aligned}
 L_{m'}(v_m; \theta) &= (\theta - 1)p_k(v_m) - m'v_m^k - m \\
 &= L_m(v_m; \theta) + (m' - m)(1 - v_m^k) \geq L_m(v_m; \theta),
 \end{aligned} \quad (6.20)$$

since $m' = q - 1 - m \geq m$ by the hypothesis of the lemma. Combining (6.19) and (6.20), we see that $L_m(v_m^{-1}; \theta) > L_m(v_m; \theta)$, which contradicts the assumption that $L_m(v_m; \theta)$ is the maximum value of the function $v \mapsto L_m(v; \theta)$.

Assume now that $v_m = 1$ for some $\theta > \theta_m$. Then

$$\left. \frac{\partial L(v; \theta)}{\partial v} \right|_{v=v_m=1} = (\theta - 1)p'_k(1) - km = (\theta - 1) \frac{k(k-1)}{2} - km = 0,$$

whence $(\theta - 1)(k - 1) = 2m$. Hence,

$$L_m(1; \theta) = (\theta - 1)(k - 1) - (q - 1) = 2m - (q - 1) \leq 0,$$

which contradicts the assumption $L_m(v_m; \theta) > 0$.

Thus, the inequality (6.18) is proved. \square

For $\theta > \theta_m$, let $w_m = w_m(\theta)$ be the point where the function $v \mapsto K_m(v; \theta)$ attains its (positive) maximum value, that is, $K_m(w_m; \theta) = \max_{v \in \mathcal{V}_m^+(\theta)} K_m(v; \theta)$. Note that $w_m(\theta_m) = v_m(\theta_m) = v_m^*$ (see Lemma 5.2(c)). The importance of the next technical lemma is pinpointed by involvement of the expression $p_k(v) - (k - 1)L_m(v; \theta)$ in the partial derivative $\partial K_m / \partial v$ (see formula (6.23) below).

Lemma 6.8. *Let $1 \leq m \leq \frac{1}{2}(q-1)$ and $\theta > \theta_m$.*

- (a) Let $w \in \mathcal{V}_m^+(\theta)$ be a critical point of the function $v \mapsto K_m(v; \theta)$, that is, any solution of the equation $\partial K_m / \partial v = 0$. Assume that either (i) $w < v_m$ and $L_m(w; \theta) < 1$, or (ii) $w \geq v_m$. Then

$$p_k(w) - (k-1)L_m(w; \theta) > 0. \quad (6.21)$$

- (b) In particular, the inequality (6.21) holds for $w = w_m$, that is,

$$p_k(w_m) - (k-1)L_m(w_m; \theta) > 0. \quad (6.22)$$

Proof. (a) From the definition (5.26), compute the partial derivative

$$\frac{\partial K_m}{\partial v} = \frac{(p_k + 1)^{k-1}}{(p_k + L_m)^{k+1}} \left((p_k + 1)(p_k - (k-1)L_m) \frac{\partial L_m}{\partial v} - kL_m(1 - L_m)p'_k \right), \quad (6.23)$$

with the shorthand notation $p_k := p_k(v)$ and $L_m := L_m(v; \theta)$. Hence, the condition $\partial K_m / \partial v = 0$ is reduced to the equality

$$(p_k + 1)(p_k - (k-1)L_m) \frac{\partial L_m}{\partial v} - kL_m(1 - L_m)p'_k = 0. \quad (6.24)$$

If $w < v_m$ then $\partial L_m / \partial v|_{v=w} > 0$, and the required inequality (6.21) readily follows from equation (6.24) using that $L_m(w; \theta) < 1$. Similarly, if $w > v_m$ then $\partial L_m / \partial v|_{v=w} < 0$ and equation (6.24) implies the inequality (6.21) provided that $L_m(w; \theta) > 1$. Alternatively, if $L_m(w; \theta) \leq 1$ then, noting that $w > v_m > 1$ (by Lemma 6.7), we obtain, in agreement with (6.21),

$$p_k(w) > p_k(1) = k-1 \geq (k-1)L_m(w; \theta), \quad (6.25)$$

because the function $w \mapsto p_k(w)$ is strictly increasing and $p_k(1) = k-1$.

Lastly, if $w = v_m$ then $\partial L_m / \partial v|_{v=v_m} = 0$ and equation (6.24) implies $L_m(v_m; \theta) = 1$. Again using Lemma 6.7, similarly to (6.25) we get

$$p_k(w) = p_k(v_m) > p_k(1) = k-1 = (k-1)L_m(w; \theta), \quad (6.26)$$

so the inequality (6.21) holds in this case as well.

- (b) Let $w = w_m$ be the point of maximum of the function $v \mapsto K_m(v; \theta)$. According to part (a), we only have to consider the case where $w_m < v_m$ and $L_m(w_m; \theta) \geq 1$.

If $L_m(w_m; \theta) > 1$, let $\bar{w} > v_m > w_m$ be such that $L_m(\bar{w}; \theta) = L_m(w_m; \theta)$, then

$$\begin{aligned} K_m(\bar{w}; \theta) &= L_m(\bar{w}; \theta) \left(1 - \frac{L_m(\bar{w}; \theta) - 1}{p_k(\bar{w}) + L_m(\bar{w}; \theta)} \right)^k \\ &= L_m(w_m; \theta) \left(1 - \frac{L_m(w_m; \theta) - 1}{p_k(\bar{w}) + L_m(w_m; \theta)} \right)^k \\ &> L_m(w_m; \theta) \left(1 - \frac{L_m(w_m; \theta) - 1}{p_k(w_m) + L_m(w_m; \theta)} \right)^k \\ &= K_m(w_m; \theta). \end{aligned} \quad (6.27)$$

Thus, $K_m(\bar{w}; \theta) > K_m(w_m; \theta)$, which contradicts the assumption that $v = w_m$ provides the maximum value of the function $v \mapsto K_m(v; \theta)$.

Lastly, suppose that, for some $\theta > \theta_m$,

$$L_m(w_m; \theta) = 1. \quad (6.28)$$

In view of the definition (5.26), condition (6.28) implies that $K_m(w_m; \theta) = 1$. Let us prove that in this case we must have $w_m > 1$, which would then automatically imply the required inequality (6.22) (cf. (6.25) and (6.26)). To the contrary, assume that

$w_m \leq 1$. If $w_m = 1$ then, using the definition (5.13) and recalling that $m + m' = q - 1$, the equation (6.28) is reduced to

$$L_m(1; \theta) = (\theta - 1)(k - 1) - (q - 1) = 1,$$

whence we find

$$\theta = 1 + \frac{q}{k - 1}. \quad (6.29)$$

Furthermore, noting that

$$p'_k(1) = \sum_{i=1}^{k-1} i = \frac{k(k-1)}{2} \quad (6.30)$$

and substituting (6.29), from (5.13) we get

$$\frac{\partial L_m(1; \theta)}{\partial v} = (\theta - 1) \frac{k(k-1)}{2} - km = k \left(\frac{q}{2} - m \right) > 0,$$

since $m \leq \frac{1}{2}(q-1) < q/2$. Thus, $w_m = 1$ is the *left root* of the equation $L_m(v; \theta) = 1$. Denote by $\bar{v} > 1$ the *right root*, that is, $L_m(\bar{v}; \theta) = 1$ and $\partial L_m / \partial v|_{v=\bar{v}} < 0$. It follows that $K_m(\bar{v}; \theta) = 1$ (see (5.26)), so the maximum value 1 of the function $v \mapsto K_m(v; \theta)$ is also attained at $v = \bar{v} > 1$. Returning to formula (6.23), observe that

$$\frac{\partial K_m(\bar{v}; \theta)}{\partial v} = \frac{p_k(\bar{v}) - (k-1)}{p_k(\bar{v}) + 1} \times \frac{\partial L_m(\bar{v}; \theta)}{\partial v} < 0, \quad (6.31)$$

because $p_k(\bar{v}) > p_k(1) = k - 1$ and, as mentioned above, $\partial L_m / \partial v|_{v=\bar{v}} < 0$. But the inequality (6.31) implies that there are points $v < \bar{v}$ such that $K_m(v; \theta) > K_m(\bar{v}; \theta)$, a contradiction. Hence, the case $w_m = 1$ is impossible.

Now, suppose that $w_m < 1$. Then $p_k(w_m) < p_k(1) = k - 1$ and, in view of the condition (6.28), from equation (6.24) it readily follows that $\partial L_m / \partial v|_{v=w_m} = 0$, that is, $L_m(w_m; \theta) = 1$ is the maximum value of the function $v \mapsto L_m(v; \theta)$. Hence, for all $v < w_m$ we have

$$L_m(v; \theta) < 1, \quad \frac{\partial L_m(v; \theta)}{\partial v} > 0. \quad (6.32)$$

On the other hand, by (6.24) and monotonicity of $p_k(v)$,

$$\begin{aligned} p_k(w_m) - (k-1)L_m(w_m; \theta) &= p_k(w_m) - (k-1) \\ &< p_k(1) - (k-1) = 0. \end{aligned} \quad (6.33)$$

By continuity of the functions $v \mapsto p_k(v)$ and $v \mapsto L_m(v; \theta)$, the inequality (6.33) is preserved for all $v < w_m$ close enough to w_m :

$$p_k(v) - (k-1)L_m(v; \theta) < 0. \quad (6.34)$$

Using (6.32) and (6.34), from (6.23) it follows that for such v we have $\partial K_m / \partial v < 0$. But this means that the function $v \mapsto K_m(v; \theta)$ is *decreasing* in the left vicinity of w_m , and thus w_m cannot be a maximum, in contradiction with our assumption. Thus, we have proved that $w_m > 1$ as required, which completes the proof of Lemma 6.8. \square

The next two lemmas provide useful bounds on $w_m = w_m(\theta)$. First, there is a simple uniform upper bound.

