

Work statistics of a projective-measurement train in every
dimension:
an exact class-wise criterion for the detailed fluctuation theorem
and the structural origin of the dimension-two exception

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Corresponding author. GeWu Solution `measurement-train-dft-dimension-split`
(internal project 23250). The verifiers `code/check_*.py` and the committed outputs
`results/check_*.txt` cited below are byte-identical to those of Solution revision
`1d3b6b98fd2a599d37c184f80d0e45d8071ec`, which Journal intake 193's record
bound as revision 1 and its round 2 reviewed; `code/check_provenance.py`
enforces that identity from the SHA-256 digests in `results/evidence_sha256.txt`.
This manuscript is the revision offered to that intake as revision 2 and changes text only.

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Abstract

A quantum system driven by a time-dependent Hamiltonian and measured projectively in its instantaneous energy eigenbasis at a finite sequence of times defines work as a random variable through the two-point-measurement scheme. Three relations are usually quoted together for such a measurement train and they are not equivalent: the integral fluctuation relation, the Crooks relation against the time-reversed process, and the detailed fluctuation theorem in its symmetric form, which is the one a single forward experiment can test. We separate them at every Hilbert-space dimension. The first two are properties of unital population dynamics: the integral fluctuation relation follows from the row sums of the composite transfer matrix alone, and the backward transfer matrix of a train is exactly the transpose of the forward one, so the Crooks relation holds without any symmetry assumption. The symmetric detailed fluctuation theorem is a different matter. We prove a necessary and sufficient class-wise criterion for it, valid at every dimension, every measurement schedule, every inverse temperature and every pair of cyclic endpoint Hamiltonians: the violation at a work value is a weighted sum, over the pairs of levels that realise that value, of the antisymmetric part of the composite transfer matrix. The violation is therefore blind to the symmetric part of that matrix, vanishes identically at zero work, and pairs opposite work values into a single condition; symmetry of the transfer matrix is sufficient at every dimension and necessary exactly when the spectral gaps are distinct. The dimension-two exception has a structural origin: the antisymmetric parts realisable by doubly stochastic matrices span a space of dimension one half of the product of one less and two less than the dimension, which vanishes only at dimension two, so there the symmetric form holds for every cyclic protocol whatever the drive, while at every higher dimension a nonzero antisymmetric direction is available. For arbitrary endpoints we prove that at dimension two the exact condition is isospectrality of the two endpoint Hamiltonians, strictly weaker than cyclicity, and we give the two drive-independent pair ratios that replace the symmetric form off isospectrality. At dimension three the whole violation is controlled by one rational scalar. We compute the worst case exactly, over all physically realisable protocols, schedules and train lengths: the total-variation violation attains its maximal value one, at every temperature, for

the two three-cycle protocols, while the pointwise worst case depends on temperature and has supremum one attained at no finite temperature; involutive protocols satisfy the theorem exactly in every dimension. We give an exact feasibility certificate at dimension three, showing that the whole one-skeleton of the Birkhoff polytope is orthostochastic while the zero set of the certificate also reaches the interior, and we exhibit a four-dimensional ray along which every necessary chain-link condition holds identically while unistochastic membership provably switches. That ray is the precise obstruction to any sufficiency theorem built on chain links in dimension four and above. Three questions are left open and are stated as such.

1 Introduction

A quantum system whose Hamiltonian is varied in time and whose energy is measured projectively at the beginning and at the end of the variation is the standard object of quantum work statistics. The two-point-measurement scheme declares the work done on the system to be the difference between the two measured energies, and the resulting random variable carries the nonequilibrium information of the protocol [3, 10]. When the energy is measured not twice but at a finite sequence of intermediate times, the object is a *measurement train*: the system is driven, dephased in its instantaneous energy eigenbasis, driven again, dephased again, and so on, until the final measurement. Each measurement resets the coherences, so the train reduces to a classical Markov chain on the energy levels whose one-step transition matrices are the entrywise squared moduli of the interval unitaries in the two energy bases. The work distribution of the train is then read off a single composite transfer matrix, the ordered product of the interval matrices.

Three relations are usually quoted for such a distribution, and they are not equivalent. The integral fluctuation relation states that the thermal average of the exponentiated minus work equals the ratio of the final to the initial partition function. The Crooks relation compares the forward work distribution with the work distribution of the time-reversed process, weighted by the free-energy difference [4]. The detailed fluctuation theorem in its symmetric form compares $P(w)$ with $P(-w)$ inside the forward process alone,

$$P(w) e^{-\beta w} = P(-w), \quad (1)$$

where β is the inverse temperature of the initial state. It is (1) that a single forward experiment can test, because it relates two quantities measured in the same run, and it is (1) that is usually meant by “the detailed fluctuation theorem” for a measurement train. The other two relations involve either a single number or a second process that has to be prepared and run separately.

For a driven two-level system the question is settled completely [5]. Every interval transfer matrix is symmetric, hence so is the composite, and (1) holds exactly for every protocol, every measurement schedule, every number of intermediate measurements and every inverse temperature, provided the two endpoint Hamiltonians have the same level spacing. When the endpoint spacings differ, (1) is replaced by two exact ratios between opposite work values, each carrying its own exponential factor and neither depending on the drive. The route to the symmetry of the interval matrices runs through an amplitude identity that is specific to two-level unitaries and has no analogue in higher dimension. Section 6 shows that the identity is not where the real reason lies: at dimension two every doubly stochastic matrix is symmetric, so nothing about the drive has to be proved at all.

At dimension three and above the situation was open. Nothing exact was known about *when* (1) holds for a measurement train, about how badly it can fail, or about which parts of the standard story survive the loss of transfer-matrix symmetry. The composite of a train is doubly stochastic,

being a product of doubly stochastic matrices, but it is in general neither symmetric nor unistochastic, and the set of composites of a long train is strictly larger than the set of unistochastic matrices. This paper closes that gap for cyclic endpoint Hamiltonians and identifies exactly where the remaining boundaries are.

The results are these.

1. *The dimension-free half.* The integral fluctuation relation follows from the row sums of the composite transfer matrix alone—equivalently, from the uniform vector being invariant, which in this convention is unitality: no symmetry, no commutation of the intervals, no assumption on the spectrum and no use of the fact that the row sums come from unitaries enters it (Theorem 4.1). The backward transfer matrix of a measurement train is exactly the transpose of the forward one, and the Crooks relation holds with that backward matrix and with the free-energy difference given by the partition-function ratio (Theorem 4.2). Both statements are valid at every dimension, every schedule, every train length, every inverse temperature and every pair of endpoint Hamiltonians.
2. *An exact class-wise criterion.* For cyclic endpoints the violation of (1) at a work value w is a weighted sum, over the pairs of levels that realise w , of the antisymmetric part of the composite transfer matrix (Theorem 5.1). The formula is necessary and sufficient, and it is affine in the composite. Four consequences follow at once: the violation is blind to the symmetric part of the composite; it vanishes identically at zero work; opposite work values carry one linear condition rather than two; and symmetry of the composite is sufficient at every dimension but necessary exactly when the spectral gaps are distinct (Corollaries 5.2–5.7).
3. *The structural origin of the dimension-two exception.* The antisymmetric parts realisable by doubly stochastic $d \times d$ matrices span the space of antisymmetric matrices with zero row sums, whose dimension is $(d-1)(d-2)/2$; that number vanishes exactly at $d=2$ (Lemma 6.1). The realised set itself is not that whole space but a compact convex body described exactly, by d linear inequalities and as the convex hull of the permutation differences (Theorem 6.2). At dimension two the symmetric form is therefore unconditional for cyclic endpoints, and for arbitrary endpoints the exact condition is isospectrality of the two endpoint Hamiltonians, strictly weaker than cyclicity (Theorems 6.3 and 6.5); off isospectrality the replacement is the pair of exact drive-independent ratios of Corollary 6.6.
4. *Dimension three is controlled by one scalar.* The antisymmetric part of a doubly stochastic 3×3 matrix is a multiple of a single fixed circulant matrix, with multiplier x equal to the difference of the two off-diagonal entries in the upper triangle. For the equally spaced spectrum the two nonzero violations are $-x(1+q)/Z$ and xq/Z , with $q = e^{-\beta}$ and Z the partition function, so the total variation distance between the two sides of (1) is exactly $|x|$ (Theorem 6.8 and Corollary 6.9). A doubly degenerate level makes (1) hold for every protocol at every temperature, symmetric or not (Theorem 6.10), and the rank of the linear map from antisymmetric parts to violations decides, exactly and at every dimension, whether symmetry is necessary (Corollary 6.11 and Table 1).
5. *The worst case, exactly.* The violation is affine in the composite and its total variation is convex, so over all realisable protocols, schedules and train lengths the worst case is attained at a vertex of the Birkhoff polytope, that is, at a deterministic protocol (Theorem 7.1). Every permutation matrix is realisable by a single unitary interval. Involutives satisfy (1) exactly at

every dimension and every spectrum (Theorem 7.2), and at dimension three with the equally spaced spectrum the two three-cycles attain total-variation violation one, the maximum possible value of a distance between two probability measures, at every temperature (Corollary 7.3). The pointwise worst case does depend on temperature: it equals $r(1+r)/(1+r+r^2)$ with $r = \max(q, 1/q)$, is strictly increasing in r , equals two thirds at infinite temperature and approaches one without ever reaching it at any finite temperature (Corollary 7.4).

6. *An exact feasibility certificate at dimension three.* The classical criterion of Au-Yeung and Poon [1] reduces, on the whole polytope, to the sign of one degree-four polynomial with integer coefficients: all six chain-link discriminants, for row pairs and for column pairs alike, are that same polynomial (Theorem 8.1). On each of the nine facets the polynomial restricts to minus a perfect square, and it vanishes identically on each of the nine edges, with an explicit closed-form real-orthogonal witness. The whole one-skeleton of the Birkhoff polytope is therefore orthostochastic (Corollary 8.2), while the zero set of the polynomial also reaches the interior of the polytope, at exactly six rational points of denominator nine and at no lattice point of smaller denominator. At dimension three the protocols that maximise the matrix asymmetry are exactly those that maximise the thermodynamic violation (Theorem 8.3).
7. *Why no sufficiency theorem built on the necessary conditions can exist in dimension four.* Along a one-parameter rational ray in the Birkhoff polytope of dimension four, all twelve necessary bracelet conditions hold identically on the whole window in which the ray lies in the polytope, while unistochastic membership provably switches: there is an explicit closed-form unitary preimage for every nonnegative parameter value and a rigorous non-membership proof at the lower endpoint (Theorem 9.2). The interior of the negative part is left open, and the exact unreduced phase system that settles it is written down (Lemma 9.1).

The composite of Corollary 6.12 deserves a separate mention because it separates two questions that are easy to conflate. At dimension four with the equally spaced spectrum the rank of the violation map drops below the dimension of the antisymmetric space, so there exist doubly stochastic composites that are asymmetric and nevertheless satisfy (1) exactly at every work value. One such composite is written down with exact rational entries. It is not unistochastic, and the bracelet conditions refute that in exact rational arithmetic. The rank deficiency of the violation map is thus a genuine feature of the polytope, and whether it has a realisation by a train with at least one intermediate measurement, rather than by a single unitary interval, is open.

Section 3 fixes the model, the conventions and the exactness regime, and Section 2 places the paper against the two literatures it draws on. Sections 4 to 8 carry the results in the order listed above, Section 9 the dimension-four ray, and Sections 10 and 11 the interpretation, the boundaries of what is established and the open questions. Appendix A records the exact recomputation behind every number quoted, and Appendix B collects the tables.

2 Relation to earlier work

This paper sits between two literatures that rarely meet: quantum fluctuation relations on one side, and the geometry of doubly stochastic matrices on the other. The connection is forced by the physics. The composite transfer matrix of a measurement train is a product of unistochastic matrices, so it lives in the Birkhoff polytope, and the question of when the symmetric detailed fluctuation theorem holds turns out to be a question about which points of that polytope carry a nonzero antisymmetric part. The second literature then supplies the feasibility certificate that the first one needs in order to say which of its extremal protocols are physically realisable.

On the fluctuation-relation side the two-point-measurement scheme and the relations it obeys are standard. Crooks derived the relation between the forward and the time-reversed work distributions together with the nonequilibrium work relation for free energy differences [4]; Tasaki established the Jarzynski relations for quantum systems [10]; the survey of Campisi, Hänggi and Talkner collects the foundations and the applications of quantum fluctuation relations [3], and the short commentary of Hänggi and Talkner [6] is cited here only as a commentary, not as a review. None of these treats the symmetric form (1) class by class, and none addresses how the answer depends on the Hilbert-space dimension. Theorem 4.1 and Theorem 4.2 restate standard material for a measurement train and prove it from the row sums of the composite alone; they appear here because separating what is dimension-free from what is not is the point of the paper, not because either relation is new. What is new on this side is Theorem 5.1, the exact class-wise criterion, and everything that follows from it.

On the matrix-geometry side the criterion used in Section 8 is classical and is not a result of this paper. That a 3×3 doubly stochastic matrix isunistochastic if and only if a certain triangle-area expression is nonnegative was established by Au-Yeung and Poon [1], in the course of studying the convexity of generalised numerical ranges. Bengtsson, Ericsson, Kuś, Tadej and Życzkowski [2] write the same condition as a triangle inequality for the three link lengths $L_k = \sqrt{B[i, k]B[j, k]}$, their equations (22) and (23), note that the six triangles built from the three row pairs and the three column pairs have the same area by unitarity, so that all six conditions reduce to one inequality $A \geq 0$, and give the phases of a preimage explicitly in their equations (24) and (25). Their Theorem 3 states that the boundary of the unistochastic set at dimension three consists of orthostochastic matrices and proves it by the observation that saturating the triangle inequality forces the phases to ± 1 ; the factorisations displayed in Theorem 8.1 below reproduce that fact symbolically from a single integer polynomial, and Corollary 8.2 sharpens it by identifying the whole one-skeleton of the polytope with an explicit closed-form witness for each of the nine edges. Nakazato studied the set of 3×3 orthostochastic matrices directly [7], and the complete description of that non-convex set in terms of the same inequalities is attributed to him by Nechita et al. [8, §3]. The definitions of the orthostochastic, unistochastic and Birkhoff sets, the inclusion chain between them, the fact that all three inclusions are proper for $N > 2$ while at $N = 2$ all three sets coincide, the polygon form of the necessary conditions at arbitrary N (their equations (4.3) and (4.4)), and the fact that the Fourier matrix has equal amplitudes and therefore maps to the van der Waerden matrix are taken from Życzkowski et al. [11]; the last of these is what identifies the explicit preimage of Theorem 9.2 at the parameter value zero, and the coincidence at $N = 2$ is the classical form of Theorem 6.3.

One classical input deserves a comment because of the way it is used. The polygon inequalities for the link lengths of a row or column pair are what the recent literature calls the *bracelet* conditions, and that they are necessary for unistochasticity at every dimension is Proposition 3.2 of Nechita et al. [8], proved there from the triangle inequality applied to row orthogonality. Lemma 6.13 below proves the same statement again, in four lines, and derives it for every index rather than only for the longest link, so that nothing in this paper rests on an external authority for a load-bearing step. What is taken from the literature is the opposite statement, which cannot be proved by the same argument: Rajchel-Mieldzioć et al. [9] show that at dimension four the bracelet conditions are necessary but not sufficient—the flat matrix lies on the boundary of the unistochastic set there while a whole ball around it satisfies the conditions—and that the unistochastic set is a proper subset of the Birkhoff polytope at every dimension three and above. Only the dimension-four case is used here, and only in the direction that keeps Corollary 6.14 one-sided: a failed bracelet condition refutes unistochasticity decisively, while a satisfied one certifies nothing. Theorem 9.2 makes that asymmetry concrete rather than merely quoting it, by exhibiting a whole segment of the dimension-four polytope on which all twelve necessary conditions hold identically

while membership switches.

The exactly solved two-level case [5] is the immediate predecessor of this work and the reason the question was asked. It establishes the symmetric form for a driven two-level system when the two endpoint level spacings agree, and replaces it by two exact drive-independent ratios when they do not. Its proof of the symmetry of each interval transfer matrix uses an amplitude identity available only for two-level unitaries, and it says so. The present paper replaces that dynamical argument by a polytope argument, which is why the two-level result becomes the $d = 2$ case of a statement about all dimensions rather than a special fact about spin one half.

3 The measurement train and its work statistics

3.1 The protocol

A d -level system is driven on the interval $[0, \tau]$ by a time-dependent Hamiltonian

$$H(t) = \sum_{j=0}^{d-1} \varepsilon_j(t) |e_j(t)\rangle \langle e_j(t)|, \quad (2)$$

where $\varepsilon_0(t) \leq \varepsilon_1(t) \leq \dots \leq \varepsilon_{d-1}(t)$ are the instantaneous eigenvalues, counted with multiplicity, and $|e_j(t)\rangle$ an orthonormal eigenbasis chosen continuously in t . No non-degeneracy is assumed: equal eigenvalues are allowed at every time, including at the endpoints. Between measurements the evolution is unitary.

The system is measured projectively in its instantaneous energy eigenbasis at the times

$$0 = t_0 < t_1 < \dots < t_N < t_{N+1} = \tau, \quad (3)$$

so that there are N intermediate measurements and $N + 1$ unitary intervals. The integer $N \geq 0$ is arbitrary and the schedule (3) is arbitrary; the endpoints $t_0 = 0$ and $t_{N+1} = \tau$ are always measured, which is what makes the object a two-point-measurement scheme when $N = 0$ and a measurement train when $N \geq 1$. Denote by U_k the unitary that carries the system from t_k to t_{k+1} . Figure 1 is a schematic of the protocol and carries no numerical content.

Because every measurement is a projective measurement in the energy basis, it fully dephases the state. The populations therefore propagate by ordinary matrix multiplication, and the one-step transition matrix of the k -th interval is

$$M_k[n, m] = |\langle e_n(t_{k+1}) | U_k | e_m(t_k) \rangle|^2, \quad k = 0, \dots, N. \quad (4)$$

Here and throughout, $M[n, m]$ is the probability of ending in level n given that the interval started in level m ; this convention fixes the order of the matrix product below and is the only place where a transposition could silently enter. Unitarity of U_k gives both $\sum_n M_k[n, m] = 1$ and $\sum_m M_k[n, m] = 1$, so each M_k is doubly stochastic. More is true: each M_k is the entrywise squared modulus of a unitary matrix written in two orthonormal bases, so each M_k isunistochastic.

Definition 3.1 (composite transfer matrix). *The composite transfer matrix from the initial to the final energy index of the train (3) is the ordered product*

$$A = M_N M_{N-1} \dots M_1 M_0, \quad \text{so that} \quad A[n, m] = \Pr(\text{final index } n \mid \text{initial index } m). \quad (5)$$

Since the set of doubly stochastic matrices is closed under multiplication, A is doubly stochastic. It is in general neither symmetric nor unistochastic, and characterising the set of composites of a train of length $N \geq 1$ is not attempted here; containment in the Birkhoff polytope and attainability of its vertices are all that is needed, and both are established in Section 7.

3.2 Work and its distribution

The initial outcome is Gibbs-distributed at inverse temperature $\beta > 0$,

$$p_m = \frac{e^{-\beta \varepsilon_m(0)}}{Z_0}, \quad Z_0 = \sum_{m=0}^{d-1} e^{-\beta \varepsilon_m(0)}, \quad Z_\tau = \sum_{n=0}^{d-1} e^{-\beta \varepsilon_n(\tau)}. \quad (6)$$

The two-point-measurement work of a trajectory that starts in m and ends in n is $w = \varepsilon_n(\tau) - \varepsilon_m(0)$, and it occurs with probability $p_m A[n, m]$. Writing

$$C_w = \{(n, m) : \varepsilon_n(\tau) - \varepsilon_m(0) = w\} \quad (7)$$

for the work class of the value w , the work distribution is

$$P(w) = \sum_{(n,m) \in C_w} p_m A[n, m]. \quad (8)$$

Throughout, $q = e^{-\beta}$, so that $e^{-\beta \varepsilon} = q^\varepsilon$ and $e^{-\beta w} = q^w$.

3.3 Three relations, distinguished

The three relations that the introduction groups together are now definitions. Each is stated with the quantifiers under which this paper proves or refutes it.

Definition 3.2 (integral fluctuation relation). *The train satisfies the integral fluctuation relation if $\langle q^W \rangle = \sum_w P(w) q^w = Z_\tau / Z_0$.*

Definition 3.3 (Crooks relation). *The backward process of the train (3) reverses the schedule and the measurement order and evolves each interval by $U_k^\dagger$; its initial state is the Gibbs state of $H(\tau)$. With $\Delta F = -\beta^{-1} \ln(Z_\tau / Z_0)$ and P_B the backward work distribution, the train satisfies the Crooks relation if $P(w) q^w (Z_0 / Z_\tau) = P_B(-w)$ for every work value w .*

Definition 3.4 (detailed fluctuation theorem, symmetric form). *The train satisfies the detailed fluctuation theorem if $P(w) q^w = P(-w)$ for every work value w . Its defect is*

$$\Delta(w) = P(w) q^w - P(-w), \quad (9)$$

and its total-variation violation is

$$V(A) = \frac{1}{2} \sum_w |\Delta(w)|. \quad (10)$$

Definition 3.4 needs a comment on the meaning of V . For a cyclic protocol both $w \mapsto P(w) q^w$ and $w \mapsto P(-w)$ are probability distributions on the work support: the first has total mass $Z_\tau / Z_0 = 1$ by the integral fluctuation relation, the second has total mass one because P is a distribution. Hence V is exactly the total variation distance between them, it satisfies $0 \leq V \leq 1$, and $V = 0$ if and only if the detailed fluctuation theorem holds at every work value. That is why V and not the ratio $P(w) q^w / P(-w)$ is the worst-case measure optimised in Section 7: the ratio has an unbounded supremum over realisable protocols, because a three-cycle protocol at dimension three gives $P(-1) = 0$ while $P(1) > 0$ at every temperature, so no finite worst-case ratio exists.

