Phase transitions in the evolution of partial orders

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Abstract

We determine the approximate number of partial orders with a fixed number of comparable pairs, give a complete description of the evolution of partial orders and prove that infinitely many phase transitions occur. This answers questions posed by Dhar, Kleitman, and Rothschild 20 years ago.

1 Introduction and Results

Let $\mathcal{P}_n$ be the set of all labeled partial orders with point set $[n] = \{1, \ldots, n\}$. In 1970, Kleitman and Rothschild [3] first gave the following bound:

$$\log_2 |\mathcal{P}_n| \;=\; \frac{1}{4}n^2 + O(n^{3/2}\log_2 n). \tag{1}$$

A few years later [4], they were able to give a considerably sharper estimate, namely

$$\log_2 |\mathcal{P}_n| \;=\; \frac{1}{4}n^2 + \frac{3}{2}n + O(\log_2 n). \tag{2}$$

The proofs of these results are considered to be the pioneers of what has become known as the Kleitman–Rothschild–method. Its underlying principle can be stated in very rough terms as follows. Find a subclass $\mathcal{Q}_n \subseteq \mathcal{P}_n$ that on the one hand has a nice structure and can therefore be enumerated easily. On the other hand it should be so large that $|\mathcal{Q}_n|$ is a good approximation for $|\mathcal{P}_n|$.

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Here Kleitman and Rothschild chose $\mathcal{Q}_n$ so that it contained only 3-*layer partial orders* – these are partial orders whose point set can be partitioned into three antichains X_1, X_2, X_3 such that no point in X_1 is above any element of X_2, no point in X_2 is above any element of X_3, and every point in X_1 is below every point in X_3. One of the particularly appealing features of this technique is that it also proves that the proportion of partial orders in $\mathcal{P}_n$ that are 3-layer partial orders tends to one as n tends to infinity – in other words, *almost all* partial orders are 3-layer partial orders. Results of this type describe the so–called *global structure* of a set. They state what properties we can expect from a *typical* (or *randomly chosen*) element of the set.

The *evolution* of a random object (chosen from a certain set) usually denotes the following 'experiment': choose a 'time'–parameter of the objects in the set and consider only one 'slice' of the set, namely only those objects where the parameter is equal to a fixed value. What is the global structure of this slice and what is its cardinality? How do global structure and cardinality evolve when the time–parameter increases? Finally, does this evolution consist of several distinct *phases*, and, if so, where do *phase transitions* occur?

When considering the evolution of partial orders, it seems natural to choose the number of comparable pairs as time–parameter. The proof in [4] immediately implies that a typical partial order in $|\mathcal{P}_n|$ has roughly $\frac{3}{16}n^2$ comparable pairs, so we can indeed expect a different global structure if we focus on the slice of all partial orders with, say, $\frac{1}{8}n^2$ comparable pairs. More precisely, for $0 < d < \frac{1}{2}$ denote by $\mathcal{P}_{n,d}$ those partial orders in $\mathcal{P}_n$ with dn^2 comparable pairs and let

$$\mathrm{c}(d) := \lim_{n\to\infty} \frac{\log_2 |\mathcal{P}_{n,d}|}{n^2}, \quad \text{in other words,} \quad |\mathcal{P}_{n,d}| = 2^{\mathrm{c}(d)n^2+o(n^2)},$$

provided the limit exists.

At first sight, determining $|\mathcal{P}_{n,d}|$ or computing $\mathrm{c}(d)$ seems to be a question of purely combinatorial interest, and it is therefore somewhat surprising that it first arose in quite a different context. In 1978, Dhar [1] suggested that partial orders can represent the states of a certain model of a lattice gas with long–range three–body interaction and energy proportional to the number of comparable pairs in the order. In this model, $\mathrm{c}(d)$ may be considered to be the entropy function of the interacting lattice gas.

Obviously, (1) implies that for any d we must have

$$\mathrm{c}(d) \;\leq\; \frac{1}{4}. \tag{3}$$

Dhar was able to show that the function $\mathrm{c}(d)/d$ is monotone nonincreasing while the function $\mathrm{c}(d)/(1-d)$ is monotone nondecreasing, which implies that $\mathrm{c}(d)$ is continuous. Moreover he proved that

$$\text{for } \frac{1}{8} \leq d \leq \frac{3}{16} \; : \qquad \mathrm{c}(d) \equiv \frac{1}{4}. \tag{4}$$

Kleitman and Rothschild [5] investigated $\mathrm{c}(d)$ in the range $0 < d \le \frac{1}{8}$. Here one can show that

$$\text{for } 0 < d \le \frac{1}{8}: \qquad \mathrm{c}(d) = \frac{1}{4} \cdot H(4 \cdot d), \tag{5}$$

where $H(x) = -x \log_2 x - (1-x)\log_2(1-x)$. For an illustration of (4) and (5) see Figure 1.

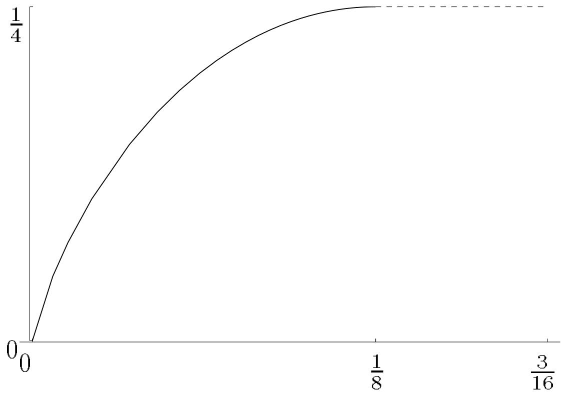

Figure 1: $\mathrm{c}(d)$ in the range $(0, \frac{3}{16})$

Not much was known for the case $d > \frac{3}{16}$. Dhar [2] conjectured that here $\mathrm{c}(d) < \frac{1}{4}$ and obtained several upper bounds for $\mathrm{c}(d)$. The central aim of this paper is to settle this question completely by describing the evolution process and the behaviour of $\mathrm{c}(d)$ in the full range $0 < d < \frac{1}{2}$.

To be able to state our results, we need a few more definitions. A partial order $P = (X, P)$ is a k-layer partial order, if there exists a partition of its point set $X = X_1 \cup \cdots \cup X_k$ into k disjoint antichains (the so–called *layers*) such that

$$\begin{array}{rcc} x < y \text{ with } x \in X_i \text{ and } y \in X_j & \Longrightarrow & i < j, \\ \text{for every } i, j \text{ with } j > i+1: \quad x \in X_i,\ y \in X_j & \Longrightarrow & x < y. \end{array}$$

For some constants $\lambda_1, \ldots, \lambda_k$ with $0 < \lambda_i < 1$ and $\sum_i \lambda_i = 1$ and a constant $0 \le p \le 1$, we say that a partial order $P \in \mathcal{P}_n$ has *configuration* $Q = (\lambda_1, \ldots, \lambda_k; p)$, if it belongs to the following set $\mathcal{P}_{n,Q}$, which is defined as the set containing all k-layer partial orders in $\mathcal{P}_n$ that have $p\,|X_i||X_{i+1}|$ comparable pairs between X_i and X_{i+1} (for all $i \in [n-1]$) and satisfy $|X_i| = \lambda_i \cdot n$ (for all $i \in [n]$).

Obviously, any two partial orders with the same configuration $Q = (\lambda_1, \ldots, \lambda_k; p)$ must have the same number of comparable pairs, namely

$$\mathrm{d}(Q)n^2 := p\sum_{i=1}^{k-1}\lambda_i\lambda_{i+1}n^2 + \sum_{i=1}^{k-2}\sum_{j\geq i+2}^{k}\lambda_i\lambda_j n^2. \tag{6}$$

On the other hand, the only degree of freedom one has when constructing a partial order in $\mathcal{P}_{n,Q}$ lies in the placement of the comparable pairs between successive layers. Thus we arrive at the following estimate.

$$|\mathcal{P}_{n,Q}| = \prod_{i=1}^{k-1}\binom{\lambda_i\lambda_{i+1}n^2}{p\cdot\lambda_i\lambda_{i+1}n^2} 2^{o(n^2)} = 2^{\sum_{i=1}^{k-1}H(p)\lambda_i\lambda_{i+1}n^2 \ +o(n^2)}. \tag{7}$$

(Here the error term $2^{o(n^2)}$ is due to the approximation of the binomial coefficient via the entropy $H(p)$ and also because we didn't care about assigning points to classes, which contributes by a factor of $O(n!) = O(2^{n\log n})$.) Letting

$$\mathrm{c}(Q) := H(p)\sum_{i=1}^{k-1}\lambda_i\lambda_{i+1},$$

we can write $|\mathcal{P}_{n,Q}| = 2^{\mathrm{c}(Q)n^2+o(n^2)}$. Using this terminology, we now state the following theorem which is proven in [6]. It forms the basis for our method of determining $\mathrm{c}(d)$.

Theorem 1.1 *For every $0 < d < \frac{1}{2}$ there exists a configuration $Q = (\lambda_1, \ldots, \lambda_k;\ p)$ with $d = \mathrm{d}(Q)$ such that*

$$|\mathcal{P}_{n,d}| = 2^{\mathrm{c}(Q)n^2+o(n^2)}, \qquad \textit{in other words,} \qquad \mathrm{c}(d) = \mathrm{c}(Q). \tag{8}$$

A configuration Q that meets the requirements of Theorem 1.1 for a fixed d will be called *d-significant* (or, if the value of d is irrelevant or clear form the context, simply *significant*). Observe that Q is significant if and only if there is no other configuration Q' with $\mathrm{d}(Q') = \mathrm{d}(Q)$ and $\mathrm{c}(Q') > \mathrm{c}(Q)$.

We will call $\mathrm{d}(Q)$ and $\mathrm{c}(Q)$ the d-*value* and the c-*value* of Q. The following lemma is proven in [6] and will be helpful when it comes to actually constructing a d-significant configuration.

Lemma 1.2 *For $\frac{1}{8} \leq d \leq \frac{1}{2}$, any d-significant configuration $Q = (\lambda_1, \ldots, \lambda_k;\ p)$ must satisfy $p \geq \frac{1}{2}$.*

Let us now review statements (4) and (5) from the point of view of significant configurations.

$$\text{For } 0 < d \le \frac{1}{8}: \qquad Q = \left(\frac{1}{2},\ \frac{1}{2};\ 4d\right) \quad \text{is } d\text{-significant,} \tag{9}$$

$$\text{for } \frac{1}{8} \le d \le \frac{3}{16}: \qquad Q = \left(\frac{1}{2} - x,\ \frac{1}{2},\ x;\ \frac{1}{2}\right) \quad \text{is } d\text{-significant,} \tag{10}$$

$$\text{where } \ x := \frac{1}{4} - \sqrt{\frac{3}{16} - d}.$$

(9) was first observed by Kleitman and Rothschild [5] and a short proof can be found in [6]. (10) is due to Dhar and easy to verify since here $c(Q) = \frac{1}{4}$ and any configuration with this c-value must be significant. The paper by Kleitman and Rothschild [5] concludes with the following remark.

> Above $\frac{3}{16}n^2$ one might guess that the dominant states have three [layers] with equal top and bottom population at least until $d = \frac{2}{9}n^2$ at which point all three [layers] would be equal in size. Eventually four and higher [layer partial orders] would dominate. Just where and what happens there is not obvious. Presumably phase transitions occur at each such point. One not only lacks a method of proof, but even sensible conjectures in this higher range.

Before we formally state our result let us explain it in a few words by illustrating what happens after d passes the point $d_3 := \frac{3}{16}$. At this point our d-significant configuration is given by $(\frac{1}{4}, \frac{1}{2}, \frac{1}{4}; \frac{1}{2})$. As d increases, the density p of relations between consecutive layers increases, the layers λ_1 and λ_3 grow at the same rate while λ_2 shrinks, and the function $c(d)$ immediately begins to decrease.

When d reaches the point $d_4' := 0.2204..$, the pattern changes dramatically: p, having reached the value $0.5827..$, now remains constant. A new fourth layer λ_4 begins to grow, λ_1 and λ_2 shrink while λ_3 grows. Perhaps most surprisingly, $c(d)$ is in this range a *linear* decreasing function. This phase ends at the point $d_4 := 0.2536..$, when $|\lambda_1| = |\lambda_4|$ and $|\lambda_2| = |\lambda_3|$. Interestingly λ_4 has now half the size of both λ_1 and λ_3 at the point d_4'.

We have tried to illustrate this in Figures 2, 3, and 4. After the point d_4' the evolution process repeats the same two–step manner an infinite number of times, as illustrated in Figure 5. Our main result can now be stated as follows.

Theorem 1.3 *There is an infinite sequence of constants*

$$0 = d_2 < d_3' < d_3 < d_4' < d_4 < \cdots < \frac{1}{2}$$

such that the following holds.

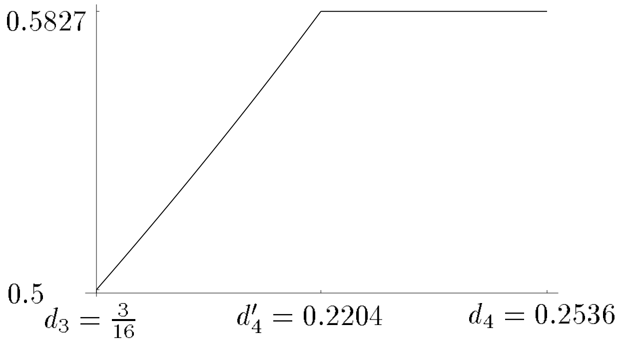

Figure 2: $p(d)$ in the range $[d_3, d_4]$.

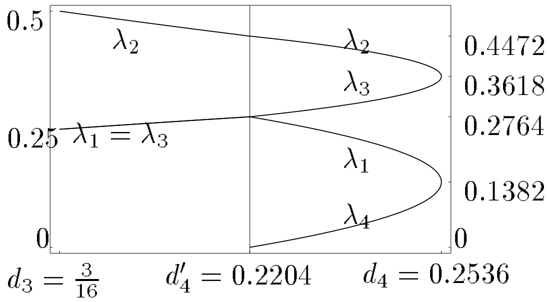

Figure 3: $\lambda_i(d)$ in the range $[d_3, d_4]$.

For every $d \in (d_k, d'_{k+1}]$ *there exists a* d*-significant configuration* $(\lambda_1, \ldots, \lambda_k; p)$. *As* d *increases from* d_k *to* d'_{k+1}
(i) the density p *increases,*
(ii) the layer sizes λ_i *change but remain symmetric:* $\lambda_i = \lambda_{k-i+1}$.
(iii) For $k \geq 3$ *the function* $\mathrm{c}(d)$ *is monotone decreasing.*

For every $d \in (d'_{k+1}, d_{k+1}]$ *there exists a* d*-significant configuration* $(\lambda_1, \ldots, \lambda_{k+1}; p)$. *As* d *increases from* d'_{k+1} *to* d_{k+1}
(iv) the density p *remains constant,*
(v) a new $(k+1)$*st layer begins to grow.*
(vi) At the end of this second phase the $(k+1)$*st layer is half as big as the* k*-th layer at the beginning of the phase. In general, the layer sizes at the end turn out to be the mean of the layer sizes at the beginning.*
(vii) The function $\mathrm{c}(d)$ *is linear in* d *and, for* $k \geq 3$, *monotone decreasing.*

In the statement of the above theorem we have been somewhat vague in that we merely stated that the constants d'_k and d_k existed. It would of course be much nicer if we could

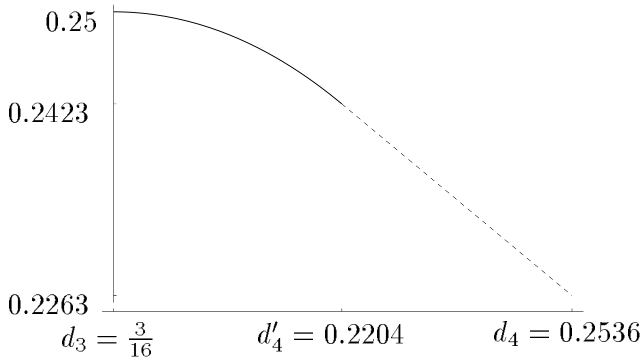

Figure 4: $c(d)$ in the range $[d_3, d_4]$.