Lemma 6.9. *For all $m \in [1, q - 2]$,*

$$w_m < \theta, \quad \theta \geq \theta_m. \quad (6.35)$$

Proof. Observe, using the definition (5.13), that

$$\begin{aligned} L_m(v; \theta)|_{v=\theta} &= (\theta - 1)p_k(\theta) - m\theta^k - m' \\ &= (\theta - 1)(\theta^{k-1} + \dots + \theta) - m\theta^k - m' \\ &= -(m - 1)\theta^k - \theta - m' < 0, \end{aligned}$$

and also (cf. (5.17))

$$\begin{aligned} \left. \frac{\partial L_m(v; \theta)}{\partial v} \right|_{v=\theta} &= (\theta - 1)p'_k(\theta) - km\theta^{k-1} \\ &= (\theta - 1)((k - 1)\theta^{k-2} + \dots + 2\theta + 1) - km\theta^{k-1} \\ &= -(km - k + 1)\theta^{k-1} - \theta^{k-2} - \dots - \theta - 1 < 0. \end{aligned}$$

Hence, the point $v = \theta$ lies to the right of the set $\mathcal{V}_m^+(\theta) = \{v > 0: L_m(v; \theta) > 0\}$ (see (2.45)). But $w_m \in \mathcal{V}_m^+(\theta)$ and therefore $w_m < \theta$, as claimed in (6.35). \square

The important lower bound for $w_m = w_m(\theta)$ is established next.

Lemma 6.10.

(a) For all m in the range $1 \leq m < \frac{1}{2}(q - 1)$, we have

$$w_m > 1, \quad \theta > \theta_m. \quad (6.36)$$

(b) If $m = \frac{1}{2}(q - 1)$ then the maximum point w_m (which may not be unique) can be chosen so that $w_m \geq 1$.

Proof. If $L_m(w_m; \theta) \geq 1$ then, by the inequality (6.22) of Lemma 6.8,

$$p_k(w_m) > (k - 1)L_m(w_m; \theta) \geq k - 1 = p_k(1),$$

which implies, due to the monotonicity of $p_k(\cdot)$, that $w_m > 1$, in line with (6.36). Thus, it remains to consider the case $L_m(w_m; \theta) < 1$.

Assume first that $w_m = 1$ for some $\theta > \theta_m$. Using the definition (5.13) and the value $p_k(1) = k - 1$, we have

$$\begin{aligned} L_m(1; \theta) &= (\theta - 1)p_k(1) - m - m' \\ &= (\theta - 1)(k - 1) - (q - 1), \end{aligned} \quad (6.37)$$

and also, recalling formula (6.30),

$$\begin{aligned} \frac{\partial L_m(1; \theta)}{\partial v} &= (\theta - 1)p'_k(1) - km \\ &= \frac{k}{2}((\theta - 1)(k - 1) - 2m) \\ &= \frac{k}{2}(L_m(1; \theta) + m' - m). \end{aligned} \quad (6.38)$$

Substituting (6.30), (6.37) and (6.38) into (6.23), it is easy to check that the condition $\partial K_m / \partial v|_{v=1} = 0$ (see (6.24)) is reduced to

$$(1 - L_m(1; \theta))(m' - m) = 0. \quad (6.39)$$

Since $L_m(1; \theta) = L_m(w_m; \theta) < 1$ by assumption, the condition (6.39) is only satisfied if $m' - m = 0$, that is, $m = \frac{1}{2}(q - 1)$. Conversely, if $m = \frac{1}{2}(q - 1)$ (i.e., $m' = m$) then, by the scaling formula (6.15) of Lemma 6.6, we have the identity

$$K_m(v^{-1}; \theta) = K_{m'}(v; \theta) = K_m(v; \theta), \quad \theta > \theta_m, \quad v > 0, \quad (6.40)$$

which implies that the maximum point $w_m = w_m(\theta)$ can always be chosen so as to satisfy the inequality $w_m \geq 1$, which proves part (b) of the lemma.

Finally, let $m < \frac{1}{2}(q-1)$ and $w_m < 1$ for some $\theta > \theta_m$. Denote $L_m^*(\theta) := L_m(v_m(\theta); \theta) = \max_{v \in \mathcal{V}_m^+(\theta)} L_m(v; \theta)$ (see Lemma 5.2 and the definition (2.45)). We need to distinguish between two subcases, (i) $L_m^*(\theta) \leq 1$ and (ii) $L_m^*(\theta) > 1$, which require a different argumentation.

(i) Assuming first that $L_m^*(\theta) \leq 1$, we will show that then

$$K_m(w_m^{-1}; \theta) > K_m(w_m; \theta), \quad (6.41)$$

which would contradict the assumption that $K_m(w_m; \theta)$ is the maximum value. By formula (6.15) of Lemma 6.6, we have $K_m(w_m^{-1}; \theta) = K_{m'}(w_m; \theta)$. Hence, recalling the definition (5.26) of the function $K_m(v; \theta)$, the inequality (6.41) is reduced to

$$\frac{L_{m'}(w_m; \theta)}{(p_k(w_m) + L_{m'}(w_m; \theta))^k} > \frac{L_m(w_m; \theta)}{(p_k(w_m) + L_m(w_m; \theta))^k}. \quad (6.42)$$

Note that (cf. (6.20))

$$\begin{aligned} L_{m'}(w_m; \theta) &= (\theta - 1)p_k(w_m) - m'w_m^k - m \\ &= L_m(w_m; \theta) + (m' - m)(1 - w_m^k) \\ &> L_m(w_m; \theta). \end{aligned}$$

Hence, for the proof of the inequality (6.42), it suffices to show that the function $L \mapsto L(p_k(w_m) + L)^{-k}$ is strictly increasing on the interval $L \in [L_m(w_m; \theta), L_{m'}(w_m; \theta)]$. Computing the derivative of this function, we see that the claim holds provided that

$$\frac{p_k(w_m)}{k-1} > L, \quad L_m(w_m; \theta) \leq L \leq L_{m'}(w_m; \theta),$$

or simply if

$$\frac{p_k(w_m)}{k-1} > L_{m'}(w_m; \theta). \quad (6.43)$$

The inequality (6.43) is easy to prove. Indeed, using the assumption $w_m < 1$, observe from the definition (5.1) that

$$\frac{p_k(w_m)}{k-1} > w_m^{k-1} > w_m^k. \quad (6.44)$$

On the other hand, according to the scaling formula (6.14) of Lemma 6.6, we have

$$L_{m'}(w_m; \theta) = w_m^k L_m(w_m^{-1}; \theta) \leq w_m^k L_m^*(\theta) \leq w_m^k, \quad (6.45)$$

by virtue of the assumption $L_m^*(\theta) \leq 1$. Now, the required inequality (6.43) readily follows from the estimates (6.44) and (6.45).

Thus, the inequality (6.41) is proved, and therefore the assumptions $w_m < 1$ and $L_m^*(\theta) \leq 1$ are incompatible.

(ii) Assume now that $L_m^*(\theta) = L_m(v_m; \theta) > 1$ and, as before, $w_m = w_m(\theta) < 1$. Denote

$$W_m = W_m(\theta) := \left\{ w > 1 : \left. \frac{\partial K_m(v; \theta)}{\partial v} \right|_{v=w} = 0 \right\},$$

that is, the set of all critical points of the function $v \mapsto K_m(v; \theta)$ (i.e., satisfying the equation (6.24)) that lie to the right of point $v = 1$. By assumption,

$$K_m(w_m; \theta) > \max_{w \in W_m} K_m(w; \theta), \quad (6.46)$$

and our aim is to show that this leads to a contradiction.

Since $\partial L_m / \partial v|_{v=v_m} = 0$ and $L_m(v_m; \theta) > 1$, formula (6.23) implies $\partial K_m / \partial v|_{v=v_m} > 0$ and, therefore, there is at least one critical point $w > v_m$, which then automatically belongs to the set W_m , because $v_m > 1$ by Lemma 6.7. There may also be critical points $w \in W_m$ such that $1 < w < v_m$; for these we may assume, without loss of generality, that $L_m(w; \theta) < 1$, for otherwise we consider the point $\bar{w} > v_m > w$ such that $L_m(\bar{w}; \theta) = L_m(w; \theta)$, and it follows (similarly to the derivation of inequality (6.27)) that $K_m(\bar{w}; \theta) \geq K_m(w; \theta)$, which means that such w can be removed from the set W_m without affecting the maximum in (6.46).