The symmetric form is the one a single forward run can test, and it is also the most demanding of the three. Definition 3.3 compares the forward process with a different, separately prepared process; Definition 3.4 compares two weights of the same forward distribution. Theorem 4.2 shows that the first comparison always succeeds for a measurement train, and Theorem 5.1 shows that the second succeeds exactly when a certain antisymmetric quantity vanishes class by class.

3.4 Conventions and the exactness regime

The following conventions are fixed here and not changed later.

The Birkhoff polytope $\mathcal{B}(d)$ is the set of $d \times d$ doubly stochastic matrices; its vertices are the $d!$ permutation matrices. The unistochastic set $\mathcal{U}(d) \subset \mathcal{B}(d)$ is the set of entrywise squared moduli of unitary matrices, and the orthostochastic set $\mathcal{O}(d) \subset \mathcal{U}(d)$ is the corresponding set for real orthogonal matrices [11]. The inclusions are strict for $d \geq 3$. I is the identity matrix and J the all-ones matrix of the size clear from the context.

A permutation σ of $\{0, \dots, d-1\}$ is represented by the matrix

$$P_\sigma[n, m] = \begin{cases} 1, & n = \sigma(m), \\ 0, & \text{otherwise,} \end{cases} \quad (11)$$

so that P_σ is the transfer matrix of the deterministic protocol that sends the initial level m to the final level $\sigma(m)$. With this convention the product $P_\sigma P_\tau$ equals $P_{\sigma\tau}$, and the cycle notation used below refers to the same σ : the permutation with $\sigma(0) = 1$, $\sigma(1) = 2$, $\sigma(2) = 0$ is the three-cycle $(0\ 1\ 2)$ and has matrix $P_{(0\ 1\ 2)}[n, m] = 1$ exactly at $(n, m) = (1, 0), (2, 1), (0, 2)$.

For a matrix M the antisymmetric part is

$$D(M) = \frac{M - M^T}{2}, \quad (12)$$

the space of antisymmetric matrices with zero row sums is

$$\mathcal{K}(d) = \{D : D^T = -D, D\mathbf{1} = 0\}, \quad (13)$$

where $\mathbf{1}$ is the all-ones vector, and the set of differences actually realised inside the polytope is

$$\mathcal{R}(d) = \{A - A^T : A \in \mathcal{B}(d)\} \subset \mathcal{K}(d). \quad (14)$$

Note the normalisation: elements of $\mathcal{R}(d)$ are the *differences*, so $D(A) = \frac{1}{2}(A - A^T)$ lies in $\frac{1}{2}\mathcal{R}(d)$. The asymmetry of a matrix is

$$\alpha(M) = \max_{k,j} |M[k, j] - M[j, k]|, \quad (15)$$

so that $\alpha(M) = 0$ exactly when M is symmetric.

Finally, the exactness regime. Every number quoted in this paper is an exact rational number or an exact radical, obtained from rational input data by rational arithmetic or by integer polynomial arithmetic, with no floating-point tolerance behind any exact claim. To keep the arithmetic exact the concrete instances use integer spectra and positive rational values of q , so that q^ε and q^w are exact rationals. This is a choice of instances and not a restriction on the theorems: every theorem is stated for arbitrary real spectra, arbitrary real $\beta > 0$, arbitrary schedules and arbitrary unitary intervals. Where a numerical search is reported rather than a proof, it is labelled as such.

4 The dimension-free half

Two of the three relations of Section 3 hold for a measurement train at every dimension, and the reason in both cases is the same: they are properties of unital classical population dynamics, and the only feature of the composite transfer matrix they use is that its columns and its rows sum to one. Nothing about the drive, the schedule, the train length, the spectrum or the dimension enters. This section separates that half of the story cleanly from the half that does depend on the dimension, so that later sections can use it without further hypotheses.

projective measurement in the instantaneous energy eigenbasis, at every t_k and at both ends

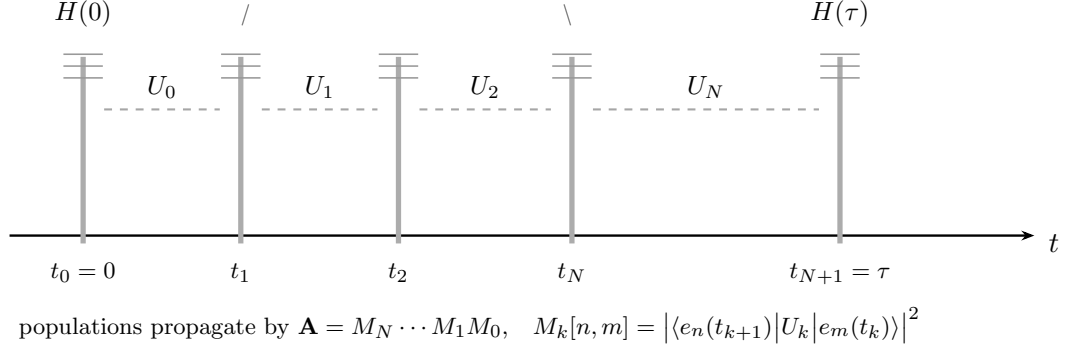


Figure 1: A measurement train. The Hamiltonian (2) is varied from $t_0 = 0$ to $t_{N+1} = \tau$; a projective measurement in the instantaneous energy eigenbasis occurs at every t_k , including both endpoints, and the evolution between t_k and t_{k+1} is the unitary U_k . Each measurement fully dephases the state, so the populations propagate by the interval transfer matrices (4) and the whole train is summarised by the composite $A = M_N \cdots M_0$ of Definition 3.1. The initial outcome is drawn from the Gibbs distribution (6) of $H(0)$, the final outcome is an eigenvalue of $H(\tau)$, and the work of a trajectory is the difference of the two. The drawing is a schematic: it carries no numerical data.

Theorem 4.1 (integral fluctuation relation). *For every d , every $N \geq 0$, every protocol and schedule (3), every $\beta > 0$ and every pair of endpoint Hamiltonians,*

$$\langle q^W \rangle = \sum_w P(w) q^w = \frac{Z_\tau}{Z_0}. \quad (16)$$

Proof. Insert (8) and (6) and sum over all pairs rather than over work classes, which is legitimate because the classes partition the pairs:

$$\begin{aligned} \sum_w P(w) q^w &= \sum_{n,m} p_m A[n, m] q^{\varepsilon_n(\tau) - \varepsilon_m(0)} = \frac{1}{Z_0} \sum_{n,m} q^{\varepsilon_m(0)} A[n, m] q^{\varepsilon_n(\tau)} q^{-\varepsilon_m(0)} \\ &= \frac{1}{Z_0} \sum_n q^{\varepsilon_n(\tau)} \left(\sum_m A[n, m] \right) = \frac{1}{Z_0} \sum_n q^{\varepsilon_n(\tau)} = \frac{Z_\tau}{Z_0}, \end{aligned} \quad (17)$$

where the third equality uses $\sum_m A[n, m] = 1$, the row sum of the composite, that is $A\mathbf{1} = \mathbf{1}$. That is the whole argument. It uses row stochasticity of A and nothing else: not symmetry, not commutation of the intervals, not degeneracy or non-degeneracy of the spectrum, not the number of measurements, and not the reason the row sums are one. They are one because each interval matrix is doubly stochastic, being the entrywise squared modulus of a unitary matrix, but the derivation above never asks where they came from: any row-stochastic A with Gibbs initial data satisfies (16). $\square$

The hypothesis really is this weak, and it is worth being explicit about what that means. A measurement train destroys the coherence that would otherwise make the dynamics non-classical, and what survives is a unital Markov chain on the energy levels. The integral fluctuation relation is a statement about unital Markov chains, so it survives the destruction of coherence completely. The verification record of Appendix A recomputes (16) exactly over 936 instances covering $d = 2, \dots, 6$, $N = 0, \dots, 6$, degenerate and non-degenerate spectra, cyclic and non-cyclic endpoints and three values of q , with maximum deficit exactly zero.

Theorem 4.2 (backward transfer matrix of a train; Crooks relation). *For the backward process of Definition 3.3 the interval matrices are $M_k^B = M_k^T$ and the composite is*

$$A_B = M_0^T M_1^T \cdots M_N^T = (M_N \cdots M_1 M_0)^T = A^T. \quad (18)$$

With the backward initial distribution $p_n^\tau = q^{\varepsilon_n(\tau)}/Z_\tau$, the Crooks relation of Definition 3.3 holds exactly for every work value w , at every d , every N , every protocol and schedule, every $\beta > 0$ and every pair of endpoint Hamiltonians.

Proof. The backward interval runs from t_{k+1} to t_k under $U_k^\dagger$, so

$$M_k^B[a, b] = |\langle e_a(t_k) | U_k^\dagger | e_b(t_{k+1}) \rangle|^2 = |\langle e_b(t_{k+1}) | U_k | e_a(t_k) \rangle|^2 = M_k[b, a], \quad (19)$$

which is $M_k^B = M_k^T$. The backward train traverses the intervals in the reverse order, applying M_N^B first and M_0^B last, so its composite is the product written in (18) and equals A^T by the anti-multiplicativity of the transpose. That identity is the only structural fact about the backward process that is needed; it is forced by the train and does not depend on any symmetry of the individual intervals.

For the relation itself, a pair $(n, m) \in C_w$ contributes to the forward distribution at w and, read backwards, to the backward distribution at $-w$ with the initial index n and the final index m . Hence

$$P_B(-w) = \sum_{(n,m) \in C_w} p_n^\tau A_B[m, n] = \frac{1}{Z_\tau} \sum_{(n,m) \in C_w} q^{\varepsilon_n(\tau)} A[n, m], \quad (20)$$

using $A_B[m, n] = A^T[m, n] = A[n, m]$. On the other hand

$$P(w) q^w \frac{Z_0}{Z_\tau} = \frac{1}{Z_\tau} \sum_{(n,m) \in C_w} q^{\varepsilon_m(0)} A[n, m] q^{\varepsilon_n(\tau) - \varepsilon_m(0)} = \frac{1}{Z_\tau} \sum_{(n,m) \in C_w} q^{\varepsilon_n(\tau)} A[n, m], \quad (21)$$

which is the same expression. With $\Delta F = -\beta^{-1} \ln(Z_\tau/Z_0)$ one has $e^{-\beta(w-\Delta F)} = q^w Z_0/Z_\tau$, so the two sides of Definition 3.3 agree for every w . $\square$

The last line deserves one clarification, because the free-energy factor is where signs are most easily lost. With $\Delta F = -\beta^{-1} \ln(Z_\tau/Z_0)$ the Crooks relation of Definition 3.3 reads $P(w) e^{-\beta(w-\Delta F)} = P_B(-w)$, and $e^{-\beta(w-\Delta F)} = q^w e^{\beta \Delta F} = q^w Z_0/Z_\tau$, which is exactly the factor used above.

Remark 4.3 (why the Crooks relation does not settle the detailed fluctuation theorem). Theorem 4.2 compares the forward distribution with the distribution of a *different* process, one that has to be prepared with the Gibbs state of $H(\tau)$ and run backwards. The symmetric form (1) compares $P(w)$ with $P(-w)$ inside the forward process alone. Substituting $A_B = A^T$ into the two sides of (1) shows what the difference is: the symmetric form asks whether A^T , weighted by the final Gibbs state, reproduces A weighted by the initial one. That is a question about the antisymmetric part of A , and it is precisely the question that fails at dimension three and above. The Crooks relation is dimension-free because it is allowed to change the process; the symmetric form is not, because it is not.

The verification record recomputes (18) and the Crooks relation exactly over the same 936 instances, including non-cyclic endpoints and non-symmetric, non-unistochastic composites, with deviation exactly zero, and checks $A_B = A^T$ entrywise for a literal three-interval train built from explicit interval matrices rather than from the transpose identity alone.

5 An exact class-wise criterion for the detailed fluctuation theorem

5.1 The criterion

The obstruction to the symmetric form lives in the work classes. Assume from here to the end of this section that the protocol is *cyclic*, $H(\tau) = H(0)$, so that $\varepsilon_n(\tau) = \varepsilon_n(0) =: \varepsilon_n$, $Z_\tau = Z_0 =: Z$ and $\Delta F = 0$. Cyclicity is exactly the regime in which (1) is the meaningful statement, since without it the two sides of (1) are weighted by different spectra; the non-cyclic case is treated separately and completely at dimension two in Theorem 6.5, and is open at higher dimension.

The obstacle to writing down a criterion is that the map $w \mapsto -w$ does not act on pairs of levels the way one first expects: the pair contributing to $P(w)$ at weight q^{ε_n} and the pair contributing to $P(-w)$ at weight q^{ε_m} are the same pair with its two indices exchanged, but the Gibbs weight attaches to different indices on the two sides. Cyclicity is what makes the exchange $(n, m) \mapsto (m, n)$ a bijection from C_w onto C_{-w} , and once that bijection is in hand the two sides can be subtracted term by term. What remains is a sum of differences $A[n, m] - A[m, n]$ over the class, which is the antisymmetric part of the composite and nothing else.

Theorem 5.1 (class-wise criterion). *Let the protocol be cyclic, let $d \geq 2$, $N \geq 0$, the schedule (3), the interval unitaries and $\beta > 0$ be arbitrary, and let $C_w = \{(n, m) : \varepsilon_n - \varepsilon_m = w\}$. Then for every work value w*

$$\Delta(w) = P(w)q^w - P(-w) = \frac{1}{Z} \sum_{(n,m) \in C_w} q^{\varepsilon_n} (A[n, m] - A[m, n]), \quad (22)$$

and the detailed fluctuation theorem (1) holds at every work value if and only if the right-hand side vanishes for every w .

Proof. From (8) with $p_m = q^{\varepsilon_m}/Z$,

$$P(w)q^w = \sum_{(n,m) \in C_w} \frac{q^{\varepsilon_m}}{Z} A[n, m] q^{\varepsilon_n - \varepsilon_m} = \frac{1}{Z} \sum_{(n,m) \in C_w} q^{\varepsilon_n} A[n, m]. \quad (23)$$

For $P(-w)$ the contributing pairs are those (a, b) with $\varepsilon_a - \varepsilon_b = -w$, that is, the class C_{-w} . Because the protocol is cyclic, $(n, m) \mapsto (m, n)$ is a bijection of C_w onto C_{-w} : if $\varepsilon_n - \varepsilon_m = w$ then $\varepsilon_m - \varepsilon_n = -w$, and the map is its own inverse. Substituting $(a, b) = (m, n)$,

$$P(-w) = \sum_{(a,b) \in C_{-w}} \frac{q^{\varepsilon_b}}{Z} A[a, b] = \frac{1}{Z} \sum_{(n,m) \in C_w} q^{\varepsilon_n} A[m, n]. \quad (24)$$

Subtracting (24) from (23) gives (22). The “if and only if” is the definition of the defect (9): (1) holds at w exactly when $\Delta(w) = 0$, and (22) expresses that number as the displayed sum. $\square$

5.2 What the criterion says

Five consequences are used repeatedly below, and all of them are immediate from (22).

Corollary 5.2 (symmetry is sufficient at every dimension). *If $A = A^T$ then $\Delta(w) = 0$ for every w , at every d , every $\beta > 0$ and every spectrum.*

Proof. $A = A^T$ makes every summand of (22) zero. No hypothesis on the spectrum, on q or on the class C_w is used. $\square$

Corollary 5.3 (zero work is vacuous). $\Delta(0) = 0$ *identically, for every cyclic protocol at every dimension.*

Proof. The exchange $(n, m) \mapsto (m, n)$ preserves C_0 , and on C_0 one has $\varepsilon_n = \varepsilon_m$, so the summands of (22) cancel in pairs. $\square$

Corollary 5.4 (w and $-w$ are one condition). $\Delta(-w) = -q^{-w}\Delta(w)$ *for every w ; in particular $\Delta(w) = 0$ if and only if $\Delta(-w) = 0$. The content of (1) is therefore one linear condition per positive work value.*

Proof. From (9), $P(-w) = P(w)q^w - \Delta(w)$, so

$$\Delta(-w) = P(-w)q^{-w} - P(w) = (P(w)q^w - \Delta(w))q^{-w} - P(w) = -q^{-w}\Delta(w), \quad (25)$$

and $q > 0$ makes the equivalence of the two vanishing statements immediate. Note that this identity is a consequence of the definition of the defect and does not use (22); it holds for non-cyclic endpoints as well. $\square$

Corollary 5.5 (the violation is a linear functional of the antisymmetric part). *With $D = D(A)$ as in (12),*

$$\Delta(w) = \frac{2}{Z} \sum_{(n,m) \in C_w} q^{\varepsilon_n} D[n, m]. \quad (26)$$

The map

$$\Phi : \mathcal{K}(d) \longrightarrow \mathbb{R}^{\#\{w>0\}}, \quad \Phi(D) = (\Delta(w))_{w>0}, \quad (27)$$

is linear, and (1) holds at every work value if and only if $\Phi(D(A)) = 0$. The detailed fluctuation theorem is blind to the symmetric part of the composite transfer matrix.

Proof. Write $A = S + D$ with $S = (A + A^T)/2$ symmetric and $D = (A - A^T)/2$ antisymmetric. Then $A[n, m] - A[m, n] = 2D[n, m]$, and (22) becomes (26), in which S does not appear. Linearity of Φ is immediate because (26) is a fixed linear combination of the entries of D for each w , with coefficients $2q^{\varepsilon_n}/Z$ on the class C_w and zero elsewhere. That $D(A) \in \mathcal{K}(d)$ is Lemma 6.1. $\square$

Corollary 5.5 is the reason the dimension analysis of Section 6 works at all. The conditions $\Delta(w) = 0$, $w > 0$, are the vanishing of a linear map on the space $\mathcal{K}(d)$, whose dimension is computed in Lemma 6.1; computing the rank of Φ exactly over the rationals therefore decides whether symmetry is necessary, and the answer depends on the endpoint spectrum and on β through the work classes. Corollary 6.11 tabulates the ranks.

Corollary 5.6 (distinct gaps make symmetry necessary as well). *Suppose the gaps are all distinct in the sense that $\varepsilon_n - \varepsilon_m = \varepsilon_{n'} - \varepsilon_{m'}$ with $(n, m) \neq (n', m')$ forces $w = 0$. Then every class C_w with $w \neq 0$ is a single pair, (22) reduces to $\Delta(w) = Z^{-1}q^{\varepsilon_n}(A[n, m] - A[m, n])$, and (1) holds at every work value if and only if A is symmetric.*

Proof. Under the hypothesis each off-diagonal pair (n, m) , $n \neq m$, lies in exactly one class C_w with $w = \varepsilon_n - \varepsilon_m \neq 0$, and that class contains no other pair, so $q^{\varepsilon_n} > 0$ and $Z > 0$ force $A[n, m] = A[m, n]$. Diagonal entries are symmetric automatically. $\square$

The hypothesis of Corollary 5.6 also implies that the spectrum is non-degenerate, since $\varepsilon_n = \varepsilon_m$ with $n \neq m$ would give $\varepsilon_n - \varepsilon_m = 0 = \varepsilon_{m'} - \varepsilon_{m'}$ for two distinct pairs. A non-degenerate spectrum with all gaps distinct is the generic situation, so generically the detailed fluctuation theorem holds exactly when the composite is symmetric. The next corollary says that degeneracy is the only way out, and that it is a way out rather than a curiosity.

Corollary 5.7 (degeneracy restores the theorem without symmetry). *If a work class C_w contains several pairs, their contributions to (22) can cancel while A remains asymmetric. At $d = 3$ with one doubly degenerate level this cancellation happens for every protocol, every schedule, every train length and every $\beta > 0$ (Theorem 6.10), and at $d = 4$ with the spectrum $(0, 0, 1, 1)$ the map Φ of (27) is identically zero on $\mathcal{K}(4)$.*

Proof. The first statement is the observation that (26) is a sum: a sum of several terms can vanish without each term vanishing, and the terms are $2q^{\varepsilon_n} D[n, m]/Z$, so pairs sharing the same final energy carry the same positive factor and cancel exactly when the corresponding entries of D are opposite.

For the $d = 4$ spectrum $(0, 0, 1, 1)$ the cancellation is forced rather than possible. The only positive work value is $w = 1$, its class is $C_1 = \{2, 3\} \times \{0, 1\}$, and every pair in it has $\varepsilon_n = 1$, so

$$\Delta(1) = \frac{2q}{Z} \sum_{n \in \{2, 3\}} \sum_{m \in \{0, 1\}} D[n, m] = \frac{q}{Z} \sum_{n \in \{2, 3\}} \sum_{m \in \{0, 1\}} (A[n, m] - A[m, n]) \quad (28)$$

with $Z = 2 + 2q$. The two sums are equal for every $A \in \mathcal{B}(4)$: the row sums at indices 2 and 3 give $\sum_{n, m} A[n, m] = 2 - (A[2, 2] + A[3, 3]) - (A[2, 3] + A[3, 2])$, and the column sums at indices 2 and 3 give the identical expression for $\sum_{n, m} A[m, n]$. Hence $\Delta(1) = 0$ for every doubly stochastic A , that is, $\Phi \equiv 0$ on $\mathcal{K}(4)$ for this spectrum. $\square$

5.3 A worked instance

The criterion is short enough to check by hand on the smallest non-trivial case, and the instance chosen here is the one that turns out to be the worst case at dimension three. Take $d = 3$ with the equally spaced spectrum $\varepsilon = (-1, 0, 1)$, inverse temperature $\beta = \ln 2$ so that $q = \frac{1}{2}$, and the deterministic protocol given by the three-cycle $\sigma = (012)$, that is, $A = P_\sigma$ with the convention (11). Then $Z = q^{-1} + 1 + q = \frac{7}{2}$ and the Gibbs weights are $p = (\frac{4}{7}, \frac{2}{7}, \frac{1}{7})$.