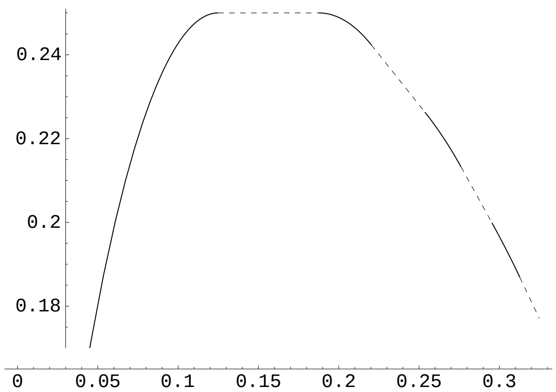

Figure 5: $c(d)$ in the range $[0.05, 0.32]$.

give an explicit formula – preferably not only for these constants but also for the density $p(d)$ and the layer sizes $\lambda_i(d)$ as functions of d, and, most importantly, the function $c(d)$. This is possible, but the formulae involved turn out to be not very attractive.

Theorem 1.4

Set

$$\begin{aligned}
\phi^k &:= \frac{k-1}{k+1}\pi, \\
\phi(p) &:= \arccos\Big(\frac{\log_2 p - \log_2(1-p)}{2\log_2 p}\Big), \\
q^k &:= \phi^{-1}(\phi^k), \\
\lambda_i^k(p) &:= \frac{(-1)^{k-i}\sin i\phi - (-1)^i \sin(k-i+1)\phi + \sin(k+1)\phi}{\frac{-(-1)^k \sin\phi + \sin k\phi + \sin(k+1)\phi}{1+\cos\phi} + k\sin(k+1)\phi}, \\
& \quad \text{where } \phi = \phi(p), \\
\mathrm{d}(p) &:= \frac{1}{2} - \frac{1}{2}\sum_{i=1}^{k}(\lambda_i^k(p))^2 - (1-p)\sum_{i=1}^{k-1}\lambda_i^k(p)\cdot\lambda_{i+1}^k(p), \\
& \quad \text{for } p \in (q^k, q^{k+1}].
\end{aligned}$$

Then

$$\begin{aligned}
\mathrm{d} &: (q^k, q^{k+1}] \to (d_k, d'_{k+1}] \ \textit{ is strictly increasing,} \\
d'_k &= \lim_{p<q^k, p\to q^k} \mathrm{d}(p), \\
d_k &= \lim_{p>q^k, p\to q^k} \mathrm{d}(p), \\
p(d) &= \begin{cases} q^k, & \text{if } d \in (d'_k, d_k], \\ \mathrm{d}^{-1}(d), & \text{if } d \in (d_k, d'_{k+1}], \end{cases} \\
\mathrm{c}(d) &= \begin{cases} r\cdot d + [c(d'_k) - r\cdot d'_k], & \text{if } d \in (d'_k, d_k], \\ H(p)\sum_{i=1}^{k-1}\lambda_i^k(p)\lambda_{i+1}^k(p), & \text{if } d \in (d_k, d'_{k+1}], \end{cases} \\
& \quad \text{where } r = -\log_2 q^k + \log_2(1-q^k) \text{ and } p = p(d).
\end{aligned}$$

Note that the concept of a significant-configuration is strong enough to determine $\mathrm{c}(d)$ but does not suffice to prove statements about the global structure. Nevertheless, we conjecture that almost all partial orders in $\mathcal{P}_{n,d}$ have the d-significant configuration described in Theorems 1.3 and 1.4.

We conclude this section with a rather philosophical than mathematical discussion on how we interpret Theorem 1.3. We view the intervals $[d_k, d'_{k+1}]$ as the evolutionary phases and the intervals $[d'_k, d_k]$ as the phase transitions. What might be held against this point of view is that phase transitions of this form are "too long", and that in fact the true phases are given by $[d'_k, d'_{k+1}]$, since for every d in this range a significant proportion of partial orders in $\mathcal{P}_{n,d}$ has k layers. But then recall that the d-significant configuration within the intervals $[d'_k, d_k]$ is not symmetric, it looks different when viewed from below or above. By the standards of theoretical physics, this indicates an unstable and therefore transitory state through which the system passes quickly. And concerning the length of the phase transitions: they are only long from the point of view of d: when viewed in terms of p, they are in fact very, very short.

2 Outline of the proof

In order to determine $\mathrm{c}(d)$, recall that for a configuration $Q = (\lambda_1, \ldots, \lambda_k; p)$ we defined $\mathrm{c}(Q) := H(p) \sum_{i=1}^{k-1} \lambda_i \lambda_{i+1}$ and (using the fact that $\sum_i \lambda_i = 1$)

$$\begin{aligned} \mathrm{d}(Q) \quad &:= \quad p \sum_{i=1}^{k-1} \lambda_i \lambda_{i+1} + \sum_{i=1}^{k-2} \sum_{j \geq i+2}^{k} \lambda_i \lambda_j \\ &= \quad \frac{1}{2} - \frac{1}{2} \sum_{i=1}^{k} (\lambda_i)^2 - (1-p) \cdot \sum_{i=1}^{k-1} \lambda_i \lambda_{i+1}. \end{aligned}$$

Observe that in view of (5) and (9), (4) and (10), and Lemma 1.2, we can and shall assume that $d \geq \frac{3}{16}$ and $p \geq \frac{1}{2}$. Finally recall that by Theorem 1.1 if for a fixed d a configuration Q satisfies $\mathrm{d}(Q) = d$ and no other configuration Q' satisfies $\mathrm{d}(Q') = d$ and $\mathrm{c}(Q') > \mathrm{c}(Q)$, then Q is called d-significant and we have $\mathrm{c}(d) = \mathrm{c}(Q)$. Hence a solution of the following constrained extremum problem must be a d-significant configuration, and it is exactly this configuration that we will be seeking.

$$\boxed{\begin{array}{lll} \text{Choose } k,\ \lambda_1, \ldots, \lambda_k,\ \text{and } p & \text{such as to maximize} & H(p) \displaystyle\sum_{i=1}^{k-1} \lambda_i \lambda_{i+1}, \\ & \text{subject to} & \displaystyle\frac{1}{2} - \frac{1}{2} \sum_{i=1}^{k} \lambda_i^2 - (1-p) \sum_{i=1}^{k-1} \lambda_i \lambda_{i+1} = d, \\ & & \displaystyle\sum_{i=1}^{k} \lambda_i = 1, \\ & & \lambda_i > 0 \qquad \text{for all } i = 1, \ldots, k, \text{ and} \\ & & \frac{1}{2} \leq p \leq 1. \end{array}} \tag{11}$$

Denote by $Q^* = (\vec{\lambda}; p)$ a solution of the above maximization problem. In the following we will derive necessary conditions that $(\vec{\lambda}; p)$ must satisfy. (Obviously the idea here is that at the end we will actually be able to deduce the values $\lambda_1, \ldots, \lambda_k, p$ from these conditions.)

From the theory of Lagrange multipliers we know that for any local extremum $z = (z_1, \ldots, z_m)$ of a function $f : \mathbb{R}^m \to \mathbb{R}$ under the side constraints $g_i(z) = 0$ for $i \in [\ell]$ there must exist real numbers t_i such that

$$\frac{\partial f}{\partial z_i}(z) = t_1 \cdot \frac{\partial g_1}{\partial z_i}(z) + \cdots + t_\ell \cdot \frac{\partial g_\ell}{\partial z_i}(z)$$

for all $i \in [m]$. Hence in our case, where $m = k+1$ and $\ell = 2$, there must be real numbers r, u such that

$$\frac{\partial}{\partial p}: \quad H'(p) \sum_{i=1}^{k-1} \lambda_i \lambda_{i+1} + \sum_{i=1}^{k-1} \lambda_i \lambda_{i+1} \cdot r = 0, \tag{12}$$

$$\frac{\partial}{\partial \lambda_i}: \quad H(p)\lambda_{i+1} + H(p)\lambda_{i-1} + \Big(- \lambda_i - (\lambda_{i-1} + \lambda_{i+1})(1-p) \Big) \cdot r + u = 0, \tag{13}$$

for all $i \in [k]$, where we set $\lambda_0 = \lambda_{k+1} = 0$ for convenience.

From (12) we obtain immediately that p and r must satisfy $H'(p) = -r$. Using this, (13) simplifies to

$$\lambda_i H'(p) + \lambda_{i-1}\Big(H(p) + (1-p)H'(p)\Big) + \lambda_{i+1}\Big(H(p) + (1-p)H'(p)\Big) = -u. \tag{14}$$

Setting

$$a(p) := -H'(p) = \log_2(p) - \log_2(1-p)$$

and

$$b(p) := -H(p) - (1-p)H'(p) = \log_2 p,$$

it is easy to see that (14) corresponds to a system of linear equations

$$T^k(p) \cdot \vec{\lambda} = \vec{u}, \qquad \text{where} \tag{15}$$

$$T^k(p) = \begin{pmatrix} a(p) & b(p) & 0 & 0 & \ldots & 0 & 0 \\ b(p) & a(p) & b(p) & 0 & \ldots & 0 & 0 \\ 0 & b(p) & a(p) & b(p) & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \ldots & b(p) & a(p) \end{pmatrix}, \qquad \vec{\lambda} = \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \vdots \\ \lambda_k \end{pmatrix}, \qquad \vec{u} = \begin{pmatrix} u \\ u \\ \vdots \\ \vdots \\ u \end{pmatrix}.$$

Before the technical details become overwhelming, let us pause here to re–evaluate our position and to sketch the line of thought in what is to come.

Let us suppose for a moment that k and p are such that $T^k(p)$ is non–singular. Then the system (15) has a unique solution $\vec{\lambda}$. In other words, for such values k and p there exists only one configuration of the form $(\lambda_1, \ldots, \lambda_k; p)$ that can possibly be the solution Q^* of (11) – call this configuration the (k,p)-*candidate* and denote it by $Q_{k,p}$. It is determined in Proposition 3.4. Since (15) is (only) a necessary condition for a configuration to be the solution of (11), it is clear that on the one hand Q^* must be a (k,p)-candidate for some k, p, but also on the other hand that not every candidate is significant, since there might well be another candidate $Q_{k',p'}$ which has the same d-value but a higher c-value.

So we are faced with the problem of comparing the c-values of candidates that have the same d-value. As the computations will show, it is relatively easy to determine $Q_{k,p}$ and hence $\mathrm{d}(Q_{k,p})$ as a function of k and p. However here we really need the inverse, i.e. for a given d we must first determine those candidates with d-value d and then compare their c-values. After a glance at the formulae needed to describe $Q_{k,p}$, this seems very hard indeed.

We therefore propose a different approach. We will prove that there is a sequence of constants $0 < q^3 < q^4 < \cdots < q^*$ so that for each k and all $p \notin [q^k, q^{k+1}]$ the respective (k,p)-candidate $Q_{k,p}$ cannot be significant. We will prove this by comparing $Q_{k,p}$ to a different configuration Q', that is obtained by slightly modifying $Q_{k,p}$, and that achieves the same d-value but a higher c-value. (Note that usually Q' will not be a (p',k')-candidate, so the idea is not to elect the best possible candidate but to simply 'dismiss' all the others.)

We have tried to illustrate this approach in Figure 6. Here we took $Q_{3,p}$ and $Q_{4,p}$ and plotted their d-value against their c-value. The dashed parts of the curves are those to be dismissed, while the solid part represents the part $p \in [q^3, q^4]$ and $p \in [q^4, q^5]$ respectively.

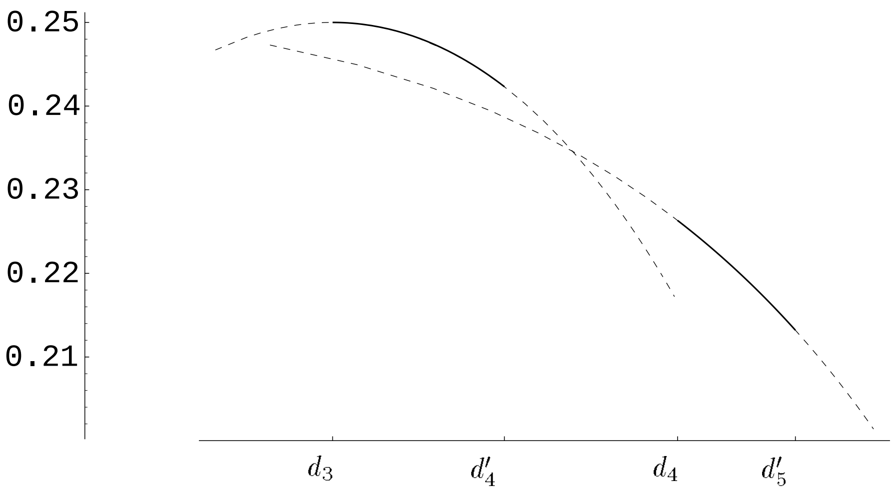

Figure 6: $Q_{3,p}$ and $Q_{4,p'}$ where $p \in [0.45, 0.68]$ and $p' \in [0.52, 0.65]$.

Let us say that as p increases from q^k to q^{k+1}, the function $\mathrm{d}(Q_{k,p})$ increases from d_k

to d'_{k+1}. What we will then have to show is that the intervals $[d_k, d'_{k+1}]$ don't overlap for different k and k', so that for $d \in [d_k, d'_{k+1}]$ the configuration $Q_{k,p}$ (where $p \in [q^k, q^{k+1}]$) is the only candidate left and must therefore be significant.

As we saw in Figure 6, not only do the intervals $[d_3, d'_4]$ and $[d_4, d'_5]$ not overlap, but there are actually gaps between them. Of course this cannot mean that we here have a total lack of significant configurations. Indeed, recall that we had assumed $T^k(p)$ to be non–singular. However there are values of p and k where this is not true. Here there is no unique solution to (15), so we can let one of the components of $\vec{\lambda}$ have some arbitrary value x, neglect one of the equations and solve the remaining system, which then always turns out to be non–singular. Denote the solution of this system by $Q_{k,p}(x)$. It is determined im Proposition 3.5. For some of these singular couples k, p (namely when $p = q^k$) the candidates $Q_{k,p}(x)$ turn out to be significant, at least for small x. Moreover, as we slowly increase x one can observe that in these cases $Q_{k,p}(x)$ beautifully builds a 'linear bridge' accross the gaps noticed above. This is illustrated by the bold line in Figure 7.

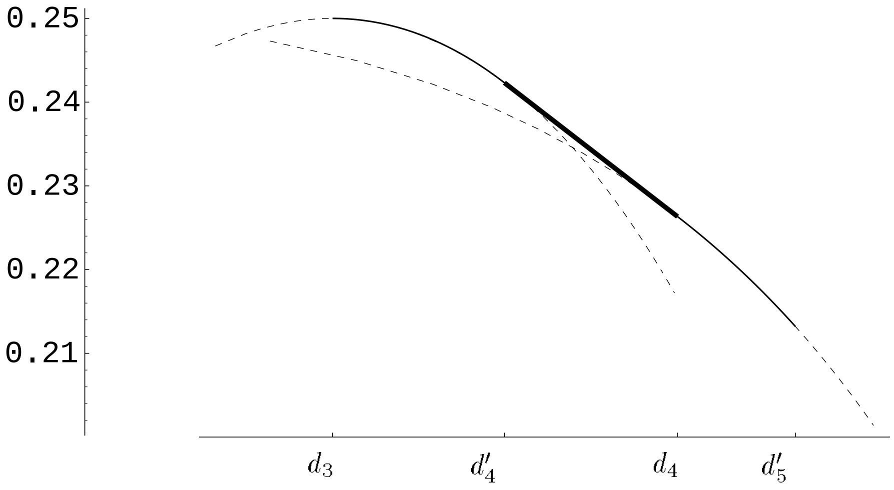

Figure 7: $Q_{3,p}$, $Q_{4,p'}$ and $Q_{4,q^4}(x)$ where $q^4 = 0.5827$ and $x \in [0, 0.1382]$.

We have subdivided the remainder of this paper into four sections. In Section 3 we determine explicit representations of the candidates $Q_{k,p}$ and $Q_{k,p}(x)$. As described above, Section 4 then shows that many of them cannot be significant. In Section 5 we then prove some facts about the behaviour of the remaining candidates and complete the proof of Theorems 1.3 and 1.4.

In the course of these three sections we will need a few lemmas and propositions whose proofs are technical in nature and do not provide any new insight. So whenever a lemma or a proposition is stated without proof, the latter can be found in Section 6. All of these proofs are elementary but we include them for completeness.

