# Permanent-on-top: a sharp vertex-cover threshold, cycles, long paths, high girth, bases and circulants

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**Abstract**

Soules conjectured in 1966 that the permanent of a positive semidefinite matrix is the largest eigenvalue of its Schur power matrix; Shchesnovich disproved this permanent-on-top conjecture in 2016 at order five. We study which zero patterns and symmetries force the property, calling a graph universal if every positive semidefinite matrix whose nonzero off-diagonal entries lie on its edges is permanent-on-top. Every graph whose edges are covered by two vertices is universal, and two is sharp: a rank-two order-five matrix on the complete graph minus an edge violates the property. Cycles are universal, and a graph is universal exactly when its blocks are. A hard-core positivity criterion for cycle coefficients shows that path bundles with long arms, graphs of maximum degree four and girth at least 197, and all sufficiently long subdivisions of any multigraph are universal. The Gram matrix of the three mutually unbiased bases of $\mathbb{C}^2$ has permanent 15 and top eigenvalue 21, the immanant of a rank-one rectangular block, which for $2n$ random unit vectors in dimension $n$ exceeds the permanent with probability at most $e^{-cn^2}$ for large $n$; Gram matrices of two bases of $\mathbb{C}^3$ with squared overlaps at most $13/20$ are permanent-on-top with gap $1/64$. Singular order-five circulant correlations and rank-two circulants of prime order satisfy the property, and all transitive order-five correlations do if order four does, as Lavi announces. Consequences include the Bapat–Sunder, Chollet and Lieb inequalities on these classes, generalized bunching bounds, and partial answers to three questions of Zhang.

**Keywords.** permanent; Schur power matrix; permanent-on-top conjecture; positive semidefinite matrix; support graph; vertex cover; cactus graph; immanant; random Gram matrix; circulant matrix; boson bunching; path bundle; girth; graph subdivision; mutually unbiased bases.
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## 1 Introduction

### 1.1 The question

For an $n \times n$ complex matrix $B = (b_{ij})$ and a permutation $\sigma \in S_n$ write

$$b_\sigma = \prod_{i=1}^{n} b_{i,\sigma(i)}, \qquad \operatorname{per} B = \sum_{\sigma \in S_n} b_\sigma .$$

The *Schur power matrix* $\Pi(B)$ is the $n! \times n!$ matrix indexed by $S_n$ with entries $\Pi(B)_{\sigma,\tau} = \prod_{i=1}^{n} b_{\sigma(i),\tau(i)}$. It is a principal submatrix of the tensor power $B^{\otimes n}$, so it is positive semidefinite when $B$ is, and each of its row sums equals $\operatorname{per} B$; hence $\operatorname{per} B$ is an eigenvalue of $\Pi(B)$. Soules

conjectured in his 1966 dissertation that it is the largest one [28, p. 3], the permanent-on-top conjecture, and later developed it as an approach to Lieb's permanental dominance conjecture [29]; the history, and the formulation below, are in Zhang's survey [32, Section 3].

**Conjecture 1.1** (Soules)**.** *If $B$ is Hermitian positive semidefinite, then $\lambda_{\max}(\Pi(B)) = \operatorname{per} B$.*

Bapat and Sunder proved Conjecture 1.1 for $n \leq 3$ [2]. Shchesnovich disproved it with a complex matrix of order five and rank two [25], Tran gave a second order-five example that can be checked by hand [30], and Drury's counterexamples to two questions of Bapat and Sunder, of orders seven and eight, and his real counterexample of order sixteen and rank three are also counterexamples to Conjecture 1.1 [6, 7, 8], [32, Section 5]. Zhang asked [32, Section 3, Question 1]:

**Question 1.2** (Zhang)**.** *Can one find a counterexample of size $n = 4$ for the permanent-on-top conjecture?*

The order-five counterexamples of Shchesnovich and Tran and Drury's order-eight matrix have no vanishing entries, and Drury's order-seven matrix has a single vanishing off-diagonal pair [6]. This leaves a natural question about zero patterns, which we describe as a gap in the comparison of these results and not as a question posed in the literature: *which graphs $G$ have the property that every positive semidefinite matrix whose off-diagonal support lies in $G$ satisfies Conjecture 1.1?* For trees the question has a classical answer: da Fonseca [5, Theorem 5.2] proves the $\mu$-permanent analogue of Conjecture 1.1 for matrices whose graph is a tree, suitably labelled, and at $\mu = 1$ this is the tree case of Conjecture 1.1. Pant and Singh prove the Bapat–Sunder inequality for real positive semidefinite matrices with nonpositive off-diagonal entries and bipartite support, and carry Chollet-type inequalities for graph Laplacians through cut vertices, cycles and cactus graphs [18, Theorems 3.1, 5.1, 5.3 and 5.4]. The results below concern Conjecture 1.1 itself, for all complex positive semidefinite matrices with a given support.

**Definition 1.3.** The *support* of a Hermitian matrix $B$ of order $n$ is the graph $\Gamma(B)$ on $[n] = \{1, \ldots, n\}$ with an edge $ij$ whenever $i \neq j$ and $b_{ij} \neq 0$. A matrix is *permanent-on-top* if it satisfies the conclusion of Conjecture 1.1. A finite simple graph $G$ on $[n]$ is *universal* if every Hermitian positive semidefinite matrix $B$ of order $n$ with $\Gamma(B) \subseteq G$ is permanent-on-top.

Every subgraph of a universal graph is universal, and Lemma 2.2 shows that adding or deleting isolated vertices does not change universality. A *vertex cover* of $G$ is a set of vertices meeting every edge, and the vertex-cover number $\tau(G)$ is the least size of one.

## 1.2 Main results

Our first theorem shows that two covering vertices suffice, however many other vertices there are.

**Theorem 1.4** (Two-vertex covers)**.** *Every graph $G$ with $\tau(G) \leq 2$ is universal. Thus every Hermitian positive semidefinite matrix whose off-diagonal nonzero entries all lie in two rows is permanent-on-top. Edge weights and complex phases are arbitrary, and the two covering vertices may be adjacent.*

The bound two cannot be raised.

**Theorem 1.5** (Sharpness at three)**.** *Let*

$$X = \begin{pmatrix} 1 & 0 & 2 & 4 & 2 \\ 0 & 1 & -1+i & 5 & -1-i \end{pmatrix}, \qquad B_5 = X^*X.$$

*Then $B_5$ is positive semidefinite of rank two, its support is the complete graph $K_5$ minus the edge 12, so $\tau(\Gamma(B_5)) = 3$, and $\lambda_{\max}(\Pi(B_5)) \geq 400112/37 > 10464 = \operatorname{per} B_5$. Consequently, for every $k \geq 3$ there is a graph with vertex-cover number $k$ that is not universal, and 2 is the largest integer $t$ such that every graph $G$ with $\tau(G) \leq t$ is universal.*

The next two theorems give universal graphs of unbounded vertex-cover number. A *block* of a graph is an isolated vertex, a bridge, or a maximal 2-connected subgraph. A *cactus* is a graph in which every block with an edge is an edge or a cycle.

**Theorem 1.6** (Block trees)**.** *A graph is universal if and only if each of its blocks is universal.*

**Theorem 1.7** (Cycles)**.** *For every $k \geq 3$ the cycle $C_k$ is universal.*

**Corollary 1.8.** *A graph is universal if each of its blocks is an edge, a cycle, or a graph with vertex-cover number at most two. In particular every cactus graph, every complete bipartite graph $K_{2,m}$ and every book $K_{1,1,m}$ is universal, and every positive semidefinite matrix of order at most four with at least one vanishing off-diagonal entry is permanent-on-top.*

The last assertion answers Question 1.2 in the negative for every matrix of order four with a vanishing off-diagonal entry: such a matrix is never a counterexample. Lavi has announced, in an unrefereed preprint, a computer-assisted proof of the full order-four case [13, Theorem 3.1]; Corollary 1.8 gives a short proof of the case with a zero entry.

Length and girth also force the property. A *path bundle* is a union of internally disjoint paths, its arms, between two hubs. Path bundles whose arms all have length at least five are universal, with any number of arms, and so are two further families of bundles (Theorem 6.1). Graphs of maximum degree at most four and girth at least 197 are universal (Theorem 7.1), as are bipartite graphs of large girth whose two sides have degrees at most $c$ and $d$ with $\sqrt{(c-1)(d-1)} < \sqrt{c-1} + \sqrt{d-1}$ (Theorem 7.2). Replacing every edge of a multigraph with at most $d$ distinct neighbours at each vertex by paths of length at least $16 + \lceil \log_2 d \rceil$ gives a universal graph, and for simple graphs of maximum degree $\Delta$ the length $20 + \lceil \frac{1}{6} \log_2 \Delta + \frac{2}{3} \log_2(1 + \log_2 \Delta) \rceil$ also suffices (Theorems 6.2 and 7.3). As $K_5$ is not universal, universality is closed under subgraphs but not under minors (Corollary 7.4). By Theorem 1.6, any graph whose blocks belong to these families or to those of Corollary 1.8 is universal.

A second obstruction, on six vertices, has a transparent structure and a large ratio.

**Theorem 1.9** (An octahedral counterexample)**.** *Let $A$ be the Gram matrix of the six unit vectors*

$$e_1, \quad e_2, \quad \tfrac{1}{\sqrt{2}}(e_1 \pm e_2), \quad \tfrac{1}{\sqrt{2}}(e_1 \pm i e_2) \qquad \text{in } \mathbb{C}^2,$$

*taken in this order. Then $A$ is a rank-two correlation matrix supported on the octahedron $K_{2,2,2}$, $\operatorname{per} A = 15$, and $\lambda_{\max}(\Pi(A)) = 21$.*

The six vectors represent the three mutually unbiased bases of $\mathbb{C}^2$, the eigenbases of the Pauli matrices; orthogonal pairs are antipodal on the Bloch sphere, which is why the support is the octahedron. The ratio $21/15 = 7/5$ is far larger than the ratios 1.0168 of Shchesnovich's matrix and 512/504 of Tran's (Section 13), and of the same size as the ratio $(525/8)/45 \approx 1.458$ that Zhang reports for Drury's order-seven matrix [32, Section 5]. The octahedron contains neither $K_4$ nor $K_5$ minus an edge, since any four of its vertices contain one of its three non-adjacent pairs. Deleting one edge of the octahedron still leaves a graph that is not universal (Proposition 8.3), with an exact certificate of rank three.

For Gram matrices of rank $r$, the block of $\Pi(B)$ indexed by a rectangular partition $(m^r)$, with $r$ parts equal to $m$, has rank at most one, and its eigenvalue is the immanant $\mathrm{Imm}_{(m^r)}(B)$, a sum of products of squared $r \times r$ determinants (Lemma 9.1). The value 21 in Theorem 1.9 is the immanant of the block $(3,3)$. For $2n$ unit vectors in dimension $n$ the block $(2^n)$ gives a probabilistic form of permanent-on-top.

**Theorem 1.10** (Random Gram matrices)**.** *Let $B = V^*V$, where the $2n$ unit columns of $V$, in $\mathbb{R}^n$ or $\mathbb{C}^n$, either form two orthonormal bases in Haar-random relative position or are independent and uniformly distributed, and let $\Upsilon$ be the largest eigenvalue of the block $(2^n)$ of $\Pi(B)$. Then $\mathbb{P}\{\Upsilon > \operatorname{per} B\} \le e^{-cn^2}$ for all large $n$, with a constant $c > 0$; for small fixed $a > 0$ the probability of $\Upsilon \ge e^{-an} \operatorname{per} B$ lies between $e^{-C_a n^2}$ and $e^{-c_a n^2}$. Theorem 9.2 gives the exact expectations of $\Upsilon$, the admissible range of $a$ and the almost sure exponential rates.*

At the order six of Theorem 1.9, Gram matrices of two orthonormal bases of $\mathbb{C}^3$ behave differently from three bases of $\mathbb{C}^2$: if $U \in U(3)$ has all squared moduli at most $13/20$, as for two mutually unbiased bases, then $B(U) = \begin{pmatrix} I & U \\ U^* & I \end{pmatrix}$ is permanent-on-top with every nonconstant eigenvalue at most $\operatorname{per} B(U) - 1/64$, and the conclusion persists for contractions within $1/50000$ of $U$ (Theorem 10.1); the block of the partition $(3,3)$ obeys the bound for every $U \in U(3)$ (Proposition 10.2).

Symmetry gives a second route at order five, the smallest order of the known counterexamples [25, 30]. A correlation matrix of order five is *transitive* if its monomial unitary symmetries permute the indices transitively; up to diagonal phases and relabeling these are the circulant correlation matrices (Lemma 11.2).

**Theorem 1.11** (Circulants of order five)**.** *Every singular circulant correlation matrix $T$ of order five is permanent-on-top, and every eigenvalue of $\Pi(T)$ on the orthogonal complement of the constants is at most $\operatorname{per} T - 1/8$ (Proposition 11.3, an exact computer-assisted certificate). If every positive semidefinite matrix of order four is permanent-on-top, as Lavi announces [13, Theorem 3.1], then every transitive correlation matrix $A \ne I$ of order five is permanent-on-top with a nonconstant gap of at least $(1 - \lambda_{\min}(A))^2/32$ (Theorem 11.4).*

For circulants of rank at most two the Schur power is diagonalized exactly in every order (Theorem 11.6); consequently every circulant, and every transitive, correlation matrix of prime order and rank at most two is permanent-on-top, and so is every circulant correlation matrix of order six and rank at most two (Corollary 11.7 and Proposition 11.8).

Universality has consequences for three classical permanental inequalities.

**Corollary 1.12.** *Let $A$ be Hermitian positive semidefinite with $\Gamma(A)$ contained in a universal graph, for instance a graph as in Corollary 1.8. Then:*

*(a)* $\operatorname{per}(A \circ C) \le \operatorname{per}(A) \prod_i c_{ii} \le \operatorname{per}(A) \operatorname{per}(C)$ *for every positive semidefinite $C$ of the same order, where $\circ$ is the entrywise product (the inequalities of Bapat–Sunder and Chollet);*

*(b)* $\mathrm{Imm}_\lambda(A) \le f^\lambda \operatorname{per} A$ *for every partition $\lambda$ of $n$, where $\mathrm{Imm}_\lambda(A) = \sum_\sigma \chi_\lambda(\sigma) a_\sigma$ and $f^\lambda = \chi_\lambda(1)$ (Lieb's permanental dominance for immanants).*

Bapat and Sunder asked for (a) for all positive semidefinite $A$ and $C$ [1], [2, Conjecture 2], and Drury showed that it fails at order seven [6], [32, Section 5]; Chollet's inequality $\operatorname{per}(A \circ C) \le \operatorname{per} A \operatorname{per} C$ is a question of Chollet [4]; and (b) is Lieb's permanental dominance conjecture for immanants [14]. The proof of Corollary 1.12 in Section 12 uses only that $A$ is permanent-on-top, so (a) and (b) also hold for every singular circulant correlation matrix of order five, for the matrices

of Theorem 10.1, Corollary 11.7 and Proposition 11.8, and, under the hypothesis of Theorem 11.4, for every transitive one. All three inequalities follow from Conjecture 1.1 by classical implications, recorded in [32, Sections 2, 3 and 5] with reference to [17, Conjecture 10], and the proof in Section 12 is the standard one; the content of Corollary 1.12 is the class of supports. Inequality (b) holds for every positive semidefinite matrix of order at most 13 by Pate's work [19, 20], [32, Section 4], and Corollary 1.12(b) extends it to every order on universal supports. Zhang also asked whether (a) has a counterexample of order less than seven, for instance of order four [32, Section 5, Question 4]. By Corollaries 1.8 and 1.12, inequality (a) holds for every pair $(A, C)$ in which $A$ has order four and a vanishing off-diagonal entry, and at orders five and six whenever $\Gamma(A)$ lies in a graph of Corollary 1.8; at order five it also holds when $A$ is a singular circulant correlation matrix, and, under the hypothesis of Theorem 11.4, when $A$ is transitive; at order six it holds when $A$ is a matrix $B(X)$ of Theorem 10.1 or a circulant correlation matrix of rank at most two (Proposition 11.8). Zhang's Question 6 [32, Section 5] asks to characterize the correlation matrices $A$ with the Hadamard-compression property $\operatorname{per}(A \circ X) \le \operatorname{per} A$ for every correlation matrix $X$. Corollary 1.12(a) with $c_{ii} = 1$ gives a sufficient condition: every correlation matrix supported in a universal graph has the property, including the graphs of Sections 6 and 7, as does every singular circulant correlation matrix of order five, every correlation matrix $B(X)$ of Theorem 10.1, every circulant correlation matrix of rank at most two and prime order or order six, and, under the hypothesis of Theorem 11.4, every transitive correlation matrix of order five. Through Shchesnovich's equivalence between Conjecture 1.1 and generalized bunching [26], the same classes give bunching bounds for photons in arbitrary joint internal states (Proposition 12.2), and Theorem 1.5 gives a further explicit five-photon violation, on a support with a missing edge; Shchesnovich's order-five matrix already gives one through the same equivalence.

### 1.3 Relation to earlier work and route of the proofs

All arguments use the Fourier form of the problem (Section 2): $\Pi(B)$ is the matrix of $T_B = \sum_\sigma b_\sigma U_\sigma$ in the regular representation, so $B$ is permanent-on-top exactly when the *deficit* $\sum_\sigma b_\sigma (I - U_\sigma)$ is positive semidefinite in every unitary representation $U$ of $S_n$. Since $U_\sigma$ is unitary, $(I - U_\sigma) + (I - U_{\sigma^{-1}}) \succeq 0$; hence the deficit is positive semidefinite whenever every coefficient $b_\sigma$ is nonnegative, and the difficulty lies in the phases of the coefficients of permutations with cycles of length at least three. When the support is a forest these do not occur (Lemma 2.2(v); compare [5, Theorem 5.2] at $\mu = 1$).

For Theorem 1.4 we call the two covering vertices hubs. The two double transpositions and the two four-cycles on a pair of leaves combine into a single operator $(\alpha I + \beta S)^* M (\alpha I + \beta S)$, where $S$ is the hub swap and $M$ a double transposition (Lemma 3.2). This bounds their joint excess by one multiple of the hub-swap deficit and retains the phase cancellation between different leaf pairs. The single transpositions and the two triangles through each leaf are bounded on the subgroup $S_3$ of that leaf and the two hubs, with an exact signed constant (Lemma 3.3). A Schur-complement estimate on the $2 \times 2$ hub block (Lemma 3.4) shows that the resulting coefficient of the hub-swap deficit is nonnegative.

Theorem 1.6 rests on two identities. Positivity lets one split a matrix along a cut vertex into positive semidefinite pieces, one per block, and the Schur power operator of the sum expands as a sum over assignments of vertices to blocks of commuting products of local operators. Pant and Singh prove a block closure of this kind for Chollet-type inequalities of graph Laplacians [18, Theorem 5.1]; Theorem 1.6 is an exact closure for the spectral property and all positive semidefinite matrices. Theorem 1.7 reduces a cycle of length $k \ge 5$ to a positive semidefinite cycle of length $\lceil k/2 \rceil$ on every second vertex, whose matching deficits are paid by disjoint families of original

matchings through a two-edge exchange inequality (Lemma 2.3).

For the obstructions we use the permutation representations on $k$-subsets, whose matrices are the permanental compounds $C_k$ of Pate [21] and Tran [30, Proposition 2.2]. Lemma 9.1 uses Schur–Weyl duality and a tight frame of antisymmetric tensors, and Theorem 9.2 combines it with moments of minors of Haar and Gaussian matrices, a Jensen lower bound for the permanent and a net argument for the lower tails. Section 11 combines an exact certificate on the singular boundary of the circulant class with the diagonal expansion (11a) and the theorem of Caputo, Liggett and Richthammer on the interchange process [3]. For long cycles, Lemmas 2.5–2.8 write $T_B^U$ as a combination of cycle packets and matchings whose coefficients are values of an independence polynomial of cycles at negative activities; their positivity follows from a site form of the criteria of Gruber–Kunz and Fernández–Procacci type [23, 11]. The required decay comes from Perron bounds on induced paths, Schur-complement loads at the hubs with a priority rule for the omitted edges (path bundles), and a nonbacktracking walk bound combined with a tree test for the matrix of moduli (high girth); the modulus bound is attained in the limit by the signings of Marcus, Spielman and Srivastava [15]. For two bases of $\mathbb{C}^3$ the blocks are identified through Schur–Weyl partial traces (Lemma 10.4), and the blocks $(3,3)$, $(4,2)$ and $(4,1,1)$ are certified by exact Bernstein expansions in the squared moduli and Jarlskog's invariant [12].

## 2 Preliminaries

Throughout, a *unitary representation* $U$ of a finite group is a homomorphism into the unitary group of a finite-dimensional Hilbert space. For a Hermitian matrix $B$ of order $n$ and a unitary representation $U$ of $S_n$ put

$$T_B^U = \sum_{\sigma \in S_n} b_\sigma U_\sigma, \qquad \Delta_B^U = (\operatorname{per} B) I - T_B^U = \sum_{\sigma \in S_n} b_\sigma \, (I - U_\sigma).$$

We write $X \preceq Y$ when $Y - X$ is positive semidefinite.

**Lemma 2.1** (Fourier form)**.** *Let $B$ be Hermitian of order $n$.*

*(i)* $b_{\sigma^{-1}} = \overline{b_\sigma}$*, so every $T_B^U$ is Hermitian.*

*(ii) For the left regular representation $L$, $\Pi(B)$ is the transpose of the matrix of $T_B^L$. Hence $\lambda_{\max}(\Pi(B)) = \max_U \lambda_{\max}(T_B^U)$, the maximum over the irreducible representations of $S_n$.*

*(iii) $B$ is permanent-on-top if and only if $\Delta_B^U \succeq 0$ for every unitary representation $U$ of $S_n$.*

*(iv) If $B \succeq 0$, then $T_B^U \succeq 0$ for every unitary representation $U$.*

*Proof.* (i) $b_{\sigma^{-1}} = \prod_i b_{\sigma(i),i} = \prod_i \overline{b_{i,\sigma(i)}}$. Hence $(T_B^U)^* = \sum_\sigma \overline{b_\sigma} U_{\sigma^{-1}} = T_B^U$. (ii) With $L_\sigma e_\tau = e_{\sigma\tau}$, the $(\pi,\tau)$ entry of $T_B^L$ is $b_{\pi\tau^{-1}}$. Substituting $j = \sigma(i)$ gives $\Pi(B)_{\sigma,\tau} = \prod_j b_{j,\tau\sigma^{-1}(j)} = b_{\tau\sigma^{-1}}$, the $(\tau,\sigma)$ entry. Every unitary representation is an orthogonal direct sum of irreducible ones, and each irreducible representation occurs in $L$. (iii) The trivial representation gives the eigenvalue $\operatorname{per} B$, so (iii) restates (ii). (iv) $\Pi(B)$ is a principal submatrix of $B^{\otimes n} \succeq 0$, so $T_B^L \succeq 0$, and every irreducible block of $T_B^L$ is positive semidefinite. □

An operator inequality among elements of the group algebra of $\mathrm{Sym}(\Omega)$, $\Omega \subseteq [n]$, that holds in every unitary representation of $\mathrm{Sym}(\Omega)$ also holds in the restriction to $\mathrm{Sym}(\Omega)$ of every unitary representation of $S_n$. We use this to prove local inequalities on small subgroups.

**Lemma 2.2** (Reductions)**.** *Let $B \succeq 0$ have order $n$.*

*(i) Let $D$ be a positive diagonal matrix and $Q$ a diagonal unitary matrix. Then*

$$\Pi(DBD) = (\det D)^2\,\Pi(B), \qquad \operatorname{per}(DBD) = (\det D)^2 \operatorname{per} B, \qquad (QBQ^*)_\sigma = b_\sigma \quad (\sigma \in S_n).$$

*(ii) If $b_{ii} = 0$ for some $i$, then all $b_\sigma$ vanish, and $B$ is permanent-on-top.*

*(iii) If $B' = B \oplus I_r$, then $B'$ is permanent-on-top if and only if $B$ is.*

*(iv) The set of permanent-on-top positive semidefinite matrices of order $n$ is closed.*

*(v) If every coefficient $b_\sigma$ is nonnegative, in particular if $\Gamma(B)$ is a forest, then $B$ is permanent-on-top.*

*Proof.* (i) The entries of $\Pi(DBD)$ carry the factor $\prod_i d_{\sigma(i)}d_{\tau(i)} = (\det D)^2$, and the same factor multiplies every $b_\sigma$. For $Q = \operatorname{diag}(q_i)$ with $|q_i| = 1$, $(QBQ^*)_\sigma = \prod_i q_i\overline{q_{\sigma(i)}}\,b_\sigma = \bigl|\prod_i q_i\bigr|^2 b_\sigma = b_\sigma$. (ii) A positive semidefinite matrix with a zero diagonal entry has a zero row, and every $b_\sigma$ contains an entry of that row. (iii) $b'_\sigma = 0$ unless $\sigma$ fixes the last $r$ points, so $T^U_{B'} = T^{U|S_n}_B$ for every unitary representation $U$ of $S_{n+r}$, and every irreducible representation of $S_n$ occurs in the restriction of the regular representation of $S_{n+r}$. (iv) Eigenvalues and permanents are continuous. (v) If every $b_\sigma \geq 0$, then $b_{\sigma^{-1}} = \overline{b_\sigma} = b_\sigma$, and $\Delta^U_B = \frac{1}{2}\sum_\sigma b_\sigma\bigl((I - U_\sigma) + (I - U_{\sigma^{-1}})\bigr) \succeq 0$ because $U_\sigma$ is unitary. If $\Gamma(B)$ is a forest, a permutation with $b_\sigma \neq 0$ has all its cycles on edges of the forest, so it is a product of disjoint transpositions and $b_\sigma = \prod |b_e|^2 \geq 0$. The forest case is the case $\mu = 1$ of [5, Theorem 5.2]. □

By (i) and (ii) we may assume, when proving that a matrix is permanent-on-top, that it is a *correlation matrix*, that is, positive semidefinite with unit diagonal. By (iii) universality of a graph is unchanged by adding or removing isolated vertices, so a graph on fewer vertices may be regarded as a graph on $[n]$.

The next inequality is the basic local tool. For distinct $a, r, b$ we write $U_{(a\,r)}$ for the operator of the transposition $(a\,r)$.

**Lemma 2.3** (Two-edge exchange)**.** *Let $a, r, b \in [n]$ be distinct and $p, q \geq 0$ with $p + q > 0$. In every unitary representation of $S_n$,*

$$p\,(I - U_{(a\,r)}) + q\,(I - U_{(r\,b)}) \succeq \frac{pq}{p+q}\,(I - U_{(a\,b)}).$$

*Consequently, if $p + q \leq 1$, then $P = pU_{(a\,r)} + qU_{(r\,b)}$ satisfies $\|P - pq\,U_{(a\,b)}\| \leq p + q - pq$.*

*Proof.* It suffices to check the inequality in the irreducible representations of $\mathrm{Sym}\{a, r, b\} \cong S_3$. In the trivial representation both sides vanish. In the sign representation every transposition acts by $-1$, and the inequality reads $2(p + q) \geq 2pq/(p + q)$. The remaining irreducible representation is contained in the permutation representation on $\mathbb{C}^{\{a,r,b\}}$, where $\langle y, (I - U_{(a\,r)})y\rangle = |y_a - y_r|^2$. There the inequality is $p|y_a - y_r|^2 + q|y_r - y_b|^2 \geq \frac{pq}{p+q}|y_a - y_b|^2$, which follows from the triangle inequality and the Cauchy–Schwarz bound $(s + t)^2 \leq (p^{-1} + q^{-1})(ps^2 + qt^2)$ (if $p$ or $q$ vanishes the right side is zero).

For the second assertion put $d = p + q$ and $u = pq \leq pq/(p + q)$. Since $I - U_{(a\,b)} \succeq 0$, the first part gives $dI - P \succeq u(I - U_{(a\,b)})$, that is $P - uU_{(a\,b)} \preceq (d - u)I$. The first part also holds in the representation $\sigma \mapsto \operatorname{sgn}(\sigma)U_\sigma$, which replaces each transposition operator by its negative; this gives $dI + P \succeq u(I + U_{(a\,b)})$, that is $P - uU_{(a\,b)} \succeq -(d - u)I$. As $P - uU_{(a\,b)}$ is Hermitian, its norm is at most $d - u$. □

Finally we record the permutation representations used for the obstructions. For $0 \le k \le n$ let $N_k$ be the representation of $S_n$ on the space with basis $e_J$, $J \subseteq [n]$, $|J| = k$, given by $\sigma e_J = e_{\sigma(J)}$. For a matrix $B$ of order $n$ let $C_k(B)$ be the matrix indexed by $k$-subsets with entries

$$C_k(B)_{I,J} = \operatorname{per} B[I,J] \operatorname{per} B[I^c, J^c],$$

where $B[I,J]$ is the submatrix with rows $I$ and columns $J$ and per of an empty matrix is 1.

**Lemma 2.4** (Permanental compounds)**.** *For every matrix $B$ of order $n$, the matrix of $T_B^{N_k}$ is $C_k(B)^{\mathsf{T}}$. If $B$ is Hermitian, $C_k(B)$ is Hermitian and every eigenvalue of $C_k(B)$ is an eigenvalue of $\Pi(B)$. In particular $x^* C_k(B) x \le \lambda_{\max}(\Pi(B))\, x^* x$ for every vector $x$.*

*Proof.* The $(I,J)$ entry of $T_B^{N_k}$ is $\sum_{\sigma(J)=I} b_\sigma$. A permutation with $\sigma(J) = I$ is a pair of bijections $J \to I$ and $J^c \to I^c$, and $b_\sigma$ factors accordingly, so the entry equals $\operatorname{per} B[J,I] \operatorname{per} B[J^c, I^c] = C_k(B)_{J,I}$. For Hermitian $B$, $\operatorname{per} B[J,I] = \overline{\operatorname{per} B[I,J]}$, so $C_k(B)$ is Hermitian, and its spectrum is that of $T_B^{N_k}$, which by Lemma 2.1 is contained in that of $\Pi(B)$. □

This is Tran's Proposition 2.2 [30] in our convention; for $k = 1$ the matrix $C_1(B)$ is the matrix $(b_{ij} \operatorname{per} B(i|j))$ of the question of Bapat and Sunder [2] that Drury's order-eight example answers [8].