The matrix A has its three ones at $(n, m) = (1, 0), (2, 1), (0, 2)$, so the work values are $\varepsilon_1 - \varepsilon_0 = 1$, $\varepsilon_2 - \varepsilon_1 = 1$ and $\varepsilon_0 - \varepsilon_2 = -2$, with probabilities $\frac{4}{7}, \frac{2}{7}$ and $\frac{1}{7}$. Hence $P(1) = \frac{6}{7}$ and $P(-2) = \frac{1}{7}$, and all other values have probability zero. The defects are

$$\Delta(1) = \frac{6}{7} \cdot \frac{1}{2} - 0 = \frac{3}{7}, \quad \Delta(2) = 0 - \frac{1}{7} = -\frac{1}{7}, \quad \Delta(-1) = -\frac{6}{7}, \quad \Delta(-2) = \frac{1}{7} \cdot 4 - 0 = \frac{4}{7}, \quad (29)$$

and $V(A) = \frac{1}{2}(\frac{3}{7} + \frac{1}{7} + \frac{6}{7} + \frac{4}{7}) = 1$.

Now the same numbers from (22). The classes are $C_1 = \{(1, 0), (2, 1)\}$ and $C_2 = \{(2, 0)\}$, and

$$\Delta(1) = \frac{2}{Z} \left[q^{\varepsilon_1} (A[1, 0] - A[0, 1]) + q^{\varepsilon_2} (A[2, 1] - A[1, 2]) \right] = \frac{2}{7} \left[1 \cdot (1 - 0) + \frac{1}{2} \cdot (1 - 0) \right] = \frac{3}{7}, \quad (30)$$

$$\Delta(2) = \frac{1}{Z} q^{\varepsilon_2} (A[2, 0] - A[0, 2]) = \frac{2}{7} \cdot \frac{1}{2} \cdot (0 - 1) = -\frac{1}{7}. \quad (31)$$

The two routes agree exactly, as they must. Corollary 5.4 is visible in the numbers: $\Delta(-1) = -q^{-1} \Delta(1) = -2 \cdot \frac{3}{7}$ and $\Delta(-2) = -q^{-2} \Delta(2) = -4 \cdot (-\frac{1}{7})$. And the antisymmetric scalar of Section 6 is $x = A[0, 1] - A[1, 0] = -1$, which reproduces both defects through the closed forms of Theorem 6.8.

6 The antisymmetric part and the dimension split

Corollary 5.5 reduced the detailed fluctuation theorem to the vanishing of a linear map on the antisymmetric part of the composite transfer matrix. This section determines which antisymmetric

parts a measurement train can produce at all, and the answer is what separates dimension two from every higher dimension.

6.1 The realised antisymmetric parts

Lemma 6.1 (dimension of the realised directions). *For every $d \geq 2$, $\mathcal{R}(d) \subset \mathcal{K}(d)$ as defined in (13) and (14), $\mathcal{K}(d)$ has dimension*

$$\dim \mathcal{K}(d) = \frac{(d-1)(d-2)}{2}, \quad (32)$$

which vanishes exactly for $d \leq 2$, and $\text{span } \mathcal{R}(d) = \mathcal{K}(d)$. More precisely, 0 is an interior point of $\mathcal{R}(d)$ relative to $\mathcal{K}(d)$: for every nonzero $D \in \mathcal{K}(d)$ and every $|t| \leq 1/\max_{i,j}|D[i,j]|$ the matrix $A_t = (J + tD)/d$ lies in $\mathcal{B}(d)$ and satisfies $A_t - A_t^T = (2t/d)D$.

Proof. If $A \in \mathcal{B}(d)$ then $A\mathbf{1} = \mathbf{1}$ by row stochasticity and $A^T\mathbf{1} = \mathbf{1}$ by column stochasticity, so $(A - A^T)\mathbf{1} = 0$; combined with antisymmetry this is $\mathcal{R}(d) \subset \mathcal{K}(d)$.

For the dimension, the space of antisymmetric $d \times d$ matrices has dimension $d(d-1)/2$, and the map $D \mapsto D\mathbf{1}$ lands in the hyperplane $\{v : \mathbf{1}^T v = 0\}$, because $\mathbf{1}^T D\mathbf{1}$ equals its own transpose and also equals minus itself. It is onto that hyperplane: given v with $\mathbf{1}^T v = 0$, the matrix $D = (v\mathbf{1}^T - \mathbf{1}v^T)/d$ is antisymmetric and satisfies $D\mathbf{1} = (vd - \mathbf{1}\mathbf{1}^T v)/d = v$. Hence $\dim \mathcal{K}(d) = d(d-1)/2 - (d-1) = (d-1)(d-2)/2$, which is zero only for $d \leq 2$.

For the span, fix a nonzero $D \in \mathcal{K}(d)$ and put $M = \max_{i,j}|D[i,j]| > 0$. For $|t| \leq 1/M$ the matrix $A_t = (J + tD)/d$ has entries $1/d + tD[i,j]/d \geq (1 - |t|M)/d \geq 0$, row sums $1 + t(D\mathbf{1})_i/d = 1$ and, by antisymmetry of D , column sums equal to the row sums of $A_t^T = (J - tD)/d$, which are also one. So $A_t \in \mathcal{B}(d)$ and $A_t - A_t^T = 2tD/d$, nonzero for $t \neq 0$. Every direction of $\mathcal{K}(d)$ is therefore realised up to a positive scale. $\square$

Lemma 6.1 is the whole dimension split. At $d = 2$ the space $\mathcal{K}(2)$ is trivial, so $A - A^T = 0$ for every $A \in \mathcal{B}(2)$ and there is no antisymmetric direction for the violation of Corollary 5.5 to use. At every $d \geq 3$ the space has positive dimension and, by the scale argument, every direction in it is available to some composite, at least up to a small multiple. What the lemma does *not* say is that $\mathcal{R}(d) = \mathcal{K}(d)$: the realised set is bounded while $\mathcal{K}(d)$ is not. The exact extent is a separate statement and it matters for Section 7, where the worst case is taken over realisable protocols.

Theorem 6.2 (exact extent of the realised set). *For every $d \geq 2$,*

$$\mathcal{R}(d) = \left\{ D \in \mathcal{K}(d) : \sum_j |D[i,j]| \leq 2 \text{ for every } i \right\} = \text{conv} \{ P_\sigma - P_\sigma^T : \sigma \in S_d \}. \quad (33)$$

At $d = 3$ this is the closed segment $[-1, 1]G$ with

$$G = \begin{pmatrix} 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & -1 & 0 \end{pmatrix}, \quad (34)$$

whose endpoints are the differences of the two three-cycle permutation matrices. At $d = 4$ it is exactly the cube section $\mathcal{K}(4) \cap \{|D[i,j]| \leq 1\}$. For every $d \geq 5$ the cube section is strictly larger than $\mathcal{R}(d)$.

Proof. $\mathcal{R}(d)$ is the image of the compact convex set $\mathcal{B}(d)$ under the linear map $A \mapsto A - A^T$, so it is a compact convex body, symmetric under $D \mapsto -D$ because $A \mapsto A^T$ preserves $\mathcal{B}(d)$, with non-empty interior in $\mathcal{K}(d)$ by Lemma 6.1. The hull identity in (33) follows immediately: $\mathcal{B}(d)$ is the convex hull of the permutation matrices and the map is linear, so the image is the convex hull of the images of the vertices.

The inequality description needs both halves. For necessity, if $A \in \mathcal{B}(d)$ then for every index i

$$\sum_j |(A - A^T)[i, j]| = \sum_j |A[i, j] - A[j, i]| \leq \sum_j (A[i, j] + A[j, i]) = 1 + 1 = 2, \quad (35)$$

the last equality being the row sum and the column sum of A at index i .

For sufficiency, let $D \in \mathcal{K}(d)$ satisfy the d inequalities (35). Set $L = |D|/2$ entrywise, $r = \mathbf{1} - L\mathbf{1}$, $s = \mathbf{1}^T r$, and

$$E = \begin{cases} rr^T/s, & s > 0, \\ 0, & s = 0, \end{cases} \quad S = L + E, \quad A = S + \frac{D}{2}. \quad (36)$$

The hypotheses give $r \geq 0$ entrywise, so $E \geq 0$ and $S \geq 0$; and $E\mathbf{1} = r$ in both branches, because if $s = 0$ then $r \geq 0$ with $\mathbf{1}^T r = 0$ forces $r = 0$. Since L and E are symmetric— $|D|$ is symmetric when D is antisymmetric— S is symmetric, and

$$A\mathbf{1} = L\mathbf{1} + E\mathbf{1} + \frac{D\mathbf{1}}{2} = (\mathbf{1} - r) + r + 0 = \mathbf{1}, \quad \mathbf{1}^T A = \mathbf{1}^T S + \frac{\mathbf{1}^T D}{2} = \mathbf{1}^T, \quad (37)$$

using $\mathbf{1}^T D = -(D\mathbf{1})^T = 0$. Entrywise,

$$A[i, j] = \frac{|D[i, j]|}{2} + \frac{D[i, j]}{2} + E[i, j] = \max(D[i, j], 0) + E[i, j] \geq 0, \quad (38)$$

and $A - A^T = D$ because S is symmetric. Hence $A \in \mathcal{B}(d)$ and $D \in \mathcal{R}(d)$.

At $d = 3$ write $x = A[0, 1] - A[1, 0]$, $y = A[0, 2] - A[2, 0]$ and $z = A[1, 2] - A[2, 1]$. Equality of the row and the column sum at index 0 gives $x + y = 0$ and at index 1 gives $z - x = 0$; the index-2 equation is their consequence. So $A - A^T = xG$ with G as in (34), and (35) at index 0 reads $2|x| \leq 2$. With $P = P_{(021)}$ and $P' = P_{(012)}$ one has $P - P' = G$, so the endpoints $x = \pm 1$ are attained, and every $x \in [-1, 1]$ is attained by $\frac{1+x}{2}P + \frac{1-x}{2}P'$.

At $d = 4$ each row of an element of $\mathcal{K}(4)$ has three entries summing to zero, so $\sum_j |D[i, j]|$ is twice the sum of the positive entries of that row and therefore at most twice the largest entry in absolute value: the cube condition $|D[i, j]| \leq 1$ already implies (35). For $d \geq 3$ the entry bound $|D[i, j]| \leq 1$ is itself attained, by any $P_\sigma - P_\sigma^T$ with $\sigma(i) = j \neq \sigma(j)$. At $d = 5$ the regular tournament $T[i, j] = 1$ for $(j - i) \bmod 5 \in \{1, 2\}$ and $T[j, i] = -T[i, j]$ lies in $\mathcal{K}(5)$ and in the cube, yet $\sum_j |T[0, j]| = 4 > 2$, so $T \notin \mathcal{R}(5)$; padding T with zero rows and columns separates $\mathcal{R}(d)$ from the cube section for every $d \geq 5$. $\square$

The dimensions (32) are 0, 1, 3, 6, 10, 15, 21 for $d = 2, \dots, 8$, and the verification record of Appendix A reproduces each of them by exact elimination. It also checks (33) from both sides. Necessity is checked on every exact lattice point of $\mathcal{B}(3)$ and $\mathcal{B}(4)$ at denominators three and two, 337 matrices, and on 81741 exact convex combinations of pairs of permutation matrices at $d = 3, 4, 5$ with weights in $\frac{1}{10}\mathbb{Z}$. Sufficiency is checked by running the construction (36) on 1263 exact elements of $\mathcal{K}(d)$ that satisfy the row bounds, at $d = 3, 4, 5$, with both branches of E exercised—116 of them have $s = 0$, and those are exactly the differences $P_\sigma - P_\sigma^T$ for which every cycle of σ has length at least three, where the construction returns P_σ itself. Of the 4245 elements of $\mathcal{K}(d)$ on that grid,

2982 violate a row bound and are rejected, and rescaling each of them by $2/\max_i \sum_j |D[i, j]|$ lands it exactly on the boundary of the set, where the construction certifies it. All 5910 permutation differences at $d = 3, \dots, 7$ satisfy the row bounds. The segment $\mathcal{R}(3) = [-1, 1]G$ is reproduced on 83 exact points of a 41-step rational grid, each written as an explicit convex combination of the two three-cycle permutation matrices; the $d = 4$ cube section on all 15 elements of $\mathcal{K}(4)$ with entries in $\{-1, 0, 1\}$; and the $d = 5$ tournament is confirmed to lie in $\mathcal{K}(5)$ and in the cube while violating the row bound by $4 > 2$, with the same separation confirmed after padding at $d = 6$ and $d = 7$.

6.2 Dimension two

Theorem 6.3 (the symmetric form is unconditional at $d = 2$). *At $d = 2$ every doubly stochastic matrix is symmetric. Consequently, for cyclic endpoint Hamiltonians, the detailed fluctuation theorem (1) holds exactly for every protocol, every schedule, every number of intermediate measurements and every $\beta > 0$. Moreover every 2×2 doubly stochastic matrix has the form $(1 - p)I + pX$ with X the swap matrix, all such matrices commute, and every composite $A = M_N \cdots M_0$ is again of that form.*

Proof. A matrix $A \in \mathcal{B}(2)$ has the form $\begin{pmatrix} a & 1-a \\ 1-b & b \end{pmatrix}$ with $a, b \in [0, 1]$; the first column sum forces $a + 1 - b = 1$, that is $b = a$, and the matrix is $\begin{pmatrix} a & 1-a \\ 1-a & a \end{pmatrix} = (1 - a)I + aX$, which is symmetric. Corollary 5.2 then gives (1) at every work value, and the commutation and closure statements are immediate from the one-parameter form. $\square$

This is the structural reason the two-level case is exceptional, and it is a statement about the polytope $\mathcal{B}(2)$ rather than about any dynamics; classically it is recorded as the coincidence $\mathcal{U}(2) = \mathcal{O}(2) = \mathcal{B}(2)$ of the unistochastic, orthostochastic and Birkhoff sets at dimension two [11]. The route usually taken at dimension two proves that each interval matrix M_k is symmetric from an amplitude identity for two-level unitaries, and then concludes that the composite is symmetric. Theorem 6.3 shows that the first step is unnecessary: $M_k \in \mathcal{B}(2)$ is already symmetric, whatever the unitary U_k and whatever the two energy bases are. The same lemma also says why no such argument can work at $d \geq 3$: there $\mathcal{K}(d)$ has positive dimension and, by the scale part of Lemma 6.1, every direction in it is available to some composite.

The cyclicity hypothesis of Theorem 6.3 is not a formality, and it cannot be replaced by symmetry of A .

Remark 6.4 (symmetry of the composite does not suffice off cyclicity). Identity (22) was derived using the bijection $(n, m) \mapsto (m, n)$ of C_w onto C_{-w} , and that bijection exists because the two endpoint spectra coincide. Symmetry of A is a statement about A alone, while $\Delta(w)$ also depends on the two endpoint spectra through the work classes, so “ A is symmetric” cannot by itself imply “ $\Delta \equiv 0$ ” when $H(\tau) \neq H(0)$. The smallest counterexample is at $d = 2$, with an A whose antisymmetric part is identically zero:

$$A = \begin{pmatrix} 2/3 & 1/3 \\ 1/3 & 2/3 \end{pmatrix} = A^T, \quad \varepsilon(0) = (0, 1), \quad \varepsilon(\tau) = (0, 2), \quad q = \frac{1}{2}, \quad Z_0 = \frac{3}{2}, \quad (39)$$

which gives

$$P = \left\{ -1 : \frac{1}{9}, 0 : \frac{4}{9}, 1 : \frac{2}{9}, 2 : \frac{2}{9} \right\}, \quad \Delta(2) = P(2)q^2 - P(-2) = \frac{1}{18} - 0 = \frac{1}{18} \neq 0. \quad (40)$$

The integral fluctuation relation holds exactly here, with $Z_\tau/Z_0 = \frac{5}{6}$ and deficit zero, and the Crooks relation holds exactly against $A_B = A^T$. The obstruction is the support: the work values

are $\{-1, 0, 1, 2\}$, the value -2 is not attainable, so $P(-2) = 0$ while $P(2) > 0$. No multiplicative correction repairs this. For every rational $c \in \{1, Z_\tau/Z_0, Z_0/Z_\tau, q, 1/q\}$ the corrected defect $P(w)q^w - cP(-w)$ at $w = 2$ equals $P(2)q^2 = \frac{1}{18}$, because c multiplies a vanishing term and drops out entirely.

The right condition turns out to be weaker and sharper than cyclicity.

Theorem 6.5 (exact $d = 2$ criterion for arbitrary endpoints). *Let $d = 2$, let $\varepsilon(0) = (a_0, a_1)$ and $\varepsilon(\tau) = (b_0, b_1)$, and let $\beta > 0$, that is, $q \neq 1$. Then $\Delta(w) = 0$ for every work value w , for every $A \in \mathcal{B}(2)$, every schedule and every number of intermediate measurements, if and only if the two endpoint Hamiltonians are isospectral, $\{b_0, b_1\} = \{a_0, a_1\}$ as multisets. Cyclicity $H(\tau) = H(0)$ is sufficient but not necessary.*

Proof. Translating both spectra by the same constant leaves every $\Delta(w)$ unchanged: the work values $b_n - a_m$ are invariant, and $p_m = q^{a_m}/Z_0$ is invariant because numerator and denominator acquire the same factor. Assume therefore $a_0 = 0$ and $a_1 = g \geq 0$, so that $p_1 = q^g p_0$, and write $s = b_0 + b_1$ and $A = (1 - p)I + pX$.

For sufficiency, if $(b_0, b_1) = (0, g)$ the protocol is cyclic and Theorem 6.3 applies. If $(b_0, b_1) = (g, 0)$ —isospectral but not cyclic, which is what following an eigenvector through a level crossing produces—the four work values are $b_0 - a_0 = g$, $b_0 - a_1 = 0$, $b_1 - a_0 = 0$ and $b_1 - a_1 = -g$. Both off-diagonal entries of A land at $w = 0$, where Δ vanishes identically by Corollary 5.3, and

$$\Delta(g) = q^g p_0 A[0, 0] - p_1 A[1, 1] = (1 - p)(q^g p_0 - p_1) = 0 \quad (41)$$

because $p_1 = q^g p_0$; then $\Delta(-g) = -q^{-g} \Delta(g) = 0$ by Corollary 5.4.

For necessity, suppose $\{b_0, b_1\} \neq \{0, g\}$. The single matrix $A = I$ already fails, at every $q \neq 1$: it gives $P(w) = p_0[w = b_0] + p_1[w = b_1 - g]$, and exactly one of three mutually exhaustive branches applies. If $b_0 \neq 0$ and $s \neq g$, then $-b_0$ is attained by neither diagonal term and $\Delta(b_0) = q^{b_0} p_0 \neq 0$. If $b_0 = 0$ and $s \neq g$, hence $b_1 \neq g$, then $w = b_1 - g$ is nonzero and $-(b_1 - g) = g - b_1$ is attained by neither term, so $\Delta(b_1 - g) = q^{b_1 - g} p_1 \neq 0$. If $b_0 \neq 0$ and $s = g$, then $b_1 - g = -b_0 \neq b_0$ and $\Delta(b_0) = q^{b_0} p_0 - p_1 = p_0(q^{b_0} - q^g) \neq 0$, because $b_0 \neq g$ —otherwise $b_0 = g$ and $b_1 = 0$, the isospectral case just excluded—and $q \neq 1$. The remaining branch, $b_0 = 0$ and $s = g$, forces $(b_0, b_1) = (0, g)$, which is isospectral. $\square$

Corollary 6.6 (the drive-independent pair ratios that replace (1) at $d = 2$). *Let $\varepsilon(0) = (0, g_0)$ and $\varepsilon(\tau) = (0, g_\tau)$ with $g_0, g_\tau \geq 1$ and $g_0 \neq g_\tau$, and let $A = (1 - p)I + pX$ be any composite. In the centred convention, with $\Omega_0 = g_0$, $\Omega_f = g_\tau$, $w_1 = (g_\tau + g_0)/2$ and $w_2 = |g_\tau - g_0|/2$,*

$$\frac{P(+w_1)}{P(-w_1)} = q^{-g_0}, \quad \frac{P(+w_2)}{P(-w_2)} = \begin{cases} q^{g_0}, & g_\tau > g_0, \\ q^{-g_0}, & g_\tau < g_0, \end{cases} \quad (42)$$

and neither ratio depends on p , hence neither depends on the drive, the schedule or the number of intermediate measurements.

Proof. In uncentred labels the $+w_1$ and $-w_1$ branches are $W = g_\tau$ and $W = -g_0$, carrying $p p_0$ and $p p_1 = p q^{g_0} p_0$, whose ratio is q^{-g_0} . For $g_\tau > g_0$ the $+w_2$ and $-w_2$ branches are $W = g_\tau - g_0$ and $W = 0$, carrying $(1 - p)p_1$ and $(1 - p)p_0$, ratio q^{g_0} ; for $g_\tau < g_0$ the two branches are exchanged and the ratio is q^{-g_0} . $\square$

The symmetric form demands $P(w)/P(-w) = q^{-w}$, that is q^{-w_1} and q^{-w_2} respectively. The first of (42) agrees with q^{-w_1} exactly when $g_0 = (g_\tau + g_0)/2$, that is when $g_\tau = g_0$, in which case

$w_2 = 0$ and the second condition is vacuous by Corollary 5.3. So (1) is the isospectral degeneration of a pair of exact ratios carrying two different exponential factors, which is what the exactly solved two-level analysis in the source record [5] states for a single interval; Corollary 6.6 establishes it for the composite of an arbitrary train.