We introduce one last definition. Observe that the candidates $Q_{k,p}$ and $Q_{k,p}(x)$ as computed in (15) and (20) respectively don't automatically satisfy the condition $0 < \lambda_i$ for all $i \in [k]$. If they do, we will call them *feasible.*

3 Determining candidates

At first it might seem as if (15) wouldn't actually produce a unique candidate $Q_{k,p}$ (even if $T^k(p)$ is non–singular), because one is allowed to choose u arbitrarily. However solutions $\vec{\lambda}$ and $\vec{\lambda}'$ of (15) are linear dependent and therefore there is only one solution that simultaneously satisfies $\sum \lambda_i = 1$. Hence for every fixed k and p where $T^k(p)$ is non-singular, $Q_{k,p}$ is given by $(\vec{\lambda}; p)$ with

$$\vec{\lambda}(p) := \frac{\vec{\xi}(p)}{|\vec{\xi}(p)|} \quad \text{and} \quad \vec{\xi}(p) := \left[T^k(p)\right]^{-1} \cdot \vec{1}. \tag{16}$$

Here $\vec{1}$ is the vector whose components are all 1, and $|\vec{v}|$ denotes the sum of the components. (This somewhat abuses the notion of a norm, since it could happen that $|\vec{v}| < 0$.)

The next two lemmas compute the determinant and inverse of a tridiagonal $k \times k$ matrix T^k with a on the main diagonal and b on the two subdiagonals for arbitrary real numbers a and b.

Lemma 3.1

$$t_k := \det(T^k) = \begin{cases} \frac{1}{D}\left[\left(\frac{a+D}{2}\right)^{k+1} - \left(\frac{a-D}{2}\right)^{k+1}\right] \textit{ where } D = \sqrt{a^2 - 4b^2} & , \textit{ if } \frac{a}{2b} \notin (-1,1) \\ b^k \sin(k+1)\phi / \sin\phi \textit{ where } \phi = \arccos\frac{a}{2b} & , \textit{ if } \frac{a}{2b} \in (-1,1). \end{cases}$$

Corollary 3.2 *$t_k = 0$ if and only if $a^2 = 4b^2$ or $\frac{a}{2b} = \cos\frac{j\pi}{k+1}$ for some $j \in \{1, \ldots, k\}$. In particular, for $-1 < a/2b < 1$ it follows from $t_k = 0$ that $t_{k-1} \neq 0$.* □

Lemma 3.3 *The inverse $M^k = (T^k)^{-1}$ is given by (m_{ij}) where*

$$m_{ij} := \begin{cases} (-1)^{i+j} b^{i-j} \frac{t_{j-1} t_{k-i}}{t_k} & , \textit{if } j < i \\ (-1)^{i+j} b^{j-i} \frac{t_{i-1} t_{k-j}}{t_k} & , \textit{if } j \geq i. \end{cases}$$

Before we use this to compute $\vec{\lambda}$, observe that in the case of our particular matrix $T^k(p)$ the function $\frac{a(p)}{2b(p)}$ is strictly decreasing for $\frac{1}{2} \leq p \leq 1$ and ranges from 0 to $-\infty$, attaining value -1 at $p = 0.682328... =: q^*$. Hence for $\frac{1}{2} \leq p \leq q^*$ the function $\phi(p) := \arccos\frac{a(p)}{2b(p)}$ is strictly increasing and ranges from $\pi/2$ to π. We will make use of the one-to-one relation between p and $\phi(p)$ and sometimes express functions in terms of $\phi = \phi(p)$ instead of p. Hopefully this will make things easier to read, as the two preceding lemmas seem to indicate.

Now Lemmas 3.1 and 3.3 enable us to give an explicit formula for $Q_{k,p}$ as suggested in (16).

Proposition 3.4 *Denote by $M^k(p) = (m^k(p)_{ij})$ the inverse of $T^k(p)$. For all k and all p with $\pi/2 < \phi < \pi$ and $\phi \neq \frac{j\pi}{k+1}$ for all $j \in \{1, \ldots, k\}$, we must have*

$$Q_{k,p} = \Big(\lambda_1^k(p), \ldots, \lambda_k^k(p);\ p\Big),$$

where

$$\lambda_i^k(p) := \frac{\xi_i^k(p)}{|\vec{\xi}^k(p)|} = \frac{(-1)^{k-i}\sin i\phi - (-1)^i \sin(k-i+1)\phi + \sin(k+1)\phi}{\frac{-(-1)^k \sin\phi + \sin k\phi + \sin(k+1)\phi}{1+\cos\phi} + k\sin(k+1)\phi},$$

$$\xi_i^k(p) := \sum_{j=1}^{k} m_{i,j}^k(p) = \frac{(-1)^{k-i}\sin i\phi - (-1)^i \sin(k-i+1)\phi + \sin(k+1)\phi}{2b(p)(1+\cos\phi)\sin(k+1)\phi}.$$

In particular, $Q_{k,p}$ is symmetric, i.e. for all $i \in [k]$ we have

$$\lambda_i^k(p) \;=\; \lambda_{k-i+1}^k(p).$$

Proof. In view of (16) it suffices to check the explicit formulae; namely

$$\sum_{j=1}^{k} m_{i,j}^k(p) \;=\; \frac{(-1)^{k-i}\sin i\phi - (-1)^i \sin(k-i+1)\phi + \sin(k+1)\phi}{2b(p)(1+\cos\phi)\sin(k+1)\phi} \tag{17}$$

and

$$|\vec{\xi}^k(p)| = \frac{\frac{-(-1)^k \sin\phi + \sin k\phi + \sin(k+1)\phi}{1+\cos\phi} + k\sin(k+1)\phi}{2b(p)(1+\cos\phi)\sin(k+1)\phi}. \tag{18}$$

This very technical task is deferred to Section 6. The symmetry of the $\lambda_i^k(p)$ is indeed obvious from the definition. □

Now we turn to the candidates $Q_{k,p}(x)$, i.e. to those pairs k, p where

$$\frac{a(p)}{2b(p)} = \cos\frac{j\pi}{k+1} \text{ for some } j \in \{1, \ldots, k\}. \tag{19}$$

Here $T^k(p)$ is singular and there is no unique solution to the system of equations (15), which we now restate as

$$T^k(p) \cdot \vec{\ell} = \vec{u}.$$

Hence we may choose one ℓ_i-value arbitrarily, say $\ell_k = x$, and neglect the last equation of the system. The requirement for the remaining ℓ_i is that there exists a u' such that

$$\begin{pmatrix} a(p) & b(p) & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ b(p) & a(p) & b(p) & 0 & \dots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & b(p) & a(p) & b(p) & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & b(p) & a(p) & b(p) \end{pmatrix} \cdot \begin{pmatrix} \ell_1 \\ \ell_2 \\ \vdots \\ \vdots \\ \ell_{k-1} \\ x \end{pmatrix} = \begin{pmatrix} u' \\ \vdots \\ \vdots \\ \vdots \\ u' \end{pmatrix}$$

which is equivalent to

$$T^{k-1}(p) \cdot \begin{pmatrix} \ell_1 \\ \vdots \\ \ell_{k-2} \\ \ell_{k-1} \end{pmatrix} = \begin{pmatrix} u' \\ \vdots \\ u' \\ u' - b(p) \cdot x \end{pmatrix}, \tag{20}$$

whose solution is uniquely determined since $\det(T_{k-1}) \neq 0$, as we saw in Corollary 3.2. Not surprisingly, the solution of (20) is related to that of (15).

Proposition 3.5 *For all $x \in (0,1)$, all k and all p with $\phi = \frac{j\pi}{k+1}$ for some $j \in \{1, \dots, k\}$*

$$Q_{k,p}(x) = \Big(\ell_1^k(p,x), \dots, \ell_k^k(p,x); p\Big),$$

where

$$\begin{aligned} \ell_i^k(p,x) &:= \lambda_i^{k-1}(p) + x \cdot \mu_i^{k-1}(p) \quad \textit{for } i = 1, \dots, k-1, \\ \ell_k^k(p,x) &:= x, \\ \mu_i^{k-1}(p) &:= -\lambda_i^{k-1}(p)\Big(1 - b(p) \cdot \xi_{k-1}^{k-1}(p)\Big) - b(p) m_{i,k-1}^{k-1} \quad \textit{for } i = 1, \dots, k-1, \\ \mu_k^{k-1}(p) &:= 1. \end{aligned}$$

Proof. For $i = 1, \dots, k-1$ denote by $\vec{r}_i$ the ith row of $T^{k-1}(p)$ and by $\vec{m}$ the $(k-1)$st column of $M^{k-1}(p)$, hence $\vec{r}_i \cdot \vec{m} = \delta_{i,k-1}$. Since $\vec{\lambda}^{k-1}(p)$ is a solution of $T_{k-1}(p) \cdot \vec{\lambda}^{k-1}(p) = \vec{u}$ for an appropriate value u, we know that $\vec{r}_i \cdot \vec{\lambda}^{k-1}(p) = u$ for all $1 \leq i \leq k-1$. Now let

$s := 1 - b(p) \cdot \xi_{k-1}^{k-1}(p)$, hence

$$\vec{r}_i \cdot \begin{pmatrix} \ell_1^k(p,x) \\ \vdots \\ \ell_{k-1}^k(p,x) \end{pmatrix} = u + x \cdot \vec{r}_i \cdot \begin{pmatrix} \mu_1^{k-1}(p) \\ \vdots \\ \mu_{k-1}^{k-1}(p) \end{pmatrix}$$

$$= u - x \cdot s \cdot \vec{r}_i \cdot \begin{pmatrix} \lambda_1^{k-1}(p) \\ \vdots \\ \lambda_{k-1}^{k-1}(p) \end{pmatrix} - x \cdot b(p) \cdot \vec{r}_i \cdot \vec{m} = u - s \cdot x \cdot u - x \cdot b(p) \cdot \delta_{i,k-1}.$$

Setting $u' := u - s \cdot x \cdot u$, this satisfies (20). Furthermore

$$\sum_{i=1}^{k-1} \mu_i^{k-1}(p) = -s \sum_{i=1}^{k-1} \lambda_i^{k-1}(p) - b(p) \cdot \sum_{i=1}^{k-1} m_{i,k-1}^{k-1}(p) = -1,$$

because

$$s = 1 - b(p) \cdot \xi_{k-1}^{k-1}(p), \quad \sum_{i=1}^{k-1} \lambda_i^{k-1}(p) = 1 \quad \text{and} \quad \sum_{i=1}^{k-1} m_{i,k-1}^{k-1}(p) = \xi_{k-1}^{k-1}(p).$$

Therefore

$$|\vec{\ell}| = \sum_{i=1}^{k} \ell_i^k(p,x) = \sum_{i=1}^{k-1} \lambda_i^{k-1}(p) + x \cdot \sum_{i=1}^{k-1} \mu_i^{k-1}(p) + x = 1.$$

$\square$

Let us introduce some definitions for those p where $T^k(p)$ is singular. Set $\phi_j^k := \frac{k-j}{k+1}\pi$ and define q_j^k by $\phi(q_j^k) = \phi_j^k$. We shall see that ϕ_1^k plays a special role, therefore let $\phi^k := \phi_1^k$ and $q^k = q_1^k$. We will often use the following trivial but helpful observation:

$$\begin{aligned} \sin(k-i)\phi_j^k &= \sin[(k+1)\tfrac{k-j}{k+1}\pi - (i+1)\phi_j^k] \\ &= (-1)^{k-j}\sin[-(i+1)\phi_j^k] = -(-1)^{k-j}\sin(i+1)\phi_j^k. \end{aligned} \tag{21}$$

In order to obtain an explicit formula for $\vec{\ell}$ as determined in Proposition 3.5, we will need the following technical lemma.

Lemma 3.6

$$m_{i,k-1}^{k-1}(q_j^k) = (-1)^{i+j} \frac{\sin i\phi_j^k}{b(q_j^k)\sin\phi_j^k}$$

$$\xi_{k-1}^{k-1}(q_j^k) = \begin{cases} \frac{1}{b(q_j^k)} & , \textit{ if } j \textit{ is odd} \\ \frac{1}{b(q_j^k)} - \frac{1}{b(q_j^k)(1+\cos\phi_j^k)} & , \textit{ if } j \textit{ is even.} \end{cases}$$

$$\mu_i^{k-1}(q_j^k) = \begin{cases} (-1)^i \frac{\sin i\phi_j^k}{\sin\phi_j^k} & , \textit{ for all } 1 \le i \le k \;\; \textit{if } j \textit{ is odd} \\ -(-1)^i \frac{\sin i\phi_j^k}{\sin\phi_j^k} - \frac{\lambda_i^{k-1}(q_j^k)}{1+\cos\phi_j^k} & , \textit{ for all } 1 \le i \le k-1 \;\; \textit{if } j \textit{ is even.} \end{cases}$$

For $1 \le i \le k-1$ *we have*

$$\ell_i^k(q_j^k, x) = \begin{cases} \lambda_i^{k-1}(q_j^k) - x \cdot b(q_j^k) \cdot m_{i,k-1}^{k-1}(q_j^k) & , \textit{ if } j \textit{ is odd} \\ (1 - \frac{x}{1+\cos\phi_j^k})\lambda_i^{k-1}(q_j^k) - x \cdot b(q_j^k) \cdot m_{i,k-1}^{k-1}(q_j^k) & , \textit{ if } j \textit{ is even.} \end{cases}$$

For an odd number j the terms $\mu_i^{k-1}(q_j^k)$ have some nice properties that we will use later, especially in the case where $j = 1$. Notice that $\mu_i^{k-1}(\phi_j^k)$ is the same as $\mu_i^{k-1}(q_j^k)$. We will frequently switch between the two expressions.

Lemma 3.7 *Now let* $j \in [k]$ *be an odd number. Then*

$$\begin{aligned} &(i) && \mu_{k+1-i}^{k-1}(\phi_j^k) = -\mu_i^{k-1}(\phi_j^k) \\ &(ii) && \sum_{i=1}^{k} \mu_i^{k-1}(\phi_j^k) = 0 \\ &(iii) && \sum_{i=1}^{k} \mu_i^{k-1}(\phi_j^k)^2 = \frac{k+1}{2\sin^2(\phi_j^k)} \\ &(iv) && \sum_{i=1}^{k-1} \mu_i^{k-1}(\phi_j^k) \cdot \mu_{i+1}^{k-1}(\phi_j^k) = -\frac{(k+1)\cos(\phi_j^k)}{2\sin^2(\phi_j^k)}. \end{aligned}$$

Let $j' \neq j$ *be another odd number in* $[k]$*. Then*

$$\begin{aligned} &(v) && \sum_{i=1}^{k} \mu_i^{k-1}(\phi_j^k) \cdot \mu_i^{k-1}(\phi_{j'}^k) = 0 \\ &(vi) && \sum_{i=1}^{k-1} \mu_i^{k-1}(\phi_j^k) \cdot \mu_{i+1}^{k-1}(\phi_{j'}^k) = 0. \end{aligned}$$

4 Dismissing candidates

In this section we follow the approach outlined in the beginning of the chapter. Namely we shall use the explicit representation just derived for $Q_{k,p}$ and show that for $p \notin [q^k, q^{k+1}]$

the candidate $Q_{k,p}$ cannot be significant. We then proceed analogously in the case of candidates $Q_{k,p}(x)$. The following lemma is our main tool in this enterprise.