## 2.1 Cycle packets and allocation

For supports with long cycles we distribute the identity and matching coefficients of $T_B^U$ among the cycles. Let $B$ be a correlation matrix with support $\Gamma = \Gamma(B)$, and write $w_e = |b_{ij}| \le 1$ for an edge $e = ij$. If $b_\sigma \ne 0$, every cycle of $\sigma$ of length two is an edge of $\Gamma$ and every longer cycle runs around a simple cycle of $\Gamma$; so $\sigma$ is determined by a family $\mathcal{A}$ of vertex-disjoint simple cycles, an orientation of each, and a matching $N$ of $\Gamma$ avoiding $V(\mathcal{A}) = \bigcup_{C \in \mathcal{A}} V(C)$, and $b_\sigma = W_N \prod_{C \in \mathcal{A}} z_C^{\pm}$, where $W_N = \prod_{e \in N} w_e^2$, $z_C$ is the coefficient of a fixed orientation $V_C$ of $C$, $z_C^+ = z_C$, and the reverse orientation has coefficient $z_C^- = \overline{z_C}$. Put $r_C = |z_C| = \prod_{e \in E(C)} w_e$, fix on each cycle $C$ an *omitted edge* $a_C$, and for a unitary representation $U$ write $S_e = U_{(i\,j)}$ for $e = ij$ and $V_C$ also for the operator of the oriented cycle.

**Lemma 2.5** (Cycle packets)**.** *Let $C$ be a simple cycle of length $k \ge 3$, and let $S_1, \dots, S_{k-1}$ be the operators of the edges of $C$ other than $a_C$, in their order along the path $C - a_C$, so that $V_C$ or $V_C^{-1}$ equals $S_1 \cdots S_{k-1}$. For a unit vector $y$ put $E_i = \langle y, (I - S_i) y \rangle \ge 0$. Then $|1 - \langle y, V_C y \rangle| \le (k-1) \sum_i E_i$. More generally, let $d_e \ge 0$, $e \in E(C) \setminus \{a_C\}$, be constants with $|1 - \langle y, V_C y \rangle| \le \sum_e d_e \langle y, (I - S_e) y \rangle$ for every unit vector $y$ in every unitary representation; the choice $d_e = k - 1$ is admissible. Then the packet*

$$\Theta_C = 2 r_C I + 2 r_C \sum_{e \in E(C) \setminus \{a_C\}} d_e S_e + z_C V_C + \overline{z_C} V_C^*$$

*satisfies $\|\Theta_C\| \le s_C$, where $s_C = 2 r_C + 2 r_C \sum_e d_e + 2 \operatorname{Re} z_C$ is its value in the trivial representation.*

*Proof.* Expanding $\prod_i (I + X_i)$ with $X_i = S_i - I$ and collecting terms by their first and last nonidentity factors gives the ordered defect identity

$$S_1 \cdots S_{k-1} - I - \sum_i (S_i - I) = \sum_{i<j} (S_i - I) S_{i+1} \cdots S_{j-1} (S_j - I).$$

The $S_i$ are unitary involutions, so $\|(I-S_i)y\|^2 = 2E_i$, and taking the inner product with $y$ gives $|1-\langle y, S_1\cdots S_{k-1}y\rangle| \le \sum_i E_i + 2\sum_{i<j}\sqrt{E_iE_j} = (\sum_i\sqrt{E_i})^2 \le (k-1)\sum_i E_i$; the same holds for the inverse product, the adjoint. For the packet,

$$\langle y, (s_C I - \Theta_C)y\rangle = 2r_C\sum_e d_e\langle y,(I-S_e)y\rangle + 2\,\mathrm{Re}\,(z_C(1-\langle y, V_C y\rangle)) \ge 0,$$

since $|z_C| = r_C$. Also $s_C I + \Theta_C = 4r_C I + 2r_C\sum_e d_e(I+S_e) + z_C(I+V_C) + \overline{z_C}(I+V_C^*)$, whose form is at least $4r_C - 4r_C = 0$. So $-s_C I \preceq \Theta_C \preceq s_C I$. □

**Definition 2.6.** Let $\mathcal{A}$ be a family of vertex-disjoint simple cycles and $N$ a matching avoiding $V(\mathcal{A})$. A simple cycle $C$ is *eligible* for $(\mathcal{A}, N)$ if it is vertex-disjoint from $\mathcal{A}$ and either no edge of $N$ has an endpoint on $C$, in which case its *charge* is $f_C(N) = 2r_C$, or exactly one edge $e$ of $N$ has an endpoint on $C$ and $e \in E(C)\setminus\{a_C\}$, in which case $f_C(N) = 2r_C d_e/w_e^2$. With $\mathcal{K}(\mathcal{A}, N)$ the set of eligible cycles, the *allocation coefficient* is

$$\gamma_{\mathcal{A}}(N) = \sum_{\mathcal{G}}(-1)^{|\mathcal{G}|}\prod_{C\in\mathcal{G}} f_C(N),$$

the sum running over the families $\mathcal{G} \subseteq \mathcal{K}(\mathcal{A}, N)$ of vertex-disjoint cycles, including $\mathcal{G} = \varnothing$.

**Lemma 2.7** (Allocation identity)**.** *In every unitary representation of $S_n$,*

$$T_B^U = \sum_{(\mathcal{A},N)} W_N\,\gamma_{\mathcal{A}}(N)\,U_N\prod_{C\in\mathcal{A}}\Theta_C,$$

*where $U_N = \prod_{e\in N} S_e$. Consequently, if every $\gamma_{\mathcal{A}}(N)$ is nonnegative, then $B$ is permanent-on-top, and if moreover $\gamma_{\varnothing}(\{e\}) > 0$ for every edge $e$ and $\Gamma$ is connected, then* $\operatorname{per} B$ *is a simple eigenvalue of $\Pi(B)$.*

*Proof.* The factors $U_N$ and $\Theta_C$, $C \in \mathcal{A}$, act on disjoint sets of vertices and commute. Expanding the packets, each term of the right side chooses for every $C \in \mathcal{A}$ the identity (weight $2r_C$), a swap $S_e$ with $e \in E(C)\setminus\{a_C\}$ (weight $2r_C d_e$), or one of the two orientations (weights $z_C, \overline{z_C}$). The resulting permutation consists of the oriented cycles of a subfamily $\mathcal{A}_0 \subseteq \mathcal{A}$ and the matching $N_0 = N \cup \{\text{chosen swap edges}\}$.

Fix a target permutation $\sigma$ with nonzero coefficient, given by an oriented family $\mathcal{A}_0$ and a matching $N_0$. The terms producing $\sigma$ correspond to the families $\mathcal{E}$ of vertex-disjoint cycles that avoid $V(\mathcal{A}_0)$, with $\mathcal{A} = \mathcal{A}_0 \cup \mathcal{E}$, where each $C \in \mathcal{E}$ contributes either the identity or a swap of an edge $e \in N_0 \cap (E(C)\setminus\{a_C\})$, and $N = N_0 \setminus \{\text{swap edges}\}$. Since $N$ must avoid $V(\mathcal{A})$, a cycle $C \in \mathcal{E}$ contributing the identity meets no edge of $N_0$, and one contributing the swap of $e$ meets no edge of $N_0$ other than $e$. So $\mathcal{E}$ ranges exactly over the vertex-disjoint families in $\mathcal{K}(\mathcal{A}_0, N_0)$, each with its determined contribution, and dividing by $b_\sigma = W_{N_0}\prod_{C\in\mathcal{A}_0} z_C^{\pm}$ (using $W_{N_0}/W_N = \prod w_e^2$ over the swap edges) the coefficient of $\sigma$ on the right is

$$\sum_{\mathcal{E}}\Big(\prod_{C\in\mathcal{E}} f_C(N_0)\Big)\gamma_{\mathcal{A}_0\cup\mathcal{E}}(N).$$

A cycle disjoint from $\mathcal{A}_0 \cup \mathcal{E}$ meets the same edges of $N$ as of $N_0$, because the removed swap edges lie on cycles of $\mathcal{E}$; hence $\mathcal{K}(\mathcal{A}_0\cup\mathcal{E}, N)$ is the set of cycles of $\mathcal{K}(\mathcal{A}_0, N_0)$ disjoint from $\mathcal{E}$, with unchanged charges. Expanding $\gamma$, the sum becomes $\sum_{\mathcal{L}}\prod_{C\in\mathcal{L}} f_C(N_0)\sum_{\mathcal{E}\subseteq\mathcal{L}}(-1)^{|\mathcal{L}\setminus\mathcal{E}|}$ over vertex-disjoint families $\mathcal{L} \subseteq \mathcal{K}(\mathcal{A}_0, N_0)$, and the inner sum is 1 for $\mathcal{L} = \varnothing$ and 0 otherwise. So the coefficient is one, which proves the identity; permutations with $b_\sigma = 0$ are not produced.

If all $\gamma_{\mathcal{A}}(N) \geq 0$, then for a unit vector $y$, by Lemma 2.5 and the commutation of the factors, $\operatorname{Re}\langle y, U_N \prod_C \Theta_C y\rangle \leq \prod_C s_C$, and the same identity in the trivial representation gives $\langle y, T_B^U y\rangle \leq \sum W_N \gamma_{\mathcal{A}}(N) \prod_C s_C = \operatorname{per} B$. Every term $W_N \gamma_{\mathcal{A}}(N)(\prod_C s_C - \operatorname{Re}\langle y, U_N \prod_C \Theta_C y\rangle)$ of $\langle y, \Delta_B^U y\rangle$ is then nonnegative, and those with $\mathcal{A} = \varnothing$, $N = \{e\}$ give $\Delta_B^U \succeq \sum_e w_e^2 \gamma_\varnothing(\{e\})(I - S_e)$; the simplicity follows as in the proof of Proposition 3.6. □

The coefficients $\gamma_{\mathcal{A}}(N)$ are values at negative activities of the independence polynomial of a hard-core gas of cycles. The following site form of the positivity criteria of Gruber–Kunz and Fernández–Procacci type [23, 11] suffices.

**Lemma 2.8** (Site criterion)**.** *Let $\mathcal{K}$ be a family of simple cycles with charges $f_C \geq 0$, and for $S \subseteq V(\Gamma)$ let $Z(S) = \sum_{\mathcal{G}} (-1)^{|\mathcal{G}|} \prod_{C \in \mathcal{G}} f_C$ over vertex-disjoint families $\mathcal{G}$ of cycles of $\mathcal{K}$ contained in $S$. If there is $\beta > 0$ with $\sum_{C \in \mathcal{K},\, C \ni v} f_C e^{\beta(|C|-1)} \leq 1 - e^{-\beta}$ for every vertex $v$, then $Z(S)/Z(S \setminus \{v\}) \geq e^{-\beta}$ for all $v \in S$; in particular $Z(V(\Gamma)) > 0$.*

*Proof.* We induct on $|S|$, with $Z(\varnothing) = 1$. At most one chosen cycle contains $v$, so $Z(S) = Z(S \setminus \{v\}) - \sum_{C \subseteq S,\, C \ni v} f_C Z(S \setminus V(C))$. Deleting the other $|C| - 1$ vertices of $C$ one at a time from $S \setminus \{v\}$, the induction hypothesis gives $Z(S \setminus V(C)) \leq e^{\beta(|C|-1)} Z(S \setminus \{v\})$ and $Z(S \setminus \{v\}) > 0$. Hence $Z(S) \geq Z(S \setminus \{v\})(1 - \sum_{C \ni v} f_C e^{\beta(|C|-1)}) \geq e^{-\beta} Z(S \setminus \{v\})$. □

Applied to $\mathcal{K}(\mathcal{A}, N)$ with $S = V(\Gamma)$, Lemma 2.8 gives $\gamma_{\mathcal{A}}(N) > 0$ whenever the criterion holds with upper bounds $F_C \geq f_C(N)$, which may depend on $N$. If every cycle has its *weakest* edge as $a_C$ and $d_e = k - 1$, the charge of an eligible cycle of length $k$ is bounded by removing two edges from its product:

$$f_C(N) \leq 2(k-1) \prod_{b \in E(C) \setminus \{e, a_C\}} w_b \tag{2a}$$

for any edge $e \neq a_C$ of $C$ in the identity case (as $w \leq 1$) and for the swap edge $e$ in the swap case, because $r_C / w_e^2 = (w_{a_C}/w_e) \prod_{b \neq e, a_C} w_b$ and $w_{a_C} \leq w_e$.

## 3 Two-vertex covers

In this section $B$ is a correlation matrix of order $n \geq 2$ whose support has a vertex cover $\{a, b\}$. We call $a, b$ the *hubs* and the other vertices, numbered $1, \dots, m$, the *leaves*; no two leaves are adjacent. By Lemma 2.2(i) we may conjugate by a diagonal unitary matrix so that $h := b_{ab} \in [0, 1]$. If $h = 1$, the matrices $(1-t)B + tI$, $0 < t < 1$, are correlation matrices with the same support and hub entry less than one, so by Lemma 2.2(iv) we may assume $0 \leq h < 1$. Put

$$G_h = \begin{pmatrix} 1 & h \\ h & 1 \end{pmatrix}, \qquad \ell = 1 - h^2, \qquad \xi_i = \begin{pmatrix} b_{ai} \\ b_{bi} \end{pmatrix}, \qquad v_i = b_{ai}\, \overline{b_{bi}}, \qquad u_i = |v_i|, \qquad V = \sum_{i=1}^{m} v_i,$$

and $p_i = |b_{ai}|^2$, $q_i = |b_{bi}|^2$, so that $u_i^2 = p_i q_i$. Let $X$ be the $2 \times m$ matrix with columns $\xi_i$. Since the leaf block of $B$ is the identity, the Schur complement shows that $B \succeq 0$ is equivalent to $XX^* \preceq G_h$.

**Lemma 3.1** (Supported permutations)**.** *If $b_\sigma \neq 0$ and $\sigma \neq 1$, then $\sigma$ is one of: a transposition $(a\,i)$, $(b\,i)$ or $(a\,b)$; a product $(a\,i)(b\,j)$ with $i \neq j$; a three-cycle through $a$, $b$ and one leaf; or a four-cycle through $a$, $i$, $b$, $j$ in this cyclic order, $i \neq j$. The coefficients are*

$$b_{(a\,i)} = p_i, \quad b_{(b\,i)} = q_i, \quad b_{(a\,b)} = h^2, \quad b_{(a\,i)(b\,j)} = p_i q_j, \quad b_{a \to i \to b \to a} = h\, v_i, \quad b_{a \to i \to b \to j \to a} = v_i \overline{v_j},$$

*and the reversed cycles have the conjugate coefficients.*

*Proof.* Every cycle of $\sigma$ of length at least two runs along edges of the support. Since leaves are pairwise nonadjacent, consecutive vertices of a cycle are never two leaves, so a cycle of length at least three contains both hubs and at most two leaves. Every cycle of length at least two contains a hub, so $\sigma$ has at most two such cycles, and if it has two, they are transpositions through different hubs. The coefficients follow from $b_\sigma = \prod_j b_{j,\sigma(j)}$; for instance $b_{ai}b_{ib}b_{ba} = b_{ai}\overline{b_{bi}}\,h = hv_i$. □

Fix a unitary representation $U$ of $S_n$ and write $A_i = U_{(a\,i)}$, $L_i = U_{(b\,i)}$, $S = U_{(a\,b)}$.

**Lemma 3.2** (Leaf pairs)**.** *For leaves $i \neq j$ let $\Delta_{ij}$ be the sum of $b_\sigma(I - U_\sigma)$ over the four permutations $(a\,i)(b\,j)$, $(a\,j)(b\,i)$ and the two four-cycles through $a, b, i, j$. Then $\Delta_{ij} \succeq 2\,\mathrm{Re}(v_i\overline{v_j})\,(I - S)$, and*

$$\sum_{i<j} \Delta_{ij} \succeq \Big(|V|^2 - \sum_i u_i^2\Big)(I - S).$$

*Proof.* Let $M = A_iL_j$. Then $SMS = A_jL_i$, and $SM$ is the operator of the four-cycle $a \to i \to b \to j \to a$ (apply $(b\,j)$, then $(a\,i)$, then $(a\,b)$), while $MS = (SM)^{-1}$. Put $\alpha = b_{ai}b_{bj}$ and $\beta = b_{aj}b_{bi}$, so $|\alpha|^2 = p_iq_j$, $|\beta|^2 = p_jq_i$ and $\alpha\bar\beta = v_i\overline{v_j}$. Expanding with $Y = \alpha I + \beta S$,

$$Y^*MY = |\alpha|^2 M + |\beta|^2 SMS + \alpha\bar\beta\, SM + \bar\alpha\beta\, MS$$

is exactly the sum of $b_\sigma U_\sigma$ over the four permutations, by Lemma 3.1. Their coefficients sum to $|\alpha|^2 + |\beta|^2 + 2\,\mathrm{Re}(v_i\overline{v_j})$. Since $M$ is a unitary involution, $M \preceq I$ and $Y^*MY \preceq Y^*Y = (|\alpha|^2 + |\beta|^2)I + 2\,\mathrm{Re}(v_i\overline{v_j})S$. Subtracting from the scalar gives the first claim. Summing over $i < j$ and using $\sum_{i<j} 2\,\mathrm{Re}(v_i\overline{v_j}) = |V|^2 - \sum_i u_i^2$ gives the second. □

**Lemma 3.3** (Leaves)**.** *For a leaf $i$ let $\Lambda_i$ be the sum of $b_\sigma(I - U_\sigma)$ over $\sigma = (a\,i)$, $(b\,i)$ and the two three-cycles through $a, i, b$. Put $c_i = 2h\,\mathrm{Re}\,v_i$, $\kappa_i = \xi_i^* G_h \xi_i = p_i + q_i + c_i$, and*

$$d_i = \frac{u_i^2(\kappa_i - \ell)}{\kappa_i} \quad \text{if } u_i > 0, \qquad d_i = 0 \quad \text{if } u_i = 0.$$

*If $u_i > 0$ then $\kappa_i \geq 2(1-h)u_i > 0$. In every case $\Lambda_i \succeq (u_i^2 + c_i - d_i)(I - S)$.*

*Proof.* If $u_i = 0$, the three-cycles have coefficient zero, $c_i = d_i = 0$, and $\Lambda_i = p_i(I - A_i) + q_i(I - L_i) \succeq 0$. Let $u_i > 0$ and drop the index $i$. Since $p + q \geq 2u$ and $|c| \leq 2hu$, $\kappa \geq 2(1-h)u > 0$. Write $z = hv$ for the coefficient of one of the two three-cycles, $\tau$, so that the other has $\bar z$; then $|z| = hu$ and $c = 2\,\mathrm{Re}\,z$. It suffices to prove $\Lambda \succeq (u^2 + c - d)(I - S)$ in the irreducible representations of $\mathrm{Sym}\{a, i, b\}$. In the trivial one both sides vanish.

In the sign representation transpositions act by $-1$ and three-cycles by 1, so the claim is $p + q \geq u^2 + c - d$, that is $p + q - c \geq u^2 - d = \ell u^2/\kappa$. Since $\kappa = p + q + c > 0$, this is $(p + q)^2 - c^2 \geq \ell u^2$, which holds because $(p + q)^2 - c^2 \geq 4u^2 - 4h^2u^2 = 4\ell u^2$.

The remaining irreducible representation lies in the permutation representation on $\mathbb{C}^{\{a,i,b\}}$. All forms $\langle y, (I - U_\sigma)y\rangle$ are unchanged by adding a constant vector to $y$, so we may take $y_i = 0$ and write $P = y_a$, $Q = y_b$. Then $\langle y, (I - A_i)y\rangle = |P|^2$, $\langle y, (I - L_i)y\rangle = |Q|^2$, $\langle y, (I - S)y\rangle = |P - Q|^2$, and the two three-cycles give $|P|^2 + |Q|^2 - \bar PQ$ and $|P|^2 + |Q|^2 - \bar QP$. Replacing $z$ by $\bar z$ exchanges the two three-cycles and leaves $u, c, \kappa, d$ unchanged, so we may assume that $\tau$ gives the first of these forms. Then $\langle y, \Lambda y\rangle - (u^2 + c)|P - Q|^2$ is the Hermitian form in $(P, Q)$ with matrix

$$N = \begin{pmatrix} p - u^2 & u^2 + \bar z \\ u^2 + z & q - u^2 \end{pmatrix}.$$

Using $pq = u^2$ and $|z|^2 = h^2u^2$, $\det N = u^2(\ell - \kappa)$. Adding $d|P-Q|^2$ adds $d\,ww^{\mathsf{T}}$ with $w = (1,-1)^{\mathsf{T}}$, and since $w^{\mathsf{T}}\operatorname{adj}(N)w = p + q + c = \kappa$, the determinant becomes $u^2(\ell-\kappa) + d\kappa = 0$. The value of the new form at $(P,Q) = (1,1)$ is $\kappa > 0$. A Hermitian $2\times 2$ matrix with zero determinant and a positive value of its form has eigenvalues 0 and a positive number, so $N + d\,ww^{\mathsf{T}} \succeq 0$, which is the claim. □

**Lemma 3.4** (Hub estimate)**.** *Let $0 \le h < 1$ and let $X \in \mathbb{C}^{2\times m}$ satisfy $XX^* \preceq G_h$. With the notation above, $\sum_i d_i \le |V+h|^2$.*

*Proof.* Write $XX^* = \begin{pmatrix} \rho_a & V \\ \overline{V} & \rho_b \end{pmatrix}$ with $\rho_a = \sum_i p_i$ and $\rho_b = \sum_i q_i$. Positivity of $G_h - XX^*$ means $\rho_a, \rho_b \le 1$ and $(1-\rho_a)(1-\rho_b) \ge |h-V|^2$.

Suppose first that $\operatorname{Re} V \le 0$. Then $|h+V| \le |h-V|$, so $G_h' - XX^* \succeq 0$ for $G_h' = \begin{pmatrix} 1 & -h \\ -h & 1 \end{pmatrix} = \ell G_h^{-1}$. Congruence by $G_h^{1/2}$ gives $G_h^{1/2}XX^*G_h^{1/2} \preceq \ell I$, and since $G_h^{1/2}\xi_i\xi_i^*G_h^{1/2} \preceq G_h^{1/2}XX^*G_h^{1/2}$, each $\kappa_i = \|G_h^{1/2}\xi_i\|^2 \le \ell$. Hence every $d_i \le 0$.

Suppose now that $R = \operatorname{Re} V > 0$, and put $s = \sum_i u_i$, $z = |V|$, $\delta = |V+h|$ and $K = 1 - |V-h| + hR$. If $s = 0$ all $d_i$ vanish, so let $s > 0$. By the arithmetic–geometric mean inequality, $2 - \rho_a - \rho_b \ge 2\sqrt{(1-\rho_a)(1-\rho_b)} \ge 2|V-h|$, and $\rho_a + \rho_b = \sum_i (p_i + q_i) \ge 2s$; hence $s \le 1 - |V-h| \le 1$ and $K \ge s$. Next, $\sum_i \kappa_i = \rho_a + \rho_b + 2hR \le 2K$, and every $\kappa_i \ge 0$ because $G_h \succeq 0$. Bounding each cross term of $|V|^2$ below by $-u_iu_j$ gives $z^2 \ge 2\sum_i u_i^2 - s^2$. By Cauchy–Schwarz over the leaves with $u_i > 0$, $s^2 \le (\sum u_i^2/\kappa_i)(\sum \kappa_i) \le 2K \sum u_i^2/\kappa_i$. Therefore

$$\sum_i d_i = \sum_i u_i^2 - \ell \sum_{u_i>0} \frac{u_i^2}{\kappa_i} \le \frac{z^2+s^2}{2} - \frac{\ell s^2}{2K} = \frac{z^2}{2} + \frac{s^2}{2K}(K-\ell).$$

Note $\delta^2 = z^2 + 2hR + h^2 \ge z^2$. If $K \le \ell$ the right side is at most $z^2/2 \le \delta^2$. If $K > \ell$, then $K - \ell = h^2 + hR - |V-h| \le h^2 + hR \le \delta^2$ and $s^2/(2K) \le s/2 \le 1/2$, so the right side is at most $z^2/2 + \delta^2/2 \le \delta^2$. □

*Proof of Theorem 1.4.* Let $\Gamma(B) \subseteq G$ with $\tau(G) \le 2$. If $n = 1$ there is nothing to prove; otherwise choose two vertices $a, b$ containing a vertex cover. By Lemma 2.2 and the reductions at the start of this section, $B$ is a correlation matrix with $0 \le h < 1$. By Lemma 3.1, $\Delta_B^U$ is the sum of $h^2(I-S)$, the $\Lambda_i$ and the $\Delta_{ij}$. Lemmas 3.2 and 3.3 give

$$\Delta_B^U \succeq \Big(h^2 + \sum_i (u_i^2 + c_i - d_i) + |V|^2 - \sum_i u_i^2\Big)(I-S) = \Big(|V+h|^2 - \sum_i d_i\Big)(I-S),$$

since $\sum_i c_i = 2hR$. The coefficient is nonnegative by Lemma 3.4 and $I - S \succeq 0$, so $\Delta_B^U \succeq 0$ for every $U$, and Lemma 2.1(iii) completes the proof. □

*Remark* 3.5. For $K_{2,m}$, that is $h = 0$, the proof simplifies: $\ell = 1$, $\kappa_i = p_i + q_i \le 1$, so every $d_i \le 0$ and Lemma 3.4 is not needed. The bound of Lemma 3.2 keeps the cross terms $2\operatorname{Re}(v_i\overline{v_j})$ with their signs; a bound applied to each four-cycle separately would lose the cancellation between pairs.

**Proposition 3.6** (Simple top eigenvalue on $K_{2,m}$)**.** *Let $B$ be a correlation matrix supported on $K_{2,m}$ with nonadjacent hubs, with $\Gamma(B)$ connected, and with $p_i + q_i < 1$ for every leaf $i$ adjacent to both hubs. Then* per $B$ *is a simple eigenvalue of* $\Pi(B)$.

*Proof.* Here $h = 0$, $c_i = 0$ and $d_i \le 0$, so the proof of Theorem 1.4 only needs $\Lambda_i \succeq u_i^2(I - S)$ for each leaf. For a leaf $i$ adjacent to both hubs put $\theta_i = 1 - p_i - q_i \in (0, 1)$. Lemma 2.3 applied to the weights $(1 - \theta_i)p_i$ and $(1 - \theta_i)q_i$ gives

$$\Lambda_i = \theta_i\big(p_i(I-A_i)+q_i(I-L_i)\big)+(1-\theta_i)\big(p_i(I-A_i)+q_i(I-L_i)\big) \succeq \theta_i\big(p_i(I-A_i)+q_i(I-L_i)\big)+u_i^2(I-S),$$

because $(1 - \theta_i)p_iq_i/(p_i + q_i) = p_iq_i = u_i^2$. A leaf with one edge has $u_i = 0$ and $\Lambda_i = p_i(I - A_i)$ or $q_i(I - L_i)$. With Lemma 3.2 this gives $\Delta_B^U \succeq c\sum_{e\in E(\Gamma(B))}(I - U_e)$ in every unitary representation, where $U_e$ is the transposition of the edge $e$ and $c > 0$ is the smallest of the numbers $\theta_ip_i$, $\theta_iq_i$ and the single-edge weights. In the regular representation a vector $v$ in the kernel of $\sum_e(I-U_e)$ satisfies $U_ev = v$ for every edge, because each $I-U_e \succeq 0$. The transpositions along the edges of a connected graph generate $S_n$, so $v$ is invariant under $S_n$, hence constant. Thus the eigenvalue $\operatorname{per} B$ of $\Pi(B)$ has multiplicity one. □

# 4 Block trees

**Lemma 4.1** (Positive splitting)**.** *Let $B \succeq 0$ have support in a graph $G$ whose blocks with an edge are $K_1, \dots, K_r$. Then $B = \sum_{t=1}^r B^{(t)} + D_0$, where $D_0 \succeq 0$ is diagonal and each $B^{(t)} \succeq 0$ is supported on $V(K_t) \times V(K_t)$, with off-diagonal entries equal to those of $B$ on the edges of $K_t$ and zero elsewhere.*

*Proof.* Put the diagonal entries of the isolated vertices of $G$ into $D_0$ and delete these vertices; we induct on the number of blocks with an edge. If there is none, $B$ is diagonal and $B = D_0$. If there is exactly one, $K_1$, let $B^{(1)}$ be the principal submatrix of $B$ on $V(K_1)$, extended by zero. If $G$ is disconnected, $B$ is the direct sum of its principal submatrices on the components, each with fewer blocks with an edge, and we apply the induction hypothesis to each. Otherwise $G$ is connected with at least two blocks, so it has a cut vertex $v$; let $W_1$ be the vertex set of one component of $G - v$ and $W_2$ the union of the others. There are no edges between $W_1$ and $W_2$, so in the order $v, W_1, W_2$,

$$B = \begin{pmatrix} d & f_1^* & f_2^* \\ f_1 & A_1 & 0 \\ f_2 & 0 & A_2 \end{pmatrix}.$$

For a positive semidefinite matrix $\begin{pmatrix} d & f^* \\ f & A \end{pmatrix}$ one has $f \in \operatorname{ran} A$ and $d \ge f^*A^+f$, with $A^+$ the Moore–Penrose inverse. Applying this with $A = A_1 \oplus A_2$ gives $f_t \in \operatorname{ran} A_t$ and $d \ge f_1^*A_1^+f_1 + f_2^*A_2^+f_2$. The matrices $\begin{pmatrix} f_t^*A_t^+f_t & f_t^* \\ f_t & A_t \end{pmatrix} = R_t^*R_t$, $R_t = \begin{pmatrix} (A_t^+)^{1/2}f_t & A_t^{1/2} \end{pmatrix}$, are positive semidefinite, because $A_t^{1/2}(A_t^+)^{1/2}$ is the projection onto $\operatorname{ran} A_t$, which fixes $f_t$. Thus $B$ is the sum of these two matrices, extended by zero, and the diagonal matrix $(d - f_1^*A_1^+f_1 - f_2^*A_2^+f_2)e_ve_v^*$. The two summands are supported on $\{v\}\cup W_1$ and $\{v\}\cup W_2$, the induced subgraphs there have the blocks of $G$ distributed between them, and the induction hypothesis applies to each. □

*Proof of Theorem 1.6.* A block is a subgraph, so universality of $G$ implies that of its blocks. Conversely let every block be universal and let $B \succeq 0$ have $\Gamma(B) \subseteq G$. Write $B = \sum_{K\in\mathcal{K}} B^{(K)}$ as in Lemma 4.1, where $\mathcal{K}$ consists of the blocks with an edge and one singleton $\{v\}$ for each vertex, carrying the entry $(D_0)_{vv}$. Every off-diagonal entry of $B$ lies in exactly one piece. If $b_\sigma \ne 0$, each cycle of $\sigma$ of length at least two runs along edges of $G$, hence lies in a unique block. Call a map $\alpha$ from $[n]$ to $\mathcal{K}$ with $v \in \alpha(v)$ an *assignment*, and call it compatible with $\sigma$ if every vertex moved by

$\sigma$ is assigned the block of its cycle. Expanding the diagonal factors $b_{vv} = \sum_{K \ni v} B^{(K)}_{vv}$ of the fixed points of $\sigma$ gives

$$b_\sigma = \sum_{\alpha \text{ compatible with } \sigma} \prod_{K \in \mathcal{K}} \left(B^{(K)}[\alpha^{-1}(K)]\right)_{\sigma|_{\alpha^{-1}(K)}},$$

where $\sigma$ restricts to a permutation of each $\alpha^{-1}(K)$. Conversely, for a fixed assignment, a family of permutations $\sigma_K$ of $\alpha^{-1}(K)$ with nonzero coefficients in $B^{(K)}[\alpha^{-1}(K)]$ has all cycles inside $K$, and its product is compatible with $\alpha$. Hence, for every unitary representation $U$ of $S_n$,

$$T^U_B = \sum_\alpha \prod_{K \in \mathcal{K}} T^U_{B^{(K)}[\alpha^{-1}(K)]},$$

where $T^U_{B'}$ for a principal submatrix $B'$ on a vertex set $\Omega$ is $\sum_{\pi \in \mathrm{Sym}(\Omega)} b'_\pi U_\pi$. The factors act on disjoint vertex sets and commute. Each $B^{(K)}[\alpha^{-1}(K)]$ is positive semidefinite with support in the universal graph $K$, so by Lemma 2.1(iv) and Lemma 2.2(iii) its operator satisfies $0 \preceq T^U_{B^{(K)}[\alpha^{-1}(K)]} \preceq \operatorname{per}\left(B^{(K)}[\alpha^{-1}(K)]\right) I$. Commuting positive semidefinite operators can be diagonalized simultaneously, so each product is at most the product of the permanents times $I$. Summing over $\alpha$ and using the same identity in the trivial representation, $T^U_B \preceq (\operatorname{per} B) I$. □

# 5 Cycles

*Proof of Theorem 1.7.* We use strong induction on $k$. The cycles $C_3$ and $C_4$ have vertex-cover number two, so Theorem 1.4 applies. Let $k \geq 5$ and let $B$ be a correlation matrix with $\Gamma(B) \subseteq C_k$; if an edge of the cycle carries a zero entry, the support is a forest and Lemma 2.2(v) applies, so all $k$ edge entries are nonzero. Label the cycle $w_0, w_1, \ldots, w_{k-1}$ in cyclic order, indices modulo $k$. Put $m = \lceil k/2 \rceil$, call $a_t = w_{2t}$ $(0 \leq t < m)$ the *original* vertices and $r_t = w_{2t+1}$ $(0 \leq t < \lfloor k/2 \rfloor)$ the *intermediate* vertices. For even $k$ every original $a_t$ is followed by $r_t$; for odd $k$ the last original $a_{m-1} = w_{k-1}$ is adjacent to $a_0$, and we write $h = |b_{a_{m-1}a_0}|$.