Now, the idea is to increase the index m . Namely, treating m as a continuous parameter (see Remark 6.3), differentiate the function $m \mapsto K_m(w_m(\theta); \theta)$ to obtain

$$\begin{aligned} \frac{\partial K_m(w_m; \theta)}{\partial m} &= \frac{\partial K_m(v; \theta)}{\partial v} \Big|_{v=w_m} \times \frac{\partial w_m(\theta)}{\partial m} \\ &\quad + \frac{\partial K_m(w_m; \theta)}{\partial L} \Big|_{L=L_m(w_m; \theta)} \times \frac{\partial L_m(v; \theta)}{\partial m} \Big|_{v=w_m} \\ &= \frac{(p_k(w_m) + 1)^k (p_k(w_m) - (k-1)L_m(w_m; \theta))}{(p_k(w_m) + L_m(w_m; \theta))^{k+1}} \times (1 - w_m^k), \end{aligned} \quad (6.47)$$

where we used the condition $\partial K_m / \partial v|_{v=w_m} = 0$ and the definitions (5.13) and (5.26). Owing to Lemma 6.8(b), the right-hand side of (6.47) is positive and, therefore, the function $m \mapsto K_m(w_m; \theta)$ is monotone *increasing* as long as $w_m < 1$ and $m < m_0 := \frac{1}{2}(q-1)$. Likewise, every critical point $w = w^{(i)}$ from the original (finite) set W_m generates a continuously differentiable branch $m \mapsto w_m^{(i)}$ as a function of the increasing variable m , and an argument similar to (6.47), now based on Lemma 6.8(a), yields that the corresponding function $m \mapsto \max_{w \in W_m} K_m(w; \theta)$ is monotone *decreasing* up to $m = m_0$.

If for some $\tilde{m} \in (m, m_0)$ it occurs that $w_{\tilde{m}} = 1$ then, by continuity, $\partial K_{\tilde{m}} / \partial v|_{v=1} = 0$, which implies, as was shown before (see (6.39)), that $L_{\tilde{m}}(w_{\tilde{m}}; \theta) = 1$ and therefore $K_{\tilde{m}}(w_{\tilde{m}}; \theta) = 1$ is the maximum value of the function $v \mapsto K_{\tilde{m}}(v; \theta)$. Moreover, combining the monotonicity properties established above with the hypothetical inequality (6.46), this implies

$$1 = K_{\tilde{m}}(w_{\tilde{m}}; \theta) > K_m(w_m; \theta) > \max_{w \in W_m} K_m(w; \theta) > \max_{w \in W_{\tilde{m}}} K_{\tilde{m}}(w; \theta),$$

that is,

$$\max_{w \in W_{\tilde{m}}} K_{\tilde{m}}(w; \theta) < 1. \quad (6.48)$$

But this cannot be true, because there is $\bar{w} > v_{\tilde{m}}$ where $L_{\tilde{m}}(\bar{w}; \theta) = 1$, so that $K_{\tilde{m}}(\bar{w}; \theta) = 1$ is another maximum and, hence, $\bar{w} \in W_{\tilde{m}}$, thus contradicting (6.48).

This shows that we can exploit the monotonicity properties with respect to variable m up to the final value $m = m_0 = \frac{1}{2}(q-1)$, so that

$$K_m(w_m; \theta) < K_{m_0}(w_{m_0}; \theta) \quad (6.49)$$

and also

$$\max_{w \in W_{m_0}} K_{m_0}(w; \theta) < \max_{w \in W_m} K_m(w; \theta). \quad (6.50)$$

Combining (6.49) and (6.50) with (6.46), it follows that

$$\max_{w \in W_{m_0}} K_{m_0}(w; \theta) < K_{m_0}(w_{m_0}; \theta). \quad (6.51)$$

But this is impossible, since $m_0 = m'_0$ and, by the scaling relation (6.15) of Lemma 6.6, $K_{m_0}(v; \theta) \equiv K_{m_0}(v^{-1}; \theta)$ (see (6.40)), which implies that the maximum values of the function $v \mapsto K_{m_0}(v; \theta)$ over $v < 1$ and $v > 1$ must be the same, in contradiction with the inequality (6.51).

Thus, the hypothesis (6.46) is false, together with the assumption $w_m < 1$ under case (ii) (i.e., with $L_m^*(\theta) > 1$). This completes the proof of Lemma 6.10. \square

6.3. Properties of θ_m and $\alpha_m(\theta)$.

Proposition 6.11. *For each $m = 1, \dots, q-2$ and $m' = q-1-m$, we have*

$$\theta_m = \theta_{m'}. \quad (6.52)$$

Moreover, the functions $\theta \mapsto \alpha_m(\theta)$ (see (2.46)) satisfy the symmetry relation

$$\alpha_{m'}(\theta) \equiv \alpha_m(\theta), \quad \theta > \theta_m. \quad (6.53)$$

Proof. Like in Lemma 5.2(c), denote $v_m^* := v_m(\theta_m)$. Observe that v_m^* satisfies the conjugation property

$$v_{m'}^* = \frac{1}{v_m^*}, \quad m = 1, \dots, q-2, \quad (6.54)$$

where $m' = q-1-m$. Indeed, computing the left-hand side of (5.16) for $v = 1/v_m^*$ and with m replaced by m' , we get, due to Lemma 5.2(c),

$$m' \sum_{i=1}^{k-1} i \left(\frac{1}{v_m^*} \right)^{k-i} - m \sum_{i=1}^{k-1} i \left(\frac{1}{v_m^*} \right)^{i-k} = - \left(m \sum_{i=1}^{k-1} i (v_m^*)^{k-i} - m' \sum_{i=1}^{k-1} i (v_m^*)^{i-k} \right) = 0,$$

whence (6.54) follows due to the uniqueness of solution.

Now, using (6.54) and the scaling property (6.14), we have

$$\begin{aligned} L_{m'}(v_{m'}^*; \theta_m) &= L_{m'}((v_m^*)^{-1}; \theta_m) \\ &= (v_m^*)^{-k} L_m(v_m^*; \theta_m) = 0, \end{aligned}$$

according to (5.15), and by the uniqueness of solution to the equation $L_{m'}(v_{m'}(\theta); \theta) = 0$ (see Lemma 5.2(b)), the equality (6.52) follows.

Finally, the identity (6.53) is valid due to the definition (2.46) and formula (6.15). \square

Proposition 6.12. *Let $q \geq 5$, and set $m_0 := \lfloor \frac{1}{2}(q-1) \rfloor$. Then for $m = 1, \dots, m_0 - 1$*

$$\theta_m < \theta_{m+1}, \quad (6.55)$$

$$\alpha_m(\theta) > \alpha_{m+1}(\theta), \quad \theta > \theta_{m+1}. \quad (6.56)$$

Proof. Treating m as a continuous parameter (see Remark 5.2), differentiate the identity (5.15) to obtain

$$\begin{aligned} \frac{dL_m(v_m^*; \theta_m)}{dm} &= \frac{\partial L_m(v; \theta_m)}{\partial v} \Big|_{v=v_m^*} \times \frac{dv_m^*}{dm} \\ &\quad + \frac{\partial L_m(v_m^*; \theta)}{\partial \theta} \Big|_{\theta=\theta_m} \times \frac{d\theta_m}{dm} + \frac{\partial L_m(v; \theta)}{\partial m} \Big|_{v=v_m^*, \theta=\theta_m} \equiv 0. \end{aligned}$$

Using (5.13) and (5.18), the last identity is reduced to

$$p_k(v_m^*) \frac{d\theta_m}{dm} + 1 - (v_m^*)^k = 0,$$

which yields

$$\frac{d\theta_m}{dm} = \frac{(v_m^*)^k - 1}{p_k(v_m^*)}. \quad (6.57)$$

Recalling that $v_m^* > 1$ for all $m < \frac{1}{2}(q-1)$ (see Lemma 5.2(c)), from (6.57) it follows that $d\theta_m/dm > 0$ for $m < \frac{1}{2}(q-1)$. For integer $m = 1, \dots, m_0$, this transcribes as the inequality (6.55).