Remark 6.7 (infinite temperature is the boundary of the scope). The hypothesis $\beta > 0$ in Theorem 6.5 is needed, and it is used at exactly one place: the third branch of the necessity proof, through $q \neq 1$. At $q = 1$ the Gibbs weights are uniform, $\Delta(w) = d^{-1}(\sum_{C_w} A - \sum_{C_{-w}} A)$, and the criterion degenerates into a symmetry of class sums that does not require isospectrality. For $\varepsilon(0) = (0, 2)$, $\varepsilon(\tau) = (1, 1)$ and $A = I$ one has $\Delta \equiv 0$ exactly at $q = 1$, while $\Delta(-1) = -\frac{2}{5}$ at $q = \frac{1}{2}$. Infinite temperature is the boundary of the stated scope, not part of it.

6.3 Dimension three

Theorem 6.8 (one scalar controls the whole violation). *At $d = 3$ the antisymmetric part of any doubly stochastic matrix is one-dimensional: $A - A^T = xG$ with G as in (34) and*

$$x = A[0, 1] - A[1, 0] \in [-1, 1], \quad (43)$$

so the entire detailed-fluctuation-theorem violation of any three-level measurement train is controlled by the single rational number x . For the equally spaced spectrum $\varepsilon = (-1, 0, 1)$,

$$\Delta(1) = -\frac{x(1+q)}{Z}, \quad \Delta(2) = \frac{xq}{Z}, \quad Z = q^{-1} + 1 + q, \quad (44)$$

and both are nonzero multiples of x for every $q > 0$. Hence for a non-degenerate three-level spectrum the detailed fluctuation theorem holds for a protocol if and only if its composite is symmetric.

Proof. The dimension count is the $d = 3$ specialisation of Theorem 6.2: with $x = A[0, 1] - A[1, 0]$, $y = A[0, 2] - A[2, 0]$ and $z = A[1, 2] - A[2, 1]$, equality of row and column sums at index 0 gives $x + y = 0$ and at index 1 gives $z - x = 0$, so $y = -x$, $z = x$ and $A - A^T = xG$.

For (44), the classes are $C_1 = \{(1, 0), (2, 1)\}$ and $C_2 = \{(2, 0)\}$, and (22) gives

$$\Delta(1) = \frac{1}{Z} [q^{\varepsilon_1} (A[1, 0] - A[0, 1]) + q^{\varepsilon_2} (A[2, 1] - A[1, 2])] = \frac{1}{Z} [-x + q(-x)] = -\frac{x(1+q)}{Z}, \quad (45)$$

$$\Delta(2) = \frac{1}{Z} q^{\varepsilon_2} (A[2, 0] - A[0, 2]) = \frac{1}{Z} q x = \frac{xq}{Z}, \quad (46)$$

using $A[1, 0] - A[0, 1] = -x$, $A[2, 1] - A[1, 2] = -z = -x$ and $A[2, 0] - A[0, 2] = -y = x$. Both coefficients are strictly positive for $q > 0$ and $Z > 0$, so each defect vanishes exactly when x does.

For the last statement, let the spectrum be non-degenerate and relabel so that $\varepsilon_0 < \varepsilon_1 < \varepsilon_2$. The largest work value $w_{\max} = \varepsilon_2 - \varepsilon_0$ is attained by the single pair $(2, 0)$, so (22) gives $\Delta(w_{\max}) = Z^{-1} q^{\varepsilon_2} (A - A^T)[2, 0] = x q^{\varepsilon_2} / Z$ because $G[2, 0] = 1$. If (1) holds at every work value then $\Delta(w_{\max}) = 0$, hence $x = 0$, hence $A = A^T$; the converse is Corollary 5.2. $\square$

Corollary 6.9 (the total-variation violation is exactly $|x|$). *For $d = 3$ with the equally spaced spectrum $\varepsilon = (-1, 0, 1)$ and any $q > 0$,*

$$V(A) = |x| = |A[0, 1] - A[1, 0]|. \quad (47)$$

Proof. The work values are $-2, -1, 0, 1, 2$, and $\Delta(0) = 0$ by Corollary 5.3. Corollary 5.4 gives $\Delta(-1) = -q^{-1}\Delta(1)$ and $\Delta(-2) = -q^{-2}\Delta(2)$, so with (44)

$$2V(A) = |\Delta(1)|(1 + q^{-1}) + |\Delta(2)|(1 + q^{-2}) = \frac{|x|}{Z} \left[(1 + q) \frac{1 + q}{q} + q \frac{1 + q^2}{q^2} \right] \quad (48)$$

$$= \frac{|x|}{Z} \cdot \frac{(1 + q)^2 + 1 + q^2}{q} = \frac{|x|}{Z} \cdot \frac{2(1 + q + q^2)}{q} = 2|x|, \quad (49)$$

because $Z = q^{-1} + 1 + q = (1 + q + q^2)/q$. $\square$

Theorem 6.10 (a doubly degenerate level makes the theorem unconditional at $d = 3$). *If the three-level spectrum has a doubly degenerate level, then $\Delta(w) = 0$ for every protocol, every schedule, every train length and every $\beta > 0$, whether or not the composite is symmetric.*

Proof. Take $\varepsilon = (0, 0, 1)$; the case $(0, 1, 1)$ is the same after relabelling. The only nonzero work values are $w = \pm 1$ and $C_1 = \{(2, 0), (2, 1)\}$, so (22) gives

$$\Delta(1) = \frac{q}{Z} \left[(A[2, 0] - A[0, 2]) + (A[2, 1] - A[1, 2]) \right] = \frac{q}{Z} (x - z) = 0, \quad (50)$$

using $A - A^T = xG$, which gives $A[2, 0] - A[0, 2] = x$ and $A[2, 1] - A[1, 2] = -z = -x$; and $\Delta(-1) = -q^{-1}\Delta(1) = 0$ by Corollary 5.4. Here $Z = 2 + q$. $\square$

The physical content is worth stating, because it explains why the cancellation is not a coincidence. When the final Hamiltonian has a degenerate doublet, work resolves only “inside the doublet” against “outside it”; the two pairs that contribute share the same final energy, hence the same Gibbs factor, and the single available antisymmetric degree of freedom cancels between them. The correct criterion is therefore the class-wise one of Theorem 5.1, not “ A symmetric”: symmetry is sufficient at every dimension, necessary when the gaps are distinct by Corollary 5.6, and not necessary in general.

6.4 The rank of the violation map decides

Corollary 6.11 (rank criterion). *For cyclic endpoints the conditions $\Delta(w) = 0$, $w > 0$, are exactly the vanishing of the linear map Φ of (27) on the space $\mathcal{K}(d)$ of dimension $(d - 1)(d - 2)/2$. Computing $\text{rank } \Phi$ exactly over the rationals therefore decides whether symmetry is necessary: $\text{rank } \Phi = \dim \mathcal{K}(d)$ forces $D(A) = 0$, that is, A symmetric, while $\text{rank } \Phi < \dim \mathcal{K}(d)$ leaves a nonzero kernel whose sufficiently small multiples are realised inside $\mathcal{B}(d)$ by Lemma 6.1 and are detailed-fluctuation-theorem exact while asymmetric.*

Proof. Linearity of Φ is Corollary 5.5 and $\dim \mathcal{K}(d) = (d - 1)(d - 2)/2$ is Lemma 6.1, so rank-nullity gives $\dim \ker \Phi = \dim \mathcal{K}(d) - \text{rank } \Phi$. If $\text{rank } \Phi = \dim \mathcal{K}(d)$ then $\ker \Phi = \{0\}$, and $\Phi(D(A)) = 0$ forces $D(A) = 0$, that is $A = A^T$; together with Corollary 5.2 this is the equivalence. If $\text{rank } \Phi < \dim \mathcal{K}(d)$ choose a nonzero $u \in \ker \Phi$ and put $M = \max_{i,j} |u[i, j]| > 0$. For every t with $0 < |t| \leq 1/M$ the matrix $A_t = (J + tu)/d$ lies in $\mathcal{B}(d)$ by the scale argument of Lemma 6.1, and $A_t - A_t^T = (2t/d)u$, so $D(A_t) = (t/d)u \in \ker \Phi$ and $\Phi(D(A_t)) = 0$; theorem (1) holds exactly for the composite A_t while A_t is asymmetric because $t \neq 0$ and $u \neq 0$. $\square$

Table 1 gives the ranks for the spectra that matter here. The pattern is structural rather than accidental. An equally spaced d -level spectrum has only $d - 1$ positive work values, which is fewer than $(d - 1)(d - 2)/2$ as soon as $d \geq 4$, so the map Φ cannot be injective there. A spectrum with

Table 1: Exact rank of the violation map Φ of (27) over the rationals, for cyclic endpoint Hamiltonians, as a function of the endpoint spectrum. The third column is $\dim \mathcal{K}(d) = (d-1)(d-2)/2$, the fourth the number of positive work values, that is, the number of independent conditions by Corollary 5.4. The ranks are independent of q on the three values tested, $q = \frac{1}{2}, \frac{2}{3}, 3$. The last column abbreviates the conclusion of Corollary 6.11: “ $\Leftrightarrow$ symmetry” means the detailed fluctuation theorem holds exactly when the composite is symmetric, “asymmetric exact” means asymmetric composites satisfy the theorem exactly, and “every protocol” means every cyclic protocol satisfies it whatever its composite.

d	spectrum	$\dim \mathcal{K}(d)$	$\#\{w > 0\}$	rank Φ	conclusion
3	$(-1, 0, 1)$, equally spaced	1	2	1	$\Leftrightarrow$ symmetry
3	$(0, 1, 3)$, distinct gaps	1	3	1	$\Leftrightarrow$ symmetry
3	$(-2, 0, 5)$, distinct gaps	1	3	1	$\Leftrightarrow$ symmetry
3	$(0, 0, 1)$, degenerate	1	1	0	every protocol
3	$(0, 1, 1)$, degenerate	1	1	0	every protocol
4	$(0, 1, 2, 3)$, equally spaced	3	3	2	asymmetric exact
4	$(0, 1, 3, 7)$, distinct gaps	3	6	3	$\Leftrightarrow$ symmetry
4	$(0, 0, 1, 1)$, degenerate	3	1	0	every protocol
5	$(0, 1, 2, 3, 4)$, equally spaced	6	4	3	asymmetric exact
5	$(0, 2, 3, 7, 11)$, distinct gaps	6	9	6	$\Leftrightarrow$ symmetry

all gaps distinct has $d(d-1)/2$ positive work values, which exceeds $(d-1)(d-2)/2$ for every $d \geq 2$, and Φ is generically injective. A degenerate spectrum collapses the number of work values and can make Φ identically zero.

6.5 Dimension four: an asymmetric composite that satisfies the theorem exactly

The rank deficiency at $d = 4$ with the equally spaced spectrum is not a formal curiosity, because it can be written down.

Corollary 6.12 (an exact asymmetric detailed-fluctuation-theorem composite at $d = 4$). *For $\varepsilon = (0, 1, 2, 3)$ and $q = \frac{1}{2}$, rank $\Phi = 2 < 3 = \dim \mathcal{K}(4)$, the kernel of Φ is one-dimensional, and with D_0 spanning it the matrix $A = J/4 + D_0/4$ is*

$$A = \begin{pmatrix} 1/4 & 1/8 & 3/8 & 1/4 \\ 3/8 & 1/4 & 3/8 & 0 \\ 1/8 & 1/8 & 1/4 & 1/2 \\ 1/4 & 1/2 & 0 & 1/4 \end{pmatrix}, \quad A[0, 1] - A[1, 0] = -\frac{1}{4}, \quad \max_{i,j} |(A - A^T)[i, j]| = \frac{1}{2}, \quad (51)$$

where the maximum is attained at the four ordered pairs $(1, 3)$, $(3, 1)$, $(2, 3)$ and $(3, 2)$. A is doubly stochastic with exact rational entries, is asymmetric, and satisfies $\Delta(w) = 0$ for every $w \in \{-3, -2, -1, 0, 1, 2, 3\}$. Symmetry is therefore provably not necessary at $d \geq 4$ either.

Proof. The row sums of (51) are $\frac{1}{4} + \frac{1}{8} + \frac{3}{8} + \frac{1}{4} = \frac{3}{8} + \frac{3}{8} + \frac{1}{4} = 1$, $\frac{3}{8} + \frac{1}{4} + \frac{3}{8} + 0 = 1$, $\frac{1}{8} + \frac{1}{8} + \frac{1}{4} + \frac{1}{2} = 1$ and $\frac{1}{4} + \frac{1}{2} + 0 + \frac{1}{4} = 1$, and the column sums are $\frac{1}{4} + \frac{3}{8} + \frac{1}{8} + \frac{1}{4} = 1$, $\frac{1}{8} + \frac{1}{4} + \frac{1}{8} + \frac{1}{2} = 1$, $\frac{3}{8} + \frac{3}{8} + \frac{1}{4} + 0 = 1$ and $\frac{1}{4} + 0 + \frac{1}{2} + \frac{1}{4} = 1$; all entries are nonnegative, so $A \in \mathcal{B}(4)$. Asymmetry is $A[0, 1] - A[1, 0] = \frac{1}{8} - \frac{3}{8} = -\frac{1}{4} \neq 0$, and the largest entry of $A - A^T$ in absolute value is $\frac{1}{2}$, attained at the four ordered pairs $(1, 3)$, $(3, 1)$, $(2, 3)$ and $(3, 2)$.

For the defects, set $D_0 = 4A - J$, which is

$$D_0 = \begin{pmatrix} 0 & -1/2 & 1/2 & 0 \\ 1/2 & 0 & 1/2 & -1 \\ -1/2 & -1/2 & 0 & 1 \\ 0 & 1 & -1 & 0 \end{pmatrix}, \quad (52)$$

antisymmetric with zero row sums, so $D_0 \in \mathcal{K}(4)$, and $A = J/4 + D_0/4$ gives $D(A) = D_0/4$. Since $J/4$ is symmetric, (26) becomes $\Delta(w) = \frac{1}{2Z} \sum_{C_w} q^{\varepsilon_n} D_0[n, m]$ with $Z = 1 + q + q^2 + q^3 = \frac{15}{8}$ at $q = \frac{1}{2}$. The three positive classes are $C_1 = \{(1, 0), (2, 1), (3, 2)\}$, $C_2 = \{(2, 0), (3, 1)\}$ and $C_3 = \{(3, 0)\}$, and

$$\begin{aligned} \frac{1}{2}D_0[1, 0] + \frac{1}{4}D_0[2, 1] + \frac{1}{8}D_0[3, 2] &= \frac{1}{4} - \frac{1}{8} - \frac{1}{8} = 0, \\ \frac{1}{4}D_0[2, 0] + \frac{1}{8}D_0[3, 1] &= -\frac{1}{8} + \frac{1}{8} = 0, \\ \frac{1}{8}D_0[3, 0] &= 0, \end{aligned} \quad (53)$$

so $\Delta(w) = 0$ for $w = 1, 2, 3$, and $\Delta(0) = 0$ by Corollary 5.3 while $\Delta(-w) = -q^{-w}\Delta(w) = 0$ by Corollary 5.4. The three class sums above are the components of $\Phi(D_0)$, so D_0 spans $\ker \Phi$ and $\text{rank } \Phi = 2$. $\square$

Whether such a composite is physically realisable is a different question, and the answer for (51) is no, at least for a single unitary interval.

Lemma 6.13 (bracelet, or chain-link, conditions are necessary at every dimension). *Let U be unitary and let $B = |U|^2$ entrywise. For every pair of distinct rows $i \neq j$ the d lengths*

$$\ell_k = \sqrt{B[i, k] B[j, k]} = |U[i, k]| |U[j, k]|, \quad k = 0, \dots, d-1, \quad (54)$$

satisfy the polygon inequalities

$$\ell_{k_0} \leq \sum_{k \neq k_0} \ell_k \quad \text{for every } k_0, \quad (55)$$

and likewise for every pair of distinct columns.

Proof. Row orthogonality gives $\sum_k U[i, k] \overline{U[j, k]} = 0$. Isolating the term $k = k_0$ and applying the triangle inequality,

$$\ell_{k_0} = |U[i, k_0]| |U[j, k_0]| = \left| \sum_{k \neq k_0} U[i, k] \overline{U[j, k]} \right| \leq \sum_{k \neq k_0} |U[i, k]| |U[j, k]| = \sum_{k \neq k_0} \ell_k. \quad (56)$$

Column orthogonality gives the identical statement for column pairs. No dimension enters the argument and no membership criterion from the literature is used. $\square$

The inequalities (55) are the bracelet conditions of Nechita et al. [8], Rajchel-Mieldzioć et al. [9]; at $d = 3$ they are the three-term triangle inequality that Bengtsson et al. [2] call the chain-link condition, and the name is kept in Section 8 for that case. The statement is classical [8, Prop. 3.2] and is proved here only so that the corollary below rests on no external authority. What is taken from the literature is the converse failure: at $d \geq 4$ the conditions (55) are necessary but not sufficient [9], so they can refute unistochasticity decisively and can never certify it.

Corollary 6.14 (the composite (51) is not unistochastic). *The matrix A of (51) is not unistochastic. Of its twelve index pairs—six row pairs and six column pairs, forty-eight polygon inequalities (55) in all—exactly two inequalities fail, one in the row pair (1, 3) and one in the column pair (2, 3), both by the exact rational margin $\frac{1}{8} - \frac{3}{32} = \frac{1}{32}$. On the other hand the four-cycle permutation matrix P is asymmetric, is unistochastic by construction, and satisfies the detailed fluctuation theorem exactly for the degenerate spectrum $\varepsilon = (0, 0, 1, 1)$ at every $\beta > 0$.*

Proof. For the row pair (1, 3) the four products $a_k = A[1, k]A[3, k]$ are $(\frac{3}{32}, \frac{1}{8}, 0, 0)$, so the lengths (54) are $(\sqrt{3/32}, \sqrt{1/8}, 0, 0)$ and the polygon inequality (55) at $k_0 = 1$ reads $\sqrt{1/8} \leq \sqrt{3/32}$. Because two of the four products vanish this is the rational comparison $\frac{1}{8} \leq \frac{3}{32}$, which is false since $\frac{4}{32} > \frac{3}{32}$; the decision uses no radicals and no tolerance. The column pair (2, 3) gives the products $(\frac{3}{32}, 0, \frac{1}{8}, 0)$ and fails at $k_0 = 2$ by the same margin. The remaining forty-six inequalities hold.

For the second statement, $P = |U|^2$ with $U = P$ the permutation unitary, so $P \in \mathcal{U}(4)$ without appeal to any criterion; $\alpha(P) = 1$ by (15), so P is maximally asymmetric; and at $\varepsilon = (0, 0, 1, 1)$ Table 1 gives $\text{rank } \Phi = 0$, so $\Delta(w) = 0$ for every doubly stochastic A and every $\beta > 0$, in particular for P . $\square$

The asymmetry of the argument in Corollary 6.14 is the point. Had all forty-eight inequalities held, nothing would have followed, because they are only necessary at $d \geq 4$; failing two is decisive. So the rank deficiency of Φ at $d = 4$ is a genuine feature of the polytope $\mathcal{B}(4)$ and has a thermodynamic realisation in the degeneracy-protected regime, but the composite (51) itself is not realisable by a single unitary interval. Whether it is realisable by a train with at least one intermediate measurement, that is, whether it is a product of unistochastic matrices, is open; that set strictly contains $\mathcal{U}(4)$ and is not characterised here.

7 The worst-case violation

The criterion of Section 5 says when the symmetric detailed fluctuation theorem holds. This section asks the quantitative question behind criterion (c) of the introduction: when it fails, how badly can it fail, over every protocol, every schedule, every train length and every temperature? The answer is exact and closed-form, and the reason it can be exact is that the violation is affine in the composite transfer matrix.

7.1 The worst case is a deterministic protocol

Two algebraic facts make the optimisation finite. The first is that (22) writes each defect as a linear functional of A :

$$\Delta(w) = \sum_{n,m} K_w[n, m] A[n, m], \quad K_w[n, m] = \frac{1}{Z} \left(q^{\varepsilon_n} \mathbf{1}[(n, m) \in C_w] - q^{\varepsilon_m} \mathbf{1}[(n, m) \in C_{-w}] \right), \quad (57)$$

so $V(A)$ of (10) is a sum of absolute values of affine functionals and is therefore convex on $\mathcal{B}(d)$. The second is that the feasible set is controlled: every realisable composite lies in $\mathcal{B}(d)$, because each M_k is doubly stochastic and $\mathcal{B}(d)$ is closed under multiplication, and every vertex of $\mathcal{B}(d)$ is realisable, because a permutation matrix P_σ is $|U|^2$ for the permutation unitary $U = P_\sigma$, and a train of k identical such intervals gives $A = P_\sigma^k$, again a permutation matrix.

Table 2: The six deterministic protocols at $d = 3$ with the equally spaced spectrum $\varepsilon = (-1, 0, 1)$ at $\beta = \ln 2$, that is, $q = \frac{1}{2}$, so that $Z = \frac{7}{2}$ and the Gibbs weights are $(\frac{4}{7}, \frac{2}{7}, \frac{1}{7})$. Cycle type is given in cycle notation for the permutation σ with $P_\sigma[n, m] = 1$ exactly when $n = \sigma(m)$. The first four protocols satisfy (1) exactly; the two three-cycles violate it maximally, with $V = 1$, the largest possible value of a total variation distance between two probability distributions. Every one of the six has $Q(P_\sigma) = 0$ in the certificate of Theorem 8.1, hence is unistochastic and physically realisable by one unitary interval.