Lemma 4.1 *Consider an arbitrary configuration* $(\lambda_1, \ldots, \lambda_r; p)$ *where* $p < 1$ *is a fixed constant. Let* $(\nu_1, \ldots, \nu_{r'})$ *be a vector with* $|\vec{\nu}| = 0$, $r \leq r'$ *and* $\nu_i \geq 0$ *for all* $r < i \leq r'$. *Set* $\lambda_{r+1} = \cdots = \lambda_{r'} = 0$ *and define*

$$\alpha_1 := 2 \sum_{i=1}^{r'} \lambda_i \nu_i \quad \textit{and} \quad \beta_1 := \sum_{i=1}^{r'} \nu_i^2,$$

$$\alpha_2 := \sum_{i=1}^{r'-1} (\nu_i \lambda_{i+1} + \nu_{i+1} \lambda_i) \quad \textit{and} \quad \beta_2 := \sum_{i=1}^{r'-1} \nu_i \nu_{i+1}.$$

If

$$-b(p) \cdot \alpha_2 - \frac{a(p)}{2} \cdot \alpha_1 \; > \; 0, \tag{22}$$

or

$$\alpha_1 = \alpha_2 = 0 \textit{ and } - b(p) \cdot \beta_2 - \frac{a(p)}{2} \cdot \beta_1 > 0, \tag{23}$$

then $(\lambda_1, \ldots, \lambda_r; p)$ *cannot be significant.*

Proof. Suppose to the contrary that $(\lambda_1, \ldots, \lambda_r; p)$ were significant. Define

$$\lambda_i' := \lambda_i + \epsilon \cdot \nu_i \quad \text{ for all } i = 1, \ldots, r',$$

$$\gamma_1 := \alpha_1 + \epsilon \cdot \beta_1, \qquad \gamma_2 := \alpha_2 + \epsilon \cdot \beta_2,$$

$$p' := p + \epsilon \cdot q, \text{ where } q := \frac{(1-p)\gamma_2 + \frac{\gamma_1}{2}}{\sum_{i=1}^{r-1} \lambda_i \lambda_{i+1} \; + \epsilon \gamma_2}.$$

We claim that $\mathrm{d}(\lambda_1, \ldots, \lambda_r; p) = \mathrm{d}(\lambda_1', \ldots, \lambda_r'; p')$, which is verified as follows.

$$\begin{aligned}
\sum_{i=1}^{r'} (\lambda_i')^2 - \sum_{i=1}^{r} (\lambda_i)^2 \;&=\; \sum_{i=1}^{r'} \left(\lambda_i^2 + \epsilon^2 \nu_i^2 + 2\epsilon \lambda_i \nu_i - \lambda_i^2 \right) \\
&=\; \epsilon \sum_{i=1}^{r'} \left(\epsilon \nu_i^2 + 2 \lambda_i \nu_i \right) \;=\; \epsilon \gamma_1,
\end{aligned}$$

$$\sum_{i=1}^{r'-1} \lambda'_i\lambda'_{i+1} - \sum_{i=1}^{r-1} \lambda_i\lambda_{i+1} \;=\; \sum_{i=1}^{r'-1} ((\lambda_i + \epsilon\nu_i)(\lambda_{i+1} + \epsilon\nu_{i+1}) - \lambda_i\lambda_{i+1})$$

$$= \epsilon \sum_{i=1}^{r'-1} (\epsilon\nu_i\nu_{i+1} + \nu_i\lambda_{i+1} + \nu_{i+1}\lambda_i) \;=\; \epsilon\gamma_2.$$

$$\mathrm{d}(\lambda'_1, \ldots, \lambda'_{r'}; p') = \frac{1}{2} - \frac{1}{2}\sum_{i=1}^{r'}(\lambda'_i)^2 - (1 - p - \epsilon q) \cdot \sum_{i=1}^{r'-1}(\lambda'_i\lambda'_{i+1})$$

$$= \frac{1}{2} - \frac{1}{2}\sum_{i=1}^{r} \lambda_i^2 - \frac{\epsilon\gamma_1}{2} - (1-p)(\sum_{i=1}^{r-1} \lambda_i\lambda_{i+1} + \epsilon\gamma_2) + \epsilon q(\sum_{i=1}^{r-1} \lambda_i\lambda_{i+1} \; + \epsilon\gamma_2)$$

$$= \mathrm{d}(\lambda_1, \ldots, \lambda_r; p) - \frac{\epsilon\gamma_1}{2} - (1-p)\epsilon\gamma_2 + \epsilon\Big((1-p)\gamma_2 + \frac{\gamma_1}{2}\Big) \;= \mathrm{d}(\lambda_1, \ldots, \lambda_r; p).$$

Thus we have shown that the configurations $(\vec{\lambda}; p)$ and $(\vec{\lambda}'; p')$ have the same d-value. Furthermore, if ϵ is sufficiently small and $(\vec{\lambda}; p)$ is a feasible configuration, then so must be $(\vec{\lambda}'; p')$. Moreover we have $|\vec{\lambda}'| = |\vec{\lambda}| + \epsilon|\vec{\nu}| = |\vec{\lambda}| = 1$. Hence if we now prove that for all small enough ϵ the c-value of $(\vec{\lambda}'; p')$ is greater than that of $(\vec{\lambda}; p)$, the latter cannot be significant.

We will use the Taylor expansion of $H(p)$ to compute the value of $H(p')$: there exists a $0 \leq \eta' \leq 1$ such that

$$H(p') = H(p + \epsilon q) = H(p) + \epsilon q H'(p) + \frac{\epsilon^2 q^2}{2} H''(p + \eta'\epsilon q),$$

therefore there exists a positive constant η, such that for all sufficiently small ϵ we have $H(p') \geq H(p) + \epsilon q H'(p) - \eta\epsilon^2 q^2$. This implies

$$\mathrm{c}(\lambda'_1, \ldots, \lambda'_{r'}; p') - \mathrm{c}(\lambda_1, \ldots, \lambda_r; p) = H(p')\sum_{i=1}^{r'-1}(\lambda'_i\lambda'_{i+1}) \;-\; H(p)\sum_{i=1}^{r-1}(\lambda_i\lambda_{i+1})$$

$$\geq (H(p) + \epsilon q H'(p) - \eta\epsilon^2 q^2)(\sum_{i=1}^{r-1} \lambda_i\lambda_{i+1} + \epsilon\gamma_2) \;-\; H(p)\sum_{i=1}^{r-1} \lambda_i\lambda_{i+1}$$

$$= \epsilon\gamma_2 H(p) + q(\epsilon H'(p) - \eta\epsilon^2 q)(\sum_{i=1}^{r-1} \lambda_i\lambda_{i+1} + \epsilon\gamma_2)$$

$$= \epsilon\gamma_2 H(p) + (\epsilon H'(p) - \eta\epsilon^2 q)((1-p)\gamma_2 + \frac{\gamma_1}{2})$$

$$= \epsilon\gamma_2\big(H(p) + (1-p)H'(p)\big) + \epsilon H'(p)\frac{\gamma_1}{2} - \eta\epsilon^2 q((1-p)\gamma_2 + \frac{\gamma_1}{2}).$$

$$= \epsilon\Big(- \gamma_2 b(p) - a(p)\frac{\gamma_1}{2} - \epsilon \cdot \eta q((1-p)\gamma_2 + \frac{\gamma_1}{2})\Big).$$

Now either of the two conditions (22) or (23) immediately guarantees that we can choose ϵ so small that the last expression certainly becomes positive, which completes the proof of this lemma. □

Corollary 4.2 *No configuration* $(\lambda_1, \ldots, \lambda_k, p)$ *with*

$$b(p) \cdot \lambda_{k-2} + a(p) \cdot \lambda_{k-1} > 0$$

is significant.

Proof. We would like to apply Lemma 4.1 with $r := k$, $r' := k+1$ and

$$\nu_{k-1} := -1,\ \nu_{k+1} := 1, \quad \text{and} \quad \nu_i := 0 \ \text{ for } i = 1, \ldots, k-2, k.$$

Then

$$\alpha_1 = -2\lambda_{k-1} \quad \text{and} \quad \alpha_2 = -\lambda_{k-2} - \lambda_k + \lambda_k = -\lambda_{k-2},$$

hence

$$-b(p)\alpha_2 - \frac{a(p)}{2}\alpha_1 = b(p)\lambda_{k-2} + a(p)\lambda_{k-1} > 0,$$

which means that (22) is satisfied. Hence Lemma 4.1 can be applied and $(\lambda_1, \ldots, \lambda_k, p)$ is not significant. □

Proposition 4.3 *For* $p < q^k$ *no configuration* $(\lambda_1, \ldots, \lambda_k; p)$ *that is symmetric (i.e. one that satisfies* $\lambda_i = \lambda_{k+1-i}$ *for* $i = 1, \ldots, k$*) can be significant.*
In particular, for $p < q^k$ *the configuration* $Q_{k,p} = (\lambda_1^k(p), \ldots, \lambda_k^k(p); p)$ *is not significant.*

Proof. We apply Lemma 4.1 with $r := r' := k$ and $\nu_i := \mu_i^{k-1}(q^k)$ and claim that (23) holds.

First we use the properties of ν_i as guaranteed by Lemma 3.7 to see that indeed $\alpha_1 = \alpha_2 = 0$:

$$\alpha_1 = 2\sum_{i=1}^{k} \lambda_i \nu_i = 0$$

because of $\lambda_i = \lambda_{k-i+1}$ and $\nu_i = -\nu_{k-i+1}$. Similarly

$$\alpha_2 = \sum_{i=1}^{k-1} (\nu_i \lambda_{i+1} + \nu_{i+1}\lambda_i) = 0,$$

since $\nu_{i+1}\lambda_i = \nu_{i+1}\lambda_{k-i+1} = -\nu_{k-(i+1)+1}\lambda_{k-i+1} = -\nu_{k-i}\lambda_{k-i+1}$.

Again using Lemma 3.7 now observe that

$$-\frac{\beta_2}{\beta_1} = -\frac{\sum_{i=1}^{k-1} \nu_i \nu_{i+1}}{\sum_{i=1}^{k} \nu_i^2} = \cos\phi^k.$$

Since $\beta_1 > 0$ and $b(p) < 0$, it now follows that

$$\begin{aligned} -b(p)\beta_2 - \frac{a(p)}{2}\beta_1 > 0 \quad &\Leftrightarrow \quad \frac{a(p)}{2b(p)} > -\frac{\beta_2}{\beta_1} \\ &\Leftrightarrow \quad \cos\phi > \cos\phi^k, \end{aligned}$$

which is true, because $p < q_k$ is equivalent to $\phi < \phi^k \leq \pi$. □

Proposition 4.4 *For $p > q^{k+1}$ the configuration $Q_{k,p} = (\lambda_1^k(p), \ldots, \lambda_k^k(p); p)$ is not significant.*

Proof. We would like to apply Corollary 4.2 and therefore need to show that for a fixed $p > q^{k+1}$

$$b(p)\lambda_{k-2}^k(p) + a(p)\lambda_{k-1}^k(p) > 0. \tag{24}$$

First we consider the case $q^{k+1} < p < q^*$. Since $a(p) > 0$ for $p > \frac{1}{2}$ and since we can assume that $\lambda_{k-1}^k(p) > 0$ (otherwise $Q_{k,p}$ wouldn't even be feasible), (24) is equivalent to

$$1 > -\frac{b(p)}{a(p)} \frac{\lambda_{k-2}^k(p)}{\lambda_{k-1}^k(p)}.$$

Using the explicit formula in Proposition 3.4 (observe that the denominator is the same for all λ_i and therefore cancels) we have to show that

$$1 > \frac{\sin(k-2)\phi - (-1)^k \sin 3\phi + \sin(k+1)\phi}{-2\cos\phi(-\sin(k-1)\phi + (-1)^k \sin 2\phi + \sin(k+1)\phi)} \quad \text{for } \frac{k}{k+2}\pi < \phi < \pi. \tag{25}$$

We defer this hardly interesting computation to Section 6.

Now consider the case $p \geq q^*$. Here $a(p)/2b(p) \leq -1$ and by Lemma 3.1

$$t_i(p) = \det(T^i(p)) > 0. \tag{26}$$

Recall that

$$\lambda_i^k(p) = \frac{\xi_i^k(p)}{|\vec{\xi}^k(p)|} \quad \text{and} \quad T^k(p) \cdot \vec{\xi}^k = \vec{1},$$

which implies that $b(p)\xi^k_{k-2}(p) + a(p)\xi^k_{k-1}(p) + b(p)\xi^k_k(p) = 1$ and therefore

$$b(p)\lambda^k_{k-2}(p) + a(p)\lambda^k_{k-1}(p) = \frac{1 - b(p)\xi^k_k(p)}{|\vec{\xi}^k(p)|}. \tag{27}$$

By Lemma 3.3 together with the fact that $t_0 = 1$ it follows that

$$\xi^k_k(p) = \sum_{j=1}^{k} m^k_{k,j}(p) = \frac{(-b(p))^k}{t_k(p)} \sum_{j=1}^{k} (-1)^j b(p)^{-j} t_{j-1}(p).$$

We use this to prove that the recursion

$$\xi^{i+1}_{i+1}(p) \cdot t_{i+1}(p) = t_i(p) - b(p) \cdot \xi^i_i(p) \cdot t_i(p) \tag{28}$$

holds for all $i \in \mathbb{N}$, which is easily verified as follows:

$$\begin{aligned} t_i(p) - b(p)\xi^i_i(p)t_i(p) &= t_i(p) + (-b(p))^{i+1} \sum_{j=1}^{i} (-1)^j b(p)^{-j} t_{j-1}(p) \\ &= (-b(p))^{i+1} \sum_{j=1}^{i+1} (-1)^j b(p)^{-j} t_{j-1}(p) \\ &= \xi^{i+1}_{i+1}(p) t_{i+1}(p) \ . \end{aligned}$$

Now coming back to our aim (24), we use (27) to obtain

$$b(p)\lambda^k_{k-2}(p) + a(p)\lambda^k_{k-1}(p) = \frac{t_k(p) - b(p)\xi^k_k(p)t_k(p)}{|\vec{\xi}^k(p)|t_k(p)} = \frac{\xi^{k+1}_{k+1}(p)t_{k+1}(p)}{|\vec{\xi}^k(p)|t_k(p)}.$$

We claim that this term is always positive. First observe that by (26), $t_i(p) > 0$ for all $i \in \mathbb{N}$. Furthermore this implies that the matrix $T^k(p)$ is positive definite, hence $M^k(p) = (T^k(p))^{-1}$ is also positive definite, thus $|\vec{\xi}^k(p)| = \vec{1}^T \cdot M^k(p) \cdot \vec{1}$ is positive. Hence if the configuration is feasible we must have $\xi^1_1(p) > 0$, thus the recursion (28) and the fact that $b(p) < 0$ imply that $\xi^i_i(p) > 0$ for all $i \in [k+1]$ and therefore $\xi^{k+1}_{k+1}(p) \cdot t_{k+1}(p)$ must also be positive. □

Now we move on to dismissing candidates $Q_{k,p}(x)$, which means dealing with those special cases, where $p = q^k_j$ for some integer $0 \leq j \leq k$. Recall that here

$$Q_{k,q^k_j}(x) = \left(\ell^k_1(q^k_j, x), \ldots, \ell^k_k(q^k_j, x); q^k_j\right),$$

as stated in Proposition 3.5. Note that the layer sizes $\lambda_i^k(p)$ are not defined for $p = q_j^k$, since here the matrix $T^k(p)$ is singular. Nevertheless we need $\lambda_i^k(q_j^k)$ when working with $\ell_i^k(q_j^k, x)$. This motivates the following definition:

$$\lambda_i^k(q_j^k) := \lim_{p \to q_j^k,\ p \geq q_j^k} \lambda_i^k(p).$$

The following proposition states some very useful facts about $\lambda_i^k(q_j^k)$ and $\ell_i^k(q_j^k, x)$.

Proposition 4.5 *Let $j \in [k]$ be an odd number and denote by $x^* := \lambda_k^k(q_j^k)$. Then*

$$\begin{array}{rl}
(i) & \lambda_i^{k-1}(q_j^k) = \dfrac{\sin\phi_j^k - (-1)^i(\sin i\phi_j^k + \sin(i+1)\phi_j^k)}{(k+1)\sin\phi_j^k} \\
(ii) & \lambda_i^k(q_j^k) = \dfrac{1 + (-1)^{i+1}\cos i\phi_j^k}{k+1} \\
(iii) & \lambda_{k-1}^{k-1}(q_j^k) = 2\lambda_k^k(q_j^k) \\
(iv) & \lambda_{i-1}^{k-1}(q_j^k) + \lambda_i^{k-1}(q_j^k) = 2\lambda_i^k(q_j^k) \\
(v) & \ell_i^k(q_j^k, x^*) = \lambda_i^k(q_j^k) \\
(vi) & \ell_i^k(q_j^k, x^* + x) = \ell_{k-i+1}^k(q_j^k, x^* - x).
\end{array}$$

This proposition has several important consequences. First, (v) states that at the point $x = x^*$ the configurations $Q_{k,p}(x)$ and $Q_{k,p}$ 'meet'. Moreover, it is equivalent to

$$\lambda_i^k(q_j^k) - x^* \cdot \mu_i^{k-1}(q_j^k) = \lambda_i^{k-1}(q_j^k),$$

which implies that

$$\ell_i^k(q_j^k, x) = \lambda_i^{k-1}(q_j^k) + x \cdot \mu_i^{k-1}(q_j^k) = \lambda_i^k(q_j^k) + (x - x^*) \cdot \mu_i^{k-1}(q_j^k). \tag{29}$$

This will turn out to be useful, since it will allow us to use the symmetry of $\vec{\lambda}$ to partly cover for the lack of symmetry in $\vec{\ell}$.