Turning to the proof of (6.56), for a given $\theta \geq \theta_1$ let $m^* \geq 1$ be the root of the equation $\theta_m = \theta$. We shall prove a (stronger) *continuous version* of the inequality (6.56), namely, that the function $m \mapsto \alpha_m(\theta)$ (defined for $m \geq m^*$) is monotone decreasing. As before, denote by $w_m = w_m(\theta)$ the point where the function $v \mapsto K_m(v; \theta)$ attains its maximum value, and set $K_m^*(\theta) := K_m(w_m(\theta); \theta)$. Differentiating the function $m \mapsto K_m^*(\theta)$, we obtain (see (6.47))

$$\frac{\partial K_m^*}{\partial m} = \frac{(p_k(w_m) + 1)^k (p_k(w_m) - (k-1)L_m(w_m; \theta))}{(p_k(w_m) + L_m(w_m; \theta))^{k+1}} \times (1 - w_m^k). \quad (6.58)$$

Now, owing to Lemmas 6.8 and 6.10 (see also Remark 6.3), the right-hand side of (6.58) is negative for all $m \in [m^*, \frac{1}{2}(q-1))$ and, therefore, the function $m \mapsto K_m^*(\theta)$ is monotone decreasing in the closed interval $[m^*, \frac{1}{2}(q-1)]$. By the definition (2.46), the same holds for the function $m \mapsto \alpha_m(\theta)$, as claimed. \square

Proposition 6.13. *For all $m = 1, \dots, q-2$, the functions $\theta \mapsto \alpha_m(\theta)$ defined by formula (2.46) satisfy the upper bound*

$$\alpha_m(\theta) < k-1, \quad \theta > \theta_m. \quad (6.59)$$

Moreover, they have the following “boundary” values,

$$\lim_{\theta \downarrow \theta_m} \alpha_m(\theta) = -\infty, \quad \lim_{\theta \uparrow \infty} \alpha_m(\theta) = k-1. \quad (6.60)$$

Proof. Let $w_m = w_m(\theta)$ be the point of maximum of the function $v \mapsto K_m(v; \theta)$, so that $K_m^*(\theta) = K_m(w_m; \theta)$. Treating the term $L_m = L_m(v; \theta)$ in the expression (5.26) as an independent parameter $L \geq 0$, we can write

$$K_m^*(\theta) \leq (p_k(w_m) + 1)^k \max_{L \geq 0} \frac{L}{(p_k(w_m) + L)^k}. \quad (6.61)$$

By differentiation, it is easy to verify that the maximum on the right-hand side of (6.61) is attained at $L_0 := p_k(w_m)/(k-1)$, hence

$$\begin{aligned} K_m^*(\theta) &\leq (p_k(w_m) + 1)^k \frac{L}{(p_k(w_m) + L)^k} \Big|_{L=L_0} \\ &= \left(\frac{k-1}{k}\right)^k \left(1 + \frac{1}{p_k(w_m)}\right)^k \frac{p_k(w_m)}{k-1} \\ &\leq \frac{p_k(w_m)}{k-1}. \end{aligned} \quad (6.62)$$

Furthermore, $w_m < \theta$ by Lemma 6.9, so that

$$p_m(w_m) < p_m(\theta) < (k-1)\theta^{k-1}.$$

Substituting this estimate into the right-hand side of (6.62), we obtain

$$K_m^*(\theta) < \theta^{k-1},$$

and therefore (see (2.46))

$$\alpha_m(\theta) = \frac{\ln K_m^*(\theta)}{\ln \theta} < k - 1,$$

which proves the bound (6.59). In particular, this implies that

$$\limsup_{\theta \rightarrow \infty} \alpha_m(\theta) \leq k - 1. \quad (6.63)$$

To obtain a matching lower bound, take a specific value

$$v = v_0 := \frac{t}{m} \left(1 - \frac{\ln t}{t} \right), \quad t := \theta - 1,$$

then, as $t \rightarrow \infty$,

$$\begin{aligned} p_k(v_0) &= \frac{t^{k-1}}{m^{k-1}} \left(1 - \frac{\ln t}{t} \right)^{k-1} + O(t^{k-2}) \\ &= \frac{t^{k-1}}{m^{k-1}} \left(1 - \frac{(k-1) \ln t}{t} \right) + O(t^{k-2}) \end{aligned}$$

and

$$\begin{aligned} L_m(v_0; \theta) &= t p_k(v_0) - m v_0^k - m' \\ &= \frac{t^k}{m^{k-1}} \left(1 - \frac{(k-1) \ln t}{t} \right) - \frac{t^k}{m^{k-1}} \left(1 - \frac{k \ln t}{t} \right) + O(t^{k-1}) \\ &= \frac{t^{k-1} \ln t}{m^{k-1}} + O(t^{k-1}). \end{aligned}$$

Hence,

$$p_k(v_0) + L_m(v_0; \theta) \sim \frac{t^{k-1} \ln t}{m^{k-1}}$$

and

$$K_m(v_0; \theta) = \frac{L_m(v_0; \theta) (p_k(v_0) + 1)^k}{(p_k(v_0) + L_m(v_0; \theta))^k} \sim \left(\frac{t}{m \ln t} \right)^{k-1}.$$

Therefore,

$$\ln K_m(v_0; \theta) \sim (k-1) \ln t \sim (k-1) \ln \theta, \quad \theta \rightarrow \infty,$$

so that

$$\liminf_{\theta \rightarrow \infty} \alpha_m(\theta) \geq \lim_{\theta \rightarrow \infty} \frac{\ln K_m(v_0; \theta)}{\ln \theta} = k - 1. \quad (6.64)$$

Thus, combining (6.63) and (6.64), we obtain the second limit in (6.60).

Finally, we turn to the proof of the first limit in (6.60). By virtue of Proposition 6.11, we may assume that $m \leq \frac{1}{2}(q-1)$. Then, by Lemma 6.10, $w_m \geq 1$ and therefore $p_k(w_m) \geq k-1$. Hence, from the definition (5.26) we get

$$\begin{aligned} 0 < K_m^*(\theta) &\leq L_m(w_m; \theta) \left(1 + \frac{1}{p_k(w_m)} \right)^k \\ &\leq L_m^*(\theta) \left(\frac{k}{k-1} \right)^k, \end{aligned} \quad (6.65)$$

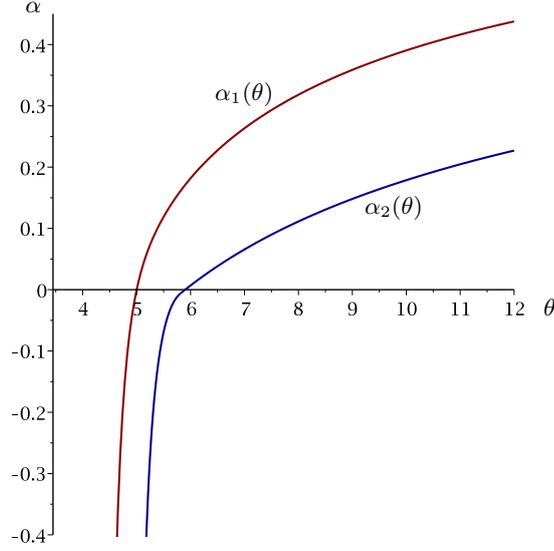


FIGURE 7. The graphs of the functions $\alpha_m(\theta)$ ($\theta > \theta_m$) for $k = 2$, $q = 5$ and $m = 1, 2$ (see the definition (2.46)). According to formula (2.47) (with $q = 5$), $\theta_1 = 1 + 2\sqrt{3} \doteq 4.4641 < \theta_2 = 5$. Note that $\theta_1^0 = 5$ and $\theta_2^0 = 1 + 2\sqrt{6} \doteq 5.8990$ are the zeros of $\alpha_1(\theta)$ and $\alpha_2(\theta)$, respectively (see Example 6.1). Note that the graphs are monotone increasing in line with Conjecture 6.2.

where $L_m^*(\theta) = L_m(v_m(\theta); \theta) = \max_{v>0} L_m(v; \theta)$. By continuity,

$$\lim_{\theta \downarrow \theta_m} L_m^*(\theta) = L_m^*(\theta_m) = 0,$$

and it follows from the bound (6.65) that $\lim_{\theta \downarrow \theta_m} K_m^*(\theta) = 0$, which implies the first limit in (6.60). Thus, the proof of Proposition 6.13 is complete. \square

Proposition 6.14. *For each $m = 1, \dots, q - 2$, the function $\theta \mapsto K_m^*(\theta)$ is monotone increasing for $\theta > \theta_m$.*

Proof. By virtue of Lemma 6.6, $K_m^*(\theta) = K_{m'}^*(\theta)$, where $m' = q - 1 - m$; hence, it suffices to prove the claim for m in the range $1 \leq m \leq \frac{1}{2}(q - 1)$. Using the definitions (5.13) and (5.26), differentiate with respect to θ to obtain

$$\begin{aligned} \frac{dK_m^*}{d\theta} &= \frac{\partial K_m}{\partial v} \Big|_{v=w_m} \times \frac{dw_m}{d\theta} + \frac{\partial K_m}{\partial L} \Big|_{v=w_m, L=L_m(w_m; \theta)} \times \frac{\partial L_m}{\partial \theta} \Big|_{v=w_m} \\ &= \frac{(p_k(w_m) + 1)^k (p_k(w_m) - (k - 1)L_m(w_m; \theta))}{(p_k(w_m) + L_m(w_m; \theta))^{k+1}} \times p_k(w_m), \end{aligned} \quad (6.66)$$

on account of the identity $\partial K_m / \partial v|_{v=w_m} \equiv 0$. To complete the proof, it remains to notice that the right-hand side of (6.66) is positive due to Lemma 6.8(b). \square

Remark 6.4. The result of Proposition 6.14 is not trivial (unlike the similar statement for $L_m^*(\theta)$, see the footnote in the proof of Lemma 5.2(b)), because, for each $v > 0$, we have that $L_m(v; \theta) \rightarrow \infty$ and, therefore, $K_m(v; \theta) \rightarrow 0$ as $\theta \rightarrow \infty$ (see formula (5.26)).