*Supported permutations.* The only cycles of $C_k$ are the two orientations of the whole cycle, so every $\sigma$ with $b_\sigma \neq 0$ is either a matching $N$ (a product of disjoint edge transpositions), with $b_N = W_N := \prod_{e \in N} |b_e|^2$, or the rotation $\omega : w_t \mapsto w_{t+1}$ with coefficient $z = \prod_t b_{w_t w_{t+1}}$, or $\omega^{-1}$ with coefficient $\bar{z}$.

*The cycle packet.* Fix a unitary representation $U$. Let $s$ be the cyclic permutation $a_t \mapsto a_{t+1}$ of the originals (indices modulo $m$), $\phi = \prod_t (a_t\, r_t)$ and $\nu = s\phi s^{-1} = \prod_t (a_{t+1}\, r_t)$, the two alternating matchings, and put $S = U_s$, $M = U_\phi$. One checks on $w_{2t}$ and $w_{2t+1}$ that $s\phi = \omega$, so $U_\omega = SM$ and $U_{\omega^{-1}} = MS^{-1}$. The modulus of $z$ is $\sqrt{W_\phi W_\nu}$ for even $k$ and $h\sqrt{W_\phi W_\nu}$ for odd $k$. Choose $\alpha, \beta$ with $|\alpha|^2 = W_\phi$ and $\alpha\bar{\beta} = z$; then $|\beta|^2 \leq W_\nu$. With $Y = \alpha I + \beta S^{-1}$,

$$Y^*MY = W_\phi U_\phi + |\beta|^2 U_\nu + z\, U_\omega + \bar{z}\, U_{\omega^{-1}}, \qquad Y^*Y = (W_\phi + |\beta|^2) I + zS + \bar{z} S^{-1}.$$

As $M \preceq I$, the contribution $W_\phi(I - U_\phi) + |\beta|^2(I - U_\nu) + z(I - U_\omega) + \bar{z}(I - U_{\omega^{-1}})$ to $\Delta^U_B$ is at least

$$z(I - S) + \bar{z}(I - S^{-1}). \tag{5a}$$

*The halved cycle.* Let $B_L$ be the principal submatrix of $B$ on the originals, $X = B[L, R]$ the block from originals to intermediates, and $\widehat{B} = B_L + \operatorname{off}(XX^*)$, where off sets the diagonal to zero. The intermediates are pairwise nonadjacent, so the Schur complement gives $B_L - XX^* \succeq 0$. The matrix $B_L - \operatorname{diag}(XX^*)$ is diagonal except, for odd $k$, at the pair $a_0, a_{m-1}$; since $m \geq 3$, these two vertices have no common intermediate neighbour, so on that pair it agrees with the principal

submatrix of $B_L - XX^*$. Hence $B_L - \mathrm{diag}(XX^*) \succeq 0$ and $\widehat{B} = (B_L - \mathrm{diag}(XX^*)) + XX^* \succeq 0$. The matrix $\widehat{B}$ has unit diagonal. Two originals $a_t, a_{t+1}$ have the unique common neighbour $r_t$ (except the directly adjacent pair for odd $k$), so

$$\widehat{B}_{a_t a_{t+1}} = b_{a_t r_t} b_{r_t a_{t+1}}, \qquad \widehat{B}_{a_{m-1} a_0} = b_{a_{m-1} a_0} \quad (k \text{ odd}),$$

and all other off-diagonal entries of $\widehat{B}$ vanish. Thus $\widehat{B}$ is a correlation matrix supported on the $m$-cycle $a_0 a_1 \cdots a_{m-1}$, and its coefficient on $s$ is $\prod_t \widehat{B}_{a_t a_{t+1}} = z$. Its matchings are the sets $Q$ of disjoint *virtual edges* $\epsilon_t = \{a_t, a_{t+1}\}$, with coefficients $W_Q^{\widehat{B}} = \prod_{\epsilon \in Q} g_\epsilon$, where $g_{\epsilon_t} = p_t q_t$ with $p_t = |b_{a_t r_t}|^2$, $q_t = |b_{r_t a_{t+1}}|^2$, and $g = h^2$ for the direct edge. Since $3 \le m < k$, the induction hypothesis and Lemma 2.1(iii), applied to the restriction of $U$ to $\mathrm{Sym}(L)$, give

$$z(I - S) + \bar{z}(I - S^{-1}) + \sum_{Q \neq \varnothing} W_Q^{\widehat{B}} \, (I - U_Q) \succeq 0, \tag{5b}$$

where $U_Q$ is the operator of the product of the transpositions $(a_t\, a_{t+1})$, $\epsilon_t \in Q$.

*Paying the virtual matchings.* For a virtual edge $\epsilon_t$ through $r_t$ put $P_t = p_t U_{(a_t\, r_t)} + q_t U_{(r_t\, a_{t+1})}$, $D_t = p_t + q_t$. The originals $a_t, a_{t+1}$ are not adjacent, so the principal $3 \times 3$ submatrix of $B$ on $a_t, r_t, a_{t+1}$ gives $D_t \le 1$, and Lemma 2.3 gives $\|P_t - g_{\epsilon_t} U_{(a_t\, a_{t+1})}\| \le D_t - g_{\epsilon_t}$. For the direct edge put $P = h^2 U_{(a_{m-1}\, a_0)}$ and $D = g = h^2$. For a virtual matching $Q$ the vertex sets of the $P_\epsilon$, $\epsilon \in Q$, are disjoint, so these Hermitian operators commute, and expanding $\prod_\epsilon \left(g_\epsilon U_\epsilon + (P_\epsilon - g_\epsilon U_\epsilon)\right)$ shows that $\prod_\epsilon P_\epsilon - \prod_\epsilon g_\epsilon U_\epsilon$ has norm at most $\prod_\epsilon D_\epsilon - \prod_\epsilon g_\epsilon$. Hence

$$\Big(\prod_{\epsilon \in Q} D_\epsilon\Big) I - \prod_{\epsilon \in Q} P_\epsilon \succeq W_Q^{\widehat{B}} \, (I - U_Q).$$

Expanding the product, the left side is $\sum_{N \in \mathcal{N}_Q} W_N (I - U_N)$, where $\mathcal{N}_Q$ is the family of matchings of $C_k$ obtained by choosing, for each $\epsilon_t \in Q$, one of the two edges $a_t r_t$, $r_t a_{t+1}$, together with the direct edge if it lies in $Q$. A matching in $\mathcal{N}_Q$ determines $Q$ (through the intermediates it covers and the direct edge), so the families $\mathcal{N}_Q$ are pairwise disjoint. Their matchings have at most $\lfloor m/2 \rfloor$ edges, while $\phi$ and $\nu$ have $\lfloor k/2 \rfloor > \lfloor m/2 \rfloor$ edges for $k \ge 5$, so no $\mathcal{N}_Q$ contains $\phi$ or $\nu$.

*Assembly.* Split $\Delta_B^U$ into the four terms of (5a), the term $(W_\nu - |\beta|^2)(I - U_\nu) \succeq 0$, the matchings in $\bigcup_{Q \neq \varnothing} \mathcal{N}_Q$, and the remaining matchings, whose terms $W_N(I - U_N)$ are positive semidefinite. By (5a), the previous paragraph and (5b),

$$\Delta_B^U \succeq z(I - S) + \bar{z}(I - S^{-1}) + \sum_{Q \neq \varnothing} W_Q^{\widehat{B}} (I - U_Q) \succeq 0.$$

This holds for every $U$, so $B$ is permanent-on-top. □

*Proof of Corollary 1.8.* Edges and graphs with $\tau \le 2$ are universal by Theorem 1.4, cycles by Theorem 1.7, and Theorem 1.6 combines the blocks. The graphs $K_{2,m}$ and $K_{1,1,m}$ have vertex-cover number two. A graph on at most four vertices other than $K_4$ is contained in $K_4$ minus an edge, whose two vertices of degree three cover all edges. □

*Remark* 5.1. Among the 34 graphs on five vertices, Theorem 1.4 applies to the 20 with vertex-cover number at most two, and Corollary 1.8 adds five more: $K_3 \cup K_2$, a triangle with a pendant path of length two, $C_5$, two triangles sharing a vertex, and $K_4$ minus an edge with a pendant edge at a vertex of degree two. Theorem 1.5 and Shchesnovich's example show that $K_5$ minus an edge and $K_5$ are not universal. Combined with Theorem 1.6, the order-four theorem announced by Lavi [13, Theorem 3.1] would extend this to $K_4 \cup K_1$ and to $K_4$ with a pendant edge.

# 6 Path bundles

A *path bundle* with hubs $u \neq v$ is a union of internally vertex-disjoint paths from $u$ to $v$, called *arms*, possibly including the edge $uv$ as an arm of length one. Every cycle of a path bundle consists of two arms and contains both hubs. Bundles all of whose arms have length two are the graphs $K_{2,m}$ of Theorem 1.4; the cycles of length at least five are the bundles with two arms (Theorem 1.7). Here the number of arms is arbitrary.

**Theorem 6.1** (Path bundles)**.** *A path bundle is universal in each of the following cases:*

*(a) every arm has length at least five;*

*(b) one arm has length at most four and every other arm has length at least ten;*

*(c) there are exactly three arms, and either every cycle has length at least nine, or exactly one cycle has length eight and the other two have length at least nine.*

*If $B$ is positive semidefinite and $\Gamma(B)$ is the whole bundle, then* $\operatorname{per} B$ *is a simple eigenvalue of $\Pi(B)$.*

**Theorem 6.2** (Subdivided multigraphs)**.** *Let $G_0$ be a finite loopless multigraph in which every vertex has at most $d \geq 1$ distinct neighbours, and let $G$ be obtained by replacing every edge of $G_0$ by a path of length at least $16 + \lceil \log_2 d \rceil$, the paths being internally disjoint. Then $G$ is universal, with a simple top eigenvalue on connected supports.*

For simple graphs Theorems 6.2 and 7.3 together show that replacing every edge of a graph of maximum degree $\Delta$ by paths of length at least $\min\{16 + \lceil \log_2 \Delta \rceil, L(\Delta)\}$ gives a universal graph; the first bound is the smaller one for $\Delta \leq 64$ and for $87 \leq \Delta \leq 128$, the two agree for $65 \leq \Delta \leq 86$ and for $129 \leq \Delta \leq 256$, and $L(\Delta)$ is smaller for $\Delta \geq 257$. Theorem 6.2 also allows parallel edges in any multiplicity.

## 6.1 Adjacent-swap constants

The proofs use Lemmas 2.5–2.8 with uniform constants $d_e = d_k$ on a cycle of length $k$, where $d_k$ is any constant with $|1 - \langle y, Vy\rangle| \leq d_k \sum_i \langle y, (I - S_i)y\rangle$ for the product $V = S_1 \cdots S_{k-1}$ of the transpositions along a path of $k$ vertices, in every unitary representation. Lemma 2.5 gives $d_k = k - 1$; we improve this by grouping.

**Lemma 6.3** (Grouped swaps)**.** *One can take $d_k = \frac{3k-2}{4}$ for odd $k$, $d_k = \frac{3k-1}{4}$ for even $k$, and, writing $k - 1 = 3a + b$ with $0 \leq b \leq 2$, $d_k = 2a + \rho_b + \frac{1}{4}$ with $\rho_0 = 0$, $\rho_1 = 1$, $\rho_2 = \frac{3}{2}$. In particular $d_{10} = \frac{25}{4}$, $d_{12} = \frac{31}{4}$ and $d_k \leq \frac{2(k-1)}{3} + \frac{7}{12} < \frac{2k}{3}$. Moreover $d_8 = \frac{17}{4}$ and $d_9 = \frac{19}{4}$ are admissible.*

*Proof.* Split $S_1, \ldots, S_{k-1}$ into consecutive groups with products $W_1, \ldots, W_t$ and swap energies $E_i = \sum_{j \in \text{group } i} \langle y, (I - S_j)y\rangle$, and suppose that $\operatorname{Re}\langle y, (I - W_i)y\rangle \leq \rho_i E_i$ and $|\langle y, (I - W_i)y\rangle| \leq (\rho_i + \frac{1}{4})E_i$. The ordered defect identity of Lemma 2.5 for the unitaries $W_i$ gives

$$|1 - \langle y, Vy\rangle| \leq \sum_i \Big(\rho_i + \tfrac{1}{4}\Big) E_i + \sum_{i<j} \|(I - W_i^*)y\| \, \|(I - W_j)y\|,$$

and $\|(I - W_i)y\|^2 = \|(I - W_i^*)y\|^2 = 2\operatorname{Re}\langle y, (I - W_i)y\rangle \leq 2\rho_i E_i$. Hence $|1 - \langle y, Vy\rangle| \leq \frac{1}{4}\sum E_i + (\sum_i \sqrt{\rho_i E_i})^2 \leq (\sum_i \rho_i + \frac{1}{4}) \sum_i E_i$ by the Cauchy–Schwarz inequality. It remains to give the constants for groups of one, two and three swaps; by restriction it suffices to check them in the irreducible

representations of $S_2$, $S_3$ and $S_4$ (the modulus bound passes to direct sums because $E$ is block diagonal).

A single swap has $\langle y, (I - S)y\rangle = E$, so $\rho = 1$ with modulus constant 1. For two swaps $W = S_1S_2$ is a three-cycle. In the trivial and sign representations of $S_3$, $I - W = 0$. In the two-dimensional representation $W$ is a rotation by $2\pi/3$, so $\mathrm{Re}(I - W) = \frac{3}{2}I$ and $\|I - W\| = \sqrt{3}$, while $(I - S_1) + (I - S_2)$ is twice the sum of the projections onto two lines at angle $\pi/3$, with eigenvalues 1 and 3, so it is at least $I$; this gives $\rho = \frac{3}{2}$ and modulus constant $\sqrt{3} \le \frac{7}{4}$. For three swaps $W = S_1S_2S_3$ is a four-cycle, and with $E$ the sum of the three swap deficits the inequalities

$$\mathrm{Re}(I - W) \preceq 2E, \qquad -E \preceq \mathrm{Im}\, W \preceq E$$

hold in the regular representation of $S_4$; the program `verify_three_adjacent_swap_defect.py` checks them in exact rational arithmetic by Gaussian elimination. So $\rho = 2$ with modulus constant $\sqrt{5} \le \frac{9}{4}$. Grouping into pairs, or into triples followed by a pair or a single swap, gives the stated $d_k$.

The values $d_8 = 17/4$ and $d_9 = 19/4$ are computer-assisted: for every nontrivial irreducible representation of $S_8$ and $S_9$ in Young's orthogonal form, the program `verify_short_cycle_defect.py` certifies $d_kE - s\,\mathrm{Re}(I - V) \mp t\,\mathrm{Im}(I - V) \succeq 0$ at the vertices $(s, t)$ of a rational polygon containing the quarter circle $\{s, t \ge 0,\ s^2 + t^2 = 1\}$, which bounds $|\langle y, (I - V)y\rangle|$ because $\mathrm{Re}\langle y, (I - V)y\rangle \ge 0$; the certificate is an integer Cholesky factorization of a rounded matrix with an explicit bound for every rounding error. □

Numerically the best uniform constant is $(k-1)/2$ for $3 \le k \le 7$, below each value of Lemma 6.3 (`verify_m1_bundles.py`).

## 6.2 Path products

**Lemma 6.4** (Path products)**.** *Let $B$ be a correlation matrix, and let the vertices of a path with $\ell$ edges induce a path in $\Gamma(B)$. Then the product of the moduli of its edges is at most $2^{1-\ell}$. A union of $h$ such induced paths with $s$ edges in total has product at most $2^{h-s}$.*

*Proof.* The principal submatrix on the path is a tridiagonal correlation matrix; a diagonal unitary conjugation makes its off-diagonal entries $-w_{ij} \le 0$, so $I - W' \succeq 0$ and $\varrho(W') \le 1$. If some modulus vanishes the claim is trivial. Otherwise let $h'$ be a positive Perron vector of $W'$ and $p_{ij} = w_{ij}h'_j/h'_i$; then $\sum_j p_{ij} = \varrho(W') \le 1$ and $w_{ij}^2 = p_{ij}p_{ji}$. The product of the squared moduli is the product over the vertices of the $p$'s leaving them; each internal vertex contributes $p_{t,t-1}p_{t,t+1} \le \frac{1}{4}$, and each end at most one. □

For an arm $i$ with $l_i \ge 2$ edges let $a_i$ and $b_i$ be the moduli of its edges at $u$ and $v$, $R_i$ the product of all its moduli and $t_i = l_iR_i$. The interior vertices of distinct arms are nonadjacent, so the principal submatrix on a hub and its neighbours on the arms gives

$$\sum_i a_i^2 \le 1, \qquad \sum_i b_i^2 \le 1. \tag{6a}$$

If all edges of arm $i$ are nonzero, its interior principal submatrix $C_i$ is positive definite: after a diagonal unitary conjugation $C_i = I - W_i$ with $W_i \ge 0$ irreducible, a vector in its kernel would be a positive Perron vector, and the range condition of positive semidefiniteness for the coupling of $C_i$ to the hubs would force $a_i$ times its first coordinate to vanish. Let $D_{u,i}$ and $D_{v,i}$ be the diagonal entries of $C_i^{-1}$ at the two interior vertices next to $u$ and $v$, and put $\alpha_i = a_i\sqrt{D_{u,i}}$, $\alpha'_i = b_i\sqrt{D_{v,i}}$.

Eliminating all arm interiors, the Schur complement at the hubs has diagonal entries $1-\sum_i a_i^2 D_{u,i}$ and $1-\sum_i b_i^2 D_{v,i}$, so

$$\sum_i \alpha_i^2 \le 1, \qquad \sum_i \alpha_i'^2 \le 1, \tag{6b}$$

also when the hubs are adjacent. Since $C_i$ has unit diagonal, $D_{u,i}, D_{v,i} \ge 1$, so $a_i \le \alpha_i$ and $b_i \le \alpha_i'$.

**Lemma 6.5** (Loaded path products)**.** *Let arm $i$ have $l = l_i \ge 3$ nonzero edges. Then $R_i \le \alpha_i\alpha_i' 2^{2-l}$. After removing one interior edge the product of the remaining moduli is at most $\alpha_i\alpha_i' 2^{3-l}$; after removing the end edge at $u$ it is at most $\alpha_i' 2^{2-l}$; after removing two interior edges, one end edge and one interior edge, or both end edges, it is at most $\alpha_i\alpha_i' 2^{5-l}$, $\alpha_i' 2^{4-l}$, and $2^{3-l}$ respectively (and symmetrically in $u, v$).*

*Proof.* Replace $a_i, b_i$ by $a' = 1/\sqrt{2D_{u,i}}$ and $b' = 1/\sqrt{2D_{v,i}}$ (with the same phases) and set the entry at $(u, v)$ to zero. The resulting matrix on the vertices of the arm is positive semidefinite: its Schur complement onto $\{u, v\}$ is $I_2$ minus a matrix with diagonal $\frac{1}{2}, \frac{1}{2}$ and off-diagonal modulus at most $a'b'\sqrt{D_{u,i}D_{v,i}} = \frac{1}{2}$. Lemma 6.4 gives $a'b' \prod_{\text{interior}} \le 2^{1-l}$, that is $R_i \le a_i b_i \cdot 2^{2-l}\sqrt{D_{u,i}D_{v,i}} = \alpha_i\alpha_i' 2^{2-l}$. For a fragment consisting of $u$ and an initial segment $F$ of the interior, the matrix with end entry $1/\sqrt{D_{u,i}}$ is positive semidefinite because $(C_F^{-1})_{11} \le (C_i^{-1})_{11}$, a consequence of the Schur complement formula for the inverse; so a fragment with $e$ edges at $u$ has product at most $\alpha_i 2^{1-e}$, and similarly at $v$. Interior fragments obey Lemma 6.4. Removing edges cuts the arm into such fragments, and multiplying the bounds gives the list. □

### 6.3 Priorities and charges

The packets are those of Lemma 2.5 with $d_e = d_k$ and with omitted edges chosen as follows. Fix $L \ge 5$, let $\varepsilon_L = L2^{2-L}$, and for an arm $i$ put $q_i = \alpha_i^2 + \alpha_i'^2$ and give its edges the *priority weights* $\nu_i(e) = 2q_i$ for interior edges and $\nu_i(e) = 1$ for the two end edges. Let $e_i$ be an edge of arm $i$ minimizing $\nu_i(e)w_e^2$, $m_i = w_{e_i}$, and $\phi_i = \nu_i(e_i)m_i^2/t_i$. On the cycle formed by arms $i$ and $j$ the omitted edge is $e_i$ if $\phi_i \le \phi_j$ and $e_j$ otherwise (ties broken by a fixed order).

**Lemma 6.6.** *If arm $i$ has length $l_i \ge L$, then*

$$t_i \le \tfrac{1}{2}\varepsilon_L q_i, \qquad t_i/\phi_i \le \varepsilon_L^2 q_i, \qquad t_i/(\nu_i(e)w_e^2) \le 3\varepsilon_L \quad (e \ne e_i).$$

*Proof.* All bounds use Lemma 6.5, $\alpha_i\alpha_i' \le q_i/2$, $\alpha_i, \alpha_i' \le \sqrt{q_i}$, and the decrease of $l2^{-l}$ for $l \ge 2$. First, $t_i \le l_i\alpha_i\alpha_i' 2^{2-l_i} \le \frac{1}{2}\varepsilon_L q_i$. Second, $t_i/\phi_i = (t_i/(m_i\sqrt{\nu_i(e_i)}))^2$; if $e_i$ is interior, $t_i/m_i \le l_i\alpha_i\alpha_i' 2^{3-l_i}$ and dividing by $\sqrt{2q_i}$ gives at most $l_i 2^{2-l_i}\sqrt{q_i}/\sqrt{2}$; if $e_i$ is an end edge, $t_i/m_i \le l_i\sqrt{q_i}\, 2^{2-l_i}$. Third, by minimality $\nu_i(e)w_e^2 \ge w_e m_i\sqrt{\nu_i(e)\nu_i(e_i)}$, and removing $e$ and $e_i$ gives at most $l_i 2^{5-l_i}\alpha_i\alpha_i'/(2q_i) \le 2\varepsilon_L$ for two interior edges, $l_i 2^{4-l_i}\sqrt{q_i}/\sqrt{2q_i} = 2\sqrt{2}\,\varepsilon_L$ for one of each kind, and $l_i 2^{3-l_i} = 2\varepsilon_L$ for two end edges. □

Fix a matching $N$. Since every cycle contains both hubs, no two cycles are vertex-disjoint, so for every $(\mathcal{A}, N)$ with $\mathcal{A} \ne \varnothing$ the eligible set is empty and $\gamma_{\mathcal{A}}(N) = 1$, while

$$\gamma_{\varnothing}(N) = 1 - \sum_{C \in \mathcal{K}(\varnothing, N)} f_C(N).$$

By Lemma 2.7 it suffices to show that this total charge is less than one for every $N$. A cycle $C$ of arms $i, j$ charges a swap only if exactly one edge $e$ of $N$ touches $C$ and $e \ne a_C$ lies on $C$, say on the *active* arm $i$, the arm $j$ then carrying no edge of $N$; the charge is

$$f_C(N) = \frac{2r_C d_k}{w_e^2} = \frac{2d_{l_i+l_j}}{l_i l_j} \cdot \frac{t_i t_j}{w_e^2}. \tag{6c}$$

If $C$ omits $e_i$, then $e \neq e_i$ and Lemma 6.6 gives $t_i t_j / w_e^2 \leq \nu_i(e) \cdot 3\varepsilon_L \cdot \frac{1}{2}\varepsilon_L q_j$. If $C$ omits $e_j$, then $\phi_j < \phi_i$ and $t_i/(\nu_i(e) w_e^2) \leq 1/\phi_i < 1/\phi_j$, so $t_i t_j / w_e^2 \leq \nu_i(e)\, t_j/\phi_j \leq \nu_i(e)\varepsilon_L^2 q_j$. In both cases

$$\frac{t_i t_j}{w_e^2} \leq \frac{3}{2}\, \nu_i(e)\, \varepsilon_L^2\, q_j. \tag{6d}$$

If no edge of $N$ is incident to a hub, then $\nu_i(e) = 2q_i$, and summing over active $i$ and arms $j$ without edges of $N$ gives at most $3\varepsilon_L^2 (\sum_{\text{active}} q_i)(\sum_{\text{inactive}} q_j) \leq 3\varepsilon_L^2$, because the two sums add to at most $\sum_i q_i \leq 2$ by (6b). If exactly one edge of $N$ is incident to a hub, it touches every cycle, so it is the only possible charged edge, $\nu_i(e) = 1$, and the sum is at most $\frac{3}{2}\varepsilon_L^2 \sum_j q_j \leq 3\varepsilon_L^2$. If two edges of $N$ are incident to hubs, no cycle is eligible. Identity charges occur only when no edge of $N$ touches $C$, and $\sum_{i<j} 2R_i R_j \leq (\sum_i R_i)^2 \leq (2^{2-L} \sum_i \alpha_i \alpha_i')^2 \leq 2^{4-2L}$ by Lemma 6.5 and the Cauchy–Schwarz inequality with (6b).

### 6.4 Proofs

*Proof of Theorem 6.1.* By Lemma 2.2 let $B$ be a correlation matrix with $\Gamma(B)$ contained in the bundle. Only arms all of whose edges are nonzero lie on cycles of $\Gamma(B)$; the other arms contribute pendant trees, whose edges at the hubs only reduce eligibility, and (6a), (6b) hold for the complete arms. So we may argue with the complete arms.

(a) Take $L = 5$, so $\varepsilon_5 = \frac{5}{8}$. For $l_i, l_j \geq 5$ the conversion factor in (6c) is at most $\frac{1}{2}$: for $l_i = l_j = 5$, $2d_{10}/25 = \frac{1}{2}$, and otherwise $2d_k/(l_i l_j) < \frac{4}{3}(\frac{1}{l_i} + \frac{1}{l_j}) \leq \frac{4}{3}(\frac{1}{5} + \frac{1}{6}) < \frac{1}{2}$ by Lemma 6.3. So the total charge is at most $\frac{1}{2} \cdot 3\varepsilon_5^2 + 2^{-6} = \frac{75}{128} + \frac{2}{128} = \frac{77}{128}$.