Also, by (vi), we know that

$$\ell_1^k(q_j^k, 2x^* + x) = \ell_k^k(q_j^k, -x) = -x,$$

hence the configuration $Q_{k,q_j^k}(x)$ is only feasible for $x \in [0, 2x^*]$, and therefore, because of the symmetry expressed in (vi), we only need to consider $x \in (0, x^*)$. Finally (iii) and (iv) prove statement (vi) of our main theorem 1.3.

Because of the different structure of $Q_{k,q_j^k}(x)$ for j odd and even, the dismissal of $Q_{k,q_j^k}(x)$ will be done separately.

Proposition 4.6 *For any even number j with $0 \leq j \leq k$ and any $x \in (0,1)$, the configuration $Q_{k,q_j^k}(x) = (\ell_1^k(q_j^k, x), \ldots, \ell_k^k(q_j^k, x); q_j^k)$ is not significant.*

Proof. Let $p := q_j^k$ and $\phi = \phi(p)$. Since we can assume that $p \geq \frac{1}{2}$, we also know that $\phi \geq \pi/2$. Recall from Lemma 3.6 that for $i \in [k-1]$,

$$\ell_i^k(p,x) = \lambda_i^{k-1}(p) + x \cdot \mu_i^{k-1}(p) = (1 - \frac{x}{1+\cos\phi})\lambda_i^{k-1}(\phi) - x \cdot b(p) \cdot m_{i,k-1}^{k-1}(p)$$

and $\ell_k^k(p,x) = x$. We consider two different cases, depending on whether

$$(1 - \frac{x}{1+\cos\phi})\frac{1}{|\vec{\xi}^{k-1}(p)|} \tag{30}$$

is positive or not.

Suppose that it is positive. Then we would like to apply Corollary 4.2 and therefore need to show that

$$b(p)\ell_{k-2}^k(p) + a(p)\ell_{k-1}^k(p) > 0. \tag{31}$$

Similarly to the proof of Proposition 4.4 we deduce from $T^{k-1}(p) \cdot \vec{\xi}^{k-1} = \vec{1}$ and $M^{k-1}(p) \cdot T^{k-1}(p) = id$ that

$$b(p)\xi_{k-2}^{k-1}(p) + a(p)\xi_{k-1}^{k-1}(p) = 1, \qquad b(p)m_{k-1,k-2}^{k-1}(p) + a(p)m_{k-1,k-1}^{k-1}(p) = 1.$$

Hence condition (31) is equivalent to

$$(1 - \frac{x}{1+\cos\phi})\frac{1}{|\vec{\xi}^{k-1}(p)|} - x \cdot b(p) > 0,$$

which is true since (30) is positive and $b(p)$ is negative.

Now suppose that (30) is negative. In this case we would like to apply Lemma 4.1 with $r := k$, $r' := k+1$, $\lambda_i := \ell_i^k(p,x)$ and

$$\nu_k := -1,\ \nu_{k+1} := 1, \ \text{ and } \ \nu_i := 0 \ \text{ for } i = 1, \ldots, k-1.$$

Then

$$\alpha_1 = -2\ell_k^k(p,x) \ \text{ and } \ \alpha_2 = -\ell_{k-1}^k(p,x) + \ell_k^k(p,x),$$

hence the condition $-b(p)\alpha_2 - \frac{a(p)}{2}\alpha_1 > 0$ now reduces to

$$\begin{aligned}
0 &\overset{!}{<} b(p) \cdot \ell_{k-1}^k(p,x) - b(p) \cdot \ell_k^k(p,x) + a(p) \cdot \ell_k^k(p,x) \\
&= b(p) \cdot (1 - \frac{x}{1+\cos\phi}) \cdot \lambda_{k-1}^{k-1}(\phi) - b(p)^2 x \cdot m_{k-1,k-1}^{k-1}(p) - b(p) \cdot x + a(p) \cdot x \\
&= b(p) \cdot \xi_{k-1}^{k-1}(p) \cdot (1 - \frac{x}{1+\cos\phi})\frac{1}{|\vec{\xi}^{k-1}(p)|} - x \cdot b(p),
\end{aligned}$$

where we used the fact (see Lemma 3.6) that

$$m_{k-1,k-1}^{k-1}(p) = (-1)^{k-1}\frac{\sin(k-1)\phi}{b(p)\sin\phi} = \frac{2\cos\phi}{b(p)} = \frac{a(p)}{b(p)^2}.$$

Since (30) is negative it therefore suffices to show that $\xi_{k-1}^{k-1}(p)$ is non–negative. Thanks to Lemma 3.6 we know that

$$\xi_{k-1}^{k-1}(p) = \frac{1}{b(p)} - \frac{1}{b(p)(1+\cos\phi)} = \frac{\cos\phi}{b(p)(1+\cos\phi)},$$

which is non–negative because $\pi \geq \phi \geq \pi/2$. □

Proposition 4.7 *For any odd number j with $1 < j \leq k$ and any $x \in (0,1)$, the configuration $Q_{k,q_j^k}(x) = (\ell_1^k(q_j^k, x), \ldots, \ell_k^k(q_j^k, x); q_j^k)$ is not significant.*

Proof. We take the same approach as in the proof of Proposition 4.3: Since $j > 1$ we have that $q_j^k < q^k$, but unfortunately the configuration $(\ell_1^k(q_j^k, x), \ldots, \ell_k^k(q_j^k, x); q_j^k)$ is not symmetric. However, recall from (29) that it can be written as

$$\ell_i^k(q_j^k, x) = \lambda_i^k(q_j^k) + (x - x^*) \cdot \mu_i^{k-1}(q_j^k)$$

where the $\lambda_i^k(q_j^k)$ are symmetric. Now we apply Lemma 4.1 with

$$r := r' := k, \qquad \nu_i := \mu_i^{k-1}(q^k) \qquad \lambda_i := \ell_i^k(q_j^k, x)$$

and claim that (23) holds.

Again we use the properties of ν_i as guaranteed by Lemma 3.7 to see that indeed $\alpha_1 = \alpha_2 = 0$:

$$\alpha_1 = 2\sum_{i=1}^{k}(\lambda_i^k(q_j^k) + (x - x^*) \cdot \mu_i^{k-1}(q_j^k))\nu_i = 0$$

because

$$\lambda_i^k(q_j^k) = \lambda_{k-i+1}^k(q_j^k), \quad \nu_i = -\nu_{k-i+1}, \quad \sum_{i=1}^{k}\mu_i^{k-1}(q_j^k) \cdot \nu_i = 0.$$

Similarly

$$\alpha_2 = \sum_{i=1}^{k-1}\Big(\nu_i[\lambda_{i+1}^k(q_j^k) + (x - x^*) \cdot \mu_{i+1}^{k-1}(q_j^k)] + \nu_{i+1}[\lambda_i^k(q_j^k) + (x - x^*) \cdot \mu_i^{k-1}(q_j^k)]\Big) = 0,$$

since $\nu_{i+1}\lambda_i^k(q_j^k) = \nu_{i+1}\lambda_{k-i+1}^k(q_j^k) = -\nu_{k-(i+1)+1}\lambda_{k-i+1}^k(q_j^k) = -\nu_{k-i}\lambda_{k-i+1}^k(q_j^k)$ and

$$\sum_{i=1}^{k} \nu_i \cdot \mu_{i+1}^{k-1}(q_j^k) = \sum_{i=1}^{k} \nu_{i+1} \cdot \mu_i^{k-1}(q_j^k) = 0$$

according to the last statement in Lemma 3.7.

The rest of the proof is identical to that of Proposition 4.3, since the ν_i are chosen in exactly the same way and because $q_j^k < q^k$. □

Thus we have dismissed all candidates $Q_{k,q_j^k}(x)$ other than $Q_{k,q^k}(x)$ in the range $x \in [0, x^*]$.

5 Linearity and monotonicity

In this section we complete the proof of Theorems 1.3 and 1.4. We start with the statement (vii) of Theorem 1.3, which we prove here in a slightly more general form.

Proposition 5.1 *For an odd number $j \in [k]$ consider a configuration $(\lambda_1, \ldots, \lambda_r; q_j^k)$ with $r \leq k$. Set $\lambda_{r+1} = \cdots = \lambda_k = 0$ and $\mu_i := \mu_i^{k-1}(q_j^k)$ for $i = 1, \ldots, k$. There exists a constant u such that for all x*

$$\mathrm{c}(\lambda_1 + x\mu_1, \ldots, \lambda_k + x\mu_k; q_j^k) \;=\; -a(q_j^k) \;\cdot\; \mathrm{d}(\lambda_1 + x\mu_1, \ldots, \lambda_k + x\mu_k; q_j^k) \;+ u \;.$$

Proof. Let $p := q_j^k$. We need to show that

$$H(p)\sum_{i=1}^{k-1}(\lambda_i + x\mu_i)(\lambda_{i+1} + x\mu_{i+1}) =$$
$$-a(p) \cdot \Big(\frac{1}{2} - \frac{1}{2}\sum_{i=1}^{k}(\lambda_i + x\mu_i)^2 - (1-p)\sum_{i=1}^{k-1}(\lambda_i + x\mu_i)(\lambda_{i+1} + x\mu_{i+1})\Big) \;+ u.$$

Both sides are polynomials in x of degree 2. We compare their coefficients:

$$x^0: \quad H(p)\sum_{i=1}^{k-1}\lambda_i\lambda_{i+1} = -a(p)\Big(\frac{1}{2}-\frac{1}{2}\sum_{i=1}^{k}\lambda_i^2-(1-p)\sum_{i=1}^{k-1}\lambda_i\lambda_{i+1}\Big)+u \tag{32}$$

$$x^1: \quad H(p)\sum_{i=1}^{k-1}(\lambda_i\mu_{i+1}+\lambda_{i+1}\mu_i) =$$

$$-a(p)\Big(-\frac{1}{2}\sum_{i=1}^{k}2\lambda_i\mu_i-(1-p)\sum_{i=1}^{k-1}(\lambda_i\mu_{i+1}+\lambda_{i+1}\mu_i)\Big) \tag{33}$$

$$x^2: \quad H(p)\sum_{i=1}^{k-1}\mu_i\mu_{i+1} = -a(p)\Big(-\frac{1}{2}\sum_{i=1}^{k}\mu_i^2-(1-p)\sum_{i=1}^{k-1}\mu_i\mu_{i+1}\Big) \tag{34}$$

Obviously u can be chosen so that (32) holds, so we only need to check (33) and (34). Comparing the coefficients of λ_i in (33) results in

$$H(p)(\mu_{i+1}+\mu_{i-1}) = -a(p)(-\mu_i-(1-p)(\mu_{i+1}+\mu_{i-1})).$$

Using the facts $H(p)=(1-p)a(p)-b(p)$ and $\frac{a(p)}{2b(p)}=\cos\phi$ this is equivalent to

$$\mu_{i+1}+\mu_{i-1} = -2\cos\phi\cdot\mu_i,$$

which is true because by Lemma 3.6

$$\begin{aligned}\mu_{i-1}+\mu_{i+1} &= (-1)^{i-1}\cdot\frac{\sin(i-1)\phi+\sin(i+1)\phi}{\sin\phi} = (-1)^{i-1}\cdot\frac{2\sin i\phi\cdot\cos\phi}{\sin\phi}\\ &= -2\cos\phi\cdot\mu_i.\end{aligned}$$

Applying the same facts as above, (34) is equivalent to

$$-\sum_{i=1}^{k-1}\mu_i\cdot\mu_{i+1} = \cos\phi\sum_{i=1}^{k}\mu_i^2,$$

which can be seen to be true using Lemma 3.7. □

To complete the proof of the main result there is now only one piece missing: we still need to prove that as x increases $\mathrm{d}(Q_{k,q^k}(x))$ increases, and that as p increases $\mathrm{d}(Q_{k,p})$ increases. This will be done in the following two propositions. The proof of the latter is very technical and hence postponed to Section 6. For the proof of the first, recall that in the case of $q_j^k = q^k$ we have $x^* = \lambda_k^k(q^k)$.

Proposition 5.2 *As x increases from 0 to x^*, the function*

$$\mathrm{d}(Q_{k,q^k}(x)) = \mathrm{d}(\ell_1^k(q^k,x),\ldots,\ell_k^k(q^k,x),q^k)$$

is strictly increasing.

Proof. Let us abbreviate $\ell_i(x) := \ell_i^k(q^k,x)$, $\lambda_i := \lambda_i^k(q^k)$ and $\mu_i := \mu_i^{k-1}(q^k)$. Then recall that by (29) we can write

$$\ell_i(x) = \lambda_i - x^* \cdot \mu_i + x \cdot \mu_i,$$

(where we will make use of the fact that the λ_i are symmetric) and that the function under consideration is given by

$$\mathrm{d}(\ell_1^k(q^k,x),\ldots,\ell_k^k(q^k,x),q^k) = \frac{1}{2} - \frac{1}{2}\sum_{i=1}^{k}\ell_i(x)^2 - (1-q^k)\sum_{i=1}^{k-1}\ell_i(x)\ell_{i+1}(x). \tag{35}$$

We claim that the derivatives of the two sums involved are negative. Since $\lambda_i = \lambda_{k-i+1}$ and $\mu_i = -\mu_{k-i+1}$ we can use that

$$\sum_{i=1}^{k}\lambda_i\mu_i = 0 = \sum_{i=1}^{k-1}(\lambda_i\mu_{i+1} + \lambda_{i+1}\mu_i).$$

Thus the derivative of the first sum is given by

$$\sum_{i=1}^{k}\left(2[\lambda_i - x^*\mu_i]\mu_i + 2x\cdot\mu_i^2\right) = 2(x-x^*)\sum_{i=1}^{k}\mu_i^2,$$

which is easily seen to be negative, because $x < x^*$.

Similarly, the derivative of the second sum in (35) is

$$\sum_{i=1}^{k-1}\left([\lambda_i - x^*\mu_i]\mu_{i+1} + [\lambda_{i+1} - x^*\mu_{i+1}]\mu_i + 2x\cdot\mu_i\mu_{i+1}\right)$$

$$= 2(x-x^*)\sum_{i=1}^{k-1}\mu_i\mu_{i+1},$$

which is negative by Lemma 3.7. □

Proposition 5.3 *As p increases from q^k to q^{k+1}, the function*

$$\mathrm{d}(Q_{k,p}) = \mathrm{d}(\lambda_1^k(p),\ldots,\lambda_k^k(p),p)$$

is strictly increasing, while

$$\mathrm{c}(Q_{k,p}) = \mathrm{c}(\lambda_1^k(p),\ldots,\lambda_k^k(p),p)$$

is strictly decreasing.

We close this section with the proof of the main theorems. The only thing we have to do is to assemble all the information gathered so far. While doing so, we will refer to previous theorems, lemmas or propositions by simply mentioning their reference numbers in brackets.

Proof of Theorems 1.3 and 1.4. We know that $\mathrm{c}(d) = \mathrm{c}(Q)$ if Q is a d-significant configuration [1.1]. We have determined a family $\mathcal{C}$ of candidates $Q_{k,p}$ and $Q_{k,p}(x)$, of which we know that for every d there exists a d-significant configuration in $\mathcal{C}$. We have defined constants q^k and x^* (depending on k) and have proved [Section 4] that $Q_{k,p}$ can only be significant if $p \in [q^k, q^{k+1}]$, and that $Q_{k,p}(x)$ can only be significant if $p = q^k$ and $x \in [0, x^*]$. Let us denote the subfamily formed by these remaining configurations by $\mathcal{C}'$. We have seen that the configurations 'meet' at the beginning (by definition of $Q_{k,p}(x)$) and end (by [4.5]) of their intervals:

$$Q_{k-1,q^k} = Q_{k,q^k}(0) \quad \text{ and } \quad Q_{k,q^k}(x^*) = Q_{k,q^k}.$$

We have shown [5.2,5.3] that $\mathrm{d}(Q_{k,p})$ is strictly increasing as a function in p, and that $\mathrm{d}(Q_{k,q^k}(x))$ is strictly increasing as a function in x. We may therefore deduce that the infinite sequence of constants defined by

$$d'_k := \mathrm{d}(Q_{k-1,q^k}) \quad \text{ and } \quad d_k := \mathrm{d}(Q_{k,q^k})$$

does indeed satisfy

$$d_2 < d'_3 < d_3 < d'_4 < d_4 < \cdots < \frac{1}{2}$$

which in turn implies that for every d there exists only one configuration Q^* in $\mathcal{C}'$ with $\mathrm{d}(Q^*) = d$. We can therefore conclude that it must be d-significant. Now it only remains to check that in the above intervals the configurations and their parameters [3.4, 3.5, 5.1] are as stated in the theorems. This completes the proof of our main result as stated in Theorems 1.3 and 1.4. □

6 Technical computations

This section contains the proofs of those lemmas and propositions that we stated in the previous sections but didn't prove there. All of them are fairly technical and hence probably not very easy to read. In the course of the following computations, we will very often use trigonometric identities such as $\sin(x \pm y) = \sin x \cos y \pm \cos x \sin y$ or $\sin x \sin y = \frac{1}{2}(\cos(x-y) - \cos(x+y))$, for example, without referring to them explicitly.