Conjecture 6.2. For each $m = 1, \dots, q - 2$, the function $\theta \mapsto \alpha_m(\theta) = \ln K_m^*(\theta) / \ln \theta$ is monotone increasing.

This conjecture is confirmed by computer plots (see Figure 7) and is easy to prove at least for $\theta \leq \theta_m^0$, where θ_m^0 is the root of the equation $K_m^*(\theta) = 1$ (cf. Proposition 6.16(a)); that is, $\alpha_m(\theta) \leq 0$ for $\theta \leq \theta_m^0$. Indeed, for any $\theta \in (\theta_m, \theta_m^0]$, we have

$$\frac{d\alpha_m(\theta)}{d\theta} = \frac{dK_m^*(\theta)}{d\theta} \times \frac{1}{\ln \theta \cdot K_m^*(\theta)} - \frac{\ln K_m^*(\theta)}{\theta \ln^2 \theta} > 0,$$

because $dK_m^*/d\theta > 0$ (Proposition 6.14), whereas $\ln K_m^*(\theta) \leq \ln K_m^*(\theta_m^0) = 0$.

6.4. Zeros of $\alpha_{\pm}(\theta)$ and $\alpha_m(\theta)$. Recall that the functions $\alpha_{\pm}(\theta)$ and $\alpha_m(\theta)$ are defined in (2.41) and (2.46), respectively. As was observed in numerical examples (see Figure 3 and also Figures 6 and 7), the functions $\alpha_{-}(\theta)$ and $\alpha_1(\theta)$ have the same zero, $\theta_0^- = \theta_1^0$, whereas $\alpha_{+}(\theta) = 0$ at $\theta_0^+ = 1 + q/(k-1)$. In this subsection, we give a proof of these observations.

Let us first state and prove a lemma. Recall the notation $L_m^*(\theta) = \max_{v \in \mathcal{V}_m^+(\theta)} L_m(v; \theta)$ and $K_m^*(\theta) = \max_{v \in \mathcal{V}_m^+(\theta)} K_m(v; \theta)$.

Lemma 6.15. *Let $q \geq 3$ and $k \geq 2$.*

- (a) *For any $m \in [1, q-2]$, if $L_m(v; \theta) < 1$ for some $v \geq 1$ and $\theta > \theta_m$ then $K_m(v; \theta) < 1$.*
- (b) *Let $1 \leq m \leq \frac{1}{2}(q-1)$. If $L_m^*(\theta) < 1$ for some $\theta > \theta_m$ then $K_m^*(\theta) < 1$. In particular, $L_m^*(\theta) = 1$ if and only if $K_m^*(\theta) = 1$.*

Proof. (a) Denoting $s := (L_m(v; \theta))^{1/k} < 1$ and using the definition (5.26), the required inequality $K_m(v; \theta) < 1$ can be rewritten as

$$p_k(v) > \frac{s - s^k}{1 - s} = p_k(s),$$

and the last inequality holds by monotonicity of $p_k(v)$, since $v \geq 1 > s$.

(b) Let $v = w_m$ be such that $K_m(w_m; \theta) = K_m^*(\theta) < 1$; by Lemma 6.10, $w_m \geq 1$. On the other hand, $L_m(w_m; \theta) \leq L_m^*(\theta) < 1$, and by part (a) it follows that $K_m(w_m; \theta) < 1$. The last claim in part (b) then follows by continuity and monotonicity of both $L_m^*(\theta)$ and $K_m^*(\theta)$ (see Lemma 5.2(b) and Proposition 6.14, respectively), also recalling that $L_m(v; \theta) = 1$ implies $K_m(v; \theta) = 1$ (see (5.26)). \square

Proposition 6.16. *Let $q \geq 3$, and set $m_0 := \lfloor \frac{1}{2}(q-1) \rfloor$.*

- (a) *For each m in the range $1 \leq m \leq m_0$, the function $\alpha_m(\theta)$ has a unique zero given by*

$$\theta_m^0 = \frac{m(v_m^0)^k + m' + 1}{p_k(v_m^0)}, \quad (6.67)$$

where $v_m^0 > 1$ is a sole positive root of the equation

$$m \sum_{i=1}^{k-1} i v^{k-i} - (m' + 1) \sum_{i=1}^{k-1} i v^{i-k} = 0. \quad (6.68)$$

- (b) (i) *The function $\alpha_{+}(\theta)$ has a unique zero given by $\theta_0^+ = 1 + \frac{q}{k-1}$. Moreover, $\alpha_{+}'(\theta_0^+) = 0$.*
- (ii) *The function $\alpha_{-}(\theta)$ has a unique zero θ_0^- , which coincides with the zero θ_1^0 of the function $\alpha_1(\theta)$.*

(c) The zeros $\theta_1^0, \dots, \theta_{m_0}^0$ follow in ascending order and are strictly below θ_0^+ ,

$$\theta_1^0 < \dots < \theta_{m_0}^0 < \theta_0^+ = 1 + \frac{q}{k-1}. \quad (6.69)$$

Proof. (a) By the definition (2.46), the condition $\alpha_m(\theta) = 0$ means that $K_m^*(\theta) = 1$ and hence, by Lemma 6.15(b), $L_m^*(\theta) = 1$. Eliminating θ from the system of equations $L_m(v; \theta) = 1$, $\partial L_m(v; \theta)/\partial v = 0$ gives for the root $v = v_m^0$ the equation (cf. (5.21))

$$mkv^{k-1}p_k(v) - (mv^k + m' + 1)p_k'(v) = 0,$$

which can be rearranged to the form (6.68). Uniqueness of positive solution v_m^0 of the equation (6.68) is obvious, noting that the left-hand side of (6.68) is a continuous, increasing function in $v > 0$, with the range from $-\infty$ to $+\infty$. To show that $v_m^0 > 1$, it suffices to check that the left-hand side of (6.68) at $v = 1$ is negative, which is indeed true since $2m \leq q - 1 < q$. Expressing θ from the equation $L_m(v_m^0; \theta) = 1$, we obtain formula (6.67).

(b) In the limit $\alpha \rightarrow 0$, the equation (5.4) always has root $u = 1$, while for $u \neq 1$, by virtue of the identity (5.1), it is reduced to equation (5.3) with $m = 1$. Using the notation (5.13), the latter equation can be rewritten as $L_1(u; \theta) = 1$, which in turn has up to two (positive) roots (see Lemma 5.2). In total, there are three positive roots, and for this number to reduce to *two* (which is the condition of belonging to the curves $y = \alpha_{\pm}(\theta)$), either (i) one zero of the function $u \mapsto L_1(u; \theta) - 1$ must coincide with $u = 1$, or (ii) the equation $L_1(u; \theta) = 1$ must have a double root, thus also satisfying the condition $\partial L_1(u; \theta)/\partial u = 0$.

In case (i), the condition $L_1(u; \theta)|_{u=1} = 1$ transcribes as $(\theta - 1)(k - 1) - (q - 1) = 1$, which immediately yields the root $\theta_0^+ = 1 + q/(k - 1)$. According to the substitution (5.8) (with $\alpha = 0$), the corresponding root of the quadratic equation (2.37) is given by $x = \theta_0^+/(q - 1)$, which appears to be the *smaller* of the two roots, $x = x_-$. Therefore, in view of formulas (2.40) and (2.41), the value θ_0^+ is a zero of the function $\alpha_+(\theta)$. Indeed, using the definition (2.36) of $b = b(\theta)$, the second root of (2.37) is found to be

$$x_+ = \frac{b}{x_-} = \frac{\theta_0^+(\theta_0^+ + q - 2)}{q - 1} \cdot \frac{q - 1}{\theta_0^+} = \theta_0^+ + q - 2 > \frac{\theta_0^+}{q - 1} = x_-,$$

as claimed.

In case (ii), according to the proof of part (a), the unique solution of the system $L_1(u; \theta) = 1$, $\partial L_1(u; \theta)/\partial u = 0$ is given by $(u, \theta) = (v_1^0, \theta_1^0)$, where

$$\theta_1^0 = 1 + \frac{(v_1^0)^k + 2}{p_k(v_1^0)} \quad (6.70)$$

and $v_1^0 > 1$ is a sole root of the equation (6.68) with $m = 1$, that is,

$$\sum_{i=1}^{k-1} iv^{k-i} - (q-1) \sum_{i=1}^{k-1} iv^{i-k} = 0. \quad (6.71)$$

Again by the substitution (5.8) with $\alpha = 0$, the corresponding root of the quadratic equation (2.37) is given by

$$x = \frac{\theta_1^0(v_1^0)^k}{q-1},$$

and we wish to prove that this is the *bigger* of the two roots, $x = x_+$, which would imply like before that θ_1^0 is a zero of the function $\alpha_-(\theta)$. Since the other root of (2.37)

equals b/x , with $b = b(\theta)$ defined in (2.36), our claim is expressed as $x > b/x$, that is,

$$(v_1^0)^{2k} > (q-1) \left(1 + \frac{q-2}{\theta_1^0} \right). \quad (6.72)$$

Furthermore, recalling that $\theta_1^0 > 1$ (see (6.70)), we have

$$1 + \frac{q-2}{\theta_1^0} > q-1,$$

so for the proof of (6.72) it suffices to show that

$$v_1^0 \geq (q-1)^{1/k}. \quad (6.73)$$

Since the function on the left-hand side of (6.71) is monotone increasing, we only need to check that its value at $v = (q-1)^{1/k}$ is non-positive, that is,

$$\sum_{i=1}^{k-1} i v^{k-i} - \sum_{i=1}^{k-1} i v^{i-k} \leq 0.$$

which can be rewritten as

$$\sum_{i=1}^{k-1} (2i-k) v^{i-k/2} \geq 0.$$

Now, the latter inequality holds because the left-hand side is obviously monotone increasing as a function of $v \geq 1$, being equal to 0 at $v = 1$. Hence, (6.73) follows.