(b) Let arm 0 have length $s \leq 4$ and the others length at least $L = 10$, so $\varepsilon_{10} = \frac{5}{128}$. Give every edge of arm 0 the priority weight $\nu_0 = s/\varepsilon_L$ and choose $e_0$, $\phi_0$ as before. As all moduli are at most one, $t_0 \leq s$, $t_0/\phi_0 \leq s\varepsilon_L$ and $t_0/(\nu_0 w_e^2) \leq \varepsilon_L$ for $e \neq e_0$. For a cycle of arms 0 and $i$ charging an edge $e$ of arm $i$, the two priority cases give $t_i t_0 / w_e^2 \leq 3\varepsilon_L s\, \nu_i(e)$; the eligible $\nu_i(e)$ sum to at most $2\sum q_i \leq 4$, or to one if $N$ meets a hub; and $2d_{s+l}/(sl) < \frac{4}{3s}(1 + \frac{s}{L})$. These charges total at most $16\varepsilon_L(1 + \frac{s}{L}) \leq \frac{7}{8}$. If instead the charged edge lies on arm 0, the pair product is at most $s\varepsilon_L q_i$, and these charges total at most $\frac{8}{3}\varepsilon_L(1 + \frac{s}{L})$; the two kinds exclude each other, since an edge of $N$ on arm 0 touches every cycle through arm 0. Charges between long arms total at most $\frac{3}{2}\varepsilon_L^2$ by (a), and identity charges at most $2^{4-2L} + 2\sum_i R_i \leq 2^{4-2L} + 2^{3-L}$. The sum is below 0.886.

(c) Use the weakest edge of each cycle as its omitted edge. Deleting two edges from an induced cycle of length $k$ leaves at most two induced paths with $k-2$ edges, so a swap charges at most $2d_k 2^{4-k}$, since $w_{a_C}/w_e \leq 1$; with Lemma 6.3 this is at most $\frac{25}{64}$ for $k \geq 9$. If one arm is the edge $uv$, the cycle of the other two arms has the chord $uv$; it has length at least 16, and splitting the remaining path that contains both hubs at an interior vertex costs a factor two, which keeps the bound below $\frac{25}{64}$. An identity charge is $2r_C \leq 2 \cdot 2^{3-k} \leq \frac{1}{32}$, since removing the two edges at $u$ leaves an induced path. At most two cycles charge swaps for a given $N$. Indeed, let $C_{12}, C_{13}, C_{23}$ be the cycles, $C_{ij}$ formed by arms $i$ and $j$, and suppose all three charge swaps, with charged edges $e_{12}, e_{13}, e_{23}$. If $e_{12}$ lies on arm 1, it touches $C_{13}$, so $e_{13} = e_{12}$; the edge $e_{23}$ lies on arm 2 or 3, hence on $C_{12}$ or $C_{13}$, which is then touched by two distinct edges of $N$, a contradiction; the case of arm 2 is symmetric. Hence the total is at most $2 \cdot \frac{25}{64} + 3 \cdot \frac{1}{32} = \frac{7}{8}$. If exactly one cycle has length eight, its swap charge is at most $2d_8/16 = \frac{17}{32}$ and its identity charge at most $\frac{1}{16}$; at length nine $2d_9/32 \leq \frac{5}{16}$, at length at least ten $2 \cdot \frac{2k}{3}\, 2^{4-k} \leq \frac{5}{16}$, and the chorded cycle, of length at least 15, stays below $\frac{5}{16}$ with the factor two. The total is at most $\frac{17}{32} + \frac{5}{16} + \frac{1}{16} + \frac{2}{32} = \frac{31}{32}$.

In each case the total charge is less than one for every matching, so all allocation coefficients are positive, and Lemma 2.7 gives the conclusion, including simplicity when $\Gamma(B)$ is the whole, connected, bundle. □

*Proof of Theorem 6.2.* Let $B$ be a correlation matrix with $\Gamma(B) \subseteq G$; as before only paths with all edges nonzero carry cycles. Call the vertices of $G_0$ hubs. Put $L = 16 + \lceil \log_2 d \rceil$, $\beta = 1/L$, $b = e\,2^{3-L}$ and $\varepsilon = Lb$. For a path $i$ of length $l_i \geq L$ use the raw end moduli $a_i, b_i$, $q_i = a_i^2 + b_i^2$, priority weights $4q_i$ on interior edges and 1 on end edges, and the weighted products $t_i = l_i R_i e^{\beta l_i}$; omit on each cycle the edge $e_i$ of the path of least $\phi_i$. As in Lemma 6.6, using Lemma 6.4 directly and the decrease of $le^{l/L}2^{-l}$ for $l \geq L$,

$$t_i \leq \tfrac{1}{2}\varepsilon q_i, \qquad t_i/\phi_i \leq \varepsilon^2 q_i, \qquad t_i/(\nu_i(e) w_e^2) \leq 2\varepsilon \quad (e \neq e_i).$$

Over the paths parallel to one edge $xy$ of $G_0$, (6a) at $x$ and $y$ gives $\sum_i t_i \leq \varepsilon$ and $\sum_i t_i/\phi_i \leq 2\varepsilon^2$, and for a fixed matching $N$ the priority weights $\nu_i(e)$ of the paths in this class carrying a unique edge $e$ of $N$ sum to at most $8 + 2 = 10$ (interior edges contribute $4q_i$, and at most two end edges, one at each of $x$ and $y$, lie in $N$).

A cycle of $G$ runs along $m \geq 2$ paths over a closed walk of $G_0$: two parallel paths, or the paths over the edges of a cycle of length $m \geq 3$ of the underlying simple graph. Fix such a closed walk, the slot carrying the charged edge and the slot supplying the omission. If the two slots coincide, the sum over the choices of paths of $\prod t_i/w_e^2$ is at most $10 \cdot 2\varepsilon \cdot \varepsilon^{m-1}$; otherwise the priority rule bounds it by $10 \cdot 2\varepsilon^2 \cdot \varepsilon^{m-2}$. The conversion factor is $2d_k/\prod_i l_i \leq \frac{4}{3}\sum_i l_i/\prod_i l_i \leq \frac{4m}{3L^{m-1}}$ by Lemma 6.3, and $e^{\beta(k-1)} \leq e^{\beta k}$ is absorbed in the $t_i$. So the weighted swap charges of one closed walk sum to at most $m^2 \cdot 20\varepsilon^m \cdot \frac{4m}{3L^{m-1}} = \frac{80}{3}m^3 L b^m$, and the identity charges to at most $2\prod(\sum_i t_i/l_i) \leq 2b^m$. A hub lies on at most $d^{m-1}$ closed walks of length $m \geq 3$ and in at most $d$ parallel classes; an interior vertex lies only on cycles through an end of its path. Hence for every vertex and matching

$$\sum_{C \ni v} f_C(N) e^{\beta(|C|-1)} \leq \frac{27L}{d} \sum_{m \geq 2} m^3 (db)^m \leq \frac{243L}{d}(db)^2,$$

since $db \leq e/8192 < 3/8192$ and consecutive terms have ratio at most $(3/2)^3 db$. As $L^2/d \leq 256$ for every $d \geq 1$, $\frac{243L}{d}(db)^2 \leq \frac{1}{2L} \cdot 486 \cdot 256 \cdot (3/8192)^2 < \frac{1}{2L} \leq 1 - e^{-\beta}$. Lemmas 2.8 and 2.7 complete the proof. □

# 7 High girth and long subdivisions

Theorems 1.6 and 1.7 give universal graphs of every girth; here universality comes from the girth itself, or from long subdivisions of an arbitrary graph. The *girth* of a graph is the length of its shortest cycle.

**Theorem 7.1** (Degree four)**.** *Every graph of maximum degree at most four and girth at least* 197 *is universal. If $B$ is a positive semidefinite matrix with connected support of this kind,* $\operatorname{per} B$ *is a simple eigenvalue of* $\Pi(B)$*.*

**Theorem 7.2** (Bipartite degree caps)**.** *Let $c, d \geq 2$ satisfy $\sqrt{(c-1)(d-1)} < \sqrt{c-1} + \sqrt{d-1}$. There is an explicit $g(c,d)$, given by* (7b) *and computed in Table 1 for the listed pairs, such that every bipartite graph of girth at least $g(c,d)$ whose vertices on the two sides have degrees at most $c$ and $d$ is universal, with a simple top eigenvalue on connected supports. In particular, if a graph of maximum degree $d$ has girth at least $g(2,d)/2$, the graph obtained by subdividing each of its edges once is universal.*

**Theorem 7.3** (Long subdivisions)**.** *Let $G_0$ be a simple graph of maximum degree $\Delta \geq 2$ and any girth, and let $G$ be obtained by replacing each edge of $G_0$ by a path of length at least*

$$L(\Delta) = 20 + \left\lceil \tfrac{1}{6}\log_2 \Delta + \tfrac{2}{3}\log_2(1 + \log_2 \Delta) \right\rceil.$$

*Then $G$ is universal, with a simple top eigenvalue on connected supports.*

**Corollary 7.4.** *The class of universal graphs is closed under subgraphs but not under minors: $K_5$ and $K_5$ minus an edge are not universal, while the graphs obtained from them by replacing every edge by a path of length at least 18 are universal and have them as minors.*

*Proof.* $K_5$ is not universal by Shchesnovich's example [25], whose off-diagonal entries are all nonzero, and $K_5$ minus an edge by Theorem 1.5. Theorem 6.2 with $d = 4$, whose length is $16 + \lceil \log_2 4 \rceil = 18$, applies to their subdivisions. □

## 7.1 Walks and the modulus of a positive semidefinite matrix

Let $W$ be the matrix of moduli, $W_{ij} = w_{ij}$ for $i \neq j$ and $W_{ii} = 0$, of a correlation matrix $B$ whose support has maximum degree at most $\Delta$, and let $\varrho = \varrho(W) > 0$ be its spectral radius. On each component choose a positive Perron vector $h$ and put $p_{vu} = \varrho^{-1} w_{vu} h_u / h_v$, so that $\sum_u p_{vu} = 1$ and $p_{vu} p_{uv} = (w_{uv}/\varrho)^2$. On the space indexed by the ordered pairs $(v, u)$ with $uv$ an edge, let $R$ be the flip $(v, u) \leftrightarrow (u, v)$, let $J$ map $x \in \mathbb{C}^V$ to $(Jx)(v, u) = \sqrt{p_{vu}}\, x_v$, and let $\Sigma = \bigoplus_v \Sigma_v$, where $\Sigma_v$ acts on the pairs at $v$ with zero diagonal and entries $\sqrt{p_{vu} p_{vx}}$, $u \neq x$. For $\ell \geq 1$ let $Q_\ell$ be the matrix whose $(v, u)$ entry is the sum over nonbacktracking walks of length $\ell$ from $v$ to $u$ of the products of the moduli $w$ along the walk, and $Q_0 = I$.

**Lemma 7.5** (Nonbacktracking walks)**.** *$Q_\ell = \varrho^\ell J^* R (\Sigma R)^{\ell-1} J$ and $\|\Sigma_v\| \leq (\deg v - 1)/\deg v$. Hence $\|Q_\ell\| \leq \varrho\, \vartheta^{\ell-1}$ for $\ell \geq 1$, with $\vartheta = \varrho\, \eta$ and $\eta = (\Delta - 1)/\Delta$. If the support is bipartite with degrees at most $c$ and $d$ on the two sides, then $\|Q_\ell\| \leq K \varrho\, \vartheta^{\ell-1}$ with $\vartheta = \varrho \sqrt{\eta_L \eta_R}$, $\eta_L = (c-1)/c$, $\eta_R = (d-1)/d$ and $K = \max(\eta_L, \eta_R)/\sqrt{\eta_L \eta_R}$.*

*Proof.* In $J^* R (\Sigma R)^{\ell-1} J$ the factor $J$ enters an edge with weight $\sqrt{p_{vu}}$, each $R$ crosses an edge, each $\Sigma_u$ turns to a different edge at $u$ with weight $\sqrt{p_{uv} p_{ux}}$, and $J^*$ exits with the last weight; every edge of the walk thus receives $\sqrt{p_{vu} p_{uv}} = w_{uv}/\varrho$, and the zero diagonal of $\Sigma_u$ forbids backtracking. Write $\Sigma_v = a a^{\mathsf{T}} - \mathrm{diag}(p)$ with $a_u = \sqrt{p_{vu}}$; for $\eta_v = (\deg v - 1)/\deg v$, $\eta_v I - \Sigma_v \succeq 0$ is equivalent to $\sum_u p_{vu}/(\eta_v + p_{vu}) \leq 1$, which holds by concavity of $x \mapsto x/(\eta_v + x)$ and $\sum_u p_{vu} = 1$: the sum is at most $\deg v \cdot \frac{1/\deg v}{\eta_v + 1/\deg v} = 1$. As $\Sigma_v$ is symmetric with nonnegative entries, its norm is its largest eigenvalue. Since $\|J\| \leq 1$ and $R$ is unitary, $\|Q_\ell\| \leq \varrho^\ell \eta^{\ell-1}$. In the bipartite case $\Sigma R$ maps the pairs based on one side to the pairs based on the other, so the norm of $(\Sigma R)^{\ell-1}$ is at most the larger of the two alternating products of $\eta_L$ and $\eta_R$, which is at most $K(\eta_L \eta_R)^{(\ell-1)/2}$. □

**Lemma 7.6** (Modulus radius at high girth)**.** *Let $B$ be a correlation matrix whose support has maximum degree at most $\Delta \geq 2$ and girth greater than $2R + 1$, $R \geq 2$. Then*

$$\varrho(W) \leq \frac{\Delta}{2\sqrt{\Delta - 1}\, \cos(\pi/(R+1))}.$$

*Proof.* Put $\delta = \Delta - 1$. Attach to every vertex of degree below $\Delta$ infinite rooted $\delta$-ary trees to obtain a $\Delta$-regular graph $\widehat{\Gamma}$; this creates no new cycles. Let $h \geq 0$ be a Perron vector of $W$, extended by zero. For a vertex $\varpi$ of $\widehat{\Gamma}$ put $f_\varpi(v) = h_v\, b_{\mathrm{dist}(\varpi, v)}$, where $b_0 = 0$, $b_j = \delta^{-j/2} \sin(j\pi/(R+1))$ for $1 \leq j \leq R$ and $b_j = 0$ for $j > R$; only finitely many $f_\varpi$ are nonzero. Balls of radius $R$ in $\widehat{\Gamma}$ induce trees, so $f_\varpi$ is supported on vertices of $\Gamma$ that induce a forest. A positive semidefinite matrix with unit diagonal and forest support can be conjugated by a diagonal unitary matrix to $I - W'$ with $W' \geq 0$ entrywise, so $f_\varpi^{\mathsf{T}} W f_\varpi \leq \|f_\varpi\|^2$. With $s_j = \sin(j\pi/(R+1))$, a vertex $v$ has $\Delta \delta^{j-1}$ vertices of $\widehat{\Gamma}$ at distance $j \leq R$, so $\sum_\varpi \|f_\varpi\|^2 = \frac{\Delta}{\delta} \sum_{j=1}^R s_j^2 \, \|h\|^2$. For an edge $uv$ of $\Gamma$,

the vertices at distance $j$ from $u$ and $j+1$ from $v$ number $\delta^j$, and symmetrically, with no others within distance $R$, by the girth; so $\sum_\varpi f_\varpi^{\mathsf T} W f_\varpi = 2\delta^{-1/2}\sum_{j=1}^{R-1} s_j s_{j+1}\, h^{\mathsf T} W h$. The sine vector satisfies $s_{j-1}+s_{j+1} = 2\cos(\pi/(R+1))s_j$ with $s_0 = s_{R+1} = 0$, so $\sum_j s_j s_{j+1} = \cos(\pi/(R+1))\sum_j s_j^2$. Summing the inequalities and using $h^{\mathsf T} W h = \varrho\|h\|^2$ gives the claim. □

**Lemma 7.7** (Bipartite modulus radius)**.** *Let $B$ be a correlation matrix with bipartite support, of degrees at most $c$ on one side and $d$ on the other, and girth greater than $4m+1$, $m \ge 1$. Then*

$$\varrho(W) \le \frac{\sqrt{cd}}{\sqrt{d-1}+\sqrt{c-1}\cos(\pi/(m+1))},$$

*and the same with $c$ and $d$ interchanged.*

*Proof.* Pad to a $(c,d)$-biregular graph as before and let $z = (c-1)(d-1)$. Take roots $\varpi$ on the $c$-side only. A vertex on the $c$-side has $n_{2j} = cz^j/(c-1)$ roots at distance $2j \ge 2$, and a vertex on the $d$-side has $n_{2j+1} = dz^j$ roots at distance $2j+1$. Put $f_\varpi(v) = h_v\varphi_t/\sqrt{n_t}$ with $t = \operatorname{dist}(\varpi, v)$, $\varphi_0 = 0$, $\varphi_{2j-1} = \varphi_{2j} = s_j = \sin(j\pi/(m+1))$ for $1 \le j \le m$ and $\varphi_t = 0$ for $t > 2m$. The supports induce forests by the girth. For a Perron vector the two sides carry equal mass $\|h_L\|^2 = \|h_R\|^2$, from the coupled equations $Xh_R = \varrho h_L$, $X^{\mathsf T} h_L = \varrho h_R$, so $\sum_\varpi \|f_\varpi\|^2 = \|h\|^2\sum_j s_j^2$. Across an edge $uv$ with $u$ on the $c$-side there are $z^j$ roots at distances $(2j, 2j+1)$ and $(d-1)z^j$ at distances $(2j+2, 2j+1)$ from $(u,v)$, and after the normalization these contribute the coefficients $a_{2j} = \sqrt{(c-1)/(cd)}$ and $a_{2j+1} = \sqrt{(d-1)/(cd)}$ to the pairs $(\varphi_{2j}, \varphi_{2j+1})$ and $(\varphi_{2j+1}, \varphi_{2j+2})$. Hence $\sum_\varpi f_\varpi^{\mathsf T} W f_\varpi = \varrho\|h\|^2(a_{\mathrm{odd}}\sum_j s_j^2 + a_{\mathrm{even}}\sum_j s_j s_{j+1})$, and the inequalities $f_\varpi^{\mathsf T} W f_\varpi \le \|f_\varpi\|^2$ give $\varrho(\sqrt{(d-1)/(cd)} + \sqrt{(c-1)/(cd)}\cos(\pi/(m+1))) \le 1$. □

*Remark* 7.8. The constant of Lemma 7.6 is the best possible as $R \to \infty$ on any family of $\Delta$-regular bipartite graphs of girth tending to infinity. Marcus, Spielman and Srivastava show that every graph has a signing whose adjacency eigenvalues are at most the spectral radius of its universal cover [15]; for a bipartite graph the spectrum of a signing is symmetric, so $B = I - A_s/(2\sqrt{\Delta-1})$ is positive semidefinite with $\varrho(W) = \Delta/(2\sqrt{\Delta-1})$. The same construction with $\sqrt{c-1}+\sqrt{d-1}$ gives $\varrho(W) = \sqrt{cd}/(\sqrt{c-1}+\sqrt{d-1})$ on $(c,d)$-biregular graphs, the limit of Lemma 7.7; such graphs of large girth are obtained by subdividing $d$-regular graphs of large girth when $c = 2$. For $\Delta \ge 3$ these values exceed one, so the matrices covered by Theorems 7.1 and 7.2 include matrices that are not diagonally dominant after any diagonal scaling.

## 7.2 Proofs of the high-girth theorems

In this section and in Theorem 7.3 every packet uses an edge of smallest modulus as its omitted edge $a_C$ and the constants $d_e = k-1$ of Lemma 2.5. Let $B$ be a correlation matrix whose support has girth $g$ and maximum degree at most $\Delta$, let $C$ be an eligible cycle of length $k$ through a vertex $v$, and remove the two edges $e, a_C$ of (2a). Traversing $C$ from $v$ in one direction, the remaining edges form three nonbacktracking walks of lengths $\ell_1, \ell_2, \ell_3 \ge 0$ with $\ell_1+\ell_2+\ell_3 = k-2$, joined by the two removed edges. Let $D$ be the 0–1 adjacency matrix of the support. The product $\prod_{b\ne e,a_C} w_b$ is one of the terms of the diagonal entry $(Q_{\ell_1} D Q_{\ell_2} D Q_{\ell_3})_{vv}$, and there are $\binom{k}{2}$ triples $(\ell_1,\ell_2,\ell_3)$. All terms are nonnegative, so

$$\sum_{C\ni v} F_C e^{\beta(|C|-1)} \le \sum_{k\ge g} k(k-1)^2\, \mathcal{M}\, \vartheta^{k-5} e^{\beta(k-1)}, \qquad F_C = 2(k-1)\prod_{b\ne e,a_C} w_b, \tag{7a}$$

where $\mathcal{M} = \max(1, K\varrho)^3\|D\|^2$ and $\|Q_\ell\| \le \max(1, K\varrho)\vartheta^{\ell-1}$ for all $\ell \ge 0$ when $\vartheta < 1$ (with $K = 1$ outside the bipartite case), by Lemma 7.5.

*Proof of Theorem 7.1.* By Lemma 2.2 let $B$ be a correlation matrix; if $W = 0$ there is nothing to prove. Padding to degree four, Lemma 7.6 with $\Delta = 4$ and $R = 87$ (girth $197 > 175$) gives $\varrho \le 1.15544$ and $\vartheta = \frac{3}{4}\varrho \le 0.86658$, and $\|D\| \le 4$. With $e^{\beta} = 1 + 1/190$, the right side of (7a) at $g = 197$ is less than $1 - e^{-\beta}$; this is checked in interval arithmetic by `verify_m5_constants.py`, using $\sum_{k\ge g} k(k-1)^2 y^k \le g^3 y^g/(1 - y(1 + 1/g)^3)$ for $y = \vartheta e^{\beta}$. Lemma 2.8 gives $\gamma_{\mathcal{A}}(N) > 0$ for all $(\mathcal{A}, N)$, and Lemma 2.7 completes the proof. □

With the cruder choices $R = 8$ and $e^{\beta} = 65/64$ the same computation succeeds from girth 440.

*Proof of Theorem 7.2.* By the hypothesis, $\sqrt{(c-1)(d-1)}/(\sqrt{c-1} + \sqrt{d-1}) < 1$, which is the limit as $m \to \infty$ of the bound for $\vartheta = \varrho\sqrt{\eta_L \eta_R}$ given by Lemma 7.7. Fix $m$ with $\vartheta_m < 1$, put $\mathcal{M} = \max(1, K\varrho_m)^3 cd$ (Schur's test gives $\|D\|^2 \le cd$), and let $g(c, d)$ be the least even $g \ge 4m + 2$ for which some $\beta > 0$ satisfies

$$\mathcal{M}\,\vartheta_m^{-5} e^{-\beta} \sum_{k\ge g} k(k-1)^2 (\vartheta_m e^{\beta})^k \le 1 - e^{-\beta}, \tag{7b}$$

with $m$ and $\beta$ chosen to make $g$ small. Then Lemmas 2.8 and 2.7 apply as before. For the last statement, the once-subdivided graph is bipartite with degree caps 2 and $d$ and has twice the girth. □

| $d$ | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $g(2,d)$ | 32 | 44 | 52 | 60 | 68 | 74 | 82 | 88 | 94 | 98 | 104 |
| $g(3,d)$ | | 70 | 104 | 146 | 202 | 280 | 396 | 580 | 918 | 1714 | 5262 |
| $g(4,d)$ | | | 198 | 432 | 1588 | | | | | | |

Table 1: Girths $g(c, d)$ certified in Theorem 7.2. The criterion holds for $c = 2$ and every $d$, for $c = 3$ and $d \le 12$, and for $c = 4$ and $d \le 6$, and fails for $(5, 5)$.

*Proof of Theorem 7.3.* Let $B$ be a correlation matrix with support in $G$. Every simple cycle of $G$ replaces the edges of a cycle of $G_0$ of length $m \ge 3$ by their paths, so its length is $k \ge Lm$. For a base vertex $u$ and a base edge $e \ni u$ let $a_{u,e}$ be the modulus of the first edge of the path of $e$ at $u$. The first vertices of these paths are pairwise nonadjacent, so the principal submatrix on $u$ and them gives $\sum_{e\ni u} a_{u,e}^2 \le 1$.

*Paths.* If the vertices of a path of $\ell$ edges induce a path in $G$, the principal submatrix is a tridiagonal correlation matrix, which after a diagonal unitary conjugation is $I - W'$ with $W' \ge 0$ and $\varrho(W') \le 1$. With a Perron vector $h'$ and $p_{ij} = w_{ij} h'_j / h'_i$ (so $\sum_j p_{ij} \le 1$ and $w_{ij}^2 = p_{ij} p_{ji}$), the product of the squared moduli is a product over the vertices, in which each internal vertex contributes $p_{t,t-1} p_{t,t+1} \le 1/4$; so the product of the moduli is at most $2^{1-\ell}$. Now let $C$ be eligible and remove its two edges $e$ and $a_C$ (in the identity case, no edges). On the path of a base edge of length $\ell$ carrying $q \in \{0, 1, 2\}$ removed edges, keep the two end factors $a_{u,e}, a_{v,e}$ that are not removed; the other edges form at most $q + 1$ induced runs with at least $\ell - 2 - q$ edges in all, so their product is at most $2^{3+2q-\ell}$. Over the $m$ paths of $C$, $f_C(N) \le 2(k-1)\, 2^{3m+4-k}\, \mathcal{E}_C$, where $\mathcal{E}_C$ is the product of the kept end factors.

*Transfers.* On the base vertices let $W_0$ have entries $a_{u,e} a_{v,e}$ for $e = uv$; by $2a_{u,e}a_{v,e}|x_u x_v| \le a_{u,e}^2 |x_u|^2 + a_{v,e}^2 |x_v|^2$, $\|W_0\| \le 1$. The transfer with the end at $u$ removed, $(E_1)_{uv} = a_{v,e}$, has norm at most $\sqrt{\Delta}$ by the Cauchy–Schwarz inequality on each row. Fix the matching $N$. The transfer $(E_N)_{uv} = a_{v,e}$ if the first edge of the path of $e = uv$ at $u$ lies in $N$, and 0 otherwise, has at most one entry in each row, as $N$ is a matching, and squared column sums at most one, so $\|E_N\| \le 1$;

the 0–1 matrix $(E_{NN})_{uv} = 1$ under the same condition has at most one entry in each row and at most $\Delta$ in each column, so $\|E_{NN}\| \le \sqrt{\Delta}$. Transposes have the same norms. Write $C$ as a closed walk of length $m$ in $G_0$ through a base vertex $u_0$: if $v$ is a base vertex take $u_0 = v$, and otherwise one end of the path containing $v$, which every cycle through $v$ contains. Then $\mathcal{E}_C$ is a term of the diagonal entry at $u_0$ of a product of $m$ transfers: $W_0$ at paths whose ends are both kept; $E_N$ or $E_1$ (suitably oriented) where only the end edge $e \in N$, respectively only $a_C$, is removed; and $E_{NN}$ where both ends of one path are removed, which requires one of them to be $e \in N$. In each case the product of the norms is at most $\sqrt{\Delta}$. The type of a term is the choice of no removal, or of the positions of $e$ and $a_C$ on the walk together with a label (interior, first end, last end) for each, so there are at most $1 + 9m(m-1) + 9m \le 32m^2$ types.

*Site sum.* Take $\beta = 1/L$. For $k \ge Lm$, $L \ge 20$ and $m \ge 3$, the function $k \mapsto ke^{(k-1)/L}2^{-k}$ decreases, so $2(k-1)2^{3m+4-k}e^{\beta(k-1)} \le 32Lm(8e\,2^{-L})^m$. Summing over the types,

$$\sum_{C \ni v} F_C e^{\beta(|C|-1)} \le 1024\sqrt{\Delta}\,L \sum_{m \ge 3} m^3 x^m, \qquad x = 8e\,2^{-L}.$$

For $x \le 1/2$, $\sum_{m\ge3} m^3x^m \le x^3 \sum_{m\ge3} m^3 2^{-(m-3)} = 188x^3$, and $1 - e^{-1/L} \ge 1/(2L)$. With $t = \log_2 \Delta$ we have $L \le 22(1+t)$ and $\sqrt{\Delta}\,2^{-3L} \le 2^{-60}(1+t)^{-2}$, so $2 \cdot 1024 \cdot 188\,(8e)^3\sqrt{\Delta}\,L^2\,2^{-3L} \le 2048 \cdot 188 \cdot (8e)^3 \cdot 22^2 \cdot 2^{-60} < 2 \cdot 10^{-6}$. The site criterion holds for every $(\mathcal{A}, N)$, and Lemmas 2.8 and 2.7 complete the proof. □

*Remark* 7.9. The choice of the removed edge matters. Replace each edge of $K_{2,m+1}$ by a path of length $L \ge 2$, so that the two hubs are joined by $m+1$ paths of length $P = 2L$; give every internal edge the modulus $1/8$, except one internal edge $e$ of one path, which gets $1/(4\sqrt{m})$, give the end edges of that path the modulus $1/8$ and those of the other $m$ paths the modulus $1/(8\sqrt{m})$, and take all off-diagonal entries real and nonnegative. For $m > 4$ the matrix of moduli has norm at most $1/4 + \sqrt{2}/8 < 1$, so $I + W$ is a correlation matrix, permanent-on-top by Lemma 2.2(v). For $N = \{e\}$ every cycle through the distinguished path is eligible with charge $2(2P-1)r_C/w_e^2$, no two cycles are disjoint, since all of them contain the hubs, and so $\gamma_\varnothing(\{e\}) \le 1 - (2P-1)8^{3-2P}\sqrt{m}/8$, which is negative for large $m$. So with the weakest-edge rule the allocation needs a length that grows with the degree, as in Theorem 7.3.

# 8 Obstructions

*Proof of Theorem 1.5.* Direct multiplication gives

$$B_5 = \begin{pmatrix} 1 & 0 & 2 & 4 & 2 \\ 0 & 1 & -1+i & 5 & -1-i \\ 2 & -1-i & 6 & 3-5i & 4+2i \\ 4 & 5 & 3+5i & 41 & 3-5i \\ 2 & -1+i & 4-2i & 3+5i & 6 \end{pmatrix},$$

which is positive semidefinite of rank two, with the single vanishing off-diagonal pair $\{1, 2\}$. The largest independent set of $K_5$ minus an edge has two vertices, so its vertex-cover number is three. Order the 2-subsets lexicographically, $12, 13, \ldots, 45$, and let

$$x = (0,\ -1,\ 2,\ -1,\ 2+i,\ -4,\ 2-i,\ 1-i,\ -1,\ 1+i)^{\mathsf{T}}.$$

Exact Gaussian-integer arithmetic (Section 13) gives $\operatorname{per} B_5 = 10464$, $x^*x = 37$ and $x^*C_2(B_5)x = 400112$, and $400112 - 37 \cdot 10464 = 12944 > 0$. By Lemma 2.4, $\lambda_{\max}(\Pi(B_5)) \ge 400112/37 > \operatorname{per} B_5$.