Proof of Lemma 3.1. By expanding the determinant of T^k by the first row we obtain the recursion

$$t_k = at_{k-1} - b^2 t_{k-2}. \tag{36}$$

In both cases the claimed identity for t_k is then easily verified by induction on k. (In the second case use $\cos 2x = 2\cos^2 x - 1$ to verify the case $\ell = 2$ and $2\sin\frac{x+y}{2}\cos\frac{x-y}{2} = \sin x + \sin y$ for the induction step.) $\square$

Proof of Lemma 3.3. Let us first deal with the case $2 \leq i, j \leq k-1$. Here we need to show that

$$bm_{i,j-1} + am_{i,j} + bm_{i,j+1} = \delta_{i,j}.$$

If indeed $i = j$ then applying the definition of the $m^k_{i,j}$ and using the recursion (36) from the preceding proof

$$\begin{aligned} bm_{i,i-1} + am_{i,i} + bm_{i,i+1} &= -b^2\frac{t_{i-2}t_{k-i}}{t_k} + a\frac{t_{i-1}t_{k-i}}{t_k} - b^2\frac{t_{i-1}t_{k-i-1}}{t_k} \\ &= \frac{1}{t_k}\Big(- b^2 t_{i-2}t_{k-i} + t_{i-1}t_{k-i+1}\Big). \end{aligned}$$

It therefore suffices to show that for all $i = 2, \ldots, k$

$$t_k = -b^2 t_{i-2}t_{k-i} + t_{i-1}t_{k-i+1},$$

which we prove by induction on i. Since $t_0 = 1$ and $t_1 = a$, the case $i = 2$ is identical to (36). For the induction step we need to show that that

$$-b^2 t_{i-2}t_{k-i} + t_{i-1}t_{k-i+1} = t_k \stackrel{!}{=} -b^2 t_{i-1}t_{k-i-1} + t_i t_{k-i},$$

which is equivalent to

$$t_{i-1}\cdot(t_{k-i+1} + b^2 t_{k-i-1}) = t_{k-i}(t_i + b^2 t_{i-2}).$$

Once again using (36), both sides of the last equality can be seen to be equal to $a \cdot t_{i-1} \cdot t_{k-i}$.

Now suppose that $i < j$, the case $i > j$ can be dealt with analogously. Then

$$bm_{i,j-1} + am_{i,j} + bm_{i,j+1} \;=\; (-1)^{i+j} b^{j-i}\frac{t_{i-1}}{t_k}\Big(- t_{k+1-j} + at_{k-j} - b^2 t_{k-j-1}\Big) \;=0,$$

as required.

To deal with those cases where $\{i,j\} \cap \{1,k\} \neq \emptyset$, simply define $t_{-1} := 0$, and observe that this agrees with the recursion (36). Now we can extend the definition $m^k_{i,j}$ to cover those cases where $\{i,j\} \cap \{0, k+1\} \neq \emptyset$ – here $m^k_{i,j} = 0$ and the same proof as above applies. $\square$

In the following we state a number of trigonometric identities that will later turn out to be useful.

Lemma 6.1

$$(i) \quad \sum_{j=1}^{k}(-1)^j \sin j\theta = \frac{-\sin\theta + (-1)^k \sin k\theta + (-1)^k \sin(k+1)\theta}{2+2\cos\theta},$$

$$(ii) \quad \sum_{j=1}^{k}\cos(j\cdot\theta+\vartheta) = \frac{-\cos\vartheta + \cos(\theta+\vartheta) + \cos(k\cdot\theta+\vartheta) - \cos((k+1)\theta+\vartheta)}{2-2\cos\theta},$$

$$(iii) \quad \sum_{j=1}^{k}(\sin j\theta)^2 = \frac{1}{2}k + \frac{1}{4} - \frac{\sin(2k+1)\theta}{4\sin\theta},$$

$$(iv) \quad \sum_{j=1}^{k}\sin j\theta\cdot\sin(j+1)\theta = \frac{1}{2}(k+1)\cos\theta - \frac{\sin(2k+2)\theta}{4\sin\theta}.$$

Proof. All proofs use the fact that

$$\sin x = \frac{1}{2i}(e^{ix}-e^{-ix}) \qquad \text{and} \qquad \cos x = \frac{1}{2}(e^{ix}+e^{-ix}).$$

Here we only include the proof of (i). The other statements can be proven very similarly.

$$\begin{aligned}
\sum_{j=1}^{k}(-1)^j \sin j\theta &= \frac{1}{2i}\sum_{j=1}^{k}(-1)^j(e^{ij\theta}-e^{-ij\theta}) \\
&= -\frac{1}{2i}\Big[\frac{e^{i\theta}(1-(-1)^k e^{ik\theta})}{1+e^{i\theta}} - \frac{e^{-i\theta}(1-(-1)^k e^{-ik\theta})}{1+e^{-i\theta}}\Big] \\
&= -\frac{1}{2i}\frac{e^{i\theta}+1-(-1)^k e^{i(k+1)\theta}-(-1)^k e^{ik\theta}-e^{-i\theta}-1+(-1)^k e^{-i(k+1)\theta}+(-1)^k e^{-ik\theta}}{(1+e^{i\theta})(1+e^{-i\theta})} \\
&= \frac{-\sin\theta+(-1)^k\sin k\theta+(-1)^k\sin(k+1)\theta}{2+2\cos\theta}.
\end{aligned}$$

□

Proof of (17) and (18) in the proof of Proposition 3.4.

$$\begin{aligned}
\xi_i^k(p) &= \sum_{j=1}^{k} m^k(p)_{ij} = \sum_{j=1}^{i} m^k(p)_{ij} + \sum_{j=i+1}^{k} m^k(p)_{ij} \\
&= \frac{(-1)^i}{b(p)\sin\phi\sin(k+1)\phi}\cdot[\sin(k-i+1)\phi\sum_{j=1}^{i}(-1)^j\sin j\phi \\
&\qquad + \sin i\phi \underbrace{\sum_{j=i+1}^{k}(-1)^j\sin(k-j+1)\phi]}_{=(-1)^{k+1}\sum_{j=1}^{k-i}(-1)^j\sin j\phi} \\
&= \frac{(-1)^i}{b(p)\sin\phi\sin(k+1)\phi}\cdot[\sin(k-i+1)\phi\frac{-\sin\phi+(-1)^i\sin i\phi+(-1)^i\sin(i+1)\phi}{2+2\cos\phi} \\
&\qquad -(-1)^k\sin i\phi\frac{-\sin\phi+(-1)^{k-i}\sin(k-i)\phi+(-1)^{k-i}\sin(k-i+1)\phi}{2+2\cos\phi}] \\
&= \frac{-(-1)^i\sin(k-i+1)\phi\sin\phi+\sin(k-i+1)\phi\sin(i+1)\phi}{b(p)\sin\phi\sin(k+1)\phi\cdot(2+2\cos\phi)} \\
&\qquad + \frac{(-1)^{k-i}\sin\phi\sin i\phi-\sin i\phi\sin(k-i)\phi}{b(p)\sin\phi\sin(k+1)\phi\cdot(2+2\cos\phi)}.
\end{aligned}$$

Finally, observe that

$$\begin{aligned}
&\sin(k-i+1)\phi\sin(i+1)\phi-\sin i\phi\sin(k-i)\phi \\
&\quad = \sin(k-i+1)\phi\cdot[\sin i\phi\cos\phi+\cos i\phi\sin\phi] \\
&\qquad -\sin i\phi\cdot[\sin(k-i+1)\phi\cos\phi-\cos(k-i+1)\phi\sin\phi] \\
&\quad = \sin\phi\cdot[\sin(k-i+1)\phi\cos i\phi+\cos(k-i+1)\phi\sin i\phi] \\
&\quad = \sin\phi\sin(k+1)\phi,
\end{aligned}$$

which proves (17). As to the proof of (18),

$$|\vec{\xi}(p)| = \sum_{i=1}^{k}\xi_i^k(p) = \frac{\sum_{i=1}^{k}(-1)^{k-i}\sin i\phi-(-1)^i\sin(k-i+1)\phi+\sin(k+1)\phi}{2b(p)(1+\cos\phi)\sin(k+1)\phi}.$$

Consider the numerator:

$$
\begin{aligned}
< N > &= (-1)^k \sum_{i=1}^{k} (-1)^i \sin i\phi - \underbrace{\sum_{i=1}^{k} (-1)^i \sin(k-i+1)\phi}_{=(-1)^{k+1}\sum_{i=1}^{k}(-1)^i \sin i\phi} + k\sin(k+1)\phi \\
&= 2(-1)^k \sum_{i=1}^{k} (-1)^i \sin i\phi + k\sin(k+1)\phi \\
&= 2(-1)^k \frac{-\sin\phi + (-1)^k \sin k\phi + (-1)^k \sin(k+1)\phi}{2+2\cos\phi} + k\sin(k+1)\phi \\
&= \frac{-(-1)^k \sin\phi + \sin k\phi + \sin(k+1)\phi}{1+\cos\phi} + k\sin(k+1)\phi,
\end{aligned}
$$

which proves (18). □

Proof of Lemma 3.6. We have to compute the value of the functions $m_{i,k-1}^{k-1}$, ξ_{k-1}^{k-1}, μ_i^{k-1} and ℓ_i^k at the point q_j^k. To improve readability, we omit the term q_j^k in our calculations and let $\phi := \phi_j^k$. Then

$$
\begin{aligned}
m_{i,k-1}^{k-1} &= (-1)^{i+k-1} b^{k-1-i} \frac{t_{i-1}t_0}{t_{k-1}} = (-1)^{i+k-1} b^{-1} \frac{\sin i\phi}{\sin k\phi} \\
&\overset{(21)}{=} (-1)^{i+k-1} b^{-1} \frac{\sin i\phi}{-(-1)^{k-j}\sin\phi} \\
&= (-1)^{i+j} \frac{\sin i\phi}{b\sin\phi}.
\end{aligned}
$$

To compute ξ_{k-1}^{k-1}, we use the formula in Proposition 3.4 to see that

$$
\begin{aligned}
\xi_{k-1}^{k-1} &= \frac{-(-1)^{k-j}\sin 2\phi - (-1)^{k-1}\sin\phi - (-1)^{k-j}\sin\phi}{-(-1)^{k-j} 2b(1+\cos\phi)\sin\phi} \\
&= \begin{cases} \frac{2\cos\phi\sin\phi + 2\sin\phi}{2b(\cos\phi\sin\phi+\sin\phi)} = \frac{1}{b} & \text{, if } j \text{ odd,} \\ \frac{2\cos\phi\sin\phi}{2b(1+\cos\phi)\sin\phi} = \frac{1}{b} - \frac{1}{b(1+\cos\phi)} & \text{, if } j \text{ even.} \end{cases}
\end{aligned}
$$

Finally, first use (21) to see that (for j odd) the formula for μ_k^{k-1} is indeed equal to one and then observe that the above results show that the expressions for μ_i^{k-1} and ℓ_i^k follow directly from their definitions in Proposition 3.5. □

Proof of Lemma 3.7. We will use the explicit formula

$$
\mu_i^{k-1}(q_j^k) = (-1)^i \frac{\sin i\phi_j^k}{\sin \phi_j^k}
$$

from Lemma 3.6 together with the observation (21) and the abbreviations $\phi := \phi_j^k$, $\mu_i := \mu_i^{k-1}(q_j^k)$, $\phi' := \phi_{j'}^k$, $\mu_i' := \mu_i^{k-1}(q_{j'}^k)$. First

$$\mu_{k+1-i} = (-1)^{k+1-i}\frac{\sin(k-(i-1))\phi}{\sin\phi} = -(-1)^{k+1-i+k-j}\frac{\sin i\phi}{\sin\phi} = -\mu_i,$$

which proves (i). This immediately implies (ii). To prove (iii)-(vi), we apply Lemma 6.1. Hence

$$\begin{aligned}\sum_{i=1}^k \mu_i^2 &= \frac{1}{\sin^2\phi}\sum_{i=1}^k(\sin i\phi)^2 = \frac{1}{\sin^2\phi}(\frac{k}{2}+\frac{1}{4}-\frac{\sin(2k+1)\phi}{4\sin\phi})\\ &\overset{(21)}{=} \frac{1}{\sin^2\phi}(\frac{k}{2}+\frac{1}{4}+\frac{1}{4}) = \frac{k+1}{2\sin^2\phi}, \quad \text{and}\\ \sum_{i=1}^{k-1}\mu_i\mu_{i+1} &= \frac{-1}{\sin^2\phi}\sum_{i=1}^k \sin i\phi\sin(i+1)\phi = \frac{-1}{\sin^2\phi}(\frac{k+1}{2}\cos\phi - \frac{\sin(2k+2)\phi}{4\sin\phi})\\ &\overset{(21)}{=} -\frac{(k+1)\cos\phi}{2\sin^2\phi},\end{aligned}$$

which proves (iii) and (iv). To prove (v) and (vi), observe that

$$\begin{aligned}\sum_{i=1}^k \mu_i'\mu_i &= \frac{1}{\sin\phi'\sin\phi}\sum_{i=1}^k \sin i\phi'\sin i\phi\\ &= \frac{1}{\sin\phi'\sin\phi}\left(\sum_{i=1}^k\cos i(\phi'-\phi) - \sum_{i=1}^k\cos i(\phi'+\phi)\right).\end{aligned}$$

We claim that the last two sums are identical. By Lemma 6.1

$$\sum_{i=1}^k \cos i(\phi'\pm\phi) = \frac{-1+\cos(\phi'\pm\phi)+\cos k(\phi'\pm\phi)-\cos(k+1)(\phi'\pm\phi)}{2-2\cos(\phi'\pm\phi)}.$$

Notice that

$$\phi'-\phi = \frac{j-j'}{k+1}\pi, \qquad \phi'+\phi = \frac{2k-j'-j}{k+1}\pi,$$

As j and j' are odd, we know that $(k+1)(\phi'\pm\phi)$ is an even multiple of π and hence $\cos(k+1)(\phi'\pm\phi) = 1$ and $\cos k(\phi'\pm\phi) = \cos((k+1)(\phi'\pm\phi)-(\phi'\pm\phi)) = \cos(\phi'\pm\phi)$. Therefore

$$\sum_{i=1}^k \cos i(\phi'\pm\phi) = \frac{-2+2\cos(\phi'\pm\phi)}{2-2\cos(\phi'\pm\phi)} = -1,$$

which completes the proof of (v). Similarly for the proof of (vi)

$$\sum_{i=1}^{k-1} \mu'_{i+1}\mu_i = \sum_{i=1}^{k} \mu'_{i+1}\mu_i = \frac{-1}{\sin\phi' \sin\phi} \left(\sum_{i=1}^{k} \cos[i(\phi'-\phi)+\phi'] - \sum_{i=1}^{k} \cos[i(\phi'+\phi)+\phi'] \right),$$

$$\begin{aligned} \sum_{i=1}^{k} \cos[i(\phi' \pm \phi)+\phi'] &= \frac{-\cos\phi' + \cos((\phi'\pm\phi)+\phi') + \cos(-(\phi'\pm\phi)+\phi') - \cos\phi'}{2-2\cos(\phi'\pm\phi)} \\ &= \frac{-2\cos\phi' + 2\cos(\phi'\pm\phi)\cos\phi'}{2-2\cos(\phi'\pm\phi)} = -\cos\phi'. \end{aligned}$$

□

Proof of (25) in the proof of Proposition 4.4. Recall that

$$(1-\frac{2}{k+2})\pi < \phi < \pi$$

and hence

$$(r-1)\cdot\pi < r\cdot\phi < r\cdot\pi \qquad \text{for } r \in (0, \frac{k+2}{2}]. \tag{37}$$

Observe that

$$\begin{aligned} &\frac{\sin(k-2)\phi - (-1)^k \sin 3\phi + \sin(k+1)\phi}{-2\cos\phi(-\sin(k-1)\phi + (-1)^k \sin 2\phi + \sin(k+1)\phi)} \\ = &\frac{(-1)^{k+1}\sin 3\phi + \sin(k-2)\phi + \sin(k+1)\phi}{(-1)^{k+1}(\sin 3\phi + \sin\phi) + \sin(k-2)\phi - \sin(k+2)\phi} \quad =: \frac{A(k,\phi)}{B(k,\phi)}. \end{aligned}$$

In order to prove (25), we need to show that $B(k,\phi) > A(k,\phi)$ or $B(n,\phi) < A(n,\phi)$, depending on whether $B(n,\phi)$ is positive or negative. This is done in the following two claims.