Thus, we have proved that $\theta_0^+ = 1 + q/(k-1)$ and $\theta_0^- = \theta_1^0$ are the sole roots of the functions $\alpha_+(\theta)$ and $\alpha_-(\theta)$, respectively.

Finally, since the function $\alpha_+(\theta)$ is known to be positive both at $\theta_c < \theta_0^+$ and at infinity (see Proposition 6.4), it readily follows that it has a minimum value 0 at $\theta = \theta_0^+$, hence $\alpha'_+(\theta) = 0$, as claimed in part (b)(i).

(c) The ordering inequalities between (θ_m^0) in (6.69) readily follow from the monotonicity property (6.56) proved in Proposition 6.55. Thus, it remains to show that $\theta_m^0 < \theta_0^+$. Observe that the value $L_m(v; \theta)|_{v=1} = (\theta-1)(k-1) - (q-1)$ does not depend on m . Recalling that $L_1(1; \theta_0^+) = 1$ (see the proof of part (a)), we get that $L_m(1; \theta_0^+) = 1$, but

$$\begin{aligned} \left. \frac{\partial L_m(v; \theta_0^+)}{\partial v} \right|_{v=1} &= (\theta_0^+ - 1) p'_k(1) - mk \\ &= \frac{q}{k-1} \cdot \frac{k(k-1)}{2} - mk \\ &= k \left(\frac{q}{2} - m \right) > 0, \end{aligned}$$

since $m \leq \frac{1}{2}(q-1) < q/2$. Hence, $L_m^*(\theta_0^+) > L_m(1; \theta_0^+) = 1$, and by monotonicity of the function $\theta \mapsto L_m(v; \theta)$ it follows, according to the proof in part (a), that $\theta_m^0 < \theta_0^+$.

An alternative simple argument is that, as shown in part (a), the maximum value of $v \mapsto L_m(v; \theta_m^0) = 1$ is attained at $v = v_m^0 > 1$, hence $L_m(1; \theta_m^0) < 1$ and, again by monotonicity, it follows that $\theta_0^+ > \theta_m^0$. \square

A version of Proposition 6.16(b) for $q = 2$ is easy to obtain.

Proposition 6.17. *In the case $q = 2$, the functions $\alpha_{\pm}(\theta)$ have a unique zero at $\theta_c = \frac{k+1}{k-1}$, which coincides with $\theta_0^+ = 1 + 2/(k-1)$. Moreover, $\alpha'_{\pm}(\theta_c) = 0$.*

Proof. By Lemma 6.3 with $q = 2$, we have $\alpha_-(\theta) = -\alpha_+(\theta)$ for all $\theta \geq \theta_c = \frac{k+1}{k-1}$. Thus, it suffices to consider the function $\alpha_+(\theta)$. Treating the index $q \geq 2$ as a continuous variable and taking the limit from the domain $q > 2$ as $q \rightarrow 2+$, we see that the unique zero of $\alpha_+(\theta)$, given by $\theta_0^+(k, q) = 1 + q/(k-1)$, converges to $1 + 2/(k-1) = \frac{k+1}{k-1} = \theta_c$. On the other hand, the derivative α'_+ vanishes at $\theta_0^+(k, q)$ for each $q > 2$, hence its limiting value at θ_c is also zero, that is, $\alpha'_+(\theta_c+) = 0$, as claimed.

This result can also be obtained by a direct calculation. Namely, for $q = 2$ the definition (2.36) is reduced to $b(\theta) = \theta^2$. From equation (2.37) with $q = 2$, it is easy to see that $x_{\pm}(\theta) \rightarrow \theta_c$ as $\theta \rightarrow \theta_c+$. Moreover, a simple asymptotic analysis shows that

$$x_{\pm}(\theta) = \theta_c \pm \sqrt{2k\theta_c(\theta - \theta_c)} + (k+1)(\theta - \theta_c) + o(\theta - \theta_c), \quad \theta \rightarrow \theta_c + .$$

Hence, from (2.40) it follows

$$\ln a_{\pm}(\theta) = -(k+1)\ln \theta_c - (k-1)(\theta - \theta_c) + o(\theta - \theta_c), \quad \theta \rightarrow \theta_c + .$$

Finally, substituting this into (2.41) we obtain

$$\begin{aligned} \alpha_{\pm}(\theta) &= -(k+1) + \frac{(k+1)\ln \theta_c + (k-1)(\theta - \theta_c) + o(\theta - \theta_c)}{\ln \theta_c + \theta_c^{-1}(\theta - \theta_c) + o(\theta - \theta_c)} \\ &= \frac{\theta - \theta_c}{\ln \theta_c} \left((k-1) - \frac{k+1}{\theta_c} \right) + o(\theta - \theta_c) \\ &= o(\theta - \theta_c), \quad \theta \rightarrow \theta_c + , \end{aligned}$$

which implies that $\alpha' \pm -(\theta_c+) = 0$, as claimed. \square

Example 6.1. Consider the case $k = 2$. Then the zero of the function $\alpha_+(\theta) = 0$ specializes to $\theta_0^+ = 1 + q$. Furthermore, the equation (6.68) is easily solved to yield $v_m^0 = \sqrt{(q-m)/m}$, and from (6.67) we readily find

$$\theta_m^0 = 1 + 2\sqrt{m(q-m)}, \quad 1 \leq m \leq \frac{1}{2}(q-1). \quad (6.74)$$

It is of interest to note, by comparing (6.74) with (2.47), that $\theta_m^0 = \theta_{m+1}$ (cf. [30, equation (2.1), page 192]). Finally, taking $m = 1$ in (6.74) gives $\theta_0^- = \theta_1^0 = 1 + 2\sqrt{q-1}$.

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APPENDIX A. PROOF OF PROPOSITION 2.6

Necessity. Assume that the measure μ^h is translation invariant, that is, the condition (2.25) holds. Pick the set $A \subset V$ to be the unit ball $V_1 \equiv V_1(x_o) = \{x_o, x_1, \dots, x_{k+1}\}$ centred at the root x_o , with $\partial\{x_o\} = \{x_1, \dots, x_{k+1}\}$, where the numbering in (x_j) is consistent with the bijection $\mathbf{b}: V \rightarrow \mathcal{A}_k$, that is, $x_j = \mathbf{b}^{-1}(a_j)$ (see Section 2.3.1). For $z \in V$, the shifted set $V_1(z) := \tilde{T}_z(V_1) = \{z, z_1, \dots, z_{k+1}\}$ (where $z_j = \tilde{T}_z(x_j)$,

$j = 1, \dots, k+1$) is the unit ball centred at $z = \tilde{T}_z(x_o)$, so that $\partial\{z\} = \{z_1, \dots, z_{k+1}\}$. Consider an arbitrary configuration $\varsigma \in \Phi^{V_1}$, with spin values

$$\varsigma(x_o) = i_0, \quad \varsigma(x_j) = i_j, \quad j = 1, \dots, k+1.$$

Note that if $y = \tilde{T}_z(x)$ then, according to (2.24),

$$(\tilde{T}_z \varsigma)(y) = \varsigma(\tilde{T}_z^{-1}(y)) = \varsigma(x). \quad (\text{A.1})$$

Hence, the property (2.25) of translation invariance of μ^h specializes as follows,

$$\begin{aligned} \mu^h(\sigma \in \Phi^V: \sigma(z) = i_0, \sigma(z_1) = i_1, \dots, \sigma(z_{k+1}) = i_{k+1}) \\ = \mu^h(\sigma \in \Phi^V: \sigma(x_o) = i_0, \sigma(x_1) = i_1, \dots, \sigma(x_{k+1}) = i_{k+1}). \end{aligned} \quad (\text{A.2})$$

Using formulas (1.3) and (1.15), and cancelling the common term $\beta \sum_{j=1}^{k+1} J \delta_{i_0, i_j}$, the equality (A.2) is reduced to

$$\sum_{j=1}^{k+1} [\xi_{i_j}(z_j) + h_{i_j}^\dagger(z_j, z)] + \xi_{i_0}(z) = \sum_{j=1}^{k+1} [\xi_{i_j}(x_j) + h_{i_j}^\dagger(x_j, x_o)] + \xi_{i_0}(x_o) + \frac{1}{\beta} \ln \frac{Z_{V_1(z)}}{Z_{V_1(x_o)}}. \quad (\text{A.3})$$

Varying $i_0 \in \Phi$ in (A.3) (whilst keeping all other i_j fixed) shows that the difference $\xi_{i_0}(z) - \xi_{i_0}(x_o)$ does not depend on i_0 . More precisely, on subtracting from (A.3) the same equality with $i_0 = q$, we obtain

$$\xi_i(z) - \xi_q(z) = \xi_i(x_o) - \xi_q(x_o), \quad i = 1, \dots, q-1. \quad (\text{A.4})$$

Since (A.4) holds for any $z \in V$, this proves (2.26) in view of the notation (2.2).