σ	cycle type	$P(w)$	$\Delta(w)$	V
(0)(1)(2)	1, 1, 1	$\{0 : 1\}$	all zero	0
(01)	2, 1	$\{-1 : \frac{2}{7}, 0 : \frac{1}{7}, 1 : \frac{4}{7}\}$	all zero	0
(02)	2, 1	$\{-2 : \frac{1}{7}, 0 : \frac{2}{7}, 2 : \frac{4}{7}\}$	all zero	0
(12)	2, 1	$\{-1 : \frac{1}{7}, 0 : \frac{4}{7}, 1 : \frac{2}{7}\}$	all zero	0
(012)	3	$\{-2 : \frac{1}{7}, 1 : \frac{6}{7}\}$	$\{-2 : \frac{4}{7}, -1 : -\frac{6}{7}, 1 : \frac{3}{7}, 2 : -\frac{1}{7}\}$	1
(021)	3	$\{-1 : \frac{3}{7}, 2 : \frac{4}{7}\}$	$\{-2 : -\frac{4}{7}, -1 : \frac{6}{7}, 1 : -\frac{3}{7}, 2 : \frac{1}{7}\}$	1

Theorem 7.1 (the worst case is attained at a vertex). *Fix $\beta > 0$, the endpoint spectra and d . Then*

$$\sup_{\text{protocols, schedules, } N} \max_w |\Delta(w)| = \max_{\sigma \in S_d} \max_w |\Delta(w)|(P_\sigma), \quad \sup_{\text{protocols, schedules, } N} V(A) = \max_{\sigma \in S_d} V(P_\sigma), \quad (58)$$

and both suprema are maxima, attained by deterministic protocols realisable by a single unitary interval. Both are exactly computable by enumerating the $d!$ permutation matrices at that value of q .

Proof. $A \mapsto \max_w |\Delta(w)|$ is a maximum of absolute values of affine functionals, hence convex on $\mathcal{B}(d)$, and $A \mapsto V(A)$ is convex by (10) and (57). A convex function on a compact convex polytope attains its maximum at a vertex, and the vertices of $\mathcal{B}(d)$ are exactly the $d!$ permutation matrices, each of which is realisable. The containment of the feasible set in $\mathcal{B}(d)$ gives one inequality and the realisability of the vertices gives the other. $\square$

The qualifier “at fixed β ” in (58) is load-bearing for the first maximum and not for the second. As Corollary 7.4 shows, the pointwise maximum depends on q , while $\max V = 1$ does not.

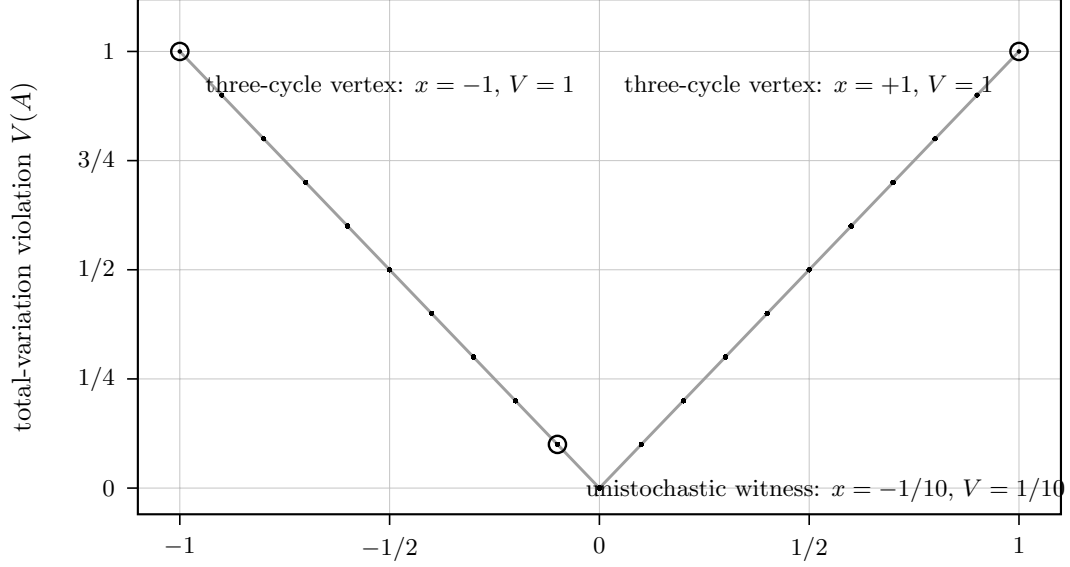
Theorem 7.1 converts an optimisation over an infinite-dimensional space of drives and schedules into a finite exact enumeration. Table 2 carries out that enumeration at $d = 3$ for the equally spaced spectrum at $\beta = \ln 2$, and Figure 2 plots the resulting identity $V(A) = |x|$ of Corollary 6.9 against an exhaustive rational grid of the polytope.

7.2 Which deterministic protocols satisfy the theorem

Theorem 7.2 (involutions satisfy the theorem exactly, at every dimension). *If $\sigma^2 = \text{id}$ then the deterministic protocol $A = P_\sigma$ satisfies (1) exactly, at every d , every endpoint spectrum and every $\beta > 0$.*

Proof. With the convention (11), (22) becomes

$$Z \Delta(w) = \sum_{m: \varepsilon_{\sigma(m)} - \varepsilon_m = w} q^{\varepsilon_{\sigma(m)}} - \sum_{n: \varepsilon_n - \varepsilon_{\sigma(n)} = w} q^{\varepsilon_n}, \quad (59)$$



$x = A[0, 1] - A[1, 0]$, the single antisymmetric scalar of a $d = 3$ train
all 2211 points of the exhaustive $\frac{1}{10}$ grid of $\mathcal{B}(3)$ at $q = \frac{1}{2}$, each exactly on $V(A) = |x|$

Figure 2: The total-variation violation $V(A)$ of (10) against the single antisymmetric scalar $x = A[0, 1] - A[1, 0]$ of (43), for all 2211 points of the exhaustive rational grid of $\mathcal{B}(3)$ at step $\frac{1}{10}$, with the equally spaced spectrum $\varepsilon = (-1, 0, 1)$ and $q = \frac{1}{2}$. Every point of the grid lies exactly on the line $V = |x|$ predicted by Corollary 6.9, so the plot is a verification of an identity rather than a fit. The two marked vertices at $x = \pm 1$ are the three-cycle permutation matrices, where V attains its maximal value one; the marked interior point at $x = -\frac{1}{10}$ is the certified unistochastic witness M_8 of Section 8, with $V = \frac{1}{10}$. Horizontal axis: the scalar x , dimensionless, ranging over $[-1, 1]$ by Theorem 6.2. Vertical axis: the total variation distance $V(A)$, dimensionless, ranging over $[0, 1]$.

the first sum from $P_\sigma[n, m] = 1$ if and only if $n = \sigma(m)$ and the second from $P_\sigma[m, n] = 1$ if and only if $m = \sigma(n)$. In the second sum substitute $n = \sigma(m)$: because $\sigma^2 = \text{id}$ this is a bijection of the summation set onto itself, the condition $\varepsilon_n - \varepsilon_{\sigma(n)} = w$ becomes $\varepsilon_{\sigma(m)} - \varepsilon_m = w$, which defines the first sum, and the summand q^{ε_n} becomes $q^{\varepsilon_{\sigma(m)}}$. The two sums are term by term identical, so $\Delta(w) = 0$ for every w . $\square$

The converse fails in general, because a permutation may satisfy (1) for a degenerate spectrum through the cancellation of Theorem 6.10 without being an involution. At $d = 3$ with the equally spaced spectrum the converse does hold, and the two three-cycles are the exact worst case at every temperature.

Corollary 7.3 (the maximal violation at $d = 3$ is temperature-independent). *At $d = 3$ with the equally spaced spectrum $\varepsilon = (-1, 0, 1)$, $V(P_\sigma) = 1$ for both three-cycles and $V(P_\sigma) = 0$ for all four involutions, for every $q > 0$. Hence $\max_\sigma V(P_\sigma) = 1$ independently of β .*

Proof. For $\sigma = (012)$ the work values are $+1$, from $m = 0$ and $m = 1$, and -2 , from $m = 2$, so P is supported on $\{+1, -2\}$. The tilted measure $w \mapsto P(w)q^w$ is therefore supported on $\{+1, -2\}$ while the reflected measure $w \mapsto P(-w)$ is supported on $\{-1, +2\}$. The two supports are disjoint at every $q > 0$, and two probability measures with disjoint supports are at total variation distance one. No value of q enters the argument. The involutive cases are Theorem 7.2. $\square$

7.3 The pointwise worst case depends on temperature

The total-variation worst case is temperature-independent; the pointwise worst case is not, and the difference is worth stating precisely because a single number quoted without its temperature is misleading.

Corollary 7.4 (exact pointwise worst case). *At $d = 3$ with the equally spaced spectrum, put $D(q) = 1 + q + q^2$ and $r = \max(q, 1/q) \geq 1$. At fixed $q > 0$,*

$$\max_{\text{protocols, schedules, } N} \max_w |\Delta(w)| = \frac{r(1+r)}{1+r+r^2} = 1 - \frac{1}{1+r+r^2}, \quad (60)$$

attained by both three-cycles, at $w = -1$ for $0 < q \leq 1$ and at $w = +1$ for $q \geq 1$. The function (60) is strictly increasing in $r \geq 1$, equals $\frac{2}{3}$ at $r = 1$, that is at $\beta = 0$, and tends to 1 as $r \rightarrow \infty$ without attaining it at any finite temperature. In particular the value $\frac{6}{7}$ belongs to $q = \frac{1}{2}$ and to $q = 2$ alone, and is neither an upper nor a lower bound across temperatures.

Proof. $A \mapsto \max_w |\Delta(w)|$ is convex on $\mathcal{B}(3)$, so by Theorem 7.1 the supremum over realisable protocols is the maximum over the six vertices. Theorem 7.2 gives $\Delta \equiv 0$ for the four involutions. Substituting the two three-cycles into (22) gives both the same multiset of absolute values, $\{1, 1+q, q(1+q), q^2\}/D(q)$: for $\sigma = (012)$ the four defects are $\Delta(1) = -x(1+q)/Z$, $\Delta(2) = xq/Z$, $\Delta(-1) = -q^{-1}\Delta(1)$ and $\Delta(-2) = -q^{-2}\Delta(2)$ with $x = -1$ and $Z = D(q)/q$, which are exactly those four numerators over $D(q)$.

For $0 < q \leq 1$ the largest numerator is $1+q$, because $1+q-1 = q > 0$, $1+q-q^2 = 1+q(1-q) > 0$ and $1+q-q(1+q) = (1+q)(1-q) \geq 0$; for $q \geq 1$ it is $q(1+q)$, because $q(1+q)-q^2 = q > 0$, $q(1+q)-(1+q) = (q-1)(q+1) \geq 0$ and $q(1+q)-1 > 0$. The two cases give $(1+q)/D(q)$ and $q(1+q)/D(q)$, which are both (60), the first with $r = 1/q$ and the second with $r = q$. The identity $r(1+r)/(1+r+r^2) = 1 - 1/(1+r+r^2)$ and the derivative $(2r+1)/(1+r+r^2)^2 > 0$ give strict monotonicity in $r \geq 1$, the range $[\frac{2}{3}, 1)$ and the limit 1. Solving $r(1+r)/(1+r+r^2) = \frac{6}{7}$ gives $7r(1+r) - 6(1+r+r^2) = r^2 + r - 6 = (r-2)(r+3) = 0$, so $r = 2$, that is $q = \frac{1}{2}$ or $q = 2$. $\square$

Figure 3 plots (60) against temperature together with the exact rational values at which it was recomputed, and Table 6 of Appendix B lists all fourteen with both the closed form and the enumerated maximum. The shape of the result is the interesting part: the pointwise violation is bounded away from one at every finite temperature, with $1 - f(r) = 1/(1+r+r^2)$ strictly positive, and reaches two thirds already at infinite temperature. The total-variation violation, by contrast, is exactly one for the two three-cycle protocols at every temperature including $\beta = 0$. The two measures answer different questions, and the gap between them is the difference between “some work value is mispredicted by a bounded amount” and “the two sides of (1) have disjoint supports”.

Remark 7.5 (the ratio is the wrong worst-case measure). The ratio $R(w) = P(w)q^w/P(-w)$ has an unbounded supremum over realisable protocols. The three-cycle protocol of Table 2 has $P(-1) = 0$ while $P(1) = (1+q)/D(q) > 0$, so $R(1) = \infty$ at every temperature. That is a property of the measure rather than of the protocol: a ratio between a positive number and zero is infinite whatever the positive number is. This is why the defect $\Delta(w)$ and the total variation $V(A)$ are the quantities optimised here, and why no finite worst-case ratio is claimed anywhere in this paper. The only temperature-free pointwise bound available is the trivial $|\Delta(w)| \leq 1$, since $\Delta(w) = P(w)q^w - P(-w)$ is a difference of two numbers in $[0, 1]$: Theorem 4.1 gives $\sum_v P(v)q^v = Z_\tau/Z_0 = 1$ for a cyclic protocol, and $\sum_v P(-v) = 1$ because P is a distribution.

The exhaustive rational grids of $\mathcal{B}(3)$ at $q = \frac{1}{2}$ with steps $\frac{1}{5}$, $\frac{1}{10}$, $\frac{1}{20}$ and $\frac{1}{30}$ —231, 2211, 26796 and 123256 exact points respectively—never exceed either tabulated maximum and attain both,

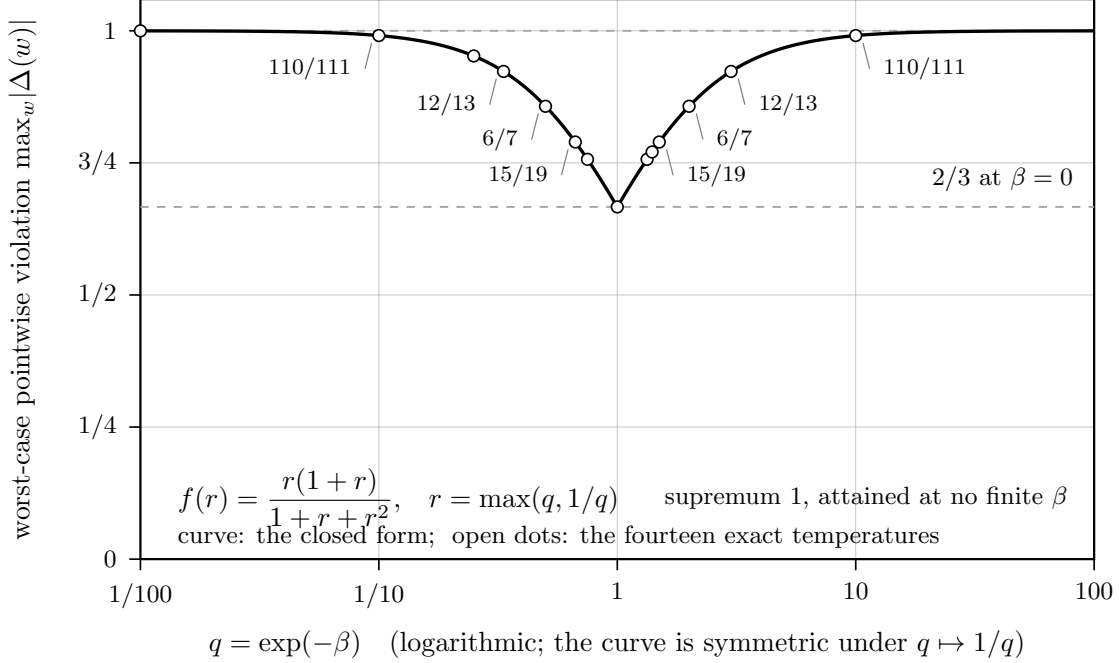


Figure 3: The worst-case pointwise violation (60) as a function of temperature. Horizontal axis: $q = e^{-\beta}$ on a logarithmic scale, dimensionless; the curve is symmetric under $q \mapsto 1/q$ because (60) depends only on $r = \max(q, 1/q)$, so β and $-\beta$ give the same value. Vertical axis: the maximum of $|\Delta(w)|$ over all work values and over all protocols, schedules and train lengths at that temperature, dimensionless. The curve is the closed form $f(r) = r(1+r)/(1+r+r^2)$ of Corollary 7.4, an analytic function and not a measurement; the dots are the fourteen exact rational temperatures at which it was recomputed in rational arithmetic, including $\beta = 0$ where $f = \frac{2}{3}$, $q = \frac{1}{10}$ where $f = \frac{110}{111}$, $q = \frac{1}{4}$ where $f = \frac{12}{13}$, $q = \frac{1}{2}$ and $q = 2$ where $f = \frac{6}{7}$, and $q = \frac{2}{3}$ where $f = \frac{15}{19}$. The dashed level marks the supremum 1, which is approached as $\beta \rightarrow \infty$ and attained at no finite temperature; the total-variation worst case, by contrast, equals one at every temperature by Corollary 7.3.

and the same holds on exhaustive grids of step $\frac{1}{10}$ at $q = \frac{1}{3}$ and $q = 3$, with 2211 exact points each. That is a brute-force confirmation of the vertex argument at this dimension and these temperatures, not a substitute for it: Theorem 7.1 is what makes the grids unnecessary.

8 Feasibility at dimension three

The worst-case analysis of Section 7 needs to know which points of $\mathcal{B}(3)$ are physically realisable, and the witnesses of this section need to know whether a given rational matrix is unistochastic. At $d = 3$ there is a complete classical answer, and it reduces to the sign of a single polynomial.

8.1 The classical criterion and its exact reduction

The criterion is classical and is not a result of this paper: a matrix $M \in \mathcal{B}(3)$ is unistochastic if and only if $Q(M) \geq 0$, where

$$Q(M) = 4a_0a_1 - (a_0 + a_1 - a_2)^2, \quad a_k = M[0, k] M[1, k], \quad (61)$$

the expression being sixteen times the square of the area of the triangle with side lengths $\sqrt{a_0}, \sqrt{a_1}, \sqrt{a_2}$ [1]. The same condition appears in chain-link form in [2], where the three link lengths are their equation (22), the chain-link condition is their equation (23) and the explicit phase solution their equations (24) and (25); the equivalence of the two forms follows from Heron's formula, $4a_0a_1 - (a_0 + a_1 - a_2)^2 = 2\sum_{i<j} a_i a_j - \sum_i a_i^2$. Three facts about (61) are needed below, and all three are established here by exact integer polynomial arithmetic rather than quoted.

Theorem 8.1 (the exact certificate at $d = 3$). *Work in the chart $(x_{00}, x_{01}, x_{10}, x_{11})$ of $\mathcal{B}(3)$, in which the remaining five entries are*

$$\begin{aligned} x_{02} &= 1 - x_{00} - x_{01}, & x_{12} &= 1 - x_{10} - x_{11}, & x_{20} &= 1 - x_{00} - x_{10}, \\ x_{21} &= 1 - x_{01} - x_{11}, & x_{22} &= x_{00} + x_{01} + x_{10} + x_{11} - 1. \end{aligned} \quad (62)$$

Then:

- (a) *All six chain-link discriminants of a matrix in $\mathcal{B}(3)$ —three unordered row pairs and three unordered column pairs—are the same degree-four polynomial with integer coefficients,*

$$Q = 4x_{00}x_{10}x_{01}x_{11} - (x_{00}x_{10} + x_{01}x_{11} - x_{02}x_{12})^2, \quad (63)$$

so the column pairs add nothing and membership of a rational matrix is an exact sign test in integer arithmetic.

- (b) *On each of the nine facets $\{M[k, j] = 0\}$ of $\mathcal{B}(3)$ the polynomial Q restricts to minus a perfect square; the nine square roots are listed in Table 4 of Appendix B. Hence $Q \geq 0$ on a facet forces $Q = 0$, and every boundary point of $\mathcal{B}(3)$ that is unistochastic is orthostochastic, that is, $\mathcal{U}(3) \cap \partial\mathcal{B}(3) \subset \mathcal{O}(3)$ [7].*

- (c) *Every permutation matrix has $Q = 0$, so all six vertices of $\mathcal{B}(3)$ are orthostochastic and the vertex maximum of Theorem 7.1 is attained by an actual unitary protocol.*

Proof. (a) By Lemma 6.13 and the classical criterion of Au-Yeung and Poon [1], Bengtsson et al. [2] quoted in Theorem 6.8, a matrix $M \in \mathcal{B}(3)$ is unistochastic exactly when, for each of the six unordered index pairs $\{i, j\}$, the three nonnegative numbers $\ell_k = \sqrt{M[i, k]M[j, k]}$, $k = 0, 1, 2$, satisfy the triangle inequalities. For nonnegative ℓ_k , not all zero, at most one of the last three factors below can be negative, so those inequalities are equivalent to the nonnegativity of

$$(\ell_0 + \ell_1 + \ell_2)(-\ell_0 + \ell_1 + \ell_2)(\ell_0 - \ell_1 + \ell_2)(\ell_0 + \ell_1 - \ell_2) = 2\sum_{k<l} a_k a_l - \sum_k a_k^2 = 4a_0a_1 - (a_0 + a_1 - a_2)^2, \quad (64)$$

where $a_k = \ell_k^2 = M[i, k]M[j, k]$ and the last identity is a polynomial identity in a_0, a_1, a_2 .