Claim 1: If $\phi^{k+1} < \phi < \pi$, then $B(k,\phi)$ is positive for odd k and negative for even k.

Claim 2: If $\phi^{k+1} < \phi < \pi$, then $B(k,\phi) - A(k,\phi)$ is positive for odd k and negative for even k.

Proof of Claim 1: Rearranging the terms involved in $B(k,\phi)$, we get

$$\begin{aligned} B(k,\phi) &= (-1)^{k+1} 2\sin 2\phi\cos\phi - 2\cos k\phi \sin 2\phi \\ &= 2\sin 2\phi\Big((-1)^{k+1}\cos\phi - \cos k\phi\Big) \\ &= \begin{cases} 2\sin 2\phi \cdot 2\sin\frac{k+1}{2}\phi \sin\frac{k-1}{2}\phi & , k \text{ odd} \\ -2\sin 2\phi\cdot 2\cos\frac{k+1}{2}\phi\cos\frac{k-1}{2}\phi & , k \text{ even.} \end{cases} \end{aligned}$$

Now with the help of (37)

$$\pi < 2\phi < 2\pi, \quad (\frac{k-1}{2} - 1)\pi < \frac{k-1}{2}\phi < \frac{k-1}{2}\pi < \frac{k+1}{2}\phi < \frac{k+1}{2}\pi$$

and thereby Claim 1 follows, because $\sin 2\phi$ is negative, and each of the pairs $\sin\frac{k-1}{2}\phi$, $\sin\frac{k+1}{2}\phi$ and $\cos\frac{k-1}{2}\phi$, $\cos\frac{k+1}{2}\phi$ has opposite signs.

Proof of Claim 2:

$$\begin{aligned}
B(k,\phi) - A(k,\phi) &= -\sin(k+2)\phi - \sin(k+1)\phi + (-1)^{k+1}\sin\phi \\
&= -2\sin(k+\frac{3}{2})\phi\cos\frac{1}{2}\phi + 2(-1)^{k+1}\sin\frac{1}{2}\phi\cos\frac{1}{2}\phi \\
&= \begin{cases} 2\cos\frac{1}{2}\phi\cdot(\sin\frac{1}{2}\phi - \sin(k+\frac{3}{2})\phi) & ,k \text{ odd} \\ 2\cos\frac{1}{2}\phi\cdot(-\sin\frac{1}{2}\phi - \sin(k+\frac{3}{2})\phi) & ,k \text{ even} \end{cases} \\
&= \begin{cases} -4\cos\frac{1}{2}\phi\cos\frac{k+2}{2}\phi\sin\frac{k+1}{2}\phi & ,k \text{ odd} \\ -4\cos\frac{1}{2}\phi\sin\frac{k+2}{2}\phi\cos\frac{k+1}{2}\phi & ,k \text{ even.} \end{cases}
\end{aligned}$$

Moreover, again with the help of (37)

$$-\frac{1}{2}\pi < \frac{1}{2}\phi < \frac{1}{2}\pi, \quad \frac{k-1}{2}\pi < \frac{k+1}{2}\phi < \frac{k+1}{2}\pi, \quad \frac{k}{2}\pi < \frac{k+2}{2}\phi < \frac{k+2}{2}\pi$$

and thereby Claim 2 follows, because $\cos\frac{1}{2}\phi$ is positive, $\cos\frac{k+2}{2}\phi$ and $\sin\frac{k+1}{2}\phi$ have opposite signs and $\sin\frac{k+2}{2}\phi$ and $\cos\frac{k+1}{2}\phi$ have the same sign. □

Proof of Proposition 4.5. We use the shorthand $\phi := \phi_j^k$, $\lambda_i^r := \lambda_i^r(q_j^k)$ and $\mu_i^r := \mu_i^r(q_j^k)$ for $r = k-1, k$. Moreover, observation (21) and the analogue for cos, namely

$$\cos(k-i)\phi_j^k = (-1)^{k-j}\cos(i+1)\phi_j^k, \tag{38}$$

will prove to be useful. Recall that, by Proposition 3.4, $\lambda_i^k = \frac{\eta_i^k(\phi)}{\psi^k(\phi)}$, where

$$\eta_i^k(\phi) := (-1)^{k-i}\sin i\phi - (-1)^i\sin(k-i+1)\phi + \sin(k+1)\phi,$$

$$\psi^k(\phi) := \frac{-(-1)^k\sin\phi + \sin k\phi + \sin(k+1)\phi}{1+\cos\phi} + k\sin(k+1)\phi.$$

To prove part (i), we repeatedly use (21) together with the fact that j is odd.

$$\begin{aligned}
\eta_i^{k-1}(\phi) &= (-1)^{k-1-i}\sin i\phi - (-1)^{k+i}\sin(i+1)\phi + (-1)^k\sin\phi \\
\psi^{k-1}(\phi) &= \frac{-(-1)^{k-1}\sin\phi + (-1)^k\sin 2\phi + (-1)^k\sin\phi}{1+\cos\phi} + (k-1)(-1)^k\sin\phi \\
&= (-1)^k\Big(\frac{2\sin\phi + 2\sin\phi\cos\phi}{1+\cos\phi} + (k-1)\sin\phi\Big) \\
&= (-1)^k(k+1)\sin\phi.
\end{aligned}$$

For the proof of (ii), notice that $\eta_i^k(\phi) = 0 = \psi^k(\phi)$. We therefore use L'Hôpital's rule to determine λ_i^k and differentiate $\eta_i^k(\phi)$ and $\psi^k(\phi)$ with respect to ϕ:

$$\begin{aligned}
(\eta_i^k)'(\phi) &= (-1)^{k-i} i \cos i\phi - (-1)^i (k-i+1)\cos(k-i+1)\phi + (k+1)\cos(k+1)\phi \\
&= (-1)^{k-i} i \cos i\phi + (-1)^{k+i}(k-i+1)\cos i\phi - (k+1)(-1)^k \\
&= (-1)^{k-1}(k+1)\Big(1 + (-1)^{i+1}\cos i\phi\Big).
\end{aligned}$$

Similarly,

$$\begin{aligned}
(\psi^k)'(\phi) &= \frac{\Big(-(-1)^k\cos\phi + k\cos k\phi + (k+1)\cos(k+1)\phi\Big)(1+\cos\phi)}{(1+\cos\phi)^2} \\
&\quad - \frac{\Big(-(-1)^k\sin\phi + \sin k\phi + \sin(k+1)\phi\Big)(-\sin\phi)}{(1+\cos\phi)^2} + k(k+1)\cos(k+1)\phi \\
&= \frac{\Big(-(-1)^k\cos\phi + k(-1)^{k-1}\cos\phi + (k+1)(-1)^{k-1}\Big)}{1+\cos\phi} + k(k+1)(-1)^{k-1} \\
&= \frac{(-1)^{k-1}\Big((k+1)\cos\phi + (k+1)\Big)}{1+\cos\phi} + k(k+1)(-1)^{k-1} \quad = (-1)^{k-1}(k+1)^2.
\end{aligned}$$

To prove (iii), simply observe that by (i) and (ii)

$$\lambda_{k-1}^{k-1} = \frac{\sin\phi + \sin 2\phi + \sin\phi}{(k+1)\sin\phi} = 2\cdot\frac{\sin\phi(1+\cos\phi)}{(k+1)\sin\phi} = 2\lambda_k^k.$$

Before we proceed to the proof of (iv)-(vi), we claim that

$$\lambda_i^{k-1} - \lambda_{i-1}^{k-1} \quad = \quad -2x^* \cdot \mu_i^{k-1} \qquad \text{for } i \geq 2, \tag{39}$$

which is immediately verified as follows:

$$\begin{aligned}
\lambda_i^{k-1} - \lambda_{i-1}^{k-1} &= \frac{-(-1)^i(\sin i\phi + \sin(i+1)\phi) + (-1)^{i-1}(\sin(i-1)\phi + \sin i\phi)}{(k+1)\sin\phi} \\
&= (-1)^{i-1}\frac{2\sin i\phi + \sin(i+1)\phi + \sin(i-1)\phi}{(k+1)\sin\phi} \\
&= (-1)^{i-1}\frac{2\sin i\phi + 2\sin i\phi\cos\phi}{(k+1)\sin\phi} \\
&= \frac{2(-1)^{i-1}\sin i\phi(1+\cos\phi)}{(k+1)\sin\phi} \quad = \quad -2\lambda_k^k\mu_i^{k-1} \quad = \quad -2x^*\mu_i^{k-1},
\end{aligned}$$

which proves (39). On the other hand,

$$\begin{aligned}
\lambda_i^{k-1}+\lambda_{i-1}^{k-1} &= \frac{2\sin\phi-(-1)^i(\sin i\phi+\sin(i+1)\phi)-(-1)^{i-1}(\sin(i-1)\phi+\sin i\phi)}{(k+1)\sin\phi} \\
&= \frac{2\sin\phi+(-1)^{i-1}(\sin(i+1)\phi)-\sin(i-1)\phi)}{(k+1)\sin\phi} \\
&= \frac{2\sin\phi+2(-1)^{i-1}\cos i\phi\sin\phi}{(k+1)\sin\phi} \quad = \quad 2\frac{1+(-1)^{i-1}\cos i\phi}{k+1} \quad = \quad 2\lambda_i^k,
\end{aligned}$$

which proves (iv).

The case $i=k$ of (v) follows from the definition of x^*. For $i<k$ we use (39) and (iv):

$$\begin{aligned}
\ell_i^k(x^*) &= \lambda_i^{k-1}+x^*\cdot\mu_i^{k-1} \quad = \quad \lambda_i^{k-1}-\frac{\lambda_i^{k-1}-\lambda_{i-1}^{k-1}}{2} \\
&= \frac{\lambda_i^{k-1}+\lambda_{i-1}^{k-1}}{2} \quad = \quad \lambda_i^k.
\end{aligned}$$

For the case $i=k$ of (vi) use the fact that (by Lemma 3.6) $\mu_1^{k-1}=-1$ together with (iii) to see

$$\ell_1^k(x^*-x)=\lambda_1^{k-1}+(x^*-x)\mu_1^{k-1}=\lambda_{k-1}^{k-1}-(x^*-x)=2\lambda_k^k-(x^*-x)=x^*+x=\ell_k^k(x^*+x).$$

For $i<k$ we have by Lemma 3.7

$$\begin{aligned}
\ell_{k-i+1}^k(x^*-x) &= \lambda_{k-i+1}^{k-1}+(x^*-x)\cdot\mu_{k-i+1}^{k-1} \quad = \quad \lambda_{i-1}^{k-1}-(x^*-x)\cdot\mu_i^{k-1} \\
&= \lambda_{i-1}^{k-1}+\frac{\lambda_i^{k-1}-\lambda_{i-1}^{k-1}}{2}+x\cdot\mu_i^{k-1} \quad = \quad \lambda_i^{k-1}-\frac{\lambda_i^{k-1}-\lambda_{i-1}^{k-1}}{2}+x\cdot\mu_i^{k-1} \\
&= \lambda_i^{k-1}+x^*\cdot\mu_i^{k-1}+x\cdot\mu_i^{k-1} \quad = \quad \ell_i^k(x^*+x).
\end{aligned}$$

□

We now approach the proof of Proposition 5.3, for which we need two auxiliary lemmas. First recall again that

$$\lambda_j^k(p)=\frac{\eta_j^k(p)}{\psi^k(p)},$$

where

$$\eta_j^k(p)=(-1)^{k-j}\sin j\phi-(-1)^j\sin(k-j+1)\phi+\sin(k+1)\phi.$$

Lemma 6.2

$$\eta_j^k(p)-\eta_{j+1}^k(p)=\begin{cases}4\cdot(-1)^j\cdot\cos\frac{k+1}{2}\phi\cdot\cos\frac{1}{2}\phi\cdot\sin\frac{2k-4j}{4}\phi & , \ \textit{if } k \textit{ is even} \\ 4\cdot(-1)^j\cdot\sin\frac{k+1}{2}\phi\cdot\cos\frac{1}{2}\phi\cdot\cos\frac{2k-4j}{4}\phi & , \ \textit{if } k \textit{ is odd.}\end{cases}$$

Proof. Assume that k is even. Then

$$\begin{aligned}
&\eta_j^k(p) - \eta_{j+1}^k(p) \\
&= (-1)^j \sin j\phi - (-1)^j \sin(k-j+1)\phi - [-(-1)^j \sin(j+1)\phi + (-1)^j \sin(k-j)\phi] \\
&= (-1)^j \cdot 2 \cdot \cos\frac{k+1}{2}\phi \cdot \sin(-\frac{k-2j+1}{2}\phi) - (-1)^j \cdot 2 \cdot \cos\frac{k+1}{2}\phi \cdot \sin\frac{k-2j-1}{2}\phi \\
&= -(-1)^j \cdot 2 \cdot \cos\frac{k+1}{2}\phi \cdot [\sin\frac{k-2j+1}{2}\phi + \sin\frac{k-2j-1}{2}\phi] \\
&= -(-1)^j \cdot 2 \cdot \cos\frac{k+1}{2}\phi \cdot 2 \cdot \sin\frac{2k-4j}{4}\phi \cdot \cos\frac{1}{2}\phi.
\end{aligned}$$

The proof for k odd is almost identical. □

Lemma 6.3 *Let $\phi^k < \phi < \pi$. Then for all integers i, j with $0 \le i < j < \frac{k}{2}$*

$$\begin{array}{lll}
(i) & (-1)^i \sin(\frac{k}{2} - i)\phi & \begin{cases} < 0 & , \textit{ if } k \equiv 0(4) \\ > 0 & , \textit{ if } k \equiv 2(4) \end{cases} \\
(ii) & (-1)^i \cos(\frac{k}{2} - i)\phi & \begin{cases} > 0 & , \textit{ if } k \equiv 1(4) \\ < 0 & , \textit{ if } k \equiv 3(4) \end{cases} \\
(iii) & (-1)^i \cos(\frac{k}{2} - i)\phi - (-1)^j \cos(\frac{k}{2} - j)\phi & \begin{cases} < 0 & , \textit{ if } k \equiv 0(4) \\ > 0 & , \textit{ if } k \equiv 2(4) \end{cases} \\
(iv) & (-1)^i \sin(\frac{k}{2} - i)\phi - (-1)^j \sin(\frac{k}{2} - j)\phi & \begin{cases} < 0 & , \textit{ if } k \equiv 1(4) \\ > 0 & , \textit{ if } k \equiv 3(4) \end{cases} \\
(v) & (-1)^k \cos(k - 2i - 1)\phi - \cos\phi > 0. &
\end{array}$$

Proof. Since $\frac{k-1}{k+1}\pi < \phi < \pi$ we can write

$$\phi = (1 - \frac{2\delta}{k+1})\pi, \quad \text{for some } \delta \in (0,1).$$

Hence, for all $0 \le i < \frac{k}{2}$:

$$(\frac{k}{2} - i)\phi = (\frac{k}{2} - i)\pi - \delta \cdot \underbrace{\frac{k-2i}{k+1}}_{\in (0,1)}\pi.$$

Now use the fact that $(-1)^i \sin x = \sin(x + i\pi)$ and $(-1)^i \cos x = \cos(x + i\pi)$ to see that

$$(-1)^i \sin(\frac{k}{2} - i)\phi = (-1)^i \sin\left((\frac{k}{2} - i)\pi - \delta\frac{k-2i}{k+1}\pi\right) = \sin\left(\frac{k}{2}\pi - \delta\frac{k-2i}{k+1}\pi\right)$$

and analogously $(-1)^i\cos(\frac{k}{2}-i)\phi = \cos(\frac{k}{2}\pi - \delta\frac{k-2i}{k+1}\pi)$. This already suffices to establish (i) and (ii). For (iii) and (iv) apply the same argument again together with the obvious fact that $\delta\frac{k-2i}{k+1} > \delta\frac{k-2j}{k+1}$ since $i<j$.