Furthermore, by virtue of (2.26) the equality (A.3) becomes

$$\sum_{j=1}^{k+1} h_{i_j}^\dagger(z_j, z) = \sum_{j=1}^{k+1} h_{i_j}^\dagger(x_j, x_o) + \sum_{x \in V_1(x_o)} \xi_q(x) - \sum_{y \in V_1(z)} \xi_q(y) + \frac{1}{\beta} \ln \frac{Z_{V_1(z)}}{Z_{V_1(x_o)}}. \quad (\text{A.5})$$

Similarly, varying the values i_1, \dots, i_{k+1} in (A.5) (one at a time) yields, for each $j = 1, \dots, k+1$,

$$\check{h}_i^\dagger(z_j, z) = \check{h}_i^\dagger(x_j, x_o), \quad i = 1, \dots, q-1. \quad (\text{A.6})$$

On the other hand, fix $j \in \{1, \dots, k+1\}$ and consider the shift \tilde{T}_{z_j} , resulting in

$$\tilde{T}_{z_j}(x_o) = z_j, \quad \tilde{T}_{z_j}(x_j) = z.$$

The latter equality follows by recalling the definition of conjugate translations (see (2.23)) and noting that $z_j = \tilde{T}_z(x_j) = \mathbf{b}^{-1}(\mathbf{b}(z)\mathbf{b}(x_j)) = \mathbf{b}^{-1}(\mathbf{b}(z)a_j)$ and, therefore,

$$\tilde{T}_{z_j}(x_j) = \mathbf{b}^{-1}(\mathbf{b}(z_j)\mathbf{b}(x_j)) = \mathbf{b}^{-1}(\mathbf{b}(z)a_j^2) = \mathbf{b}^{-1}(\mathbf{b}(z)) = z,$$

because $a_j^2 = e$ (see Section 2.3.1). Hence, for \tilde{T}_{z_j} the result (A.6) transforms into

$$\check{h}_i^\dagger(z, z_j) = \check{h}_i^\dagger(x_j, x_o), \quad i = 1, \dots, q-1. \quad (\text{A.7})$$

Comparing (A.6) and (A.7), we conclude that $\check{h}_i^\dagger(z_j, z) = \check{h}_i^\dagger(z, z_j)$, and the claim (2.27) follows. Finally, let $y = \tilde{T}_v(z)$ and $y_j = \tilde{T}_v(z_j)$, for some $v \in V$. Observe that

$$y = \tilde{T}_y(x_o), \quad y_j = \tilde{T}_y(x_j). \quad (\text{A.8})$$

The first equality in (A.8) is automatic; to check the second one, note that

$$\begin{aligned} \mathbf{b}(y_j) &= \mathbf{b}(v) \mathbf{b}(z_j) & [y_j = \tilde{T}_v(z_j)] \\ &= \mathbf{b}(v) (\mathbf{b}(z) \mathbf{b}(x_j)) & [z_j = \tilde{T}_z(x_j)] \\ &= (\mathbf{b}(v) \mathbf{b}(z)) \mathbf{b}(x_j) \\ &= \mathbf{b}(y) \mathbf{b}(x_j) & [y = \tilde{T}_v(z)]. \end{aligned}$$

That is, $\mathbf{b}(y_j) = \mathbf{b}(y) \mathbf{b}(x_j)$ and (A.8) follows. Thus, formula (A.6) applied to the edge $\langle y_j, y \rangle$ gives

$$\check{h}_i^\dagger(y_j, y) = \check{h}_i^\dagger(x_j, x_o), \quad i = 1, \dots, q-1.$$

Combined with (A.6), this implies

$$\check{h}_i^\dagger(z_j, z) = \check{h}_i^\dagger(y_j, y) = \check{h}_i^\dagger(\tilde{T}_v(z_j), \tilde{T}_v(z)),$$

and (2.28) follows. This completes the ‘‘only if’’ part of the proof.

Sufficiency. Suppose that the conditions (2.26), (2.27) and (2.28) are satisfied. It suffices to verify formula (2.25) for the balls V_n ($n \geq 1$). For $z \in V$, denote $\Lambda := \tilde{T}_z(V_{n-1})$, then $\bar{\Lambda} = \tilde{T}_z(V_n)$ and $\partial\Lambda = \tilde{T}_z(W_n)$. Furthermore, for $\varsigma \in \Phi^{V_n}$ set $\varsigma_z := \tilde{T}_z(\varsigma) \in \Phi^{\bar{\Lambda}}$ (see (2.24)). Observe that if $y = \tilde{T}_z(x)$ then, according to (A.1),

$$\varsigma_z(y) = \varsigma(\tilde{T}_z^{-1}(y)) = \varsigma(x). \quad (\text{A.9})$$

Hence, recalling (1.3), we have

$$\begin{aligned} H_{\bar{\Lambda}}(\varsigma_z) &= - \sum_{\langle y, y' \rangle \in E_{\bar{\Lambda}}} J \delta_{\varsigma_z(y), \varsigma_z(y')} - \sum_{y \in \bar{\Lambda}} \xi_{\varsigma_z(y)}(y) \\ &= - \sum_{\langle x, x' \rangle \in E_n} J \delta_{\varsigma(x), \varsigma(x')} - \sum_{x \in V_n} \xi_{\varsigma(x)}(\tilde{T}_z(x)) \\ &= H_n(\varsigma) + \sum_{x \in V_n} (\xi_q(x) - \xi_q(\tilde{T}_z(x))), \end{aligned}$$

where at the last step we used the property (2.26). Thus, from formula (1.15) we obtain, omitting factors not depending on ς ,

$$\mu^h(\sigma_{\bar{\Lambda}} = \varsigma_z) \propto \mu^h(\sigma_{V_n} = \varsigma) \cdot \exp \left\{ \beta \sum_{y \in \partial\Lambda} h_{\varsigma_z(y)}^\dagger(y, y_\Lambda) - \beta \sum_{x \in W_n} h_{\varsigma(x)}(x) \right\}, \quad (\text{A.10})$$

where y_Λ is the unique neighbour of $y \in \partial\Lambda$ in Λ . Note that if $y = \tilde{T}_z(x)$, with $x \in \partial V_{n-1} = W_n$, then $y_\Lambda = \tilde{T}_z(x')$, where $x' \in W_{n-1}$ is the unique vertex such that $x \in S(x')$. Thus, using (A.9), (2.28) and (2.29), we can write

$$\begin{aligned} \exp \left\{ \beta \sum_{y \in \partial\Lambda} h_{\varsigma_z(y)}^\dagger(y, y_\Lambda) \right\} &= \exp \left\{ \beta \sum_{x \in W_n} h_{\varsigma(x)}^\dagger(\tilde{T}_z(x), \tilde{T}_z(x')) \right\} \\ &\propto \exp \left\{ \beta \sum_{x \in W_n} h_{\varsigma(x)}^\dagger(x, x') \right\} \\ &\propto \exp \left\{ \beta \sum_{x \in W_n} h_{\varsigma(x)}(x) \right\}. \end{aligned}$$

Returning to (A.10), this gives $\mu^h(\sigma_{\bar{A}} = \varsigma_z) \propto \mu^h(\sigma_{V_n} = \varsigma)$, and since

$$\sum_{\varsigma \in \Phi^{V_n}} \mu^h(\sigma_{\bar{A}} = \varsigma_z) = 1 = \sum_{\varsigma \in \Phi^{V_n}} \mu^h(\sigma_{V_n} = \varsigma),$$

it follows that $\mu^h(\sigma_{\bar{A}} = \varsigma_z) = \mu^h(\sigma_{V_n} = \varsigma)$, and the proof of the ‘‘if’’ part is complete.

APPENDIX B. PROOF OF LEMMA 5.3

B.1. Proof of part (a). Denote $t := \theta - 1$. For $q = 3$ (i.e., with $m = m' = 1$), the partial derivative $\partial K_1 / \partial v$ (see (6.23)) can be represented as

$$\begin{aligned} \frac{\partial K_1}{\partial v} = \frac{(p_k + 1)^{k-1}}{(p_k + L_m)^{k+1}} & \left\{ (p_k + 1 + (1 - L_1)(k - 1)) L'_1 (p_k - (k - 1)) \right. \\ & \left. - (1 - L_1) k L_1 \left(p'_k - \frac{k(k-1)}{2} \right) + \frac{k(k-1)}{2} (1 - L_1) (2L'_1 - kL_1) \right\}, \end{aligned} \quad (\text{B.1})$$

where $L_1 = tp_k - v^k - 1$ and $L'_1 = \partial L_1 / \partial v = tp'_k - kv^{k-1}$.