For the row pair $\{0, 1\}$ one has $a = (x_{00}x_{10}, x_{01}x_{11}, x_{02}x_{12})$, and substituting the chart relations (62) into the right-hand side of (64) gives exactly the polynomial Q of (63). The same expansion for the remaining two row pairs $\{0, 2\}$, $\{1, 2\}$ and for the three column pairs $\{0, 1\}$, $\{0, 2\}$, $\{1, 2\}$ again produces Q . Those five further expansions are polynomial identities over $\mathbb{Z}$ in the four chart variables and were checked coefficient by coefficient in exact integer arithmetic, as recorded in Table 3 of Appendix A. Hence all six discriminants coincide with Q , and membership reduces to the single sign test $Q \geq 0$.

(b) Fix a facet $\{M[k, j] = 0\}$. The relation it imposes on the chart is affine and is listed in the second column of Table 4. Substituting that relation into $-Q$ and factoring over $\mathbb{Z}$ produces the polynomial in the third column of the same row; each of the nine factorisations was verified by

multiplying the square out and comparing coefficients exactly. Hence $Q = -s^2 \leq 0$ on the facet and $Q \geq 0$ there forces $s = 0$, that is, $Q = 0$. Equality in (64) means the triangle with sides ℓ_0, ℓ_1, ℓ_2 is degenerate, and the chain-link phases of Bengtsson et al. [2] are then forced to be ± 1 , which gives a real orthogonal preimage [7, 11].

(c) A permutation matrix has $d-1 = 2$ zero entries in every row and column, so it lies on several facets and (b) gives $Q(P_\sigma) = 0$. Directly, $P_\sigma = |P_\sigma|^2$ and P_σ is orthogonal, so it is orthostochastic; the vertex maximum of Theorem 7.1 is therefore attained by an actual unitary protocol. $\square$

Part (a) is what makes the certificate usable: a naive reading of the chain-link conditions suggests six two-sided triangle inequalities, twelve inequalities involving square roots, and deciding them for a rational matrix would seem to require radical arithmetic and a tolerance. That all six discriminants coincide with the single integer polynomial (63) removes both difficulties. Part (b) re-derives, symbolically and from the polynomial alone, the fact that the orthostochastic set is the boundary of the unistochastic set at $d = 3$ [7].

8.2 The whole one-skeleton is orthostochastic

Corollary 8.2 (the one-skeleton of $\mathcal{B}(3)$). *Q vanishes identically on all nine edges of $\mathcal{B}(3)$, and each edge carries an explicit closed-form real-orthogonal witness. Every point of every edge of $\mathcal{B}(3)$ is therefore orthostochastic, and the boundary of $\mathcal{U}(3)$ contains the whole one-skeleton of the Birkhoff polytope.*

Proof. An edge of $\mathcal{B}(3)$ joins P_σ to P_τ exactly when the two matrices differ in exactly two rows, equivalently when $\sigma^{-1}\tau$ is a transposition; there are $6 \cdot 3/2 = 9$ of them. Write the edge point as $M(s) = sP_\sigma + (1-s)P_\tau$ for $s \in [0, 1]$, let i and j be the two indices moved by $\sigma^{-1}\tau$ and k the fixed one, and set $a = \sigma(i) = \tau(j)$, $b = \tau(i) = \sigma(j)$, $c = \sigma(k) = \tau(k)$. Then $M(s)$ has s at (a, i) and (b, j) , $1-s$ at (b, i) and (a, j) , 1 at (c, k) and zero elsewhere, so it has the 2×2 block $\begin{pmatrix} s & 1-s \\ 1-s & s \end{pmatrix}$ on rows $\{a, b\}$ and columns $\{i, j\}$. Substituting these entries into (61) and expanding in s gives the zero polynomial; the expansion is exact and was carried out symbolically for all nine edges.

For the witness, let $u^2 = s$ and $v^2 = 1-s$ and define O by

$$O[a, i] = u, \quad O[b, i] = v, \quad O[a, j] = v, \quad O[b, j] = -u, \quad O[c, k] = -1, \quad (65)$$

with all other entries zero. Then $|O|^2 = M(s)$ entrywise. The two nontrivial rows are (u, v) and $(v, -u)$ on the columns $\{i, j\}$, which are orthonormal because $u^2 + v^2 = 1$ and $uv - vu = 0$; the remaining row is $-e_c$, supported on a column the other two do not touch; so $OO^T = I_3$. The 2×2 block $\begin{pmatrix} u & v \\ v & -u \end{pmatrix}$ has determinant $-u^2 - v^2 = -1$, so $|\det O| = 1$, and flipping the sign of the fixed row gives $\det O = +1$ without changing $|O|^2$. $\square$

Corollary 8.2 is a consequence of part (b) of Theorem 8.1 rather than an independent phenomenon: every edge lies on at least one facet, on a facet Q is minus a perfect square, and the square vanishes along the edge. Its content is the identification of the *whole* one-skeleton, together with a witness that is closed-form in s and exact in radical arithmetic, rather than one chord of it.

The converse is false and the failure is exact. The hollow matrix $H = (J - I)/2$ lies on three facets of $\mathcal{B}(3)$ and has $Q(H) = -\frac{1}{16} < 0$, so H is not unistochastic. On a facet the unistochastic locus is the zero set of the polynomial whose square is $-Q$, which is a curve; the nine edges are lines inside that curve, and H is a boundary point of $\mathcal{B}(3)$ outside it. The matrix H is therefore an exact zero-tolerance witness that $\mathcal{U}(3)$ is strictly smaller than $\mathcal{B}(3)$, needing no random search and no tolerance.

8.3 Where the zero set of the certificate sits

Two facts bound what Corollary 8.2 means, and neither follows from the other. The one-skeleton lies inside the union of the facets: the two permutations of an edge differ by a transposition, so their supports meet in exactly one cell, an interior edge point has $9 - 5 = 4$ zero entries and therefore lies on four of the nine facets. On the other hand $\{Q = 0\} \cap \mathcal{B}(3)$ is strictly larger than that union, because it reaches the interior of $\mathcal{B}(3)$: the matrix

$$M_9 = \frac{4J - 3I}{9} = \begin{pmatrix} 1/9 & 4/9 & 4/9 \\ 4/9 & 1/9 & 4/9 \\ 4/9 & 4/9 & 1/9 \end{pmatrix} \quad (66)$$

has all nine entries positive, is doubly stochastic, and has $Q(M_9) = 0$ exactly, with all six chain-link discriminants equal to zero. An exhaustive sweep of every lattice point of $\mathcal{B}(3)$ at denominators 1 through 9—6, 21, 55, 120, 231, 406, 666, 1035 and 1540 exact points, 4080 in total, the counts of Table 5 in Appendix B—shows that 9 is the smallest denominator at which $\{Q = 0\}$ reaches the interior, and that it does so at exactly the six points $(4J - 3P_\sigma)/9$ for $\sigma \in S_3$. Read together, the two facts say something neither says alone: $\{Q = 0\} \cap \mathcal{B}(3)$, which is the boundary of $\mathcal{U}(3)$ relative to $\mathcal{B}(3)$, contains the entire one-skeleton and also reaches the interior, so that boundary is neither confined to the facets nor exhausted by the skeleton. The count 231 at denominator 5 also cross-checks the step- $\frac{1}{5}$ grid used in Section 7.

8.4 Exact witnesses

Three rational matrices carry the claims of Sections 6 and 7, and each is reproduced here from the definitions by an independent exact computation.

The first is an interior unistochastic matrix that violates the detailed fluctuation theorem by a controlled amount:

$$M_8 = \begin{pmatrix} 1/2 & 1/5 & 3/10 \\ 3/10 & 1/2 & 1/5 \\ 1/5 & 3/10 & 1/2 \end{pmatrix}, \quad Q(M_8) = \frac{239}{10000} > 0, \quad \alpha(M_8) = \frac{1}{10}. \quad (67)$$

Strict positivity of Q at an interior point makes M_8 unistochastic by (61). With the equally spaced spectrum $\varepsilon = (-1, 0, 1)$, $\beta = \ln 2$ so that $q = \frac{1}{2}$, and one intermediate measurement, its work distribution is

$$P(W) = \left(\frac{3}{70}, \frac{3}{35}, \frac{1}{2}, \frac{9}{35}, \frac{4}{35} \right) \quad \text{for } W = (-2, -1, 0, +1, +2), \quad (68)$$

with the two ratios

$$\frac{P(+1)}{P(-1)} = 3 \quad \text{against} \quad e^{\beta W} = 2, \quad \frac{P(+2)}{P(-2)} = \frac{8}{3} \quad \text{against} \quad e^{2\beta W} = 4, \quad (69)$$

defects $\Delta = \{-2 : \frac{2}{35}, -1 : -\frac{3}{35}, 0 : 0, 1 : \frac{3}{70}, 2 : -\frac{1}{70}\}$, total variation $V = \frac{1}{10}$, and the integral fluctuation relation exact: $\sum_w P(w)2^{-w} = 1$. The scalar of Theorem 6.8 is $x = M_8[0, 1] - M_8[1, 0] = \frac{1}{5} - \frac{3}{10} = -\frac{1}{10}$, and the closed forms (44) reproduce both defects exactly, $\Delta(1) = -x(1 + q)/Z = \frac{3}{70}$ and $\Delta(2) = xq/Z = -\frac{1}{70}$ with $Z = \frac{7}{2}$; Corollary 6.9 gives $V = |x| = \frac{1}{10}$. The witness is thus a single rational matrix that ties the criterion, the one-scalar reduction, the total-variation identity and the integral fluctuation relation together at once.

The second is the non-membership witness $H = (J - I)/2$ with $Q(H) = -\frac{1}{16}$ already used above. The third is an exact orthogonal matrix whose square lands on a facet, as part (b) of Theorem 8.1 predicts:

$$O = \frac{1}{65} \begin{pmatrix} 15 & -52 & 36 \\ 20 & 39 & 48 \\ -60 & 0 & 25 \end{pmatrix}, \quad OO^T = O^T O = I, \quad \det O = 1, \quad (70)$$

all three exactly over the rationals. The matrix $|O|^2$ has $Q = 0$, lies on the facet $M[2, 1] = 0$, and has asymmetry $\alpha(|O|^2) = 2304/4225$, so it is an orthostochastic point on the boundary that is far from symmetric while nevertheless satisfying (1) only to the extent its scalar x allows.

8.5 The bridge between asymmetry and violation

Theorem 8.3 (maximal asymmetry and maximal violation coincide at $d = 3$). *At $d = 3$ with the equally spaced spectrum,*

$$\begin{aligned} \alpha(P_\sigma) = 1 &\iff V(P_\sigma) = 1 \iff \sigma \text{ is a three-cycle,} \\ \alpha(P_\sigma) = 0 &\iff V(P_\sigma) = 0 \iff \sigma \text{ is an involution.} \end{aligned} \quad (71)$$

Proof. Both chains are the conjunction of Theorem 7.2, Corollary 7.3 and the enumeration of the six permutations in Table 2: the four involutions are the identity and the three transpositions, for which P_σ is symmetric, so $\alpha = 0$ and $V = 0$; the two three-cycles have $\alpha = 1$ by (15) and $V = 1$ by Corollary 7.3. $\square$

The characterisation of the permutation witnesses extends to every dimension, and its hypothesis has to be stated exactly.

Remark 8.4 (which permutations are asymmetry witnesses). For a permutation matrix P_σ at any d ,

$$\begin{aligned} \alpha(P_\sigma) = 1 &\iff \sigma \text{ has a cycle of length at least three,} \\ \alpha(P_\sigma) = 0 &\iff \sigma \text{ is an involution,} \end{aligned} \quad (72)$$

which was checked by exhaustive enumeration of S_3 , S_4 and S_5 , 150 permutations, in exact integer arithmetic. A transposition *is* an involution, so its permutation matrix is symmetric and has $\alpha = 0$: a transposition is not an asymmetry witness, and any statement to that effect is wrong. The sharp hypothesis is the presence of a cycle of length at least three. At $d = 3$ the witnesses are exactly the two three-cycles, both of which have determinant $+1$ and so already lie in $SO(3)$; at $d = 4$ the four-cycle has determinant -1 , and flipping the sign of one nonzero entry gives determinant $+1$ with identical $|U|^2$ and identical $\alpha = 1$.

Theorem 8.3 is a bridge rather than a reformulation. Programs that maximise a free-energy functional over $\mathcal{U}(3)$ use α as their measure of how far a unistochastic matrix is from symmetric; Theorem 8.3 says that at $d = 3$ the extremal matrices for that purely matrix-theoretic quantity are exactly the ones that destroy the detailed fluctuation theorem most strongly. The link between the two is an identity, not an analogy, and it is available only because the equally spaced three-level spectrum makes the violation a monotone function of a single scalar.

9 A four-dimensional ray: why necessary conditions cannot certify

Corollary 6.14 used the bracelet conditions of Lemma 6.13 in the only direction in which they are decisive: a failure refutes unistochasticity. This section shows that the restriction is not a technical

convenience but an obstruction of principle. Along a one-parameter rational ray in $\mathcal{B}(4)$, all twelve necessary conditions hold *identically* on the whole window in which the ray lies in the polytope, while unistochastic membership provably switches inside that window. No sufficiency theorem built on those conditions can therefore exist at $d \geq 4$, and the exact system that would settle the remaining case is written down.

9.1 The normal form for preimages

Lemma 9.1 (normal form and the unreduced phase system). *Fix t and write*

$$a = \frac{1-3t}{4}, \quad b = \frac{1+t}{4}, \quad c = \frac{1+9t}{4}, \quad L = \frac{a}{b}, \quad \rho = \frac{c}{b} = 3 - 2L, \quad (73)$$

and let $B(t)$ be the 4×4 matrix with first row (a, a, a, c) and each remaining row (b, b, b, a) . Then $B(t)$ has a unitary preimage if and only if there exist a 3×3 complex matrix R and a vector $v \in \mathbb{C}^3$ with $|R[k, j]| = \sqrt{b}$ for all k, j and $|v_j| = \sqrt{a}$ for all j , satisfying

$$R^* R = I_3 - vv^*, \quad |(Rv)_k|^2 = ac \quad \text{for } k = 1, 2, 3. \quad (74)$$

Given such a pair (R, v) with $c > 0$, the matrix

$$U = \begin{pmatrix} \sqrt{c} & \bar{v}^T \\ -\frac{1}{\sqrt{c}} Rv & R \end{pmatrix} \quad (75)$$

is unitary and $|U|^2$ equals $B(t)$ up to exchanging columns 0 and 3. Under the gauge transformation $R \mapsto D_1 R D_2$, $v_j \mapsto (\overline{D_2})_j v_j$ by diagonal unitaries D_1, D_2 , which preserves (74), all the moduli and the matrix $|U|^2$, one may take $v = \sqrt{a}(1, 1, 1)$ and $R[k, 0] = \sqrt{b} > 0$. Writing $T = R/\sqrt{b}$, so that $T[k, 0] = 1$, $T[k, 1] = p_k$ and $T[k, 2] = q_k$ with $|p_k| = |q_k| = 1$, the system (74) becomes exactly

$$p_1 + p_2 + p_3 = -L, \quad (76)$$

$$q_1 + q_2 + q_3 = -L, \quad (77)$$

$$\overline{p_1} q_1 + \overline{p_2} q_2 + \overline{p_3} q_3 = -L, \quad (78)$$

$$|1 + p_k + q_k|^2 = \rho = 3 - 2L \quad \text{for } k = 1, 2, 3, \quad (79)$$

that is, nine real equations for six real unknowns, the six phases of p_k and q_k modulo the residual gauge. No membership criterion from the literature is used anywhere in the statement or the proof.

Proof. For necessity, leave c symbolic so that the argument also covers $c = 0$, which is the endpoint $t = -\frac{1}{9}$. Let U be a preimage, $|U|^2 = B(t)$. The pattern of $B(t)$ fixes every modulus with no permutation: set $h = U[0, 3]$, $u_j = U[0, j]$ for $j = 0, 1, 2$, $g_k = U[k, 3]$ for $k = 1, 2, 3$, $R[k, j] = U[k, j]$ for $k, j = 1, 2, 3$, and $v = \bar{u}$. Then $|h|^2 = c$, $|u_j|^2 = a$, $|g_k|^2 = a$ and $|R[k, j]|^2 = b$, which are the modulus requirements of the lemma.

Column orthogonality of columns $j \neq j'$ in $\{0, 1, 2\}$ reads $\bar{u}_j u_{j'} + \sum_k \overline{R[k, j]} R[k, j'] = 0$, that is, $(R^* R)[j, j'] = -\bar{u}_j u_{j'}$. Since $v = \bar{u}$, one has $\bar{u}_j u_{j'} = v_j \bar{v}_{j'} = (vv^*)[j, j']$, so the off-diagonal part of (74) holds. The entry $h = U[0, 3]$ belongs to column 3 alone and does not enter either inner product. The diagonal reads $a + \sum_k |R[k, j]|^2 = 1$, that is $(R^* R)[j, j] = 1 - a = 3b$, and $(I_3 - vv^*)[j, j] = 1 - |v_j|^2 = 1 - a = 3b$, using $a + 3b = 1$; hence the first identity in (74). Row orthogonality of row 0 with row k reads $\bar{h} g_k + \sum_j \bar{u}_j R[k, j] = 0$; since $v_j = \bar{u}_j$, the sum is $\sum_j R[k, j] v_j = (Rv)_k$, so $(Rv)_k = -\bar{h} g_k$ and $|(Rv)_k|^2 = |h|^2 |g_k|^2 = ca$, which is the second identity

in (74). It degenerates correctly to $(Rv)_k = 0$ when $c = 0$, so necessity is proved with no hypothesis beyond unitarity and is valid at the endpoint.

For sufficiency, assume $c > 0$ and let (R, v) satisfy (74). Set $h = \sqrt{c} > 0$, $u = \bar{v}$, $g = -(1/\sqrt{c})Rv$ and $U = \begin{pmatrix} h & u^T \\ g & R \end{pmatrix}$, so that $|g_k|^2 = ac/c = a$ and $|h|^2 = c$ and every modulus is as required. The column containing h has norm $c + \sum_k |g_k|^2 = c + 3a = 1$, and a column of the R -block has norm $|u_j|^2 + \sum_k |R[k, j]|^2 = a + 3b = 1$. Orthogonality inside the R -block is $\bar{u}_j u_{j'} + (R^* R)[j, j'] = (vv^*)[j, j'] - (vv^*)[j, j'] = 0$ by (74). Orthogonality of the h -column against the column j of the block is

$$\bar{h} u_j + \sum_k \bar{g}_k R[k, j] = \sqrt{c} \bar{v}_j - \frac{1}{\sqrt{c}} \sum_l \overline{(Rv)_l} R[l, j] = \sqrt{c} \bar{v}_j - \frac{1}{\sqrt{c}} \overline{(R^* R v)_j}, \quad (80)$$

and $(R^* R)v = (I_3 - vv^*)v = v - v \sum_l |v_l|^2 = (1 - 3a)v = cv$, so the expression is $\sqrt{c} \bar{v}_j - \sqrt{c} \bar{v}_j = 0$. A square matrix with orthonormal columns is unitary, and composing with the exchange of columns 0 and 3 puts c in position $(0, 3)$, giving $|UP_{0 \leftrightarrow 3}|^2 = B(t)$.

For the gauge, $R \mapsto D_1 R D_2$ and $v \mapsto \overline{D_2} v$ leave $R^* R$ conjugated by D_2 and vv^* conjugated by D_2 , so the first identity in (74) is preserved, and $(Rv)_k$ is multiplied by $(D_1)_k$, so the second is preserved; the moduli are unchanged and $|U|^2$ depends only on moduli. Choosing $(D_2)_j = v_j/\sqrt{a}$ gives $v = \sqrt{a}(1, 1, 1)$, and choosing D_1 then gives $R[k, 0] = \sqrt{b} > 0$. Substituting $R = \sqrt{b}T$ and $v = \sqrt{a}(1, 1, 1)$ into the first identity of (74) gives $T^* T = b^{-1}I_3 - LJ$, whose diagonal is the identity $3 = b^{-1} - L$, equivalent to $a + 3b = 1$, and whose three off-diagonal entries are (76), (77) and (78). Substituting into the second gives $ab|1 + p_k + q_k|^2 = ac$, which is (79) after division by ab and use of $\rho = c/b$. $\square$

9.2 The ray

Theorem 9.2 (an exact unistochastic ray in $\mathcal{B}(4)$). *For $t \in \mathbb{R}$ let a, b, c, L, ρ be as in (73) and let*

$$B(t) = \begin{pmatrix} a & a & a & c \\ b & b & b & a \\ b & b & b & a \\ b & b & b & a \end{pmatrix} = \frac{J}{4} + tW, \quad 4W = \begin{pmatrix} -3 & -3 & -3 & 9 \\ 1 & 1 & 1 & -3 \\ 1 & 1 & 1 & -3 \\ 1 & 1 & 1 & -3 \end{pmatrix}, \quad (81)$$

so that every row and every column of W sums to zero, which is what makes $B(t)$ doubly stochastic for every t as soon as its entries are nonnegative. Then:

- (i) $B(t) \in \mathcal{B}(4)$ if and only if $t \in [-\frac{1}{9}, \frac{1}{3}]$.
- (ii) All twelve bracelet conditions of Lemma 6.13 hold at every t in that window, identically, with the margin vanishing only at $t = \frac{1}{3}$.
- (iii) For every $t \in [0, \frac{1}{3}]$ the matrix $B(t)$ is unistochastic, with the explicit preimage

$$U(t) = \begin{pmatrix} \sqrt{a} & \sqrt{a} & \sqrt{a} & \sqrt{c} \\ \sqrt{b} & \sqrt{b} & \sqrt{b} E & z \\ \sqrt{b} E & \sqrt{b} & \sqrt{b} & z \\ \sqrt{b} & \sqrt{b} E & \sqrt{b} & z \end{pmatrix}, \quad (82)$$

$$\begin{aligned} E &= e^{ix}, & \cos x &= -\frac{1+L}{2} = \frac{t-1}{1+t}, & \sin x &= \frac{2\sqrt{t}}{1+t}, \\ z &= -\sqrt{\frac{ab}{c}}(2+E), & |z|^2 &= a, \end{aligned} \quad (83)$$

and every entry of $U(t)$ is an exact radical whenever t is rational and $t \geq 0$.