For $k \geq 3$ let $G_k$ be the disjoint union of $K_5$ minus an edge and $k-3$ disjoint edges. Then $\tau(G_k) = k$, and $G_k$ is not universal, since it contains $K_5$ minus an edge and every subgraph of a universal graph is universal. Every graph with $\tau \leq 2$ is universal by Theorem 1.4. □

*Remark* 8.1. The top eigenvalue of $C_2(B_5)$ is about 10959.06, and it is the top eigenvalue of $\Pi(B_5)$, attained in the block of the partition $(3,2)$: as in the proof of Theorem 1.9, the blocks of partitions with more than two rows vanish because $B_5$ has rank two, and the other three occur in $N_2$. Hence $\lambda_{\max}(\Pi(B_5))/\operatorname{per} B_5 \approx 1.0473$. The block $(4,1)$ has top eigenvalue about $8895.90 < \operatorname{per} B_5$, so $B_5$ satisfies $\lambda_{\max}(C_1(B_5)) \leq \operatorname{per} B_5$, the inequality of Bapat and Sunder's question on $C_1$ [2], while $C_2(B_5)$ violates Pate's conjecture $\lambda_{\max}(C_k(A)) \leq \operatorname{per} A$ [21] for $k = 2$. A local search over rank-two matrices supported on $K_5$ minus an edge reaches the ratio 1.0609 (Section 13).

*Proof of Theorem 1.9.* Positive diagonal congruence (Lemma 2.2(i)) lets us work with the unnormalized vectors $(1,0)$, $(0,1)$, $(1,\pm 1)$, $(1,\pm i)$, the columns of

$$X_6 = \begin{pmatrix} 1 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & -1 & i & -i \end{pmatrix}, \qquad B_6 = X_6^* X_6 = \begin{pmatrix} 1 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & -1 & i & -i \\ 1 & 1 & 2 & 0 & 1+i & 1-i \\ 1 & -1 & 0 & 2 & 1-i & 1+i \\ 1 & -i & 1-i & 1+i & 2 & 0 \\ 1 & i & 1+i & 1-i & 0 & 2 \end{pmatrix},$$

and $A = D^{-1/2} B_6 D^{-1/2}$ with $D = \operatorname{diag}(B_6)$, so that $\Pi(A) = \Pi(B_6)/16$ and $\operatorname{per} A = \operatorname{per} B_6/16$. The vanishing off-diagonal pairs are exactly $\{1,2\},\{3,4\},\{5,6\}$, so $\Gamma(A) = K_{2,2,2}$. Exact computation gives $\operatorname{per} B_6 = 240$. Let $x$ be the vector indexed by the 3-subsets of $[6]$ with $x_J = -3(-1)^{|J \cap \{2,4,6\}|}$ when $J$ meets each of $\{1,2\},\{3,4\},\{5,6\}$ once, and, when $J$ contains one of these pairs and one further vertex $c$,

$$x_J = \begin{cases} i & J = \{1,2,c\},\ c \in \{3,4\},\ \text{or } J = \{3,4,c\},\ c \in \{5,6\},\ \text{or } J = \{5,6,c\},\ c \in \{1,2\}, \\ -i & \text{otherwise.} \end{cases}$$

Then $C_3(B_6)x = 336\,x$ exactly, so by Lemma 2.4 $\lambda_{\max}(\Pi(A)) \geq 336/16 = 21 > 15 = \operatorname{per} A$.

The value 21 is the top eigenvalue. Let $\eta_1, \ldots, \eta_6 \in \mathbb{C}^2$ be the six unit vectors, so $a_{jk} = \langle \eta_j, \eta_k \rangle$. Then $\Pi(A)_{\sigma,\tau} = \langle w_\sigma, w_\tau \rangle$ with $w_\sigma = \eta_{\sigma(1)} \otimes \cdots \otimes \eta_{\sigma(6)}$, so $\Pi(A) = W^*W$ for the map $W : e_\sigma \mapsto w_\sigma$ into $(\mathbb{C}^2)^{\otimes 6}$. Since $w_{\sigma\pi}$ is $w_\sigma$ with its tensor factors permuted by $\pi$, $W$ intertwines the right regular representation with the action of $S_6$ on tensor positions. By Schur–Weyl duality [9, Lecture 6], only partitions with at most two rows occur in $(\mathbb{C}^2)^{\otimes 6}$, so $W$, and with it $\Pi(A)$, vanishes on the isotypic components of all other partitions. The four partitions $(6),(5,1),(4,2),(3,3)$ with at most two rows each occur exactly once in $N_3$ by Young's rule [22], since the corresponding Kostka numbers for content $(3,3)$ equal one. Finally, the polynomial $t(t-96)(t-144)(t-240)(t-336)$ annihilates $C_3(B_6)$ and the traces of its first four powers fix the multiplicities, so the characteristic polynomial of $C_3(B_6)$ is $t^{10}(t-96)^2(t-144)^3(t-240)^4(t-336)$. Hence $\lambda_{\max}(\Pi(A)) = 336/16 = 21$. □

*Remark* 8.2. The block of the partition $(3,3)$ has rank one, and its eigenvalue 21 is the immanant $\operatorname{Imm}_{(3,3)}(A)$, which Lemma 9.1 evaluates by hand. For a rank-two matrix of order $2k$ the same lemma shows that permanent-on-top requires the unnormalized inequality $\operatorname{Imm}_{(k,k)}(A) \leq \operatorname{per} A$, much stronger than Lieb's normalized $\operatorname{Imm}_{(k,k)}(A) \leq f^{(k,k)} \operatorname{per} A$. Heuristically, pairs of orthogonal Gram vectors, which are the zeros of the matrix, move the product tensor towards the $SU(2)$-invariant sector of shape $(k,k)$ and away from the symmetric sector that carries the permanent; in Theorem 1.9 all three pairs are orthogonal.

Deleting an edge of the octahedron does not restore the property.

**Proposition 8.3.** *The octahedron $K_{2,2,2}$ with one edge deleted is not universal.*

*Proof.* The certificate is exact and computer-assisted. Label the octahedron so that its non-adjacent pairs are $\{1,2\},\{3,4\},\{5,6\}$, and delete the edge 13. Take six vectors $x_1,\dots,x_6 \in \mathbb{Q}(i)^3$ with coordinates in $10^{-6}\mathbb{Z}[i]$, rounded from a numerical local maximizer of $\lambda_{\max}(\Pi)/\operatorname{per}$, and replace $x_2$, $x_3$, $x_4$, $x_6$ by their exact orthogonal projections away from $x_1$, $x_1$, $x_3$, $x_5$ respectively. The Gram matrix $B = X^*X$ is positive semidefinite, its vanishing off-diagonal pairs are exactly $\{1,2\},\{1,3\},\{3,4\},\{5,6\}$, and all other off-diagonal entries are nonzero, so its support is the octahedron minus the edge 13. An explicit vector $y$ indexed by 3-subsets, with coordinates in $10^{-6}\mathbb{Z}[i]$, satisfies $y^*C_3(B)y > \operatorname{per}(B)\, y^*y$ in exact rational arithmetic, with Rayleigh ratio about 1.000686 per $B$. Lemma 2.4 completes the proof. The data are listed in Appendix A, and the check is `verify_octahedron_minus_edge.py` (Section 13). □

# 9 Rectangular blocks and random Gram matrices

For Gram matrices of low rank some irreducible blocks of the Schur power have rank one, and then the block eigenvalue is an immanant. This explains the value 21 in Theorem 1.9 and leads to a probabilistic form of permanent-on-top on such a block.

A partition $(m^r)$ has $r$ parts equal to $m$. For $V \in \mathbb{C}^{r\times N}$ and $A \subseteq [N]$ with $|A| = r$, write $V_A$ for the $r \times r$ submatrix with the columns in $A$, in increasing order.

**Lemma 9.1** (Rectangular blocks)**.** *Let $N = mr$, let $V \in \mathbb{C}^{r\times N}$ have columns $v_1,\dots,v_N$, and let $B = V^*V$. The block $T_B^\rho$ of the irreducible representation $\rho$ of the partition $(m^r)$ has rank at most one. Hence its largest eigenvalue is*

$$\Upsilon_{(m^r)}(B) = \operatorname{Imm}_{(m^r)}(B) = \sum_{(A_1,\dots,A_m)} \prod_{i=1}^{m} |\det V_{A_i}|^2,$$

*where the sum runs over the ordered partitions of $[N]$ into $m$ sets of size $r$.*

*Proof.* Let $S_N$ act on $(\mathbb{C}^r)^{\otimes N}$ by $P_\pi(y_1\otimes\cdots\otimes y_N) = y_{\pi^{-1}(1)}\otimes\cdots\otimes y_{\pi^{-1}(N)}$, and put $w = v_1\otimes\cdots\otimes v_N$. Then $\langle w, P_\sigma w\rangle = \prod_j b_{j,\sigma^{-1}(j)} = b_{\sigma^{-1}}$. By Schur–Weyl duality [9, Lecture 6], $(\mathbb{C}^r)^{\otimes N} = \bigoplus_\nu S_\nu(\mathbb{C}^r)\otimes S^\nu$, and for $\nu = \lambda := (m^r)$ the factor $S_\lambda(\mathbb{C}^r)$ is the one-dimensional representation $\det^m$ of $GL_r$. Let $H$ be the $\lambda$-isotypic component and $E$ the orthogonal projection onto it; $H$ is an irreducible representation of $S_N$.

*Rank.* As in the proof of Theorem 1.9, $\Pi(B) = W^*W$ with $W : e_\sigma \mapsto v_{\sigma(1)}\otimes\cdots\otimes v_{\sigma(N)}$, and $W$ intertwines the right regular representation with $P$. The $\lambda$-isotypic part of $\Pi(B)$ consists of $f^\lambda$ copies of $T_B^\rho$ and is mapped by $W$ into $H$, of dimension $f^\lambda$. Hence $f^\lambda \operatorname{rank} T_B^\rho \le f^\lambda$. As $T_B^\rho \succeq 0$ (Lemma 2.1(iv)), its largest eigenvalue is its trace $\sum_\sigma \chi_\lambda(\sigma) b_\sigma = \operatorname{Imm}_\lambda(B)$.

*Formula.* The character $\chi_\lambda$ is real and constant on conjugacy classes, so $\sum_\sigma \chi_\lambda(\sigma) P_\sigma = (N!/f^\lambda)E$, and

$$\operatorname{Imm}_\lambda(B) = \sum_\sigma \chi_\lambda(\sigma)\langle w, P_\sigma w\rangle = \frac{N!}{f^\lambda}\,\|Ew\|^2.$$

Let $\varepsilon = (r!)^{-1/2}\sum_{\pi\in S_r}\operatorname{sgn}(\pi)\, e_{\pi(1)}\otimes\cdots\otimes e_{\pi(r)}$, a unit vector, and for an ordered partition $\mathcal{A} = (A_1,\dots,A_m)$ let $a_\mathcal{A}$ be the tensor carrying a copy of $\varepsilon$ on the positions of each $A_i$. Then $\|a_\mathcal{A}\| = 1$, $g^{\otimes N}a_\mathcal{A} = (\det g)^m a_\mathcal{A}$ for $g \in GL_r$, so $a_\mathcal{A} \in H$, and $\langle a_\mathcal{A}, w\rangle = (r!)^{-m/2}\prod_i \det V_{A_i}$. The operator

$F = \sum_{\mathcal{A}} a_{\mathcal{A}} a_{\mathcal{A}}^*$ commutes with every $P_\pi$, because $P_\pi a_{\mathcal{A}} = \pm a_{\pi\mathcal{A}}$ and $\mathcal{A} \mapsto \pi\mathcal{A}$ permutes the ordered partitions. It vanishes on $H^\perp$ and maps $H$ into itself, so Schur's lemma gives $F = cE$, and comparing traces gives $cf^\lambda = N!/(r!)^m$, the number of ordered partitions. Therefore

$$\sum_{\mathcal{A}} \frac{\prod_i |\det V_{A_i}|^2}{(r!)^m} = \langle w, Fw\rangle = c\|Ew\|^2 = \frac{N!}{(r!)^m f^\lambda}\|Ew\|^2 = \frac{\mathrm{Imm}_\lambda(B)}{(r!)^m},$$

which is the formula. □

For the octahedral matrix of Theorem 1.9 ($m = 3$, $r = 2$) the lemma gives the value 21 by hand. For unit vectors $|\det(\eta_i, \eta_j)|^2 = 1 - |a_{ij}|^2$, which is 1 on the three orthogonal pairs and $1/2$ on the other twelve pairs. Ordered partitions into three pairs are the 3! orderings of the 15 perfect matchings of $K_6$. The matching of the orthogonal pairs contributes 1, each of the six matchings containing exactly one orthogonal pair contributes $1/4$, and each of the remaining eight contributes $1/8$. Hence $\mathrm{Imm}_{(3,3)}(A) = 6(1 + 6/4 + 8/8) = 21$.

From now on $m = 2$ and $r = n$, so $N = 2n$, and we write

$$\Upsilon = \Upsilon_{(2^n)}(B) = \sum_{|A|=n} |\det V_A|^2\, |\det V_{A^c}|^2.$$

If $V = [I_n\ I_n]$, two copies of an orthonormal basis, then $\Upsilon = \operatorname{per} B = 2^n$; so on this block the permanent-on-top inequality $\Upsilon \le \operatorname{per} B$ can hold with equality. We compare $\Upsilon$ with $\operatorname{per} B$ for random frames of $2n$ unit vectors in $\mathbb{F}^n$, where $\mathbb{F} = \mathbb{R}$ or $\mathbb{C}$, in two models.

- *Two bases:* $V = [I_n\ U]$ with $U$ Haar distributed in the orthogonal group ($\mathbb{F} = \mathbb{R}$) or the unitary group ($\mathbb{F} = \mathbb{C}$). Then $B = \begin{pmatrix} I & U \\ U^* & I \end{pmatrix}$ is supported on the complete bipartite graph $K_{n,n}$.
- *Independent columns:* the $2n$ columns of $V$ are independent and uniform on the unit sphere of $\mathbb{F}^n$.

Put $b_0 = 3\log 3 - 2 - 2\gamma \approx 0.1414$, where $\gamma$ is Euler's constant.

**Theorem 9.2** (Random Gram matrices)**.** *(a) For two bases,* $\mathbb{E}\Upsilon = (n+2)(n+3)/6$ *over* $\mathbb{C}$ *and* $\mathbb{E}\Upsilon = (n+3)(n+4)(n+5)/60$ *over* $\mathbb{R}$*. For independent columns,* $\mathbb{E}\Upsilon = \binom{2n}{n}(n!/n^n)^2$ *over either field.*

*(b) Fix* $a$ *with* $0 < a < b_0$ *for two bases, or* $0 < a < b_0 + 2 - \log 4$ *for independent columns. There are constants* $C_a \ge c_a > 0$ *such that for all sufficiently large* $n$

$$e^{-C_a n^2} \le \mathbb{P}\{\Upsilon \ge e^{-an} \operatorname{per} B\} \le e^{-c_a n^2}.$$

*In particular the event* $\Upsilon > \operatorname{per} B$*, on which permanent-on-top fails on the block* $(2^n)$*, has probability at most* $e^{-c_a n^2}$*.*

*(c) Almost surely* $n^{-1}\log\Upsilon \to 0$ *for two bases and* $n^{-1}\log\Upsilon \to \log 4 - 2$ *for independent columns, under any coupling of the models in different dimensions.*

The two exponents in (b) are both of order $n^2$; the constants $c_a$ and $C_a$ are not equal.

## 9.1 Two permanent bounds

For any unit vectors $v_1, \dots, v_{2n} \in \mathbb{F}^n$, Wick's formula for a standard complex Gaussian vector $g$ in $\mathbb{C}^n$ ($\mathbb{E} g g^* = I$) gives $\operatorname{per} B = \mathbb{E} \prod_{j=1}^{2n} |v_j^* g|^2$, since $\mathbb{E}(v_i^* g)\overline{(v_j^* g)} = b_{ij}$. Write $g = R\theta$ with $\theta$ uniform on the unit sphere of $\mathbb{C}^n$ and $R^2$ a Gamma$(n)$ variable independent of $\theta$, so that $\mathbb{E} R^{4n} = \Gamma(3n)/\Gamma(n)$. Each $|v_j^* \theta|^2$ has the Beta$(1, n-1)$ law, with logarithmic mean $\psi(1) - \psi(n) = -H_{n-1}$, where $H_{n-1} = \sum_{j<n} 1/j$. Jensen's inequality for the logarithm gives

$$\operatorname{per} B \;\geq\; \frac{\Gamma(3n)}{\Gamma(n)}\, e^{-2nH_{n-1}} = e^{(b_0 + o(1))n}. \tag{9a}$$

Products of linear forms on the complex sphere and their relation to permanents of positive semidefinite matrices are studied by Yuan and Parrilo [31].

For two bases, $B$ is supported on $K_{n,n}$, and grouping permutations by the sets $I$ and $J$ of moved vertices on the two sides gives $\operatorname{per} B = \sum_{k=0}^{n} \sum_{|I|=|J|=k} |\operatorname{per} U[I,J]|^2$. For a fixed $k$-set $I$, let $u_i$ be the rows of $U$ and $T = \bigotimes_{i \in I} u_i \in (\mathbb{C}^n)^{\otimes k}$. Its symmetrization has squared norm $\frac{1}{k!} \sum_\pi \prod_t \langle u_{i_t}, u_{i_{\pi(t)}} \rangle = \frac{1}{k!}$, and its inner product with the unit symmetric tensor indexed by a $k$-set $J$ has squared modulus $|\operatorname{per} U[I,J]|^2/k!$. These unit tensors are orthonormal, so $\sum_J |\operatorname{per} U[I,J]|^2 \leq 1$, and

$$\operatorname{per} B \leq \sum_{k=0}^{n} \binom{n}{k} = 2^n. \tag{9b}$$

In the formula of Lemma 9.1, $V_A = [e_S, U_T]$ for $A = S \cup (n + T)$ with $S, T \subseteq [n]$; the Laplace expansion along the columns $e_S$ and Jacobi's complementary-minor identity for the unitary (or orthogonal) matrix $U$ give

$$\Upsilon = \sum_{k=0}^{n} \sum_{|I|=|J|=k} |\det U[I,J]|^4. \tag{9c}$$

In particular $\Upsilon \geq 2$, from $k = 0$ and $k = n$.

## 9.2 Moments

Put $\varkappa = 1$ over $\mathbb{C}$ and $\varkappa = 2$ over $\mathbb{R}$. In the two-bases model let $d = |\det U[I,J]|^2$ for fixed $k$-sets $I, J$. For integers $s \geq 1$,

$$\mathbb{E} d^s = \prod_{j=0}^{s-1} \frac{\binom{k+\varkappa j}{k}}{\binom{n+\varkappa j}{k}}. \tag{9d}$$

Indeed, let $\mathcal{G}$ be an $n \times k$ standard Gaussian matrix over $\mathbb{F}$ and $\mathcal{G}_0$ its first $k$ rows. The factor $Q = \mathcal{G}(\mathcal{G}^*\mathcal{G})^{-1/2}$ is uniform on the isometries $\mathbb{F}^k \to \mathbb{F}^n$ and independent of $\mathcal{G}^*\mathcal{G}$, by invariance under left multiplication. Its first $k$ rows have the law of $U[I,J]$, and $|\det \mathcal{G}_0|^2 = |\det Q_0|^2 \det(\mathcal{G}^*\mathcal{G})$. By Gram–Schmidt, $|\det \mathcal{G}_0|^2$ and $\det \mathcal{G}^*\mathcal{G}$ are products of independent Gamma variables with shapes $(k-i+1)/\varkappa$ and $(n-i+1)/\varkappa$, $1 \leq i \leq k$, and a common scale. Dividing the $s$-th moments gives $\prod_{i=1}^{k} \frac{\Gamma((k-i+1)/\varkappa + s)\Gamma((n-i+1)/\varkappa)}{\Gamma((k-i+1)/\varkappa)\Gamma((n-i+1)/\varkappa + s)}$, which equals (9d).

With $s = 2$ and the $\binom{n}{k}^2$ minors of size $k$, $Z_k = \sum_{|I|=|J|=k} |\det U[I,J]|^4$ has

$$\mathbb{E} Z_k = \frac{\binom{n}{k}\binom{k+\varkappa}{\varkappa}}{\binom{n+\varkappa}{k}} = \frac{\binom{k+\varkappa}{\varkappa}\binom{n-k+\varkappa}{\varkappa}}{\binom{n+\varkappa}{\varkappa}},$$

and the Chu–Vandermonde identity $\sum_k \binom{k+\varkappa}{\varkappa}\binom{n-k+\varkappa}{\varkappa} = \binom{n+2\varkappa+1}{2\varkappa+1}$ gives $\mathbb{E}\Upsilon = \binom{n+2\varkappa+1}{2\varkappa+1}/\binom{n+\varkappa}{\varkappa}$, the two polynomials of Theorem 9.2(a).

For independent columns and a fixed $n$-set $A$, Gram–Schmidt writes $d = |\det V_A|^2$ as a product of independent $\mathrm{Beta}(j/\varkappa, (n-j)/\varkappa)$ variables, $1 \le j \le n$ (the factor $j = n$ is the constant 1): conditionally on the span of the earlier columns, the squared length of the next column's component orthogonal to it has this law, and the law does not depend on the span. Hence

$$\mathbb{E}d^s = \prod_{i=0}^{s-1} \prod_{j=1}^{n} \frac{j + \varkappa i}{n + \varkappa i}, \qquad \mathbb{E}\Upsilon = \binom{2n}{n} (\mathbb{E}d)^2 = \binom{2n}{n} \Big(\frac{n!}{n^n}\Big)^2, \tag{9e}$$

using the independence of $V_A$ and $V_{A^c}$.

### 9.3 Upper tails

*Two bases.* For an integer $s \ge 1$ the power-mean inequality over the $n+1$ levels and over the $\binom{n}{k}^2$ minors of each level gives

$$\mathbb{E}\Upsilon^s \le (n+1)^s \max_k \binom{n}{k}^{2s} \mathbb{E}d^{2s} \le (n+1)^s \prod_{j=0}^{2s-1} \frac{(n + 2\varkappa s)^{\varkappa j}}{(\varkappa j)!},$$

because $\binom{n}{k} \le \binom{n+\varkappa j}{k}$ and $\binom{k+\varkappa j}{k} = \binom{k+\varkappa j}{\varkappa j} \le (n+2\varkappa s)^{\varkappa j}/(\varkappa j)!$ for $k \le n$ and $j < 2s$. Take $s = \lfloor \epsilon n \rfloor$. Since $\sum_{j<t} \log((\varkappa j)!) = \frac{\varkappa t^2}{2} \log(\varkappa t) - \frac{3\varkappa t^2}{4} + o(t^2)$,

$$\limsup_{n\to\infty} \frac{\log \mathbb{E}\Upsilon^s}{n^2} \le 2\varkappa\epsilon^2 \Big[ \log \frac{1 + 2\varkappa\epsilon}{2\varkappa\epsilon} + \frac{3}{2} \Big],$$

which is $o(\epsilon)$ as $\epsilon \downarrow 0$. By (9a) and Markov's inequality,

$$\mathbb{P}\{\Upsilon \ge e^{-an} \operatorname{per} B\} \le \mathbb{P}\{\Upsilon \ge e^{(b_0 - a + o(1))n}\} \le \mathbb{E}\Upsilon^s \, e^{-s(b_0 - a + o(1))n},$$

whose logarithm divided by $n^2$ has lim sup at most $2\varkappa\epsilon^2[\log((1+2\varkappa\epsilon)/(2\varkappa\epsilon)) + 3/2] - \epsilon(b_0 - a)$. For $a < b_0$ this is negative for a fixed small $\epsilon > 0$, which gives the upper bound in (b).

*Independent columns.* By the power-mean inequality over the $\binom{2n}{n}$ sets $A$ and the independence of $V_A$ and $V_{A^c}$, $\mathbb{E}\Upsilon^s \le \binom{2n}{n}^s (\mathbb{E}d^s)^2$. Bounding each factor of (9e) by $(j + \varkappa s)/n$ and using a Riemann sum,

$$\limsup_{n\to\infty} \frac{\log \mathbb{E}\Upsilon^s}{n^2} \le \epsilon \Big[ \log 4 + 2 \int_0^1 \log(x + \varkappa\epsilon)\, dx \Big]$$

for $s = \lfloor \epsilon n \rfloor$. As $\epsilon \downarrow 0$ the bracket tends to $\log 4 - 2$, so Markov's inequality with (9a) gives a negative rate $\epsilon[\log 4 - 2 - (b_0 - a) + o_\epsilon(1)]$ when $a < b_0 + 2 - \log 4$.

### 9.4 Lower tails

*Two bases.* If $\|U - I\| \le \delta < 1$, every principal submatrix $U[I, I]$ has all singular values at least $1 - \delta$, so (9c) and (9b) give $\Upsilon \ge (1 + (1-\delta)^4)^n$ and $\Upsilon / \operatorname{per} B \ge [(1 + (1-\delta)^4)/2]^n \ge e^{-an}$ for $\delta$ small enough depending on $a$. A maximal $\delta$-separated set in the group, in the operator norm, has at most $(1 + 2/\delta)^D$ points, where $D = n^2$ or $2n^2$ is the real dimension of the ambient matrix space: the balls of radius $\delta/2$ about its points are disjoint and lie in the ball of radius $1 + \delta/2$. The $\delta$-balls about these points cover the group and have equal Haar measure by invariance, so $\mathbb{P}\{\|U - I\| \le \delta\} \ge (1 + 2/\delta)^{-D} = e^{-O(n^2)}$.

*Independent columns.* Realize the two blocks $W_1, W_2$ of $n$ columns by normalizing the columns of independent $n \times n$ Gaussian matrices $\mathcal{G}_1, \mathcal{G}_2$ whose entries have $\mathbb{E}|\mathcal{G}_{ij}|^2 = 1/n$. There is an absolute

$K$ with $\mathbb{P}\{\|\mathcal{G}\| \le K\} \ge 1/2$ for all $n$, by the standard net argument (a 1/4-net of the unit sphere and Gaussian tail bounds for each value of the bilinear form). The density of $\mathcal{G}$ is proportional to $\exp(-c_{\mathbb{F}} n \|\mathcal{G}\|_F^2)$ with $c_{\mathbb{C}} = 1$, $c_{\mathbb{R}} = 1/2$. For $0 < \eta \le \delta/K$, substituting $\mathcal{G} = I + \eta Y$ (Jacobian $\eta^D$) and using $\|I + \eta Y\|_F^2 \le n(1 + \eta K)^2$ on $\{\|Y\| \le K\}$ gives $\mathbb{P}\{\|\mathcal{G} - I\| \le \delta\} \ge \frac{1}{2}\eta^D \exp(-c_{\mathbb{F}} n^2 (1 + \eta K)^2) = e^{-O(n^2)}$. On this event the column norms lie in $[1-\delta, 1+\delta]$, so $\|W_t - I\| \le e_\delta := 2\delta/(1-\delta)$. For each of the $2^n$ choices of one column of index $i$ from $W_1$ or $W_2$ for every $i$, both the chosen matrix $V_A$ and its complement satisfy $\|V_A - I\| \le \sqrt{2}\, e_\delta$, by the Cauchy–Schwarz inequality on the two groups of columns. Hence $\Upsilon \ge 2^n (1 - \sqrt{2} e_\delta)^{4n}$. For the permanent, Wick's formula and the Cauchy–Schwarz inequality give $\operatorname{per} B \le \prod_{t=1,2} \left(\mathbb{E} \prod_i |(W_t^* g)_i|^4\right)^{1/2}$. Each expectation is the permanent of $(W_t^* W_t) \otimes J_2$, with $J_2$ the $2 \times 2$ all-ones matrix, and $(W_t^* W_t) \otimes J_2 \preceq (1 + e_\delta)^2 I \otimes J_2$. The permanent is monotone on positive semidefinite matrices of order $N$, since $\operatorname{per} X = \langle s, X^{\otimes N} s \rangle$ with $s = (N!)^{-1/2} \sum_{\sigma \in S_N} e_{\sigma(1)} \otimes \cdots \otimes e_{\sigma(N)}$, and $0 \preceq X \preceq Y$ implies $X^{\otimes N} \preceq Y^{\otimes N}$ by telescoping, $Y \otimes Y - X \otimes X = (Y - X) \otimes Y + X \otimes (Y - X)$. Thus $\operatorname{per} B \le (1 + e_\delta)^{4n} 2^n$ and $\Upsilon / \operatorname{per} B \ge [(1 - \sqrt{2} e_\delta)/(1 + e_\delta)]^{4n} \ge e^{-an}$ for $\delta$ small, on an event of probability $e^{-O(n^2)}$.

### 9.5 Almost sure rates

For two bases $\Upsilon \ge 2$, while $\mathbb{E}\Upsilon$ is a polynomial, so Markov's inequality gives $\sum_n \mathbb{P}\{\Upsilon > e^{\eta n}\} < \infty$ for every $\eta > 0$, and the Borel–Cantelli lemma gives $n^{-1} \log \Upsilon \to 0$. For independent columns the same argument with (9e) gives $\limsup n^{-1} \log \Upsilon \le \log 4 - 2$. For the lower bound, Jensen's inequality over the $\binom{2n}{n}$ terms gives $\log \Upsilon \ge \log \binom{2n}{n} + 2\bar{L}$, where $\bar{L}$ is the average of $L_A = \log |\det V_A|^2$ over the $n$-sets $A$. By the Beta product, $\mathbb{E} L_A = \sum_{j=1}^n (\psi(j/\varkappa) - \psi(n/\varkappa)) = -n + O(\log n)$ and $\operatorname{Var} L_A = \sum_{j=1}^n (\psi_1(j/\varkappa) - \psi_1(n/\varkappa)) = O(\log n)$, where $\psi_1 = \psi'$; also $\operatorname{Var} \bar{L} \le \operatorname{Var} L_A$. Chebyshev's inequality at scale $\eta n$ and the Borel–Cantelli lemma give $\liminf n^{-1} \log \Upsilon \ge \log 4 - 2$. This proves Theorem 9.2.