Note that $\partial K_1 / \partial v|_{v=1} = 0$ (cf. (6.39)); this follows without calculations from the scaling property $K_1(v; t) = K_1(v^{-1}; t)$ (see (6.15)). More explicitly, using the formulas

$$p_k|_{v=1} = k - 1, \quad p'_k|_{v=1} = \frac{k(k-1)}{2}, \quad (\text{B.2})$$

it is easy to see that the terms in (B.1) vanish at $v = 1$. We will also need the formula

$$p''_k|_{v=1} = \frac{k(k-1)(k-2)}{3}. \quad (\text{B.3})$$

Such expressions can be obtained by successively differentiating (at $v = 1$) the identity

$$v^k - 1 \equiv (v - 1)(p_k + 1).$$

To compute the second-order derivative $\partial^2 K_1 / \partial v^2$ at $v = 1$, we need to differentiate in (B.1) only the factors that vanish at $v = 1$, setting $v = 1$ elsewhere. Hence,

$$\begin{aligned} \frac{\partial^2 K_1}{\partial v^2} \Big|_{v=1} = \frac{(p_k + 1)^{k-1}}{(p_k + L_1)^{k+1}} & \left\{ (p_k + 1) L'_1 p'_k \right. \\ & \left. + (1 - L_1) \left[(k - 1) L'_1 p'_k - k L_1 p''_k + \frac{k(k-1)}{2} (2L''_1 - kL'_1) \right] \right\} \Big|_{v=1}. \end{aligned} \quad (\text{B.4})$$

Using (B.2) and (B.3), we find

$$L_1|_{v=1} = tp_k(1) - 2 = t(k - 1) - 2, \quad (\text{B.5})$$

$$L'_1|_{v=1} = tp'_k(1) - k = t \frac{k(k-1)}{2} - k, \quad (\text{B.6})$$

$$L''_1|_{v=1} = tp''_k(1) - k(k-1) = t \frac{k(k-1)(k-2)}{3} - k(k-1). \quad (\text{B.7})$$

Finally, substituting formulas (B.2), (B.3) and (B.5)–(B.7) into (B.4), after simple manipulations (verified with **Maple**) we obtain

$$\begin{aligned} \frac{\partial^2 K_1}{\partial v^2} \Big|_{v=1} = & \left(\frac{k}{(k-1)(t+1) - 2} \right)^{k+1} \frac{k-1}{2} \\ & \times \left(\frac{(k-1)^2}{2} t^2 + \frac{(k-1)(7k-11)}{6} t - 3k + 1 \right). \end{aligned} \quad (\text{B.8})$$

The quadratic polynomial in (B.8) has one positive zero $t = t^*$,

$$t^* = \frac{11 - 7k + \sqrt{49k^2 + 62k + 49}}{6(k - 1)},$$

which corresponds to $\tilde{\theta}_1 = t^* + 1$ as defined in (2.48). Hence, $\partial^2 K_1 / \partial v^2|_{v=1} > 0$ for $\theta > \tilde{\theta}_1$, which implies that $v = 1$ is a local minimum of the function $v \mapsto K_1(v; \theta)$. This completes the proof of Lemma 5.3(a).

B.2. Proof of part (b). It suffices to show, for $1 \leq \theta \leq \tilde{\theta}_1$ (i.e., $0 \leq t \leq t^*$), that $v = 1$ is the sole root of the equation $\partial K_1 / \partial v = 0$. A plausible general scheme of the proof of the latter statement may be as follows.

- (1) First, the condition $\partial K_1 / \partial v = 0$ (see (6.23)) is reduced to $P(v; t) = 0$, where $P(v; t)$ is a polynomial in v (and also a quadratic polynomial in t).
- (2) Since $P(1; t) = 0$, the quotient $R(v; t) = P(v; t) / (v - 1)$ is a polynomial in v , and we wish to prove that $R(v; t) < 0$ for any $t \leq t^*$ and all $v \neq 1$.
- (3) According to the proof in Section B.1, the condition $\partial^2 K_1 / \partial v^2|_{v=1} \leq 0$ is satisfied whenever $R(1; t) \leq 0$; moreover, the critical value t^* is determined by the quadratic equation $R(1; t^*) = 0$, which implies that $R(1; t) \leq 0$ for $t \in [0, t^*]$.
- (4) Bearing in mind the invariance of $K_1(v; t)$ under the map $v \mapsto v^{-1}$, it should be possible to represent the polynomial $R(v; t)$ in the form

$$R(v; t) = \chi(v) \cdot \tilde{R}(y; t), \quad y = v + v^{-1} \geq 2,$$

where $\chi(v) > 0$ and $\tilde{R}(y; t)$ is a polynomial in y .

- (5) The crucial step is to show that, for each $t \in [0, t^*]$, the function $y \mapsto \tilde{R}(y; t)$ is *monotone decreasing*.
- (6) Finally, using steps (3) to (5), for any $y > 2$ (i.e., $v \neq 1$) we have

$$\tilde{R}(y; t) < \tilde{R}(2; t) = \frac{R(1; t)}{\chi(1)} \leq 0, \quad 0 \leq t \leq t^*.$$

Hence, for all $t \in [0, t^*]$ and $v \neq 1$, we get

$$R(v; t) = \chi(v) \cdot \tilde{R}(y; t) < 0,$$

as required.

In what follows, we implement this scheme in more detail for the cases $k = 2, 3, 4$. All calculations were done analytically and also verified using **Maple**.

B.2.1. Case $k = 2$. According to formula (2.49), $t^* = \frac{1}{2}(\sqrt{41} - 1)$. The polynomial $P(v; t)$ is found to be

$$\begin{aligned} P(v; t) &= t^2 v^2 - t^2 v - t v^3 + 4t v^2 - 4t v + t - 4v^3 + 2v^2 - 2v + 4 \\ &= (v - 1) \{ t^2 v - t(v^2 - 3v + 1) - (4v^2 + 2v + 4) \}. \end{aligned}$$

Hence,

$$\begin{aligned} R(v; t) &= t^2 v - t(v^2 - 3v + 1) - (4v^2 + 2v + 4) \\ &= v \left(t^2 - t \left(v - 3 + \frac{1}{v} \right) - 4 \left(v + \frac{1}{v} \right) - 2 \right) \\ &= v (t^2 - t(y - 3) - 4y - 2), \end{aligned}$$

where $y = v + v^{-1}$. This gives

$$\tilde{R}(y; t) = t^2 - t(y - 3) - 4y - 2 = -y(t + 4) + t^2 + 3t - 2,$$

which is clearly a decreasing function of y for any $t \geq 0$.

B.2.2. *Case $k = 3$.* By (2.49), we have $t^* = \frac{4}{3}$. The quotient $R(v; t) = P(v; t)/(v - 1)$ is explicitly given by

$$\begin{aligned} R(t, v) &= (v + 1)(t + 3)(2tv^3 + 2tv - 2v^4 - 2 + 5tv^2 - 4v^3 - 4v) \\ &= v^2(v + 1)(t + 3) \left(2t \left(v + \frac{1}{v} \right) - 2 \left(v^2 + \frac{1}{v^2} \right) + 5t - 4 \left(v + \frac{1}{v} \right) \right) \\ &= v^2(v + 1)(t + 3)(2ty - 2(y^2 - 2) + 5t - 4y). \end{aligned}$$

Thus,

$$\tilde{R}(y; t) = (t + 3)(2ty - 2(y^2 - 2) + 5t - 4y),$$

and it is easy to check that this function is decreasing in y for any $t \leq t^* = \frac{4}{3}$.

B.2.3. *Case $k = 4$.* Elementary but tedious calculations yield

$$\begin{aligned} R(v; t) &= t^2 (3v^7 + 11v^6 + 25v^5 + 30v^4 + 25v^3 + 11v^2 + 3v) \\ &\quad - t (3v^8 + v^7 - 13v^6 - 57v^5 - 72v^4 - 57v^3 - 13v^2 + v + 3) \\ &\quad - (8v^8 + 24v^7 + 48v^6 + 36v^5 + 32v^4 + 36v^3 + 48v^2 + 24v + 8). \end{aligned}$$

Rearranging under the substitution $y = v + v^{-1}$ gives $R(v; t) = v^4 \tilde{R}(y; t)$ with

$$\begin{aligned} \tilde{R}(y; t) &= t^2(3y^3 + 11y^2 + 16y + 8) \\ &\quad - t(3y^4 + y^3 - 25y^2 - 60y - 40) \\ &\quad - (8y^4 + 24y^3 + 16y^2 - 36y - 48). \end{aligned} \tag{B.9}$$

In particular, if $y = 2$ then

$$\tilde{R}(2; t) = 12(9t^2 + 17t - 22) = 0$$

for $t = \frac{1}{18}(\sqrt{1081} - 17) = t^*$ (cf. (2.49)), as it should be.

Finally, we need to verify that the function $y \mapsto \tilde{R}(y; t)$ is decreasing for any $t \in [0, t^*]$. Unfortunately (but inevitably), technicalities involved in a purely analytic check become quite substantial; however, using `Maple` to plot the graph of (B.9), with parameter t ranging from 0 to t^* , makes the monotonicity evident.

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