To prove (v), observe that

$$(-1)^k\cos(k-2i-1)\phi - \cos\phi \quad = \quad -\cos\left(2\delta\frac{k-2i-1}{k+1}\pi\right) + \cos\left(\frac{2\delta}{k+1}\pi\right).$$

But since $2\delta\frac{k-2i-1}{k+1}\pi > \frac{2\delta}{k+1}\pi$ and $2\delta\frac{k-2i-1}{k+1}\pi < 2\pi - \frac{2\delta}{k+1}\pi$, this expression is positive. □

Proof of Proposition 5.3. We will prove that for $q^k < p < q^*$ the functions

$$\mathrm{c}(Q_{k,p}) = H(p)\sum_{i=1}^{k-1}\lambda_i^k(p)\lambda_{i+1}^k(p)$$

$$1 - 2\cdot\mathrm{d}(Q_{k,p}) = \sum_{i=1}^{k}(\lambda_i^k(p))^2 + 2(1-p)\sum_{i=1}^{k-1}\lambda_i^k(p)\lambda_{i+1}^k(p)$$

are strictly decreasing. In the following we will abbreviate $\lambda_i^k(p)$ by λ_i, and set $\lambda_0 = \lambda_{k+1} = 0$ for convenience. It obviously suffices to show that both of the involved sums are strictly decreasing. Denote the sums by A and B respectively. Their derivatives are

$$A' = 2\sum_{i=1}^{k}\lambda_i\lambda_i', \quad B' = \sum_{i=1}^{k-1}(\lambda_i'\lambda_{i+1} + \lambda_i\lambda_{i+1}') = \sum_{i=1}^{k}(\lambda_{i-1}+\lambda_{i+1})\lambda_i'.$$

Notice that $\sum_{i=1}^k \lambda_i' = 0$ since $\sum_{i=1}^k \lambda_i = 1$. Recall that by the original Lagrange conditions as stated in (15) we know that there exists a u such that for all i

$$b(p)\cdot\lambda_{i-1} + a(p)\cdot\lambda_i + b(p)\cdot\lambda_{i+1} = u.$$

Combining these two facts results in

$$\sum_{i=1}^{k} b(p)\cdot(\lambda_{i-1}+\lambda_{i+1})\lambda_i' + a(p)\lambda_i\lambda_i' = 0,$$

which is the same as $b(p)B' + a(p)A'/2 = 0$. Since $b(p)$ is negative and $a(p)$ is positive, B' and A' must have the same sign. We introduce a third sum

$$C := \sum_{i=0}^{k}(\lambda_{i+1}-\lambda_i)^2 \ = 2(A-B).$$

Since

$$C' = 2A' - 2B' = A' \cdot (2 + \frac{a(p)}{b(p)})$$

and $\frac{a(p)}{b(p)} > -2$ for $p < q^*$, C' has the same sign as A' and B'. Our aim is now to show that

$$C' = 2 \sum_{i=1}^{k} (\lambda_{i+1} - \lambda_i)(\lambda'_{i+1} - \lambda'_i)$$

is indeed negative.

Recall that

$$\lambda_j = \lambda_j^k(p) = \frac{\eta_j^k(p)}{\psi^k(p)}, \quad \eta_j^k(p) = (-1)^{k-j} \sin j\phi - (-1)^j \sin(k-j+1)\phi + \sin(k+1)\phi,$$

and note that the definition also allows for $\eta_0^k(p) = \eta_{k+1}^k(p) = 0$. By Lemma 6.2

$$\eta_j^k(p) - \eta_{j+1}^k(p) = \begin{cases} 4 \cdot (-1)^j \cdot \cos \frac{k+1}{2}\phi \cdot \cos \frac{1}{2}\phi \cdot \sin(\frac{k}{2} - j)\phi & , \text{ if } k \text{ is even} \\ 4 \cdot (-1)^j \cdot \sin \frac{k+1}{2}\phi \cdot \cos \frac{1}{2}\phi \cdot \cos(\frac{k}{2} - j)\phi & , \text{ if } k \text{ is odd.} \end{cases}$$

For k even this implies that

$$\frac{\lambda_i - \lambda_{i+1}}{\lambda_0 - \lambda_1} = (-1)^i \frac{\sin(\frac{k}{2} - i)\phi}{\sin \frac{k}{2}\phi}$$

and hence, as $\lambda_0 = 0$, also

$$\lambda_{i+1} = \lambda_i + (-1)^i \frac{\sin(\frac{k}{2} - i)\phi}{\sin \frac{k}{2}\phi} \cdot \lambda_1.$$

For k odd we analogously obtain

$$\lambda_{i+1} = \lambda_i + (-1)^i \frac{\cos(\frac{k}{2} - i)\phi}{\cos \frac{k}{2}\phi} \cdot \lambda_1.$$

Moreover, induction on i gives

$$\lambda_i = (1 + \frac{\sum_{j=1}^{i-1} y_j}{y_0}) \cdot \lambda_1, \qquad \text{where } y_j := \begin{cases} (-1)^j \sin(\frac{k}{2} - j)\phi & , \text{ for } k \text{ even,} \\ (-1)^j \cos(\frac{k}{2} - j)\phi & , \text{ for } k \text{ odd.} \end{cases} \tag{40}$$

Observe that by Lemma 6.3 we know that for a given k all

$$y_i \text{ with } 0 \leq i < \tfrac{k}{2} \text{ have the same sign.} \tag{41}$$

Setting $i := k+1$ in (40), we deduce from $\lambda_{k+1} = 0$ that

$$\sum_{j=1}^{k} y_j = -y_0.$$

Taking $\sum_{i=1}^{k+1} \lambda_i = 1$ and replacing λ_i by (40) gives

$$1 = (k+1)\lambda_1 + \frac{\lambda_1}{y_0} \sum_{j=1}^{k} (k+1-j) y_j = -\frac{\lambda_1}{y_0} \sum_{j=1}^{k} j y_j,$$

and hence

$$\lambda_1 = -\frac{y_0}{\sum_{j=1}^{k} j y_j}. \tag{42}$$

Furthermore

$$\begin{aligned} \lambda_1' &= -\frac{y_0'}{\sum_{j=1}^{k} j y_j} + \frac{y_0 \cdot \sum_{j=1}^{k} j y_j'}{(\sum_{j=1}^{k} j y_j)^2} \\ &= \lambda_1 \cdot \left(\frac{y_0'}{y_0} - \frac{\sum_{j=1}^{k} j y_j'}{\sum_{j=1}^{k} j y_j}\right). \end{aligned} \tag{43}$$

Now determine λ_i' by differentiating (40)

$$\lambda_i' = \left(1 + \frac{\sum_{j=1}^{i-1} y_j}{y_0}\right) \cdot \lambda_1' + \left(\frac{\sum_{j=1}^{i-1} y_j'}{y_0} - \frac{y_0' \sum_{j=1}^{i-1} y_j}{(y_0)^2}\right) \cdot \lambda_1.$$

Hence,

$$\lambda_{i+1}' - \lambda_i' = \frac{\lambda_1'}{y_0} \cdot y_i + \frac{\lambda_1}{y_0} \cdot \left(y_i' - \frac{y_0'}{y_0} \cdot y_i\right).$$

As $\lambda_{i+1} - \lambda_i = \frac{\lambda_1}{y_0} \cdot y_i$, this implies

$$\begin{aligned}
C' = \sum_{i=0}^{k} (\lambda_{i+1} - \lambda_i)(\lambda'_{i+1} - \lambda'_i) \\
&= \sum_{i=0}^{k} \left(\frac{\lambda_1 \cdot \lambda'_1}{(y_0)^2} \cdot y_i^2 + \frac{\lambda_1 \cdot \lambda_1}{(y_0)^2} \cdot (y_i y'_i - \frac{y'_0}{y_0} \cdot y_i^2) \right) \\
&\overset{(43)}{=} \frac{(\lambda_1)^2}{(y_0)^2} \cdot \sum_{i=0}^{k} \left(y_i y'_i - y_i^2 \cdot \frac{\sum_{j=1}^{k} j y'_j}{\sum_{j=1}^{k} j y_j} \right) \\
&= \frac{(\lambda_1)^2}{(y_0)^2 \cdot \sum_{j=1}^{k} j y_j} \cdot \sum_{i=0}^{k} \sum_{j=1}^{k} (y_i y'_i j y_j - y_i^2 j y'_j) \\
&\overset{(42)}{=} -\frac{(\lambda_1)^3}{(y_0)^3} \cdot \sum_{i=0}^{k} \sum_{j=1}^{k} (y_i y'_i j y_j - y_i^2 j y'_j) \\
&= -\frac{(\lambda_1)^3}{(y_0)^3} \cdot \sum_{i=0}^{k} \sum_{j=0}^{k} (y_i y'_i j y_j - y_i^2 j y'_j)
\end{aligned}$$

Since we want to prove that $C' < 0$ and since we know that $\lambda_1 > 0$, our aim is to show that the above double sum has the same sign as y_0. To do this we first simplify this sum by grouping some terms, namely the pairs $i, k-i$ and $j, k-j$.

Observe that for k even

$$y_{k-i} = (-1)^{k-i} \cdot \sin(\frac{k}{2} - (k-i))\phi = (-1)^i \sin(-(\frac{k}{2} - i))\phi = -y_i$$

hence $y'_{k-i} = -y'_i$ and analogously for k odd. Therefore

$$j y_j + (k-j) y_{k-j} = (2j-k) y_j, \qquad j y'_j + (k-j) y'_{k-j} = (2j-k) y'_j.$$

That is, using that for k even $y_{\frac{k}{2}} = y'_{\frac{k}{2}} = 0$,

$$
\begin{aligned}
&\sum_{i=0}^{k}\sum_{j=0}^{k}(y_i y_i' j y_j - y_i^2 j y_j') = 2\sum_{0\le i<\frac{k}{2}}\ \sum_{0\le j<\frac{k}{2}} (y_i y_i'(2j-k)y_j - y_i^2(2j-k)y_j') \\
&= 2\sum_{0\le i<j<\frac{k}{2}} (y_i y_i'(2j-k)y_j - y_i^2(2j-k)y_j' + y_j y_j'(2i-k)y_i - y_j^2(2i-k)y_i') \\
&= 2\sum_{0\le i<j<\frac{k}{2}} [y_i' y_j (y_i(2j-k) - y_j(2i-k)) - y_i y_j'((2j-k)y_i - y_j(2i-k))] \\
&= 2\sum_{0\le i<j<\frac{k}{2}} (y_i' y_j - y_i y_j')\cdot(y_i(2j-k) - y_j(2i-k)).
\end{aligned}
$$

So, we have reduced the problem to the two factors $y_i' y_j - y_i y_j'$ and $y_i(2j-k) - y_j(2i-k)$ for $i < j$. We claim that the factor $y_i(2j-k) - y_j(2i-k)$ has the same sign as y_0. Consider its derivative: for k even

$$
\begin{aligned}
&(y_i(2j-k) - y_j(2i-k))' \\
&= (2j-k)(-1)^i(\frac{k}{2}-i)\cos(\frac{k}{2}-i)\phi - (2i-k)(-1)^j(\frac{k}{2}-j)\cos(\frac{k}{2}-j)\phi \\
&= -2(\frac{k}{2}-j)(\frac{k}{2}-i)\cdot[(-1)^i\cos(\frac{k}{2}-i)\phi - (-1)^j\cos(\frac{k}{2}-j)\phi].
\end{aligned}
$$

Analogously for k odd:

$$
(y_i(2j-k) - y_j(2i-k))' = 2(\frac{k}{2}-j)(\frac{k}{2}-i)\cdot[(-1)^i\sin(\frac{k}{2}-i)\phi - (-1)^j\sin(\frac{k}{2}-j)\phi].
$$

Now apply Lemma 6.3 (iii) and (iv) to see that these expressions are positive if $k \equiv 0, 3(4)$ and negative otherwise. As the value of $y_i(2j-k) - y_j(2i-k)$ is zero at $\phi = \pi$ the value has to be negative for all $\phi \in (\frac{k-1}{k+1}\pi, \pi)$ if $k \equiv 0, 3(4)$ and positive otherwise. By Lemma 6.3 (i) and (ii) we know that y_0 behaves identically.

Now consider $y_i' y_j - y_i y_j'$: we claim that it is positive for all k and all $i < j$. Since this expression is exactly the numerator of the derivative of y_i/y_j, it suffices to show that the latter is positive. Moreover observe that

$$
\begin{aligned}
&\left(\frac{y_i}{y_j}\right)' = \left(\frac{y_i}{y_{i+1}}\frac{y_{i+1}}{y_{i+2}}\cdots\frac{y_{j-1}}{y_j}\right)' \\
&= \left(\frac{y_i}{y_{i+1}}\right)'\frac{y_{i+1}}{y_{i+2}}\cdots\frac{y_{j-1}}{y_j} + \frac{y_i}{y_{i+1}}\left(\frac{y_{i+1}}{y_{i+2}}\right)'\cdots\frac{y_{j-1}}{y_j} + \cdots + \frac{y_i}{y_{i+1}}\frac{y_{i+1}}{y_{i+2}}\cdots\left(\frac{y_{j-1}}{y_j}\right)'.
\end{aligned}
$$

Due to (41), the terms y_i/y_{i+1} are all positive, and it therefore suffices to show that $(y_i/y_{i+1})' > 0$ for all $0 \leq i < \frac{k}{2} - 1$. We claim that

$$y_i' y_{i+1} - y_i y_{i+1}' = -(-1)^k \frac{1}{2} \sin(k-2i-1)\phi + \frac{1}{2}(k-2i-1)\sin\phi, \tag{44}$$

which can be checked as follows. For k even:

$$\begin{aligned} & y_i' y_{i+1} - y_i y_{i+1}' \\ = \; & -(\frac{k}{2}-i)\cos(\frac{k}{2}-i)\phi\sin(\frac{k}{2}-i-1)\phi + (\frac{k}{2}-i-1)\cos(\frac{k}{2}-i-1)\phi\sin(\frac{k}{2}-i)\phi \\ = \; & -(\frac{k}{2}-i)\frac{1}{2}[\sin(k-2i-1)\phi + \sin(-\phi)] + (\frac{k}{2}-i-1)\frac{1}{2}[\sin(k-2i-1)\phi + \sin\phi] \\ = \; & -\frac{1}{2}\sin(k-2i-1)\phi + \frac{1}{2}(k-2i-1)\sin\phi. \end{aligned}$$

For k odd:

$$\begin{aligned} & y_i' y_{i+1} - y_i y_{i+1}' \\ = \; & (\frac{k}{2}-i)\sin(\frac{k}{2}-i)\phi\cos(\frac{k}{2}-i-1)\phi - (\frac{k}{2}-i-1)\sin(\frac{k}{2}-i-1)\phi\cos(\frac{k}{2}-i)\phi \\ = \; & (\frac{k}{2}-i)\frac{1}{2}[\sin\phi + \sin((k-2i-1)\phi)] - (\frac{k}{2}-i-1)\frac{1}{2}[\sin(-\phi) + \sin(k-2i-1)\phi] \\ = \; & \frac{1}{2}\sin(k-2i-1)\phi + \frac{1}{2}(k-2i-1)\sin\phi. \end{aligned}$$

At the point $\phi = \pi$ (44) has value zero. Again we consider the derivative

$$(y_i' y_{i+1} - y_i y_{i+1}')' = -\frac{1}{2}(k-2i-1)[(-1)^k \cos(k-2i-1)\phi - \cos\phi].$$

By Lemma 6.3 (v) this is negative and therefore $y_i' y_{i+1} - y_i y_{i+1}'$ must be positive for $\phi < \pi$. $\square$

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