## 10 Two orthonormal bases of $\mathbb{C}^3$

Theorem 1.9 shows that the Gram matrix of three mutually unbiased bases of $\mathbb{C}^2$, of order six, is not permanent-on-top. Two orthonormal bases of $\mathbb{C}^3$ give Gram matrices of the same order, supported on $K_{3,3}$, and for these the property holds with a uniform gap as long as no squared overlap exceeds $13/20$; in particular it holds for two mutually unbiased bases of $\mathbb{C}^3$, whose squared overlaps all equal $1/3$.

For a $3 \times 3$ matrix $X$ put

$$B(X) = \begin{pmatrix} I_3 & X \\ X^* & I_3 \end{pmatrix}.$$

Throughout this section $U \in U(3)$, $V = [I_3 \; U]$ has columns $v_1, \dots, v_6$, so $B(U) = V^* V$ is a correlation matrix of rank three, and

$$c_{ij} = |u_{ij}|^2, \quad C = (c_{ij}), \quad S = \sum_{i,j} c_{ij}^2, \quad r = |\operatorname{per} U|, \quad q = \max_{i,j} c_{ij}, \quad p = \operatorname{per} B(U),$$

$s$ is the second singular value of the doubly stochastic matrix $C$ (its norm on the orthogonal complement of $\mathbf{1}$), $M_{ij} = \operatorname{per} U[\hat{\imath}, \hat{\jmath}]$ is the permanent of the $2 \times 2$ submatrix complementary to $(i, j)$, and

$$J = \operatorname{Im}\left(u_{11} u_{22} \overline{u_{12} u_{21}}\right)$$

is Jarlskog's invariant [12]. Indices $1, 2, 3$ label the rows of $U$ and $4, 5, 6$ its columns.

**Theorem 10.1** (Two bases of $\mathbb{C}^3$)**.** *If* $\max_{i,j}|u_{ij}|^2 \le 13/20$*, then every eigenvalue of* $\Pi(B(U))$ *on the orthogonal complement of the constants is at most* $\operatorname{per} B(U) - 1/64$*. If* $X$ *is a* $3\times 3$ *contraction with* $\max_{i,j}|x_{ij}-u_{ij}| \le 1/50000$ *for such a* $U$*, then* $\operatorname{per} B(X)$ *is a simple largest eigenvalue of* $\Pi(B(X))$*.*

**Proposition 10.2** (The block $(3,3)$ for all unitaries)**.** *For every* $U \in U(3)$ *the block of the partition* $(3,3)$ *of* $\Pi(B(U))$ *has all eigenvalues at most* $\operatorname{per} B(U)$*, with strict inequality unless* $U$ *is a monomial matrix.*

## 10.1 Scalar identities

**Lemma 10.3.** *(i)* $p = 4 + S + r^2$*,* $1 + s^2 \le S \le 3q$*,* $r \le 1$*, and* $\sum_i |M_{ij}|^2 \le 1$ *for each* $j$*.*

*(ii)* $s \le q$ *and* $s \le 3q - 1$*.*

*(iii) For distinct rows* $i,k$ *(remaining row* $m$*) and distinct columns* $j,l$ *(remaining column* $t$*),*

$$u_{ij}u_{kl}\overline{u_{il}u_{kj}} = \tfrac{1}{2}\bigl(c_{ij}c_{kl} + c_{il}c_{kj} - c_{mt}\bigr) + \mathrm{i}\,\epsilon(i,k)\epsilon(j,l)\,J,$$

*where* $\epsilon(i,k) = 1$ *if* $k \equiv i+1 \pmod 3$ *and* $-1$ *otherwise. In particular* $J^2 = c_{11}c_{22}c_{12}c_{21} - \tfrac{1}{4}(c_{11}c_{22} + c_{12}c_{21} - c_{33})^2$*, and* $|J| \le \sqrt{3}/18$*.*

*(iv) For* $\pi \in S_3$ *put* $m_\pi = \prod_i u_{i\pi(i)}$*. All six numbers* $m_\pi/\det U$ *have imaginary part* $-J$*, and* $(m_\pi - m_\rho)/\det U = \operatorname{sgn}(\pi)\,c_{i\pi(i)}$ *when* $\pi$ *and* $\rho$ *have opposite parity and agree exactly at* $i$*. Hence for* $\pi \ne \tau$ *of equal parity, with* $\delta = (m_\pi - m_\tau)/\det U \in \mathbb{R}$*,*

$$m_\pi\overline{m_\tau} = \tfrac{1}{2}\bigl(|m_\pi|^2 + |m_\tau|^2 - \delta^2\bigr) + \mathrm{i}\,J\delta.$$

*Proof.* (i) Grouping the permutations of [6] with nonzero coefficient by the sets $I \subseteq \{1,2,3\}$ and $J' \subseteq \{4,5,6\}$ of moved vertices gives, as for (9b), $p = \sum_k \sum_{|I|=|J'|=k} |\operatorname{per} U[I,J']|^2$. The terms $k = 0,1,3$ give $1$, $\sum_{ij} c_{ij} = 3$ and $r^2$. For $k=2$ and rows $a,b$, expanding $|u_{aj}u_{bl} + u_{al}u_{bj}|^2$ and using $\sum_j u_{aj}\overline{u_{bj}} = 0$ gives $\sum_{j<l} |\operatorname{per} U[\{a,b\},\{j,l\}]|^2 = 1 - 2\sum_j c_{aj}c_{bj}$, and summing over the three row pairs gives $3 - \sum_j \bigl((\sum_i c_{ij})^2 - \sum_i c_{ij}^2\bigr) = S$. The singular values of $C$ are $1 \ge s \ge \sigma_3$, so $S = \|C\|_F^2 \ge 1 + s^2$, and $S \le q\sum c_{ij} = 3q$. The bound $r \le 1$ is the case $k=3$ of the bound $\sum_{J'} |\operatorname{per} U[I,J']|^2 \le 1$ proved before (9b), and $\sum_i |M_{ij}|^2 \le 1$ is the same bound for the unitary $U^{\mathsf T}$, with $k=2$ and the fixed set $\hat\jmath$ of rows of $U^{\mathsf T}$.

(ii) For two rows of $C$ the difference $d$ has three coordinates summing to zero, so its total variation $\tfrac{1}{2}\|d\|_1$ equals $\max_j |d_j| \le q$. Hence the Dobrushin coefficients of $C$ and $C^{\mathsf T}$ are at most $q$, so $\|x^{\mathsf T}C\|_1 \le q\|x\|_1$ and $\|x^{\mathsf T}C^{\mathsf T}\|_1 \le q\|x\|_1$ for every real $x$ with $\sum x_i = 0$, and both maps preserve that condition. For a real eigenvector $x \perp \mathbf{1}$ of $C^{\mathsf T}C$ with eigenvalue $s^2$ this gives $s^2\|x\|_1 \le q^2\|x\|_1$. For the second bound, $D = (q\mathbf{1}\mathbf{1}^{\mathsf T} - C)/(3q-1)$ is doubly stochastic, so $\|D\| \le 1$ by Birkhoff's theorem, and $C = -(3q-1)D$ on $\mathbf{1}^\perp$.

(iii) For a unitary matrix the entry $\overline{u_{mt}}$ is the cofactor of $(m,t)$ divided by $\det U$, and $|\det U| = 1$, so $c_{mt} = |u_{ij}u_{kl} - u_{il}u_{kj}|^2$; expanding gives the real part. For the imaginary part let $z_j = u_{ij}\overline{u_{kj}}$; then $z_1 + z_2 + z_3 = 0$, so $\operatorname{Im}(z_j\overline{z_l})$ is the same for the three cyclically ordered pairs $(j,l)$ and changes sign under $j \leftrightarrow l$; the same argument with the columns $j,l$ and the rows shows the dependence $\epsilon(i,k)$ on the rows. As $z_j\overline{z_l} = u_{ij}u_{kl}\overline{u_{il}u_{kj}}$, the common value at $(i,k,j,l) = (1,2,1,2)$ is $J$. Then $J^2 = |u_{11}u_{22}u_{12}u_{21}|^2 - (\text{real part})^2$. Finally, for rows $1,2$ the three numbers $z_j$ form a closed triangle with perimeter $\sum_j |z_j| \le 1$ by the Cauchy–Schwarz inequality, and $|J| = |\operatorname{Im}(z_1\overline{z_2})|$ is twice its area; by Heron's formula and the arithmetic–geometric mean inequality the area is at most $\sqrt{3}/36$.

(iv) If $\pi, \rho$ have opposite parity they agree in exactly one position $i$, and the two terms $\operatorname{sgn}(\pi)m_\pi + \operatorname{sgn}(\rho)m_\rho$ of the Laplace expansion of $\det U$ along row $i$ that contain $u_{i\pi(i)}$ sum to $u_{i\pi(i)}$ times its cofactor, that is $c_{i\pi(i)} \det U$. Hence the normalized monomials $\alpha_\pi + \mathrm{i}\mu_\pi = m_\pi / \det U$ have pairwise real differences, so a common imaginary part $\mu$. For $\pi = \mathrm{id}$ and $\tau = (12)$, which agree at 3, $\alpha_{\mathrm{id}} - \alpha_{(12)} = c_{33}$ and $m_{\mathrm{id}}\overline{m_{(12)}} = c_{33}\, u_{11}u_{22}\overline{u_{12}u_{21}}$; comparing imaginary parts, $-\mu c_{33} = c_{33}J$, so $\mu = -J$ where $c_{33} \neq 0$, and everywhere by continuity. For $\pi, \tau$ of equal parity, $m_\pi \overline{m_\tau} = (\alpha_\pi - \mathrm{i}J)(\alpha_\tau + \mathrm{i}J) = \alpha_\pi\alpha_\tau + J^2 + \mathrm{i}J(\alpha_\pi - \alpha_\tau)$, which is the displayed formula. □

Every coefficient $b_\sigma$ of $B(U)$ and every product $\operatorname{per} B[A, D]\, \overline{\operatorname{per} B[A', D']}$ of permanents or determinants of its submatrices is a sum of monomials in the $u_{ij}$ and $\overline{u_{ij}}$ that are invariant under multiplying rows and columns of $U$ by phases. In such a monomial cancel each factor $u_{ij}$ against a factor $\overline{u_{ij}}$, which gives $c_{ij}$; the remaining factors form a balanced directed multigraph on $K_{3,3}$ ($u_{ij}$ an arc from row $i$ to column $j$, $\overline{u_{ij}}$ the reverse arc), which decomposes into directed simple cycles of lengths four and six. Lemma 10.3(iii) and (iv) express each such cycle as $x + \mathrm{i}Jy$ with $x, y$ polynomials in the $c_{ij}$, and products are multiplied using the polynomial $J^2$ of (iii). The value of the monomial does not depend on the decomposition. Hence each such quantity equals $R + \mathrm{i}JH$ with $R, H$ real polynomials in the four free entries $c_{11}, c_{12}, c_{21}, c_{22}$ of $C$, the others being determined by double stochasticity. The programs of this section form these polynomials exactly.

## 10.2 Blocks of the Schur power

By Schur–Weyl duality only partitions with at most three rows give nonzero blocks of $\Pi(B(U))$, as in the proof of Theorem 1.9. The nontrivial ones are $(5,1), (4,2), (4,1,1), (3,3), (3,2,1), (2,2,2)$. Three are read off permutation modules: by Young's rule [22] the representation $N_k$ on $k$-subsets contains $(6-j, j)$ once for $0 \le j \le k \le 3$, so the block $(5,1)$ is $C_1(B)$ on $\mathbf{1}^\perp$, the block $(4,2)$ is $C_2(B)$ on the kernel of the incidence map from pairs to points, and the block $(3,3)$ has $\operatorname{tr} T_{33} = \operatorname{tr} C_3(B) - \operatorname{tr} C_2(B)$ and $\operatorname{tr} T_{33}^2 = \operatorname{tr} C_3(B)^2 - \operatorname{tr} C_2(B)^2$ (Lemma 2.4). For $(4,1,1)$ we use the module $N_3^-$ with basis $e_A$, $|A| = 3$, and action $\sigma e_A = \operatorname{sgn}(\sigma|_A) e_{\sigma(A)}$, where $\operatorname{sgn}(\sigma|_A)$ is the sign of $\sigma : A \to \sigma(A)$ for the increasing orders. It is induced from the sign character of $\mathrm{Sym}(A)$ times the trivial character of $\mathrm{Sym}(A^c)$, so by Pieri's rule it is $(4,1,1) \oplus (3,1,1,1)$, and the second block vanishes. As in Lemma 2.4, the matrix of $T_B^{N_3^-}$ is the transpose of the *signed compound* $C_3^-(B)_{A,D} = \det B[A, D] \operatorname{per} B[A^c, D^c]$, which is Hermitian. For the remaining block $(3,2,1)$ we need the following form of Schur–Weyl duality.

**Lemma 10.4** (Blocks as partial traces)**.** *Let $B = V^*V$ with $V \in \mathbb{C}^{d \times N}$, let $w = v_1 \otimes \cdots \otimes v_N$, let $\lambda \vdash N$ have at most $d$ rows, and let $Q$ be the orthogonal projection, acting on tensor positions, onto the vectors that transform by a one-dimensional character $\chi$ of a Young subgroup $Y_\mu = \mathrm{Sym}(A_1) \times \cdots \times \mathrm{Sym}(A_s)$, where $|A_t| = \mu_t$. Assume that $\chi$ occurs exactly once in the restriction of $S^\lambda$ to $Y_\mu$, and let $\mathcal{O}$ be the orbit of $(A_1, \ldots, A_s)$ under $S_N$, with $m = |\mathcal{O}|$ and projections $Q_\mathcal{A}$, $\mathcal{A} \in \mathcal{O}$. Let $K_\mathcal{A}$ be the $\lambda$-isotypic part of $Q_\mathcal{A}(\mathbb{C}^d)^{\otimes N}$, an irreducible $U(d)$-module, and fix a $U(d)$-equivariant isometry $j_\mathcal{A}$ from a model $Y$ of it onto $K_\mathcal{A}$. Then the nonzero spectrum of the block $T_B^{\rho_\lambda}$ equals the nonzero spectrum of the Hermitian form*

$$y \mapsto \frac{N!}{m} \sum_{\mathcal{A} \in \mathcal{O}} \left| \langle j_\mathcal{A}(y), Q_\mathcal{A} w \rangle \right|^2 \qquad (y \in Y).$$

*Proof.* As in the proof of Theorem 1.9, $\Pi(B) = W^*W$ for $W : e_\sigma \mapsto v_{\sigma(1)} \otimes \cdots \otimes v_{\sigma(N)}$, which intertwines the right regular representation with the action $P$ of $S_N$ on tensor positions. The $\lambda$-isotypic part of $\Pi(B)$ consists of $f^\lambda$ copies of $T_B^{\rho_\lambda}$, and its nonzero spectrum is that of $WW^* =$

$\sum_\sigma P_\sigma w w^* P_\sigma^*$ on the $\lambda$-isotypic subspace $H_\lambda \cong Y_\lambda \otimes S^\lambda$, with $Y_\lambda$ the irreducible $U(d)$-module of $\lambda$ [9, Lecture 6]. Write the component $E_\lambda w = \sum_a y_a \otimes e_a$ in an orthonormal basis $(e_a)$ of $S^\lambda$, for which $P_\sigma$ acts as $I \otimes \rho_\lambda(\sigma)$ with $\rho_\lambda$ real orthogonal. The orthogonality relations give $\sum_\sigma \rho_\lambda(\sigma) e_a e_b^{\mathsf T} \rho_\lambda(\sigma)^{\mathsf T} = (N!/f^\lambda)\delta_{ab} I$, so $WW^*$ acts on $H_\lambda$ as $\Omega_\lambda \otimes I$ with $\Omega_\lambda = \frac{N!}{f^\lambda}\sum_a y_a y_a^*$. Hence the nonzero spectrum of $T_B^{\rho_\lambda}$ is that of $\Omega_\lambda$, whose form is $\langle \varphi, \Omega_\lambda \varphi\rangle = \frac{N!}{f^\lambda}\|(\varphi^* \otimes I) E_\lambda w\|^2$.

Each $Q_\mathcal{A}$ commutes with $U(d)$ and acts on $H_\lambda$ as $I \otimes u_\mathcal{A} u_\mathcal{A}^*$ for a unit vector $u_\mathcal{A} \in S^\lambda$, by the multiplicity hypothesis. The operator $\sum_{\mathcal{A}\in\mathcal{O}} u_\mathcal{A} u_\mathcal{A}^*$ commutes with $\rho_\lambda$, because $P_\pi Q_\mathcal{A} P_\pi^* = Q_{\pi\mathcal{A}}$, so by Schur's lemma it is $(m/f^\lambda) I$, comparing traces. Therefore

$$\langle \varphi, \Omega_\lambda \varphi\rangle = \frac{N!}{m}\sum_{\mathcal{A}} \big|\langle \varphi \otimes u_\mathcal{A}, E_\lambda w\rangle\big|^2 = \frac{N!}{m}\sum_{\mathcal{A}} \big|\langle \varphi \otimes u_\mathcal{A}, Q_\mathcal{A} w\rangle\big|^2,$$

since $\varphi \otimes u_\mathcal{A} \in H_\lambda \cap \operatorname{ran} Q_\mathcal{A}$. The map $\varphi \mapsto \varphi \otimes u_\mathcal{A}$ is a $U(d)$-equivariant isometry from $Y_\lambda$ onto $K_\mathcal{A}$; fixing one isometry $Y \to Y_\lambda$, Schur's lemma shows that it differs from $j_\mathcal{A}$ by a unimodular factor, which does not affect the form. □

**Lemma 10.5** (Four blocks)**.** *Let $U \in U(3)$. Then:*

*(a) every eigenvalue of the block $(5,1)$ is at most $p - (1-s) + (r - r^2)$;*

*(b) the block $(2,2,2)$ has rank one and eigenvalue $2 + 2S = p - 2P_3$, where $P_3 = 6\sum_j \prod_i c_{ij}$;*

*(c) the block $(3,2,1)$ has nonzero spectrum equal to that of the Hermitian form*

$$Y \mapsto \sum_{(A,D,c)} |\det V_A|^2 \, |v_c^* Y \ell_D|^2$$

*on traceless $3\times 3$ matrices with the Hilbert–Schmidt norm, the sum running over the 60 ordered divisions of [6] into a triple $A$, a pair $D = \{i<j\}$ and a point $c$, with $\ell_D = \overline{v_i \times v_j}$; its eigenvalues are at most $4q + (1+q)(1+s)$.*

*Proof.* (a) In $N_1$ group the permutations by the number $k$ of row indices they send to columns. For $k=1$, $\sigma = (i\ j)$ ($i$ a row, $j$ a column) has $b_\sigma = c_{ij}$, and $\sum c_{ij}(I - U_\sigma)$ is the Laplacian of the bipartite graph with weights $c_{ij}$; since $C$ is doubly stochastic it is $I - \begin{pmatrix} 0 & C \\ C^{\mathsf T} & 0 \end{pmatrix}$, whose eigenvalues on $\mathbf{1}^\perp$ are at least $1 - s$. For $k=2$ no permutation moves a row to a row, and the weight carried from row $i$ to column $j$ is the sum of $c_{ij}c_{ab}$ over the double transpositions $(i\,j)(a\,b)$, $a \neq i$, $b \neq j$, which is $c_{ij}(1 + c_{ij})$, plus the sum over the four-cycles $i \to j \to a \to b \to i$, which is $u_{ij}\sum_{a\neq i}\overline{u_{aj}}\sum_{b\neq j} u_{ab}\overline{u_{ib}} = -c_{ij}(1-c_{ij})$ by row orthogonality; so the $k=2$ deficit in $N_1$ is the Laplacian with weights $2c_{ij}^2$, which is positive semidefinite. For $k=3$ every $\sigma$ swaps the rows and the columns, the total coefficient is $r^2$, and the operator in $N_1$ is off-diagonal with blocks $\overline{\operatorname{per} U}\, K$ and its adjoint, where $K_{ij} = u_{ij} M_{ij}$. By the Cauchy–Schwarz inequality and Lemma 10.3(i), $|x^* K y| \le (\sum_{ij} c_{ij}|x_i|^2)^{1/2}(\sum_{ij}|M_{ij}|^2|y_j|^2)^{1/2} \le \|x\|\|y\|$, so this layer contributes at least $(r^2 - r)I$ to the deficit. Adding the three layers gives (a).

(b) By Lemma 9.1 with $m=2$ and by (9c), the block has rank at most one and eigenvalue

$$\sum_{|A|=3} |\det V_A|^2 |\det V_{A^c}|^2 = \sum_k \sum_{|I|=|J|=k} |\det U[I,J]|^4 = 1 + S + S + 1,$$

because the $2\times 2$ minors of a unitary matrix have the moduli of the complementary entries. For the second expression consider the cubic

$$\Phi(x)=\prod_{i=1}^{3}\Big(\sum_{j}u_{ij}x_j\Big)=\sum_{|\alpha|=3}\varphi_\alpha x^\alpha$$

and the weights $\pi_\alpha=\alpha!|\varphi_\alpha|^2$. In the Fischer inner product, in which the monomials are orthogonal with $\|x^\alpha\|^2=\alpha!$, a product of linear forms $\prod\ell_i$ has squared norm $\operatorname{per}(\langle\ell_i,\ell_k\rangle)$; the rows of $U$ are orthonormal, so $\sum_\alpha\pi_\alpha=\operatorname{per}I=1$. Here $\pi_{(1,1,1)}=|\operatorname{per}U|^2=r^2$ and $\sum_j\pi_{3e_j}=P_3$. Moreover $\sum_\alpha\pi_\alpha\alpha_j(\alpha_j-1)=\|\partial_j^2\Phi\|^2=4\sum_{i<k}c_{ij}c_{kj}$, since $\partial_j^2\Phi=2\sum_{i<k}u_{ij}u_{kj}\ell_m$ with $\ell_m$ the remaining row form. Summing $\sum_j\binom{\alpha_j}{2}$ in two ways,

$$(1-r^2-P_3)+3P_3=2\sum_j\sum_{i<k}c_{ij}c_{kj}=3-S,$$

the last equality because the columns of $C$ sum to one, so $p-(2+2S)=2+r^2-S=2P_3$.

(c) Apply Lemma 10.4 with $N=6$, $d=3$, $\lambda=(3,2,1)$, the Young subgroup of a division $(A,D,\{c\})$ and its sign character, which occurs once in $S^{(3,2,1)}$ (the Kostka number $K_{(3,2,1),(3,2,1)}$, since $(3,2,1)$ is self-conjugate). Here $m=60$. The range of $Q_{\mathcal{A}}$ is $\bigwedge^3\otimes\bigwedge^2\otimes\mathbb{C}^3$, which as a $U(3)$-module is $\det{}^2\otimes(\mathbb{C}I\oplus\mathfrak{sl}_3)$ through the isometry $\varepsilon\otimes(x\wedge y)\otimes v\mapsto v(x\times y)^{\mathsf T}$, with $\varepsilon$ the unit vector of $\bigwedge^3$ and $x\wedge y=(x\otimes y-y\otimes x)/\sqrt{2}$; the traceless part is the $(3,2,1)$-component, so $Y$ is the space of traceless matrices. The antisymmetrizations give $Q_{\mathcal{A}}w=\pm\frac{\det V_A}{\sqrt{6}}\,\varepsilon\otimes\frac{1}{\sqrt{2}}(v_i\wedge v_j)\otimes v_c$, and $\langle Y,v_c(v_i\times v_j)^{\mathsf T}\rangle_{HS}=\overline{v_c^*Y\ell_D}$. As $N!/m\cdot\frac{1}{12}=1$, the form is the displayed one.

For the bound fix $c$. The triple opposite the basis of $v_c$ has $|\det V_A|=|\det U|=1$ or $|\det I|=1$, with $D$ the other two vectors of the basis of $v_c$ and $\ell_D\ell_D^*=v_cv_c^*$; every other triple has $|\det V_A|^2$ equal to some $c_{ij}$ or to the squared modulus of a $2\times 2$ minor of $U$, which is again some $c_{ij}$, so at most $q$. The compound Cauchy–Binet formula gives $\sum_{D\subseteq[6]\setminus\{c\}}\ell_D\ell_D^*=\operatorname{adj}(VV^*-v_cv_c^*)=\operatorname{adj}(2I-v_cv_c^*)=2I+2v_cv_c^*$. So the terms with this $c$ are at most $q\operatorname{tr}\big(Y^*v_cv_c^*Y(2I+2v_cv_c^*)\big)+(1-q)|v_c^*Yv_c|^2=2q\|Y^*v_c\|^2+(1+q)|v_c^*Yv_c|^2$. Summing over $c$, $\sum_c\|Y^*v_c\|^2=\operatorname{tr}(YY^*VV^*)=2\|Y\|^2$, and $\sum_c|v_c^*Yv_c|^2=\|\Pi_1Y\|^2+\|\Pi_2Y\|^2$, where $\Pi_1,\Pi_2$ are the orthogonal projections onto the traceless matrices diagonal in the standard basis and in the basis of columns of $U$. The cosines between these two planes are the singular values of $C$ on $\mathbf{1}^\perp$, since $\langle\operatorname{diag}(a),U\operatorname{diag}(b)U^*\rangle_{HS}=a^*Cb$, so $\|\Pi_1+\Pi_2\|\le 1+s$, and the form is at most $(4q+(1+q)(1+s))\|Y\|^2$. □

## 10.3 Exact certificates

Put $t=\operatorname{tr}T_{33}$, $s_2=\operatorname{tr}T_{33}^2$ and $h=p^2+\frac14(t-p)^2-s_2$.

**Lemma 10.6.** *$t=11-\sum_{i,j}c_{ij}|M_{ij}|^2$, hence $8\le t\le 11$.*

*Proof.* The character of $(3,3)$ is the number of fixed 3-subsets minus the number of fixed 2-subsets, since $N_3=N_2\oplus(3,3)$. Its values on the cycle types that occur are:

| type | $1^6$ | $2\,1^4$ | $2^2\,1^2$ | $4\,1^2$ | $2^3$ | $4\,2$ | $6$ |
|---|---|---|---|---|---|---|---|
| $\chi_{(3,3)}$ | 5 | 1 | 1 | −1 | −3 | −1 | 0 |
| $k$ | 0 | 1 | 2 | 2 | 3 | 3 | 3 |

where $k$ is the number of rows moved to columns. The total coefficient at $k=0$ is 1, at $k=1$ it is $\sum c_{ij}=3$, and at $k=2$ it is $S$ (proof of Lemma 10.3(i)), of which the double transpositions

carry $\frac{1}{2}\sum_{ij} c_{ij}(1+c_{ij}) = (3+S)/2$ and the four-cycles $(S-3)/2$; so these layers contribute $5+3+((3+S)/2-(S-3)/2) = 11$. At $k=3$ the permutations containing a given transposition $(i\,j)$ carry total coefficient $c_{ij}|M_{ij}|^2$, and the types $2^3$, $4\,2$, $6$ contain 3, 1, 0 transpositions, so the $k=3$ contribution $-3m_{2^3} - m_{4\,2}$ equals $-\sum c_{ij}|M_{ij}|^2$. By Lemma 10.3(i) this sum is at most $\sum_j \sum_i |M_{ij}|^2 \le 3$. □

**Lemma 10.7** (Three certificates)**.** *Let $\mathcal{C}_{q_0}$ be the set of doubly stochastic $3\times 3$ matrices with entries at most $q_0$, and evaluate the polynomials $R$, $H$ and $J^2$ of the previous subsection at $C \in \mathcal{C}_{q_0}$.*

*(i) On $\mathcal{C}_{13/20}$, $h - (290+99S)J^2 \ge 1/2$.*

*(ii) Let $L$ be a rational $15\times 9$ basis matrix of the kernel of the incidence map from pairs to points, $G = L^{\mathsf{T}}L$, and $pG - L^{\mathsf{T}}C_2(B)L = R_2 + \mathrm{i}JH_2$. On $\mathcal{C}_{13/20}$, $R_2 - (\frac{137}{4} - \frac{17}{10}S)J^2G \pm \frac{\mathrm{i}}{10}H_2 \succeq G/50$.*

*(iii) With $pI - C_3^-(B) = R_3 + \mathrm{i}JH_3$, on $\mathcal{C}_{13/20}$, $R_3 - (\frac{157}{4} - \frac{17}{10}S)J^2I \pm \frac{\mathrm{i}}{10}H_3 \succeq I/2$.*

*(iv) On the set of all doubly stochastic matrices, $h - 192J^2 \ge 0$; it is positive at every point that is not a permutation matrix and is a convex combination of permutation matrices in which either at least three permutations, or two of opposite parity, have positive weight.*

*Proof.* For $q_0 \in [1/3, 1]$ the map $C \mapsto D = (q_0\mathbf{1}\mathbf{1}^{\mathsf{T}} - C)/(3q_0-1)$ is an affine bijection of $\mathcal{C}_{q_0}$ onto a subset of the doubly stochastic matrices, and by Birkhoff's theorem every doubly stochastic $D$ is $\sum_\pi u_\pi P_\pi$ with $u$ in the standard simplex $\Delta_5$ of the six permutations; so every $C \in \mathcal{C}_{q_0}$ is $C(u) = q_0\mathbf{1}\mathbf{1}^{\mathsf{T}} - (3q_0-1)\sum_\pi u_\pi P_\pi$ for some $u \in \Delta_5$, and for (iv) we use $C(u) = \sum_\pi u_\pi P_\pi$. The entries of $C(u)$ are linear in $u$. Each expression is a polynomial of degree at most six in the free entries of $C$, with scalar or Hermitian matrix coefficients; substituting $C(u)$ and multiplying lower-degree terms by powers of $\sum_\pi u_\pi = 1$ gives a homogeneous form $\sum_{|\alpha|=6} \frac{6!}{\alpha!}\beta_\alpha u^\alpha$ of degree six. If every Bernstein coefficient $\beta_\alpha$ is at least $\gamma$ (positive semidefinite after subtracting $\gamma G$ or $\gamma I$), the form is at least $\gamma(\sum u)^6 = \gamma$ on $\Delta_5$. For a Hermitian coefficient $X + \mathrm{i}Y$ the program tests the real matrix $\begin{pmatrix} X & -Y \\ Y & X \end{pmatrix}$ by exact rational Gaussian elimination with positive pivots; the sign $-\frac{\mathrm{i}}{10}$ gives the transposed real matrix, which is congruent to the same one. All arithmetic is in $\mathbb{Q}$. The programs `overlap_13_20_moments.py`, `overlap_13_20_42.py` and `overlap_13_20_411.py` check (i)–(iii) for all 462 coefficients; the exact minimum in (i) is 351859677/256000000. The program `global_unitary_33_certificate.py` computes the 462 coefficients for (iv): they are nonnegative, and exactly 54 vanish, namely the six pure powers, the exponents $(5,1)$ and $(1,5)$ on all fifteen pairs, and the exponents $(4,2), (3,3), (2,4)$ on the six pairs of equal parity. At a point $u$ of the stated kind some $u^\alpha$ with $\beta_\alpha > 0$ is positive. □

*Proof of Proposition 10.2.* Let $\lambda$ be the largest eigenvalue of the positive semidefinite $5\times 5$ block $T_{33}$. The other four eigenvalues sum to $t-\lambda$, so $s_2 \ge F(\lambda)$ with $F(x) = x^2 + \frac{1}{4}(t-x)^2$, which increases on $[t/5, \infty)$; also $\lambda \ge t/5$ and $p \ge 5 > t/5$ by Lemmas 10.3(i) and 10.6. By Lemma 10.7(iv), $F(p) - s_2 = h \ge 192J^2 \ge 0$, so $F(\lambda) \le F(p)$ and $\lambda \le p$. If $U$ is not monomial, $C$ is not a permutation matrix. If a convex decomposition of $C$ uses exactly two permutations of equal parity, their quotient is a three-cycle, so each row of $C$ has two positive entries in columns that differ from row to row, and two rows share exactly one column; orthogonality of the corresponding rows of $U$ then fails. So Lemma 10.7(iv) gives $h > 0$ and $\lambda < p$. □

*Proof of Theorem 10.1.* Let $q \le 13/20$. By Lemma 10.3, $s \le q$, $S \ge 1 + s^2$, $p \le 5 + 3q \le 139/20$ and $p \ge 5$. We bound $p$ minus the top of each nontrivial block.