- (iv) Within the class of preimages invariant under the diagonal cyclic action —rows $1 \rightarrow 2 \rightarrow 3$ and columns $0 \rightarrow 1 \rightarrow 2$, that is, $U[0, j]$ independent of $j \in \{0, 1, 2\}$, $U[k, 3]$ independent of $k \in \{1, 2, 3\}$ and $U[k, j] = w_{(k-1-j) \bmod 3}$ for $k, j \in \{1, 2, 3\}$ —a preimage exists if and only if $L \leq 1$, equivalently $t \geq 0$. So (82) exhausts that class.
- (v) $B(-\frac{1}{9})$ has no unitary preimage at all. The lower endpoint of the bistochastic window is not unistochastic, unconditionally and with no criterion from the literature used.
- (vi) For $-\frac{1}{9} < t < 0$ membership is open. Only numerical evidence is available; see the discussion below.

Proof. For (i), the row sums are $3a + c = 1$ and $3b + a = 1$ and the column sums are $a + 3b = 1$ and $c + 3a = 1$, all identities in t , so $B(t)$ is doubly stochastic exactly when it is nonnegative. That gives $t \leq \frac{1}{3}$ from $a \geq 0$, $t \geq -1$ from $b \geq 0$ and $t \geq -\frac{1}{9}$ from $c \geq 0$; the binding constraints are $t \leq \frac{1}{3}$ and $t \geq -\frac{1}{9}$.

For (ii), there are six row pairs and six column pairs, hence twelve bracelet conditions, and each carries four polygon inequalities (55), so 48 scalar inequalities in total. On the ray, row 0 is (a, a, a, c) and every row $k \geq 1$ is (b, b, b, a) , so the four products $p_k = B(t)[i, k]B(t)[j, k]$ of a pair are exactly (ab, ab, ab, ac) for the pairs $(0, k)$ and (b^2, b^2, b^2, a^2) for the pairs (k, l) with $k, l \geq 1$; the six column product vectors are the reversals of the six row ones, so the twelve conditions split into six couples. By (i) every entry is nonnegative on the window, hence every p_k is nonnegative, and since the square root is monotone and subadditive on the nonnegative reals, $p_{k_0} \leq \sum_{k \neq k_0} p_k$ implies $\ell_{k_0} \leq \sum_{k \neq k_0} \ell_k$. The polynomial margin $m(t) = \sum_{k \neq k_0} p_k(t) - p_{k_0}(t)$ is therefore an exact sufficient certificate for the radical inequality; the converse is neither needed nor claimed. The 48 margins reduce to four polynomials, with multiplicities,

$$\begin{aligned} & -\frac{(3t-1)(5t+1)}{8} \text{ (18 times),} & \frac{(3t-1)^2}{8} \text{ (6 times),} \\ & \frac{5t^2-2t+1}{8} \text{ (18 times),} & -\frac{3t^2-6t-1}{8} \text{ (6 times),} \end{aligned} \tag{84}$$

whose nonnegativity sets are $[-\frac{1}{5}, \frac{1}{3}]$, all of $\mathbb{R}$, all of $\mathbb{R}$ —the third has discriminant $4 - 20 = -16$ —and $[1 - \frac{2\sqrt{3}}{3}, 1 + \frac{2\sqrt{3}}{3}]$ respectively. Each contains the window $[-\frac{1}{9}, \frac{1}{3}]$, since $-\frac{1}{5} < -\frac{1}{9}$ and $1 - \frac{2\sqrt{3}}{3} \approx -0.155 < -\frac{1}{9}$. The check is finite and exact. The common zero set inside the window is $\{\frac{1}{3}\}$: the first polynomial also vanishes at $-\frac{1}{5}$ and the fourth at $1 \pm \frac{2\sqrt{3}}{3}$, all outside the window, and the third never vanishes. At $t = \frac{1}{3}$ one has $a = 0$, three entries of $B(\frac{1}{3})$ vanish and exactly 24 of the 48 margins are zero.

For (iii), the rows of $U(t)$ have norms $3a + c = 1$ and $3b + a = 1$, the latter using $|E| = 1$ and $|z|^2 = a$, which follows from $|2 + E|^2 = 5 + 4\cos x = 5 - 2 - 2L = 3 - 2L = \rho = c/b$. The first row is orthogonal to row k because $\sqrt{ab}(2 + \overline{E}) + \sqrt{c}\overline{z} = \sqrt{ab}(2 + \overline{E}) - \sqrt{ab}(2 + \overline{E}) = 0$, and for $k \neq l$ the inner product of rows k and l is $b(1 + E + \overline{E}) + |z|^2 = b(1 + 2\cos x) + a$, in which $b(1 + 2\cos x) = b(1 - (1 + L)) = -bL = -a$, so the sum vanishes. A square matrix with orthonormal rows is unitary, and $|U(t)|^2 = B(t)$ entrywise. The phase x is real exactly when $|-(1 + L)/2| \leq 1$, that is $-3 \leq L \leq 1$; on the window L decreases monotonically from $\frac{3}{2}$ at $t = -\frac{1}{9}$ to 0 at $t = \frac{1}{3}$, so the condition is $L \leq 1$, equivalently $t \geq 0$. At $t = 0$ one has $L = 1$, $\cos x = -1$, $E = -1$, $a = b = c = \frac{1}{4}$ and $z = -\frac{1}{2}$, so $U(0)$ is a real matrix with entries $\pm\frac{1}{2}$ and orthogonal rows, hence a Hadamard matrix of order four divided by two, whose squared moduli are the van der Waerden matrix $J/4$ [11]. At $t = \frac{1}{3}$ one has $L = 0$, $\cos x = -\frac{1}{2}$, $\sin x = \frac{\sqrt{3}}{2}$, $E = e^{2\pi i/3}$, $a = 0$, $b = \frac{1}{3}$, $c = 1$ and $z = 0$.

For (iv), write $w_d = \sqrt{b} e^{i\phi_d}$ in the invariant class, with $|U[0, j]| = \sqrt{a}$ for $j \in \{0, 1, 2\}$, $|U[0, 3]| = \sqrt{c}$ and $|U[k, 3]| = \sqrt{a}$; the row norms are then automatic. The condition that rows $k \neq l$ be orthogonal becomes $\sum_d \bar{w}_d w_{d+m} = -a$ for $m = (l - k) \bmod 3$, and the cases $m = 1$ and $m = 2$ are complex conjugates of each other with a real right-hand side, so the requirement is the single equation

$$e^{i\delta_0} + e^{i\delta_1} + e^{i\delta_2} = -L, \quad \delta_d = \phi_{d+1} - \phi_d, \quad \delta_0 + \delta_1 + \delta_2 = 0 \pmod{2\pi}. \quad (85)$$

The remaining condition, orthogonality of row 0 with row k , has modulus part $\sqrt{ab} |\sum_d e^{i\phi_d}| = \sqrt{ac}$, that is $|\sum_d e^{i\phi_d}|^2 = \rho$. Writing $e^{i\delta_0} = e^{i\delta}$, $e^{i\delta_1} = e^{i\epsilon}$ and $e^{i\delta_2} = e^{-i(\delta+\epsilon)}$, the imaginary part of (85) vanishes if and only if $2 \sin \frac{\delta+\epsilon}{2} (\cos \frac{\delta-\epsilon}{2} - \cos \frac{\delta+\epsilon}{2}) = 0$. The second factor forces $\delta = 0$ or $\epsilon = 0$ and the first forces $\delta + \epsilon = 0$ modulo 2π ; in every branch one of the δ_d vanishes and the other two are $\pm\delta$, so (85) becomes $1 + 2 \cos \delta = -L$, that is $\cos \delta = -(1 + L)/2$, solvable exactly when $-3 \leq L \leq 1$, which on the window is $L \leq 1$, equivalently $t \geq 0$. With $\phi = (0, \delta, 0)$ the modulus condition becomes $|2 + e^{i\delta}|^2 = 5 + 4 \cos \delta = 3 - 2L = \rho$, the identity $c = 3b - 2a$, so it imposes nothing further. Hence (82) exhausts the invariant class and no element of that class exists for $t < 0$.

For (v), by the necessity half of Lemma 9.1, which is the half valid at $c = 0$, a preimage of $B(-\frac{1}{9})$ would give unimodular p_k, q_k satisfying (76)–(79) at $L = \frac{3}{2}$ and $\rho = 0$. Then (79) forces $1 + p_k + q_k = 0$, that is $q_k = -1 - p_k$, and $|q_k| = 1$ gives $|1 + p_k|^2 = 2 + 2 \operatorname{Re} p_k = 1$, so $\operatorname{Re} p_k = -\frac{1}{2}$ and, since $|p_k| = 1$, $p_k = -\frac{1}{2} + i s_k \frac{\sqrt{3}}{2}$ with $s_k \in \{+1, -1\}$; that is, $p_k \in \{\omega, \omega^2\}$ for $\omega = e^{2\pi i/3}$. Then $q_k = -1 - p_k = \bar{p}_k$ exactly, and $\sum_k p_k = -\frac{3}{2} + i \frac{\sqrt{3}}{2} (s_1 + s_2 + s_3)$. But (76) requires $\sum_k p_k = -L = -\frac{3}{2} \in \mathbb{R}$, that is $s_1 + s_2 + s_3 = 0$, and with three signs each ± 1 the sum lies in $\{3, 1, -1, -3\}$ and is never zero. The eight sign patterns, which the argument above shows are exactly the admissible configurations, were enumerated in exact arithmetic and all three residuals fail for every one of them; indeed since $q_k = \bar{p}_k$ throughout, $\sum_k q_k = \sum_k \bar{p}_k$ makes the residual of (77) minus the conjugate of that of (76), and $\bar{p}_k q_k = q_k^2 = p_k$ because $\omega^3 = 1$ makes the residual of (78) equal to that of (76). The contradiction holds in every gauge, so $B(-\frac{1}{9})$ is notunistochastic. $\square$

9.3 What the ray establishes, and what it leaves open

Parts (i) to (iii) and (v) of Theorem 9.2 are proved from first principles and use no membership criterion from the literature, so they are self-contained. Their content is that the bracelet conditions, although necessary at every dimension by Lemma 6.13, are satisfied *identically* along a whole segment of $\mathcal{B}(4)$ on which membership nevertheless switches: unistochastic for every $t \in [0, \frac{1}{3}]$, provably not unistochastic at $t = -\frac{1}{9}$. Figure 4 draws the four margin polynomials over the window and shades it by membership status. That is the exact form of the obstruction to a sufficiency theorem built on those conditions in dimension four and above, and it is why Corollary 6.14 uses them only in the refuting direction. The distinction between the two endpoints is not a matter of degree. At $t \geq 0$ an explicit unitary with exact radical entries is exhibited; at $t = -\frac{1}{9}$ the non-membership is a finite enumeration of eight configurations forced by the equations themselves. Neither argument has any slack.

Part (vi) is not proved and is not claimed. For $-\frac{1}{9} < t < 0$ the system (76)–(79) is overdetermined, with nine real equations for six real unknowns, and a seeded nonlinear least-squares search with 20000 restarts per parameter value, together with an exhaustive structured scan over the branches of (76) and (79), found no unimodular solution at $t = -\frac{1}{27}$, where $L = \frac{15}{13}$ and $\rho = \frac{9}{13}$, or at $t = -\frac{1}{60}$, where $L = \frac{63}{59}$ and $\rho = \frac{51}{59}$. The minimal residuals were 0.127227745 and 0.0236626448

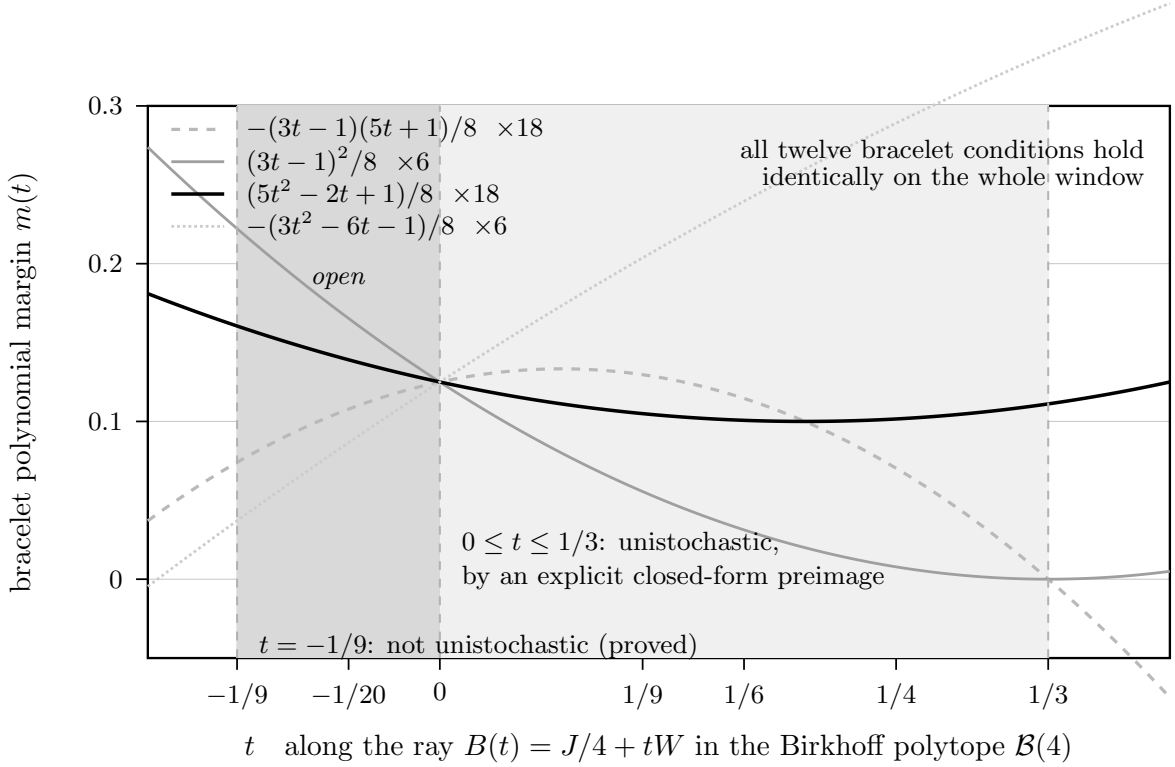


Figure 4: The ray $B(t) = J/4 + tW$ of (81) in the Birkhoff polytope $\mathcal{B}(4)$. Horizontal axis: the ray parameter t , dimensionless; the ray lies in $\mathcal{B}(4)$ exactly on the window $[-\frac{1}{9}, \frac{1}{3}]$ marked by the vertical rules (Theorem 9.2, part (i)). Vertical axis: the polynomial bracelet margin $m(t)$ of (84), dimensionless and nonnegative throughout the window; the four curves are the four distinct margins, labelled with their multiplicities 18, 6, 18 and 6 among the 48 scalar polygon inequalities. All four are nonnegative on the whole window and vanish together only at $t = \frac{1}{3}$, which is part (ii): every necessary bracelet condition holds identically along the ray. The horizontal axis is shaded by membership status: unistochastic with the explicit preimage (82) for $0 \leq t \leq \frac{1}{3}$ by part (iii), provably not unistochastic at $t = -\frac{1}{9}$ by part (v), and open for $-\frac{1}{9} < t < 0$ by part (vi). The curves are analytic functions, not measurements.

respectively, against zero required. A failed search is evidence and not proof, and this paper claims nothing for the interior.

What would settle it is either an explicit unitary preimage for some $-\frac{1}{9} < t < 0$, or a proof that (76)–(79) has no unimodular solution there. The second is the natural target, and the endpoint argument of part (v) suggests where it should go: for $t < 0$ one has $\rho = c/b < 1$ while $L > 1$, and the question is whether $|1 + p_k + q_k|^2 = \rho < 1$ is compatible with (76)–(78) as $t \rightarrow -\frac{1}{9}^+$, where the argument already closes. Lemma 9.1 is deliberately stated as an unreduced system, importing no criterion from the literature, so that an independent attempt starts from the equations themselves rather than from a reduced form whose reduction has already assumed something.

If the answer for the interior is negative, then $t = 0$ is an *interior* point of a segment of $\mathcal{B}(4)$ along which every necessary bracelet condition holds identically while membership switches on both sides of it. That would be the sharpest possible form of the obstruction, and would also mean that $\mathcal{U}(4)$ is not closed under taking such segments. The verification record of Appendix A reproduces the continuum identities of parts (i) to (iii) as symbolic identities in t , part (ii) in

full rather than by sampling, and five exact rational specialisations $t = \frac{1}{30}, \frac{1}{9}, \frac{1}{6}, \frac{1}{4}, \frac{1}{3}$, equivalently $\cos x = -\frac{29}{31}, -\frac{4}{5}, -\frac{5}{7}, -\frac{3}{5}, -\frac{1}{2}$, with $U(t)U(t)^* = I_4$, $U(t)^*U(t) = I_4$ and $|U(t)|^2 = B(t)$ checked entrywise in exact radical arithmetic.

10 Discussion

The three relations of Section 3 separate cleanly once the composite transfer matrix of a train is identified as the only object that matters. The integral fluctuation relation and the Crooks relation are properties of unital population dynamics: the first needs only that the rows of A sum to one, the second only that the backward train reverses the order of the intervals, which turns the composite into its transpose. Neither statement mentions the dimension, and neither can fail, because neither uses anything that a measurement train can destroy. The symmetric detailed fluctuation theorem is different in kind. It compares two weights of the same forward distribution, and Theorem 5.1 shows that the comparison reduces, class by class, to the antisymmetric part of A . Everything that follows is a consequence of that reduction: the violation is blind to the symmetric part of the composite, it vanishes at zero work, opposite work values carry one condition rather than two, and the question of when symmetry is necessary becomes a question about the rank of a linear map that can be computed exactly.

The dimension-two exception is then not an exception at all but the first value of a dimension count. The antisymmetric parts realisable inside $\mathcal{B}(d)$ span a space of dimension $(d-1)(d-2)/2$, which is zero only at $d=2$. At dimension two there is no antisymmetric direction for the violation to occupy, so the symmetric form holds for every cyclic protocol whatever the drive, the schedule or the number of measurements; the two-level amplitude identity usually invoked to establish the symmetry of each interval matrix is doing unnecessary work, since every matrix in $\mathcal{B}(2)$ is symmetric to begin with. At every $d \geq 3$ the count is positive and the scale argument of Lemma 6.1 makes every direction available, so a violation is always possible in principle and the question becomes quantitative.

The quantitative answer at dimension three is unusually clean, and its cleanness is what makes the worst case exactly computable. One scalar $x = A[0, 1] - A[1, 0]$ carries the whole antisymmetric part, the two nonzero defects are $-x(1+q)/Z$ and xq/Z , and the total variation distance between the two sides of the symmetric form is exactly $|x|$. Since $|x| \leq 1$ with equality only at the two three-cycle permutation matrices, and since every permutation matrix is realisable by a single unitary interval, the worst possible violation over every protocol, schedule, train length and temperature is the maximum value one of a total variation distance, attained by a deterministic three-cycle at every temperature. The pointwise worst case is a different quantity with a different behaviour: it is $r(1+r)/(1+r+r^2)$ with $r = \max(q, 1/q)$, it equals two thirds already at infinite temperature, and it approaches one without reaching it at any finite temperature. Quoting a single pointwise number without its temperature is therefore a mistake, and the value six sevenths that a fixed-temperature computation produces belongs to $q = \frac{1}{2}$ and $q = 2$ alone.

Degeneracy is the other half of the dimension-three story, and it is the part that shows why the class-wise criterion and not symmetry is the right statement. A doubly degenerate level collapses the work values to ± 1 , puts two pairs into the same class with the same final energy and hence the same Gibbs factor, and makes the single available antisymmetric degree of freedom cancel between them. The detailed fluctuation theorem then holds for every protocol at every temperature, symmetric or not, and the composite (51) at dimension four shows that the same mechanism produces asymmetric composites that satisfy the theorem exactly even when the spectrum is not degenerate, provided the rank of the violation map drops below the dimension of the antisymmetric space. Symmetry is

sufficient at every dimension, necessary when the gaps are distinct, and neither in between; Table 1 is the exact statement of where the boundary runs for the spectra computed here.

The feasibility question that the worst-case argument needs is settled exactly at dimension three and provably unsettled at dimension four. At $d = 3$ the classical criterion collapses to the sign of one integer polynomial, all six chain-link discriminants being that polynomial, and the polynomial's factorisations on the facets and on the edges give the whole one-skeleton of the polytope as orthostochastic with an explicit closed-form witness per edge. The zero set of the polynomial is larger than the skeleton: it also reaches the interior, at exactly six rational points of denominator nine and at no lattice point of smaller denominator. At $d = 4$ the ray of Theorem 9.2 shows that the same kind of necessary condition cannot be turned into a criterion, because all twelve of them hold identically along a segment on which membership switches. That is the precise sense in which the dimension-four problem is harder: not that the conditions are complicated, but that they are silent.