$(5,1)$. By Lemma 10.5(a) and $r - r^2 \le 1/4$, the gap is at least $1 - q - \frac{1}{4} \ge \frac{1}{10}$.

$(3,2,1)$. By Lemma 10.5(c), the gap is at least $5 + s^2 - 4q - (1+q)(1+s)$, which decreases in $s$ on $[0,q]$ (its derivative is $2s - 1 - q < 0$), so it is at least $4 - 6q \ge \frac{1}{10}$.

$(2,2,2)$. By Lemma 10.5(b) the gap is $2P_3$. Some column of $C$ has all entries at least $1/32$: otherwise each column has an entry below $1/32$, and these lie in distinct rows, since a row with two of them has sum below $1/16 + q < 1$. For two columns $j, l$ consider $\sum_i u_{ij}\overline{u_{il}} = 0$. In the row containing neither small entry both entries exceed $1 - q - \frac{1}{32} = \frac{51}{160}$, so that term has modulus above $51/160$, while the other two have total modulus at most $2\sqrt{q/32} < 51/160$, a contradiction. On a column with entries in $[1/32, q]$ summing to one, the concave function $\sum_i \log c_{ij}$ is minimal at a vertex of the feasible polygon, a permutation of $(\frac{1}{32}, \frac{13}{20}, \frac{51}{160})$ when $q = 13/20$ and larger for smaller $q$. Hence $2P_3 \ge 12 \cdot \frac{1}{32} \cdot \frac{13}{20} \cdot \frac{51}{160} > \frac{1}{16}$.

$(3,3)$. By Lemma 10.7(i), $h \ge 1/2$ since $290 + 99S > 0$. As in the proof of Proposition 10.2, $\lambda < p$ and $F(p) - F(\lambda) \ge h$; on $[\lambda, p]$, $F'(x) = (5x - t)/2 \le 2p$ because $p \le 139/20 < 8 \le t$. So $p - \lambda \ge h/(2p) \ge \frac{1}{4p} \ge \frac{5}{139}$.

$(4,2)$ *and* $(4,1,1)$. By Lemma 10.3(iii), $|J| \le \sqrt{3}/18 < 1/10$, so

$$R_2 + \mathrm{i}JH_2 = (\tfrac{1}{2} + 5J)(R_2 + \tfrac{\mathrm{i}}{10}H_2) + (\tfrac{1}{2} - 5J)(R_2 - \tfrac{\mathrm{i}}{10}H_2)$$

is a convex combination, and Lemma 10.7(ii), with the multiplier $\frac{137}{4} - \frac{17}{10}S > 0$ (as $S \le 3$), gives $pG - L^{\mathsf{T}}C_2(B)L \succeq G/50$. For $y = Lx$ this reads $y^*(pI - C_2(B))y \ge \|y\|^2/50$ on the kernel of the incidence map, which carries the block $(4,2)$; its gap is at least $1/50$. The same argument with Lemma 10.7(iii) gives $pI - C_3^-(B) \succeq I/2$ on $N_3^-$, so the block $(4,1,1)$ has gap at least $1/2$.

The smallest of these gaps is $1/50 > 1/64$, which proves the first assertion. For the second, $B(X) \succeq 0$ because $X$ is a contraction. A permutation with nonzero coefficient on the support $K_{3,3}$ moves $k$ rows and $k$ columns, $0 \le k \le 3$; there are $\binom{3}{k}^2 (k!)^2$ of them, with $2k$ off-diagonal factors, each of modulus at most one for both $B(X)$ and $B(U)$. Telescoping, $|b_\sigma(X) - b_\sigma(U)| \le 2k\varepsilon$ with $\varepsilon = \max|x_{ij} - u_{ij}|$, and $\sum_\sigma |b_\sigma(X) - b_\sigma(U)| \le (9 \cdot 2 + 36 \cdot 4 + 36 \cdot 6)\varepsilon = 378\varepsilon$. This bounds $|\operatorname{per} B(X) - \operatorname{per} B(U)|$ and the norm of $T^L_{B(X)} - T^L_{B(U)}$, so on the complement of the constants, which both operators preserve, the deficit decreases by at most $756\varepsilon \le 756/50000 < 1/64$. Hence every nonconstant eigenvalue of $\Pi(B(X))$ is below $\operatorname{per} B(X)$. □

*Remark* 10.8. Two mutually unbiased bases of $\mathbb{C}^3$ have $q = 1/3$, so Theorem 10.1 applies to them, while three mutually unbiased bases of $\mathbb{C}^2$ give the counterexample of Theorem 1.9, at the same order six. Since $|U|$ has row sums at least $q^{-1/2} > 1$, the matrices $B(U)$ of Theorem 10.1 are not diagonally dominant after any diagonal scaling. By Corollary 1.12, which uses only the permanent-on-top property, each matrix $A = B(X)$ of Theorem 10.1 satisfies $\operatorname{per}(A \circ C) \le \operatorname{per} A \prod_i c_{ii}$ for every positive semidefinite $C$ of order six: none is the first factor of an order-six counterexample to the inequality of Bapat and Sunder in Zhang's Question 4, and every such correlation matrix has the Hadamard-compression property of Zhang's Question 6 [32, Section 5].

## 11 Circulant correlations of order five

Order five is the smallest order of the known counterexamples to Conjecture 1.1 [25, 30], and the first order beyond the order-four case announced by Lavi [13, Theorem 3.1]. Here we prove it on the whole class of order-five correlation matrices with a transitive symmetry: unconditionally on the singular part of the class, and on the rest of the class under the hypothesis that Conjecture 1.1 holds at order four.

**Definition 11.1.** A correlation matrix $A$ of order five is *transitive* if the permutation parts of the monomial unitary matrices $W$ with $W^*AW = A$ act transitively on [5]. Let $\omega = e^{2\pi i/5}$. For $x = (x_0, \dots, x_4)$ with $x_k \geq 0$ and $\sum_k x_k = 1$, the *circulant correlation* $T(x)$ has entries $T(x)_{jl} = \sum_k x_k \omega^{k(j-l)}$, indices modulo five.

The eigenvalues of $T(x)$ are $5x_0, \dots, 5x_4$, so every circulant correlation matrix is some $T(x)$, and $T(x)$ is singular exactly when some $x_k$ vanishes.

**Lemma 11.2** (Reduction)**.** *Let $A$ be a transitive correlation matrix of order five.*

*(i) After conjugation by a diagonal unitary matrix and a relabeling, $A = T(x)$ for some $x$. Neither operation changes* $\operatorname{per} A$ *or the spectrum of* $\Pi(A)$*.*

*(ii) For $s \in \mathbb{Z}/5$ and $r \in (\mathbb{Z}/5)^\times$, the matrices $T(x_{\cdot+s})$ and $T(x_{r\cdot})$, with coordinates $x_{k+s}$ and $x_{rk}$, are obtained from $T(x)$ by a diagonal unitary conjugation and by the relabeling $j \mapsto r^{-1}j$, respectively.*

*Proof.* (i) A transitive subgroup of $S_5$ has order divisible by five and so contains a five-cycle $c$. Let $W = DP_c$ be a monomial symmetry of $A$ with permutation part $c$, where $D = \operatorname{diag}(d_j)$ is unitary. Choose a fifth root $\lambda$ of $\prod_j d_j$ and solve $e_j = \lambda^{-1} d_j e_{c^{-1}(j)}$ along the cycle; the product condition makes the five equations consistent. With $E = \operatorname{diag}(e_j)$ we get $E^*WE = \lambda P_c$. Hence $E^*AE$ commutes with $P_c$, which after relabeling along the cycle is the cyclic shift, so $E^*AE$ is circulant. Diagonal unitary conjugation preserves every $a_\sigma$ (Lemma 2.2(i)), and relabeling conjugates $\Pi(A)$ by a permutation matrix. (ii) $\operatorname{diag}(\omega^{-sj})\, T(x)\, \operatorname{diag}(\omega^{sj})$ has entries $\sum_k x_k \omega^{(k-s)(j-l)} = \sum_k x_{k+s} \omega^{k(j-l)}$, and $T(x)_{r^{-1}j, r^{-1}l} = \sum_k x_k \omega^{kr^{-1}(j-l)} = \sum_k x_{rk} \omega^{k(j-l)}$. □

**Proposition 11.3** (Singular circulants)**.** *If $T$ is a singular circulant correlation matrix of order five, every eigenvalue of* $\Pi(T)$ *on the orthogonal complement of the constant vector is at most* $\operatorname{per} T - 1/8$*. In particular $T$ is permanent-on-top with a simple top eigenvalue.*

*Proof.* The certificate is exact and computer-assisted. By Lemma 11.2(ii) we may take $T = T(x)$ with $x_4 = 0$, so that $x$ ranges over the simplex $\mathcal{S}_3 = \{(x_0, \dots, x_3) : x_k \geq 0,\ \sum x_k = 1\}$, and each coefficient $t_\sigma = \prod_j T_{j\sigma(j)}$ is a homogeneous polynomial of degree five in $x_0, \dots, x_3$ with coefficients in $\mathbb{Z}[\omega]$.

*Representations.* Let $N_2$ be the permutation representation on 2-subsets, $N_2^-$ its twist by the sign character, and $\bigwedge^2$ the exterior square of the natural permutation representation, each of dimension ten. By Young's rule [22], $N_2 \cong S^{(5)} \oplus S^{(4,1)} \oplus S^{(3,2)}$, hence $N_2^- \cong S^{(1^5)} \oplus S^{(2,1^3)} \oplus S^{(2,2,1)}$, and $\bigwedge^2 \cong \bigwedge^2(S^{(4,1)}) \oplus S^{(4,1)} \cong S^{(3,1,1)} \oplus S^{(4,1)}$. Together they contain all seven irreducible representations of $S_5$, so by Lemma 2.1 it suffices to bound the operators $F = \sum_\sigma t_\sigma \rho(\sigma)$ in these three representations, where for $N_2$ the eigenvalue $\operatorname{per} T$ of the constant vector is to be excluded.

*Translation.* Since $T_{c(j)c(l)} = T_{jl}$ for the cyclic shift $c$, we have $t_{c\sigma c^{-1}} = t_\sigma$, so $\rho(c)$ commutes with $F$. In each of the three spaces the basis vectors indexed by $\{j, j+d\}$, $d \in \{1, 2\}$ (in $\bigwedge^2$ the vector $e_j \wedge e_{j+d}$), form two orbits of length five under $c$, permuted without signs; in $N_2^-$ this uses that $c$ is even. Hence each Fourier mode $m \in \mathbb{Z}/5$ of $c$ gives a $2 \times 2$ block $F_m$ of $F$, on the $\omega^m$-eigenspace of $\rho(c)$, with entries in $\mathbb{Z}[\omega][x]$.

*Reduction between modes.* The certificate below treats all five modes directly; the following symmetry explains why the nonzero modes behave alike. Let $r \in (\mathbb{Z}/5)^\times$ and $q_r : j \mapsto rj$. Conjugating by $\rho(q_r)$ maps $F$ for $T$ to $F$ for the relabeled matrix of Lemma 11.2(ii), which is again a singular circulant correlation, and maps the mode $m$ to the mode $r^{\pm 1}m$, since $q_r c q_r^{-1} = c^r$. After the frequency shift of Lemma 11.2(ii), which restores $x_4 = 0$ and does not change any $t_\sigma$, the

relabeled matrix is again a point of $\mathcal{S}_3$. So a bound for the mode-one blocks over all of $\mathcal{S}_3$ would already cover the four nonzero modes.

*The inequalities.* With $P = \operatorname{per} T$ and $\Sigma = x_0 + x_1 + x_2 + x_3$, the program checks on $\mathcal{S}_3$ that

$$8(PI - F_m) - \Sigma^5 I \succ 0$$

for every $m \in \mathbb{Z}/5$ in each of the three representations, except that for $N_2$ at $m = 0$, whose block contains the constant vector with eigenvalue $P$, it checks the scalar $8(2P - \operatorname{tr} F_0) - \Sigma^5 > 0$ for the other eigenvalue $\operatorname{tr} F_0 - P$. Since $\Sigma = 1$ on $\mathcal{S}_3$, this gives the gap $1/8$.

*The certificate.* Each inequality states that a homogeneous Hermitian matrix polynomial of degree five, $Q(x) = \sum_\alpha Q_\alpha x^\alpha$, is positive definite on $\mathcal{S}_3$. If every coefficient $Q_\alpha$ is positive semidefinite and the four vertex coefficients $Q_{5e_k}$ are positive definite, then $Q(x) \succ 0$ on $\mathcal{S}_3$, because $Q(x) \succeq \sum_k x_k^5 Q_{5e_k}$. Otherwise the simplex is bisected along a longest edge, by the substitution $(y_i, y_j) \mapsto (y_i + y_j/2,\ y_j/2)$ in barycentric coordinates (scaled by $2^5$ to keep the coefficients integral), and the test is repeated on both halves. A real element of $\mathbb{Z}[\omega]$ is $(a + b\sqrt{5})/2$ with integers $a, b$, so its sign is decided by comparing $a^2$ with $5b^2$; a Hermitian $2 \times 2$ coefficient is tested through its diagonal entries and its determinant. All arithmetic is in integers. The numbers of accepted leaves and the maximal depths are:

| | $m = 0$ | $m = 1$ | $m = 2$ | $m = 3$ | $m = 4$ |
|---|---|---|---|---|---|
| $N_2$ | 32 (7) | 166 (11) | 131 (10) | 122 (10) | 114 (10) |
| $\bigwedge^2$ | 58 (8) | 137 (11) | 107 (10) | 99 (10) | 82 (10) |
| $N_2^-$ | 31 (7) | 38 (8) | 38 (8) | 43 (8) | 31 (7) |

All 1229 leaves pass (`verify_circulant_order_five.py`, which also replays the weaker margin $10(PI - F_m) - \Sigma^5 I$ for $m = 0, 1$ with 366 leaves). □

The same program certifies $\operatorname{per} T > 17/12$ on $\mathcal{S}_3$ with 45 leaves; this is not used. Numerically the best constant in Proposition 11.3 is about 0.15 (Section 13).

**Theorem 11.4** (Transitive correlations of order five)**.** *Assume that every positive semidefinite matrix of order four is permanent-on-top; Lavi has announced a computer-assisted proof of this statement [13, Theorem 3.1]. Let $A \neq I$ be a transitive correlation matrix of order five, $\zeta = \lambda_{\min}(A)$, and $a_1, a_2$ the entries of a circulant representative at cyclic distances one and two. Then every eigenvalue of $\Pi(A)$ on the orthogonal complement of the constants is at most $\operatorname{per} A - \Xi(A)$, where*

$$\Xi(A) = \frac{(1-\zeta)^5}{8} + \zeta^3 \frac{5 - \sqrt{5}}{2} \left(|a_1|^2 + |a_2|^2\right) \ \geq \ \frac{(1-\zeta)^2}{32}.$$

*Consequently $A$ is permanent-on-top with a simple top eigenvalue, and for every correlation matrix $C$ of order five*

$$\operatorname{per}(A \circ C) \leq \operatorname{per} A - \Xi(A)\Big(1 - \frac{\operatorname{per} C}{120}\Big),$$

*with equality in $\operatorname{per}(A \circ C) \leq \operatorname{per} A$ exactly when $C$ has rank one.*

The quantity $|a_1|^2 + |a_2|^2 = (\operatorname{tr} A^2 - 5)/10$ does not depend on the circulant representative, since $\operatorname{tr} A^2$ is invariant under relabeling and diagonal unitary conjugation. By Lemma 2.2(i) the theorem extends to every matrix $DAD$ with $D$ positive diagonal, with $\Xi(A)$ replaced by $(\det D)^2 \Xi(A)$. For singular $A$ ($\zeta = 0$) the bound is Proposition 11.3, which does not use the hypothesis.

*Proof.* By Lemma 11.2 let $A = \zeta I + (1-\zeta)T$ with $T$ a singular circulant correlation matrix; $\zeta < 1$ as $A \neq I$. Expanding each factor $a_{j\sigma(j)} = \zeta\delta_{j\sigma(j)} + (1-\zeta)t_{j\sigma(j)}$ and collecting by the set $W \supseteq \{j : \sigma(j) \neq j\}$ of coordinates where the second summand is chosen gives, in every unitary representation,

$$(\operatorname{per} A)I - T_A^U = \sum_{W \subseteq [5]} \zeta^{5-|W|}(1-\zeta)^{|W|}\Big((\operatorname{per} T[W])I - T_{T[W]}^U\Big), \tag{11a}$$

where $T_{T[W]}^U = \sum_{\pi \in \mathrm{Sym}(W)} t_\pi U_\pi$ acts through the subgroup $\mathrm{Sym}(W)$. Every summand is positive semidefinite: for $|W| \leq 3$ by Theorem 1.4, since every graph on at most three vertices has vertex-cover number at most two, for $|W| = 4$ by the hypothesis, and for $W = [5]$ by Proposition 11.3. Two summands give more. The full set $W = [5]$ contributes at least $(1-\zeta)^5/8$ on the complement of the constants, by Proposition 11.3. A two-element set $W = \{j, l\}$ contributes $\zeta^3(1-\zeta)^2|t_{jl}|^2(I - U_{(j\,l)}) = \zeta^3|a_{jl}|^2(I - U_{(j\,l)})$, and the sum of these terms is the interchange operator with edge weights $|a_{jl}|^2$. By the theorem of Caputo, Liggett and Richthammer [3, Theorem 1.1], its smallest eigenvalue on the complement of the constants in the regular representation equals the smallest nonzero eigenvalue of the weighted graph Laplacian with weights $|a_{jl}|^2$; Shchesnovich uses the same theorem to bound multiparticle indistinguishability by two-particle marginal bunching [27]. For the circulant weights $|a_1|^2$ (distance one) and $|a_2|^2$ (distance two) the Laplacian eigenvalues are $2|a_1|^2(1 - \cos\frac{2\pi k}{5}) + 2|a_2|^2(1 - \cos\frac{4\pi k}{5})$, $k = 1, \ldots, 4$, each at least $2(1 - \cos\frac{2\pi}{5})(|a_1|^2 + |a_2|^2) = \frac{5-\sqrt{5}}{2}(|a_1|^2 + |a_2|^2)$. Adding the two contributions gives the bound $\Xi(A)$ in the regular representation, hence for every nonconstant eigenvalue of $\Pi(A)$.

For the lower bound, $T$ is singular, so with eigenvalues $5x_k$ and some $x_k = 0$, $\operatorname{tr} T^2 = 25\sum_k x_k^2 \geq 25/4$. Also $\operatorname{tr} T^2 = 5 + 10(|t_1|^2 + |t_2|^2)$, so $|t_1|^2 + |t_2|^2 \geq 1/8$ and $|a_1|^2 + |a_2|^2 \geq (1-\zeta)^2/8$. Hence $\Xi(A) \geq (1-\zeta)^2[(1-\zeta)^3/8 + \zeta^3(5-\sqrt{5})/16] \geq (1-\zeta)^2((1-\zeta)^3 + \zeta^3)/8 \geq (1-\zeta)^2/32$, since $(5-\sqrt{5})/16 > 1/8$ and $t^3 + (1-t)^3 \geq 1/4$.

For the retention inequality, $\operatorname{per}(A \circ C) = \operatorname{tr}(\Pi(A)\Pi(C)^{\mathsf{T}})/120$ (Section 12). The matrix $\Pi(C)^{\mathsf{T}} \succeq 0$ has trace 120 and value $\operatorname{per} C$ on the unit constant vector, and $\Pi(A)$ is at most $\operatorname{per} A$ on that vector and at most $\operatorname{per} A - \Xi(A)$ on its complement; so $\operatorname{tr}(\Pi(A)\Pi(C)^{\mathsf{T}}) \leq \operatorname{per} A \operatorname{per} C + (\operatorname{per} A - \Xi(A))(120 - \operatorname{per} C)$. Since $\Xi(A) > 0$, equality in $\operatorname{per}(A \circ C) \leq \operatorname{per} A$ forces $\operatorname{per} C = 120 = \operatorname{tr}\Pi(C)$, so $\Pi(C)$ is supported on the constant vector, all its entries equal one, $|c_{jl}| = 1$ for all $j, l$, and $C$ has rank one; conversely a rank-one correlation matrix $C = dd^*$ with $|d_j| = 1$ gives $A \circ C = DAD^*$ with $D = \operatorname{diag}(d)$, and $\operatorname{per}(A \circ C) = \operatorname{per} A$. □

**Corollary 11.5** (A neighbourhood)**.** *Under the hypothesis of Theorem 11.4, let $C_0 \neq I$ be a transitive correlation matrix of order five and $\alpha = 1 - \lambda_{\min}(C_0)$. If a correlation matrix $A$ of order five satisfies $\|A - C_0\|_F \leq \alpha/10^4$, then every nonconstant eigenvalue of $\Pi(A)$ is at most* $\operatorname{per} A - 39\alpha^2/4000$.

*Proof.* Put $r = \|A - C_0\|_F$. The off-diagonal entries of $C_0 = \zeta I + (1-\zeta)T$ have modulus at most $\alpha = 1 - \zeta$, so those of $A$ have modulus at most $R := \alpha + r \leq 1.0001\,\alpha$. For a permutation $\sigma \neq 1$, with $c_\sigma$ the coefficient of $C_0$, telescoping $a_\sigma - c_\sigma$ over the moved coordinates gives $|a_\sigma - c_\sigma| \leq R\sum_{j:\sigma(j)\neq j} |a_{j\sigma(j)} - (c_0)_{j\sigma(j)}|$, since every term keeps another off-diagonal factor of modulus at most $R$ and all other factors have modulus at most one. Each ordered pair $j \neq l$ occurs for $4! = 24$ permutations, so $\sum_\sigma |a_\sigma - c_\sigma| \leq 24R\sum_{j\neq l} |a_{jl} - (c_0)_{jl}| \leq 24\sqrt{20}\,Rr$. This bounds both $|\operatorname{per} A - \operatorname{per} C_0|$ and the operator norm of $T_A^L - T_{C_0}^L$, so the deficit operator changes in norm by at most $48\sqrt{20}\,Rr \leq 215\,\alpha r \leq 0.0215\,\alpha^2$. The constant vector stays an eigenvector, and $\Xi(C_0) \geq \alpha^2/32$ by Theorem 11.4, so the nonconstant gap of $A$ is at least $(0.03125 - 0.0215)\alpha^2 = 39\alpha^2/4000$. □

## 11.1 Circulants of rank two in every order

For circulants of rank at most two the Schur power can be diagonalized exactly in every order. Let $n \geq 2$, let $\zeta$ be a primitive $n$-th root of unity, $z = (1, \zeta, \dots, \zeta^{n-1})^{\mathsf{T}}$ and $\mathbf{1} = (1, \dots, 1)^{\mathsf{T}}$. For $x, y \geq 0$ with $x + y = 1$ put

$$A_{x,y} = x\,\mathbf{1}\mathbf{1}^{*} + y\,zz^{*},$$

a circulant correlation matrix of rank at most two. For $0 \leq k \leq n$ let $N_k$ be the permutation representation on $k$-subsets of Section 2, let $v_k \in \mathbb{C}^{\binom{n}{k}}$ have entries $v_k(S) = \prod_{i \in S} z_i$, and recall from Young's rule [22] that $N_k$ contains each two-row irreducible representation $\rho_j$ of shape $(n-j, j)$, $0 \leq j \leq \min(k, n-k)$, exactly once; let $E_{k,j}$ be the orthogonal projection onto it and $d_j = \binom{n}{j} - \binom{n}{j-1}$ its dimension. Write $b_{\underline{r}} = b(b-1)\cdots(b-r+1)$, with $b_{\underline{0}} = 1$.

**Theorem 11.6** (Two primitive Fourier modes)**.** *Let $n \geq 2$ and $x, y \geq 0$ with $x + y = 1$. Then $\operatorname{per} A_{x,y} = n!\,(x^n + y^n)$, every block of $\Pi(A_{x,y})$ whose partition has at least three rows vanishes, and for $1 \leq j \leq n/2$ the nonzero eigenvalues of the block of $(n-j, j)$ are the numbers*

$$n!\,x^{n-k}y^{k}\,g_{\kappa,j}, \qquad j \leq k \leq n-j, \quad \kappa = \min(k, n-k), \qquad g_{\kappa,j} = \frac{n}{n-j}\,\frac{(\kappa-1)_{\underline{\kappa-j}}}{(n-j-1)_{\underline{\kappa-j}}}. \tag{11b}$$

*Consequently, with $x_+ = \max(x,y)$, $x_- = \min(x,y)$ and $h = \lfloor n/2 \rfloor$, the largest eigenvalue of $\Pi(A_{x,y})$ on the orthogonal complement of the constants is*

$$n!\,\max\Big\{\frac{n}{n-1}\,x_+^{n-1}x_-,\ \frac{n}{n-h}\,x_+^{n-h}x_-^{h}\Big\} \ \leq\ \operatorname{per} A_{x,y}, \tag{11c}$$

*with equality exactly when $n$ is even and $x = y = 1/2$. In particular $A_{x,y}$ is permanent-on-top, and its top eigenvalue is simple unless $n$ is even and $x = y$.*

*Proof. Expansion.* Write $A = A_{x,y}$, so $a_{il} = x + y\,z_i\overline{z_l}$. Expanding the product over $i$ and collecting the set $S$ of indices at which $y\,z_i\overline{z_{\pi(i)}}$ is chosen,

$$a_{\pi} = \sum_{S \subseteq [n]} x^{n-|S|}y^{|S|}\,v(S)\,\overline{v(\pi S)} = \sum_{k=0}^{n} x^{n-k}y^{k}\,v_k^{*}N_k(\pi)v_k,$$

since $(N_k(\pi)v_k)(T) = v_k(\pi^{-1}T)$, so that $v_k^{*}N_k(\pi)v_k = \sum_{|S|=k} v_k(S)\overline{v_k(\pi S)}$.

*Schur orthogonality.* Fix a two-row irreducible $\rho = \rho_j$ in Young's orthogonal form, which is real and orthogonal, of dimension $d = d_j$. For $j \leq k \leq n-j$ let $\iota_k : \mathbb{C}^d \to \mathbb{C}^{\binom{n}{k}}$ be an isometric intertwiner onto the image of $E_{k,j}$ and put $w_k = \iota_k^{*}v_k$, so $\|w_k\|^2 = \|E_{k,j}v_k\|^2$. In $v_k^{*}N_k(\pi)v_k$ only the $\rho$-isotypic part survives after multiplication by $\rho(\pi)$ and summation over $\pi$, by the orthogonality relations $\sum_{\pi} \rho'(\pi)_{ab}\rho(\pi)_{ce} = 0$ for $\rho' \not\cong \rho$ (all irreducible representations of $S_n$ are real) and $\sum_{\pi} \rho(\pi)_{ab}\rho(\pi)_{ce} = (n!/d)\delta_{ac}\delta_{be}$. Since $\iota_k^{*}N_k(\pi)\iota_k = \rho(\pi)$, the $\rho$-isotypic part of $v_k^{*}N_k(\pi)v_k$ is $\sum_{a,b} \overline{(w_k)_a}\rho(\pi)_{ab}(w_k)_b$, and this gives

$$\sum_{\pi} (v_k^{*}N_k(\pi)v_k)\rho(\pi) = \frac{n!}{d}\,\overline{w_k}\,w_k^{\mathsf{T}}.$$

Hence $T_A^{\rho} = \frac{n!}{d}\sum_{k=j}^{n-j} x^{n-k}y^{k}\,\overline{w_k}w_k^{\mathsf{T}}$, a sum of positive semidefinite operators of rank at most one. A representation with at least three rows occurs in no $N_k$, so its block vanishes. For the trivial representation only $k = 0$ and $k = n$ contribute, because the constant component of $v_k$ is proportional

to $\sum_{|S|=k} v_k(S)$, the coefficient of $t^k$ in $\prod_i(1+tz_i) = 1-(-t)^n$, which vanishes for $0<k<n$; as $|v_n|=1$ this gives $\operatorname{per} A = n!(x^n+y^n)$.

*Orthogonality across $k$.* Let $c$ be the cyclic shift $i \mapsto i+1$. Then $(N_k(c)v_k)(T) = v_k(c^{-1}T) = \zeta^{-k}v_k(T)$, so $\rho(c)w_k = \zeta^{-k}w_k$ and $\rho(c)\overline{w_k} = \zeta^k\overline{w_k}$, as $\rho(c)$ is real. For $j \ge 1$ the indices $k = j, \dots, n-j$ lie in $\{1,\dots,n-1\}$, where the numbers $\zeta^k$ are distinct because $\zeta$ is primitive. Eigenvectors of the unitary $\rho(c)$ for distinct eigenvalues are orthogonal, so the summands of $T_A^\rho$ have orthogonal ranges, and the nonzero eigenvalues of $T_A^\rho$ are $n!\,x^{n-k}y^k\,g_{k,j}$ with $g_{k,j} = \|E_{k,j}v_k\|^2/d_j$.

*The Johnson average.* The map $e_S \mapsto e_{S^c}$ is a unitary intertwiner from $N_k$ to $N_{n-k}$, and $v_k(S) = v_n\,\overline{v_{n-k}(S^c)}$ because $|z_i|=1$; the isotypic projections of a permutation representation are real matrices, so $g_{k,j} = g_{n-k,j}$ and we may take $k \le n/2$. Let $G_k = \frac{1}{n!}\sum_\pi N_k(\pi)v_kv_k^*N_k(\pi)^*$. It commutes with $N_k$, so it equals $\sum_j \gamma_j E_{k,j}$, and $\gamma_j d_j = \operatorname{tr}(E_{k,j}G_k) = \|E_{k,j}v_k\|^2$; thus $\gamma_j = g_{k,j}$. The entry $G_k(S,T)$ is the average of $v_k(S')\overline{v_k(T')}$ over the pairs $(S',T')$ with $|S'\setminus T'| = \ell := |S\setminus T|$, on which $S_n$ acts transitively. The common part of $S'$ and $T'$ cancels, so $G_k(S,T) = c_\ell/\big(\binom{n}{\ell}\binom{n-\ell}{\ell}\big)$, where $c_\ell = [u^\ell v^\ell]\prod_{i=0}^{n-1}(1+u\zeta^i+v\zeta^{-i})$. In formal power series let $a = (1+\sqrt{1-4uv})/2$, so that $a+uv/a = 1$ and $1+uw+v/w = a(1+uw/a)(1+v/(aw))$. With $\prod_i(1+t\zeta^i) = 1-(-t)^n$,

$$\prod_i(1+u\zeta^i+v\zeta^{-i}) = a^n\big(1-(-u/a)^n\big)\big(1-(-v/a)^n\big).$$

The terms with $(u/a)^n$ or $(v/a)^n$ have $u$- and $v$-degrees differing by $n$ or have total degree at least $2n$, so for $2\ell \le n$ they do not contribute, and $c_\ell = [t^\ell]a^n$ with $t = uv$. The roots of $r^2-r+t$ are $a$ and $1-a = t+O(t^2)$, so $[t^\ell]a^n$ is the coefficient of $t^\ell$ in the power sum $a^n+(1-a)^n = \sum_\ell (-1)^\ell \frac{n}{n-\ell}\binom{n-\ell}{\ell}t^\ell$ (the Girard–Waring formula). Since $\binom{n}{\ell}\frac{n-\ell}{n} = \binom{n-1}{\ell}$,

$$G_k(S,T) = \frac{(-1)^\ell}{\binom{n-1}{\ell}}, \qquad \ell = |S\setminus T|. \tag{11d}$$

*Eigenvalues of distance kernels.* For a number $q$ let $M(q)$ be the matrix on $k$-subsets with entries $q^{|S\setminus T|}$. It commutes with $N_k$, so it is a scalar $\mu_j(q)$ on the image of $E_{k,j}$. For disjoint pairs $\{a_1,b_1\},\dots,\{a_j,b_j\}$ put $f(S) = \prod_{i=1}^j(\mathbf{1}_{a_i\in S} - \mathbf{1}_{b_i\in S})$. Expanding the product shows that $f$ is a combination of the functions $S \mapsto \mathbf{1}_{R\subseteq S}$ with $|R| \le j$, which span the sum of the summands with index at most $j$; and $f$ is orthogonal to $\mathbf{1}_{R\subseteq S}$ for every $R$ with $|R| \le j-1$, because $R$ misses some pair $\{a_i,b_i\}$ and the transposition $(a_i\,b_i)$ fixes $\mathbf{1}_{R\subseteq S}$ and negates $f$. So $f$ lies in the image of $E_{k,j}$, and it is nonzero at any $S_0$ that contains every $a_i$ and no $b_i$, which exists since $j \le k \le n-j$. At $S_0$, a set $T$ with $f(T) \ne 0$ takes one element of each pair, each $b_i$ contributing the factor $-q$, and replaces $r$ of the other $k-j$ elements of $S_0$ by $r$ of the $n-k-j$ remaining elements. Hence

$$\mu_j(q) = (1-q)^j\sum_{r=0}^{k-j}\binom{k-j}{r}\binom{n-k-j}{r}q^r.$$

By the beta integral, $(-1)^\ell/\binom{n-1}{\ell} = n\int_0^1(1-s)^{n-1}\big(-s/(1-s)\big)^\ell\,ds$, so (11d) gives $G_k = n\int_0^1(1-s)^{n-1}M\big(-s/(1-s)\big)\,ds$ entrywise, and

$$g_{k,j} = n\sum_r(-1)^r\binom{k-j}{r}\binom{n-k-j}{r}\int_0^1 s^r(1-s)^{n-1-j-r}\,ds,$$

and evaluating the beta integrals,

$$g_{k,j} = \frac{n}{n-j}\sum_{r=0}^{k-j}(-1)^r\binom{k-j}{r}\frac{(n-k-j)_{\underline{r}}}{(n-j-1)_{\underline{r}}}.$$

By inclusion and exclusion the last sum is the probability that $k-j$ draws without replacement from $n-j-1$ objects, $n-k-j$ of them marked, avoid the marked ones; there are $k-1$ unmarked objects, so the sum is $(k-1)_{k-j}/(n-j-1)_{k-j}$. This is (11b).

*The top eigenvalue.* For $1 \le j \le \kappa \le n/2$, (11b) gives $g_{\kappa,\kappa} = n/(n-\kappa)$, and for $j < \kappa$ the value $g_{\kappa,j}$ is smaller: $(n-\kappa)/(n-j) < 1$ and each factor $(\kappa-1-i)/(n-j-1-i)$ is less than one because $\kappa + j < n$. So the nonconstant top is $n! \max_{1\le k\le n-1} \frac{n}{n-\kappa} x^{n-k}y^k$. By symmetry of this list under $(x,k) \leftrightarrow (y, n-k)$ we may take $x \ge y$; then the term of $k > n/2$ is at most that of $n-k$, and since $k \mapsto \log\frac{n}{n-k} + k\log(y/x)$ is convex, the maximum over $1 \le k \le h$ is attained at $k = 1$ or $k = h$. This is the left side of (11c) (if $y = 0$ both sides of the maximum vanish). Finally, by the weighted arithmetic–geometric mean inequality, for $1 \le k \le n/2$,

$$\frac{n}{n-k}\, x^{n-k}y^k \le \frac{n}{n-k}\Big(\frac{n-k}{n}x^n + \frac{k}{n}y^n\Big) = x^n + \frac{k}{n-k}y^n \le x^n + y^n,$$

and symmetrically for $k \ge n/2$. Equality forces $x^n = y^n$ and $k = n-k$, that is $n$ even, $x = y$ and $k = j = n/2$. □

At $x = y = 1/2$ and even $n \ge 4$ the endpoint $k = h = n/2$ is the strict maximizer in (11c), since $n/(n-h) > n/(n-1)$; by continuity it remains the maximizer for $x$ near $1/2$, where the nonconstant gap is $\operatorname{per} A_{x,y} - 2\,n!\,x^hy^h = n!\,(x^h - y^h)^2$.

**Corollary 11.7.** *Let $p$ be a prime. Every circulant correlation matrix of order $p$ and rank at most two, and every transitive correlation matrix of order $p$ and rank at most two, is permanent-on-top; for $p$ odd its top eigenvalue is simple.*

*Proof.* The proof of Lemma 11.2(i) applies verbatim at a prime order $p$: a transitive subgroup of $S_p$ has order divisible by $p$ and so contains a $p$-cycle. So let $A$ be circulant, $a_{jl} = \sum_k x_k\omega^{k(j-l)}$ with $\omega = e^{2\pi i/p}$, $x_k \ge 0$, $\sum_k x_k = 1$; rank at most two means that at most two weights, say $x_a$ and $x_b$, are nonzero. The diagonal unitary conjugation of Lemma 11.2(ii), which works in every order, shifts the frequencies so that $a = 0$, and $A = x_0\mathbf{1}\mathbf{1}^* + x_d ww^*$ with $w_j = \omega^{dj}$, $d = b - a \not\equiv 0$. As $p$ is prime, $d$ is invertible modulo $p$, and the relabeling $j \mapsto d^{-1}j$ turns $w$ into $z$ with $\zeta = \omega$. Neither operation changes $\operatorname{per} A$ or the spectrum of $\Pi(A)$, and Theorem 11.6 applies. □

At order five, Corollary 11.7 covers the transitive correlation matrices of rank two without the hypothesis of Theorem 11.4; they are singular, so they also lie in the class of Proposition 11.3, and Theorem 11.6 gives their nonconstant gap $120\big(x^5 + y^5 - \max\{\frac{5}{4}x_+^4x_-, \frac{5}{3}x_+^3x_-^2\}\big)$ exactly.

**Proposition 11.8** (Order six, rank two)**.** *Every circulant correlation matrix of order six and rank at most two is permanent-on-top. Its top eigenvalue is simple except when its two Fourier weights are equal and their frequencies differ by $\pm1$ or by 3 modulo 6.*

*Proof.* As in the proof of Corollary 11.7 we may take $A = x\mathbf{1}\mathbf{1}^* + y\,ww^*$, $w_j = \omega^{dj}$, $\omega = e^{2\pi i/6}$, $d \in \{1,\dots,5\}$. Complex conjugation, which conjugates $\Pi(A)$ entrywise and keeps its spectrum, replaces $d$ by $6-d$, so $d \in \{1,2,3\}$. For $d = 1$ Theorem 11.6 applies. For $d = 3$, $a_{jl} = x + y(-1)^{j-l}$ equals 1 within the two parity classes and $x - y$ across them; conjugation by a diagonal sign matrix makes all entries nonnegative, so every $a_\sigma \ge 0$ and Lemma 2.2(v) applies. If $x \ne y$, every off-diagonal entry is nonzero, so every transposition $(j\,l)$ has coefficient $|a_{jl}|^2 > 0$; as in the proof of Lemma 2.2(v), $\Delta_A^U \succeq \sum_{j<l} |a_{jl}|^2 (I - U_{(j\,l)})$, which vanishes only on the constants because the transpositions generate $S_6$, and the top eigenvalue is simple. If $x = y$, $A$ is the direct sum of two all-ones blocks.

Let $d = 2$. As $A$ has rank at most two, only blocks of partitions with at most two rows are nonzero (as in the proof of Theorem 1.9), and $(6), (5,1), (4,2), (3,3)$ each occur once in $N_3$; by Lemma 2.4 it suffices to show that $\operatorname{per} A\, I - C_3(A)$ is positive semidefinite on the orthogonal complement of the constants. Replacing $(x, y)$ by $(y, x)$ is a frequency shift followed by complex conjugation, so we may assume $x \geq y$ and write $x = z_0 + w_0$, $y = w_0$ with $z_0, w_0 \geq 0$. Then $L^*(\operatorname{per} A\, I - C_3(A))L$, with $L$ the $20 \times 19$ matrix of columns $e_J - e_{J_0}$, is a homogeneous polynomial of degree six in $(z_0, w_0)$ whose coefficients are Hermitian matrices over $\mathbb{Z}[\omega]$. The program `verify_order_six_rank_two_circulant_schur_power.py` computes all of them exactly and shows, by fraction-free Hermitian elimination in $\mathbb{Z}[\omega]$, that every coefficient is positive semidefinite and that the coefficient of $z_0^6$ is positive definite; it does the same for $d = 1$ and $d = 3$ as a check. The ranks of the coefficients of $z_0^{6-k} w_0^k$, $k = 0, \ldots, 6$, are $19, 19, 19, 19, 19, 18, 19$ for $d = 2$ (and $19, 19, 19, 19, 19, 16, 18$ for $d = 1$, $19, 19, 19, 19, 19, 16, 16$ for $d = 3$). Hence the deficit is positive definite on the complement of the constants when $z_0 > 0$, and also at $z_0 = 0$ for $d = 2$, since the coefficient of $w_0^6$ then has full rank. □

# 12 Consequences for permanental inequalities

*Proof of Corollary 1.12.* This is the classical argument, recorded in [32, Sections 3 and 5]; we include it for completeness. (a) For matrices $P, Q$ indexed by $S_n$, $\sum_{\sigma,\tau} P_{\sigma\tau} Q_{\sigma\tau} = \operatorname{tr}(PQ^{\mathsf{T}})$, and

$$\sum_{\sigma,\tau} \Pi(A)_{\sigma,\tau} \Pi(C)_{\sigma,\tau} = \sum_{\sigma,\tau} \prod_i (a \circ c)_{\sigma(i),\tau(i)} = n!\, \operatorname{per}(A \circ C).$$

The matrix $\Pi(C)^{\mathsf{T}} = \Pi(C^{\mathsf{T}})$ is positive semidefinite with trace $n! \prod_i c_{ii}$, and $\operatorname{tr}(PQ) \leq \lambda_{\max}(P) \operatorname{tr} Q$ for Hermitian $P$ and $Q \succeq 0$. With $\lambda_{\max}(\Pi(A)) = \operatorname{per} A$ this gives the first inequality. The second is the inequality $\prod_i c_{ii} \leq \operatorname{per} C$ of Marcus [16]. (b) In Young's orthogonal form $\rho_\lambda$, $\operatorname{Imm}_\lambda(A) = \operatorname{tr} T_A^{\rho_\lambda} \leq f^\lambda \lambda_{\max}(T_A^{\rho_\lambda}) \leq f^\lambda \operatorname{per} A$. □

*Remark* 12.1. Corollary 1.12 needs the support hypothesis only for $A$; the second matrix $C$ is arbitrary. Pant and Singh prove (a) for real symmetric $A$ with nonpositive off-diagonal entries and bipartite support [18, Theorem 3.1], a class in which every coefficient $a_\sigma$ is nonnegative, and Chollet-type inequalities for Laplacians of cycles and cactus graphs [18, Theorems 5.3 and 5.4]. Corollary 1.12(a) gives the Bapat–Sunder inequality for every complex positive semidefinite $A$ supported on a cycle, a cactus or a graph with $\tau \leq 2$.

## 12.1 Generalized bunching

Shchesnovich showed that Conjecture 1.1 is equivalent to a statement about generalized bunching of bosons [26], and Seron, Novo and Cerf showed that boson bunching is not maximized by indistinguishable particles [24]; Geller and Knill write the bunching probability of a permutation-invariant internal state as a convex combination of immanants of a Gram matrix [10, Appendix C]. We record the form we use, with its convention derived from first principles, because the sign convention decides the value of the witness below.

Let $n$ photons enter distinct input modes $1, \ldots, n$ of a linear interferometer, photon $j$ in internal (for instance polarization) states from a Hilbert space $\mathcal{H}$ with orthonormal basis $(f_k)$, and let $O$ be a set of output modes. With joint internal state $\psi = \sum_{\mathbf{k}} \psi_{\mathbf{k}} f_{k_1} \otimes \cdots \otimes f_{k_n}$ the input is $\sum_{\mathbf{k}} \psi_{\mathbf{k}} \prod_j a^\dagger_{j,k_j} |0\rangle$. Projecting onto the event that every photon leaves through $O$ replaces $a^\dagger_{j,k}$ by $c^\dagger_{j,k} = \sum_{o \in O} u_{oj} b^\dagger_{o,k}$, where $u$ is the unitary of the interferometer. Since $[c_{j,k}, c^\dagger_{l,k'}] = \delta_{kk'} (G_O)_{jl}$ with $G_O = u_O^* u_O$, that

is $(G_O)_{jl} = \sum_{o\in O} \overline{u_{oj}}\, u_{ol}$, the Gram matrix of the restricted input columns, Wick's theorem gives the probability

$$\Big\| \sum_{\mathbf{k}} \psi_{\mathbf{k}} \prod_j c^\dagger_{j,k_j} |0\rangle \Big\|^2 = \sum_{\sigma\in S_n} g_\sigma \langle \psi, R_\sigma \psi\rangle, \qquad g_\sigma = \prod_j (G_O)_{j\sigma(j)}, \tag{12a}$$

where $(R_\sigma\psi)_{\mathbf{k}} = \psi_{\mathbf{k}\circ\sigma^{-1}}$: in the squared norm the annihilator of photon $j$, carrying the label $k'_j$ of the bra, is contracted with the creator of photon $\sigma(j)$, carrying the label $k_{\sigma(j)}$ of the ket, which requires $\mathbf{k}' = \mathbf{k}\circ\sigma$. The map $\sigma \mapsto R_\sigma$ is a unitary anti-representation of $S_n$, so (12a) is $\langle\psi, T\psi\rangle$ for an operator $T$ whose spectrum on each isotypic component is that of the corresponding block of $\Pi(G_O)$, and every block occurs once $\dim \mathcal{H} \geq n$. Indistinguishable photons, $\psi = f_1^{\otimes n}$, give $\operatorname{per} G_O$. Hence, for mixed internal states as well by convexity:

**Proposition 12.2.** *If $G_O = u_O^* u_O$ is permanent-on-top, in particular if $\Gamma(G_O)$ lies in a universal graph, then for every joint internal state the probability that all $n$ photons leave through $O$ is at most its value* $\operatorname{per} G_O$ *for indistinguishable photons. If $\Pi(G_O)$ has a nonconstant eigenvalue above* $\operatorname{per} G_O$ *and* $\dim \mathcal{H} \geq n$*, some internal state exceeds* $\operatorname{per} G_O$*.*

Applied to Shchesnovich's order-five counterexample [25], the second statement gives a five-photon violation; applied to Theorem 1.5 it gives an explicit witness on a support with a missing edge. Since $B_5$ has largest eigenvalue $(55+\sqrt{1049})/2 < 64$, the $7\times 5$ matrix with rows $X/8$ and $(I - B_5/64)^{1/2}$ is an isometry; complete it to a unitary $u$ on seven modes and let $O$ be the first two output modes, so $G_O = B_5/64$. Give photon $j$ the label 1 if $j \in J$ and 0 otherwise, and superpose over the 2-subsets $J$ with the coefficients $x_J/\sqrt{37}$ of Theorem 1.5. By (12a), only permutations with $\sigma(J) = J'$ contribute to the $(J, J')$ term, and their sum is $\operatorname{per} G_O[J, J']\operatorname{per} G_O[J^c, J'^c]$; so the probability is $x^* C_2(G_O) x/37 = 400112/(37\cdot 64^5)$, which exceeds $\operatorname{per} G_O = 10464/64^5$. With the conjugate coefficients $\bar{x}_J$ the same computation gives $237296/(37\cdot 64^5)$, below $\operatorname{per} G_O$; the convention in (12a) therefore matters, and `verify_five_photon_witness.py` confirms both values by expanding the Fock states directly and by evaluating (12a).

# 13 Computations

The proofs above are complete without computation, except for the exact finite certificates in Theorems 1.5, 1.9 and 10.1, Propositions 8.3, 11.3, 10.2 and 11.8, the swap constants $d_8, d_9$ and the three-swap inequality of Lemma 6.3, and the interval evaluations of the girth bounds in Theorems 7.1 and 7.2. All programs are run from the folder `verification` with `python -I`, and each writes a file `.out.txt` next to it.

*Exact certificates.* `verify_k5e_certificate.py` evaluates $B_5$, the matrix $C_2(B_5)$, $\operatorname{per} B_5$ and the Rayleigh quotient of Theorem 1.5 in exact Gaussian-integer arithmetic. `verify_octahedron.py` does the same for $C_3(B_6)$, checks $C_3(B_6)x = 336x$, certifies the spectrum of $C_3(B_6)$ by the annihilating polynomial and the traces of its powers, and computes $\operatorname{Imm}_{(3,3)}(B_6) = 336$. `verify_octahedron_minus_edge.py` checks the certificate of Proposition 8.3 in exact rational arithmetic. `verify_circulant_order_five.py` is the self-contained integer certificate of Proposition 11.3, and `verify_five_photon_witness.py` expands the Fock states of Section 12.1 exactly.

*Harness and validation.* The library `potlib.py` builds the irreducible representations of $S_n$ in Young's orthogonal form and the blocks $T_B^{\rho\lambda}$, summing only over permutations with $b_\sigma \neq 0$. `verify_harness.py` checks the homomorphism property for $n \leq 6$, agreement with the dense $n!\times n!$ Schur power for $n = 4, 5$ to $10^{-11}$, and reproduces the published counterexamples: Shchesnovich's

matrix gives per = 814016640 and top eigenvalue 827687908.5 in the block $(3,2)$ (ratio 1.016795); Tran's matrix gives 504 and 512; Drury's order-eight matrix gives the cofactor ratio 1.01707.

*Local lemmas.* `verify_lemmas.py` checks the operator identity of Lemma 3.2 in all irreducible representations of $S_4$, the inequalities of Lemmas 2.3 and 3.3 on $2\times10^4$ random parameter sets in all irreducible representations of $S_3$, the determinant identities of Lemma 3.3 symbolically, Lemma 3.4 on $10^5$ random boundary instances together with a local minimization of its slack, and the cycle factorization $s\phi=\omega$ for $5\le k\le 8$.

*Section 9.* `verify_rect_identity.py` checks Lemma 9.1 for $(m,r)=(2,2),(2,3),(2,4),(3,2)$ over $\mathbb{R}$ and $\mathbb{C}$ (the second eigenvalue of the block vanishes and the top eigenvalue equals the determinant sum to relative error $4\cdot10^{-15}$), the two-bases forms of $\Upsilon$ and $\operatorname{per}B$, the bound $\operatorname{per}B\le 2^n$ and the equality case $U=I$. `verify_rect_moments.py` checks (9d), the formulas for $\mathbb{E}Z_k$ and $\mathbb{E}\Upsilon$ in exact rational arithmetic for $n\le 30$, the expectations by Monte Carlo, the bound (9a) on random samples, the constant $b_0$, the Stirling sum and the negativity of both tail rates for small $\epsilon$.

*Section 11.* `verify_circulant_numerics.py` computes all irreducible blocks of $\Pi$ for random circulant correlation matrices of order five: the smallest nonconstant gap over 3000 singular ones is $0.154\ge 1/8$, the gap minus $\Xi(A)$ over 2000 nonsingular ones is at least $2.9\cdot10^{-3}$, and the retention inequality of Theorem 11.4 holds for 300 random pairs up to rounding (equality for rank-one partners); it also checks the expansion (11a).

*Sections 6, 7, 10 and Subsection 11.1.* `verify_m5_allocation.py` checks the allocation identity of Lemma 2.7 coefficient by coefficient on nine graphs, among them $K_4$, $K_5$ minus an edge and the triangular prism, and the packet bound in all irreducible representations of $S_3,\dots,S_7$; `verify_m5_walks.py` checks Lemmas 7.5–7.7 on the Heawood graph and its subdivision; `verify_m5_constants.py` certifies the girths of Theorems 7.1 and 7.2 in interval arithmetic and the arithmetic of Theorem 7.3. `verify_three_adjacent_swap_defect.py` and `verify_short_cycle_defect.py` are the certificates of Lemma 6.3, and `verify_m1_bundles.py` checks the remaining facts of Section 6 and every budget. The exact certificates of Section 10 are `overlap_13_20_moments.py`, `overlap_13_20_42.py`, `overlap_13_20_411.py` and `global_unitary_33_certificate.py`, the last with argument `1`; `verify_m6_blocks.py` checks every analytic identity of that section and the polynomial inputs of the certificates against the actual blocks, and `verify_m6_global_zeros.py` checks the zero pattern used for Proposition 10.2. `verify_m8_two_mode.py` checks Theorem 11.6 against the full block spectra for $n\le 7$ and in exact arithmetic for $n\le 40$, and `verify_order_six_rank_two_circulant_schur_power.py` is the certificate of Proposition 11.8. The shell scripts `run_m1_certs.sh` and `run_m6_certs.sh` run the certificates of Lemma 6.3 and of Section 10, which import one another, with `python -I`.

*Searches.* `verify_random_supports.py` tests random and locally optimized correlation matrices on $K_{2,3}$, $K_{2,5}$, the books $K_{1,1,m}$ for $m=2,3,4,6$, the cycles $C_5,\dots,C_9$ (for $C_9$ random draws only) and two graphs glued at a cut vertex; all ratios $\lambda_{\max}(\Pi)/\operatorname{per}$ are at most one up to rounding, while the control, $K_5$ minus an edge, exceeds one. The programs in the folder `searches` run a local optimizer (`potsearch.py`: BFGS, then Nelder–Mead, from seeded random starts) over Gram matrices of prescribed rank whose columns are kept orthogonal on the non-edges, or over contractions $X$ in $B=\begin{pmatrix} I & X\\ X^* & I\end{pmatrix}$ for $K_{3,m}$. The search sizes and results are as follows; these are search results, not theorems.

- The fourteen graphs with five vertices and vertex-cover number at least three: ranks two, three and four, complex and real, 36 starts per graph (`search_g5.py`). The ratio exceeded one only for $K_5$ (largest value 1.0617) and $K_5$ minus an edge (1.0609), only with complex

entries, and these values are attained already at rank two.

- $K_{3,3}$: 48 starts at ranks three to six (`search_k3m.py`) and 60 starts over contractions (`search_bip.py`), complex and real; largest ratio one.
- $K_{3,4}$: 12 complex contraction starts (`search_bip.py`); largest ratio one.
- $K_{1,2,2}$: the 36 starts above and 20 more at ranks two and three (`search_n6.py`); largest ratio one.
- The octahedron: 20 starts at ranks two and three (`search_n6.py`), which found the ratio 7/5 and led to the exact form of Theorem 1.9. The octahedron minus an edge: 36 starts at ranks three to five (`search_octa_minus.py`), which found the ratio 1.000686 at rank three and led to Proposition 8.3.

The folder also holds `search_quick2.py`, a short preliminary run of the same optimizer on $K_4$ at ranks two and three and on $K_5$ and $K_5$ minus an edge at rank two (largest ratios 1, 1.0617 and 1.0609), and `explore_octahedron.py`, which prints the numerical block spectra of the matrix of Theorem 1.9.

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**Competing interests.** The author owns Luminary Oddities and has no other relevant competing interests.

**Data and code availability.** The verification scripts cited in the text are included with this article.

**AI assistance.** OpenAI ChatGPT and OpenAI Codex working notes and manuscripts were the source of the arguments of Sections 3–5, 6, 7 and 10, of Subsections 2.1 and 11.1, of the example of Theorem 1.5, of the moment and tail estimates in Section 9, of Section 11 and its certificate program, of Proposition 3.6, of the five-photon witness, and of the certificate programs of Lemma 6.3, Section 10 and Proposition 11.8. Anthropic Claude verified and rewrote these proofs, gave the proof of Lemma 9.1, found and certified the examples of Theorem 1.9 and Proposition 8.3, replayed the certificate program of Section 11, replayed the certificate programs of Sections 6 and 10 and of Proposition 11.8, derived the normalizations of Lemma 10.4, wrote the other verification programs, and checked the sources. Scott Schubr directed the research and is responsible for the content.

# A Data for Proposition 8.3

All coordinates below are to be multiplied by $10^{-6}$. The vectors $x_1, \dots, x_6 \in \mathbb{Q}(i)^3$, before the projections described in the proof, are:

$$
\begin{aligned}
x_1 &\quad (-491769 + 3281i, -670427 - 92557i, -540610 + 88625i)\\
x_2 &\quad (-50535 - 151584i, -362160 - 423111i, 647718 + 494720i)\\
x_3 &\quad (278413 - 302465i, -643202 + 347117i, 427837 - 337280i)\\
x_4 &\quad (-109549 + 52893i, 22073 - 583450i, -17401 - 802495i)\\
x_5 &\quad (-201637 - 117493i, -34095 + 659111i, 564535 + 437320i)\\
x_6 &\quad (43094 + 282918i, -587249 + 463996i, -40519 - 596913i)
\end{aligned}
$$

The projections are, in this order, $x_2 \mapsto x_2 - \frac{\langle x_1, x_2\rangle}{\langle x_1, x_1\rangle} x_1$, the same for $x_3$ against $x_1$, then $x_4$ against $x_3$ and $x_6$ against $x_5$, all in exact arithmetic. The vector $y$, indexed by the 3-subsets of [6] in lexicographic order, is:

| | |
|---|---|
| 123: $259278 + 46768i$ | 124: $-265180 + 105493i$ |
| 125: $-325162 - 104962i$ | 126: $331064 - 47299i$ |
| 134: $-259278 - 46768i$ | 135: $-409658 - 531i$ |
| 136: $409658 + 531i$ | 145: $1000000$ |
| 146: $-475541 - 58725i$ | 156: $-265180 + 105493i$ |
| 234: $265180 - 105493i$ | 235: $475541 + 58725i$ |
| 236: $-1000000$ | 245: $-409658 - 531i$ |
| 246: $409658 + 531i$ | 256: $259278 + 46768i$ |
| 345: $-331064 + 47299i$ | 346: $325162 + 104962i$ |
| 356: $265180 - 105493i$ | 456: $-259278 - 46768i$ |

With these data, exact computation in $\mathbb{Q}(i)$ (the program `verify_octahedron_minus_edge.py`) gives $\operatorname{per} B = 15.1617076538\ldots$ and $y^* C_3(B) y - \operatorname{per}(B)\, y^* y = 0.0436048514\ldots > 0$; the Rayleigh ratio is $1.000686216\ldots \operatorname{per} B$.

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