Several boundaries of this work should be stated where a reader will meet them. There is no membership criterion for $\mathcal{U}(d)$ at $d \geq 4$ here. Lemma 6.13 proves the bracelet conditions necessary at every dimension and Rajchel-Mieldzioć et al. [9] that they are insufficient at $d = 4$, so they can refute membership and never certify it; Corollary 6.14 uses exactly that one-sided power to settle the single matrix constructed here and nothing beyond it. There is no characterisation of the set of composites of a train of length $N \geq 1$. That set is the set of products of $N + 1$ unistochastic matrices, it strictly contains $\mathcal{U}(d)$, it grows with N , and Theorem 7.1 does not need it: containment in $\mathcal{B}(d)$ together with attainability of the vertices is all the worst-case argument uses. Whether the composite (51) is such a product is open. The supremum of the ratio $P(w)q^w/P(-w)$ over realisable protocols is infinite, not a finite number, for the reason given in Remark 7.5, and no finite worst-case ratio is claimed anywhere. Non-cyclic protocols are classified completely only at $d = 2$; at $d \geq 3$ the class-wise criterion for two different endpoint spectra is not derived here, because the work classes would have to be rebuilt from two spectra and the violation map would no longer factor through the antisymmetric part of A alone. The measurements are projective and in the energy basis and the intervals are unitary: open-system dynamics between measurements, general instruments, positive-operator-valued measurements, feedback and measurement-apparatus energetics are all outside the model. Finally, the pattern of ranks in Table 1 is structural and the eight spectra there are computed exactly, but the general statement that an equally spaced spectrum has rank $\Phi = d - 2$ for $d \geq 4$, or that a spectrum with all gaps distinct has rank $\Phi = \dim \mathcal{K}(d)$, is not proved here; it is a conjecture supported by the computed cases.

Four questions remain open, and each is a question this paper creates rather than one it inherits. The first is whether the composite (51) is realisable by a train with at least one intermediate measurement rather than by a single unitary interval. An explicit factorisation into unistochastic matrices would show that the rank deficiency of the violation map at a gap-non-degenerate four-level spectrum has a genuine thermodynamic realisation requiring more than one interval; a proof that no factorisation exists would show that the deficiency is visible only through degeneracy, which Corollary 6.14 already realises with the four-cycle at the spectrum $(0, 0, 1, 1)$. Either answer is informative, and the matrix is a favourable test case: it has a zero entry, only four distinct entry values, and two failed bracelet inequalities that constrain any candidate factorisation strongly.

The second is whether $B(t)$ is unistochastic for $-\frac{1}{9} < t < 0$. Theorem 9.2 settles both ends of the ray and leaves the interior of its negative part open, with a failed numerical search as the only evidence. Lemma 9.1 gives the exact unreduced system that any attempt should start from.

The third is whether the composite set of a long measurement train can be characterised at all. Its exact description, or even a proof that its closure is the whole of $\mathcal{B}(d)$ for N large enough, would upgrade Theorem 7.1 from a maximum over the polytope to a maximum over the realisable

set with no vertex-realizability argument, and would identify which intermediate violation values are physically reachable at a given train length. That matters experimentally: Theorem 7.1 shows the maximal violation $V = 1$ is reachable with a single interval, and says nothing about which violations strictly between zero and one require a long train.

The fourth is whether degeneracy-protected exactness extends to every dimension. Theorem 6.10 shows a doubly degenerate level makes the theorem unconditional at $d = 3$, and Table 1 shows the violation map vanishes identically for the spectrum $(0, 0, 1, 1)$ at $d = 4$. Whether there is a clean condition on the endpoint spectrum that forces $\text{rank } \Phi = 0$ at every dimension is open. Such a condition would be the exact higher-dimensional analogue of Theorem 6.3 and would have direct experimental content: degenerate multiplets would protect the fluctuation theorem against the loss of transfer-matrix symmetry, whatever the drive.

11 Conclusion

A projective-measurement train on a driven quantum system defines work through the two-point-measurement scheme, and the three relations usually quoted for that work distribution are not equivalent. Two of them are dimension-free. The integral fluctuation relation follows from the row sums of the composite transfer matrix alone, and the backward transfer matrix of a train is exactly the transpose of the forward one, so the Crooks relation holds against it with the free-energy difference given by the partition-function ratio. Neither statement uses symmetry, commutation of the intervals, degeneracy or the dimension, and neither needs to know that the composite came from unitaries. The third relation, the detailed fluctuation theorem in the symmetric form that a single forward experiment can test, is a statement about the antisymmetric part of the composite: its violation at a work value is a weighted sum, over the pairs of levels realising that value, of exactly that antisymmetric part. That identity is necessary and sufficient, affine in the composite, and valid at every dimension, every schedule, every train length, every inverse temperature and every pair of cyclic endpoint Hamiltonians.

The dimension-two exception follows from it as the first value of a dimension count. The antisymmetric parts realisable by doubly stochastic matrices span a space of dimension $(d-1)(d-2)/2$, zero only at $d = 2$, so at dimension two the symmetric form holds for every cyclic protocol whatever the drive, while at every higher dimension an antisymmetric direction is available and the theorem becomes a quantitative question. For arbitrary endpoints at dimension two the exact condition is isospectrality of the two endpoint Hamiltonians, strictly weaker than cyclicity, and off isospectrality the symmetric form is replaced by two exact drive-independent ratios carrying different exponential factors. At dimension three a single rational scalar controls the entire violation and the total variation distance equals its absolute value; the worst case over all physically realisable protocols, schedules, train lengths and temperatures is attained by a deterministic three-cycle and equals one at every temperature, while the pointwise worst case depends on temperature, equals two thirds at infinite temperature and approaches one without ever attaining it. Involution protocols satisfy the theorem exactly in every dimension, and at dimension three the protocols of maximal matrix asymmetry are exactly those of maximal thermodynamic violation.

Two structural facts complete the picture. At dimension three the classical feasibility criterion reduces to the sign of one integer polynomial, and the factorisations of that polynomial on the facets and on the edges show that the whole one-skeleton of the Birkhoff polytope is orthostochastic with an explicit closed-form orthogonal witness per edge, while its zero set also reaches the interior of the polytope at exactly six rational points of denominator nine. At dimension four a rational ray exhibits the obstruction to any sufficiency theorem built on the necessary bracelet conditions: all

twelve of them hold identically along the ray while unistochastic membership switches, proved positively by an explicit closed-form unitary preimage for nonnegative parameter values and negatively by a finite enumeration at the lower endpoint. The interior of the negative part is left open, with the exact unreduced phase system written down as the starting point for settling it, and three further questions are stated as open rather than resolved.

A Exact verification

Every number quoted in this paper is an exact rational number or an exact radical. This appendix records the arithmetic regime that makes that possible, what was recomputed independently of the derivations in the body, and where a numerical search rather than a proof is the only evidence available.

A.1 The arithmetic regime

Two layers of exact arithmetic are used. The first is rational arithmetic with arbitrary-precision integer numerator and denominator: every transfer matrix, work distribution, defect, total variation, rank and witness is computed in that ring, and every comparison against a claimed value is a comparison of exact rationals, so a deficit of zero means zero and not “below tolerance”. No floating-point value is evidence for any exact claim anywhere in this paper. The second layer is multivariate polynomial arithmetic with integer coefficients, used for the algebraic facts of Sections 8 and 9: products of polynomials are formed exactly, two polynomials are equal exactly when all their coefficients agree, and an integer polynomial square root is extracted by a graded-lexicographic long division that either terminates with an exact root or reports failure. The instances use integer spectra and positive rational values of q , so that q^ε and q^w are exact rationals; as Section 3 states, this is a choice of instances and not a restriction on the theorems, all of which are stated for arbitrary real spectra and arbitrary real $\beta > 0$.

A.2 What was recomputed

The verification was organised so that each claim in the body is reproduced from the definitions rather than from the derivation that proved it. The work distribution is recomputed from the composite transfer matrix and the Gibbs weights; the defect from the work distribution; the total variation from the defects; the certificate from the chart; the ranks from an explicit basis of $\mathcal{K}(d)$; and the backward process from a literal reversal of the schedule and the interval unitaries, so that $A_B = A^T$ is confirmed entrywise rather than assumed. Table 3 lists the groups, the number of exact instances in each, and the outcome. All 226 checks passed with zero failures; the full output is part of the record accompanying this paper [5].

Table 3: Independent exact recomputation behind the claims of the body. “Instances” counts exact cases, not floating-point samples; every entry is a comparison of exact rationals or of integer polynomial coefficients against the value claimed in the body.

claim checked	instances	result
Integral fluctuation relation (16), $d = 2, \dots, 6$, $N = 0, \dots, 6$, degenerate and non-degenerate spectra, cyclic and non-cyclic endpoints, three values of q	936 exact trains	deficit exactly 0
Crooks relation and $A_B = A^T$ (18), same sweep, plus a literal three-interval train built from explicit unitaries	936 exact trains	deviation exactly 0; transpose identity confirmed entrywise
Class-wise formula (22) against the definition (9)	41880 work classes	maximum difference exactly 0
Corollaries 5.3 and 5.4, and symmetry implies exactness	systematic sweep over $d = 2, \dots, 6$	both identities exact; $\Delta \equiv 0$ for symmetric A
$\dim \mathcal{K}(d) = (d-1)(d-2)/2$ by elimination, and $(A - A^T)\mathbf{1} = 0$	$d = 2, \dots, 8$	0, 1, 3, 6, 10, 15, 21
$\mathcal{R}(d)$: the construction (36) certified on exact elements of the set; elements outside it rejected by the row bound and rescaled onto its boundary; $\mathcal{R}(3) = [-1, 1]G$; the $d = 4$ cube section; the $d = 5$ tournament and its padding	337 exact lattice points of $\mathcal{B}(3)$, $\mathcal{B}(4)$; 81741 exact convex combinations at $d = 3, 4, 5$; 1263 elements of $\mathcal{K}(d)$ inside the row bounds, 116 of them with $s = 0$; 2982 outside, each rescaled; 5910 permutation differences at $d = 3, \dots, 7$; 83 points of $\mathcal{R}(3)$; 15 elements of the $d = 4$ cube section; the tournament at $d = 5, 6, 7$	all certified or rejected exactly, in rational arithmetic
rank Φ of Table 1 from an explicit basis of $\mathcal{K}(d)$	8 spectra $\times$ 3 values of q	all ten ranks reproduced exactly
Theorem 6.3 and Theorem 6.5: isospectrality necessary and sufficient	120 endpoint pairs, symbolic in p and q	no exception
Corollary 6.6: drive independence of the two ratios	1350 exact cases	ratios exactly $q^{\mp g_0}$
Remark 6.4: the symmetric counterexample, and that no rational correction factor repairs it	1 matrix, 5 correction factors	$\Delta(2) = \frac{1}{18}$; integral fluctuation relation and Crooks both exact
Remark 6.7: the $q = 1$ boundary	1 endpoint pair, 2 temperatures	$\Delta \equiv 0$ at $q = 1$, $\Delta(-1) = -\frac{2}{5}$ at $q = \frac{1}{2}$

claim checked	instances	result
Theorem 6.8, Corollary 6.9: the closed forms and $V = x $	5 temperatures; exhaustive grid of 2211 points of $\mathcal{B}(3)$ at $q = \frac{1}{2}$ and $q = \frac{1}{3}$	both reproduced exactly on every grid point
Theorem 6.10: $\Delta \equiv 0$ for degenerate three-level spectra	9 spectra and temperatures	exactly 0 for asymmetric A
Theorem 7.2: involutions satisfy (1)	224 cases	exactly 0
Remark 8.4: $\alpha(P_\sigma) = 1$ exactly for permutations with a cycle of length at least three	all of S_3, S_4, S_5 , 150 permutations	confirmed by exhaustive enumeration
Theorem 7.1 and Corollary 7.4: vertex enumeration at 14 exact temperatures, and the closed form $f(r)$	14 temperatures $\times$ 6 vertices; exhaustive grids of 231, 2211, 26796 and 123256 points at $q = \frac{1}{2}$; 2211 points each at $q = \frac{1}{3}$ and $q = 3$	$f(r)$ matched at every temperature; no grid point above the vertex bound; both bounds attained
The witnesses M_8, H, M_9, O of Section 8	4 matrices	every quoted entry, Q value, defect, ratio and asymmetry reproduced
Corollaries 6.12 and 6.14: the asymmetric exact composite, its defects, $\dim \mathcal{K}(4)$ and rank Φ , and its failed bracelet inequalities	1 matrix, all 48 polygon inequalities; 3×3 rank system; 4-cycle and two further asymmetric matrices at 3 temperatures and the spectrum $(0, 0, 1, 1)$	$\Delta \equiv 0$; $\dim \mathcal{K}(4) = 3$, rank $\Phi = 2$, $\Phi(D_0) = 0$; exactly the row pair $(1, 3)$ at $k_0 = 1$ and the column pair $(2, 3)$ at $k_0 = 2$ fail, each by margin $\frac{1}{32}$; the other 46 hold
Theorem 8.1(a): all six chain-link discriminants are one integer polynomial	symbolic, in the chart	identical, degree 4, 26 terms, integer coefficients
Theorem 8.1(b): the nine facet factorisations	symbolic	$-Q$ is a perfect square on each facet; each root verified by exact multiplication
Corollary 8.2: the nine edge identities and their witnesses	symbolic, in the ring modulo $u^2 = s, v^2 = 1 - s$	Q identically zero on each edge; $OO^T = I$ and $ O ^2 = M(s)$ on each edge
The lattice sweep of $\mathcal{B}(3)$ and the interior witness M_9	denominators $1, \dots, 9$, 4080 exact lattice points	the nine counts of Table 5; denominator 9 minimal; exactly the six points $(4J - 3P_\sigma)/9$

claim checked	instances	result
Theorem 9.2(i),(ii): the window and the 48 bracelet margins	symbolic in t , plus 15 exact probes	four distinct margin polynomials with multiplicities 18, 6, 18, 6; all non-negative on the window; common zero set $\{\frac{1}{3}\}$; exactly 24 of 48 vanish there
Theorem 9.2(iii): the algebraic identities behind the explicit preimage	5 exact rational values of t	$b(1 + 2 \cos x) = -a$, $ z ^2 = a$, $\cos x = (t - 1)/(1 + t)$ and row norms 1, all exact; $\cos x$ equals $-\frac{29}{31}$, $-\frac{4}{5}$, $-\frac{5}{7}$, $-\frac{3}{5}$, $-\frac{1}{2}$
Theorem 9.2(v): the eight admissible configurations at $t = -\frac{1}{9}$	exact enumeration	all eight fail; a sum of three signs never vanishes

A.3 One correction found by the recomputation

The recomputation corrected one statement about the ray direction W of (81). Its rows and columns each sum to zero, which is the property that makes $B(t)$ doubly stochastic, but W is not traceless: $\text{Tr}W = -1$ and $\text{Tr}(4W) = -4$. Nothing in the argument uses the trace, and no claim in the body depends on it, but the property is stated here as it is rather than as it was first written, because a reader checking W entry by entry would otherwise find a false statement.

A.4 The figures

The four figures were drawn from exactly computed data and are vector graphics. Figure 1 is a schematic of the protocol and carries no numerical content. Figure 2 plots the 2211 points of the exhaustive rational grid of $\mathcal{B}(3)$ at step $\frac{1}{10}$ together with the three marked matrices $x = -1$, $x = -\frac{1}{10}$ and $x = 1$; every plotted coordinate is an exact rational converted to a drawing position. Figure 3 plots the closed form (60) as an analytic curve, densely sampled for drawing only, together with the fourteen exact rational temperatures of Table 6 as individual points; the curve is a function, not a measurement, and the caption says so. Figure 4 plots the four margin polynomials (84) as analytic curves over the window, with the membership status of each part marked. No figure contains an error bar, a fitted form or a value that was not computed.

A.5 What is numerical rather than exact

Exactly one item in this paper rests on numerical evidence, and it is labelled as such wherever it appears. For $-\frac{1}{9} < t < 0$ the membership of $B(t)$ in $\mathcal{U}(4)$ is open. A seeded nonlinear least-squares search over the six phases of (76)–(79), with 20000 restarts per parameter value, together with an exhaustive structured scan over the branches of (76) and (79), found no unimodular solution at $t = -\frac{1}{27}$ or $t = -\frac{1}{60}$; the minimal residuals were 0.127227745 and 0.0236626448 against the required zero. Those residuals are floating-point quantities and are reported to the precision at which they were obtained, not as exact rationals. A failed search is evidence and not proof, and

Theorem 9.2(vi) states the interior as open. The radical arithmetic of the explicit preimage (82) is not part of this item: part (iii) of Theorem 9.2 is proved by the algebraic identities listed in Table 3, which are exact, and no floating-point value supports it.

B Tables

B.1 The nine facet factorisations

Table 4 lists the perfect square whose negative is the restriction of the certificate polynomial (63) to each of the nine facets of $\mathcal{B}(3)$. The chart is $(x_{00}, x_{01}, x_{10}, x_{11})$ with the five derived entries given by (62); the second column records the relation that the facet imposes inside that chart. Each root was verified by exact integer polynomial multiplication, that is, by checking that the square of the listed polynomial equals $-Q$ after the substitution, coefficient by coefficient.

Table 4: The restriction of $-Q$ to each facet of $\mathcal{B}(3)$ is a perfect square, as Theorem 8.1(b) states. The square root is given in the chart $(x_{00}, x_{01}, x_{10}, x_{11})$ after the substitution recorded in the second column, and is unique up to sign. Consequence: on a facet, $Q \geq 0$ forces $Q = 0$, so every boundary point of $\mathcal{B}(3)$ that is unistochastic is orthostochastic.

facet	substitution in the chart	square root s with $-Q = s^2$
$M[0, 0] = 0$	$x_{00} = 0$	$x_{01}x_{10} - x_{01} - x_{10} - x_{11} + 1$
$M[0, 1] = 0$	$x_{01} = 0$	$x_{00}x_{11} - x_{00} - x_{10} - x_{11} + 1$
$M[0, 2] = 0$	$x_{01} = 1 - x_{00}$	$x_{00}x_{10} + x_{00}x_{11} - x_{11}$
$M[1, 0] = 0$	$x_{10} = 0$	$x_{00}x_{11} - x_{00} - x_{01} - x_{11} + 1$
$M[1, 1] = 0$	$x_{11} = 0$	$x_{01}x_{10} - x_{00} - x_{01} - x_{10} + 1$
$M[1, 2] = 0$	$x_{11} = 1 - x_{10}$	$x_{00}x_{10} + x_{01}x_{10} - x_{01}$
$M[2, 0] = 0$	$x_{00} = 1 - x_{10}$	$x_{01}x_{10} + x_{10}x_{11} - x_{01}$
$M[2, 1] = 0$	$x_{01} = 1 - x_{11}$	$x_{00}x_{11} + x_{10}x_{11} - x_{00}$
$M[2, 2] = 0$	$x_{11} = 1 - x_{00} - x_{01} - x_{10}$	$x_{00}^2 + x_{00}x_{01} + x_{00}x_{10} + x_{01}x_{10} - x_{00}$

B.2 The lattice sweep of the Birkhoff polytope at dimension three

Table 5 is the exhaustive sweep quoted in Section 8. A lattice point of denominator n is a matrix in $\mathcal{B}(3)$ all of whose entries are integer multiples of $1/n$; the enumeration is over all such matrices, with no sampling. The last column counts those with all nine entries strictly positive and $Q = 0$, that is, the points at which the zero set of the certificate reaches the interior of the polytope.

B.3 The fourteen exact temperatures

Table 6 is the enumeration behind Figure 3 and Corollary 7.4. At each temperature the maximum of $|\Delta(w)|$ over all work values and over the six vertices of $\mathcal{B}(3)$ was computed exactly by the vertex enumeration of Theorem 7.1, and compared with the closed form (60); the two agree at all fourteen temperatures with no mismatch. The maximum of V is one at every one of them, by Corollary 7.3.

Table 5: Exhaustive enumeration of the lattice points of $\mathcal{B}(3)$ at denominators 1 through 9, and the number of them at which the certificate polynomial Q of (63) vanishes while all nine entries are strictly positive. The counts in the second column are the exact numbers of lattice points of $\mathcal{B}(3)$ at each denominator; their total is 4080. The last column is zero through denominator 8 and equals six at denominator 9, where the six points are exactly $(4J - 3P_\sigma)/9$ for $\sigma \in S_3$, one of which is the witness M_9 of (66). Denominator 9 is therefore the smallest at which the boundary of $\mathcal{U}(3)$ relative to $\mathcal{B}(3)$ reaches the interior, and the count 231 at denominator 5 cross-checks the step- $\frac{1}{5}$ grid of Section 7.

denominator n	lattice points of $\mathcal{B}(3)$	interior points with $Q = 0$
1	6	0
2	21	0
3	55	0
4	120	0
5	231	0
6	406	0
7	666	0
8	1035	0
9	1540	6
total	4080	6

Table 6: Exact worst-case violation at $d = 3$ with the equally spaced spectrum $\varepsilon = (-1, 0, 1)$, over all protocols, schedules and train lengths, at fourteen exact rational temperatures. The fourth column is the closed form $f(r) = r(1+r)/(1+r+r^2)$ of Corollary 7.4 and the fifth the maximum obtained by exact vertex enumeration; they agree in every row. The sixth column names the work value at which the pointwise maximum is attained, always by both three-cycle protocols. The seventh column is $\max V$, which equals one at every temperature. Values are exact rationals, dimensionless.

q	$\beta = \ln(1/q)$	$r = \max(q, 1/q)$	$f(r)$	$\max_w \Delta(w) $	attained at	$\max V$
1/100	$\ln 100$	100	10100/10101	10100/10101	$w = -1$	1
1/10	$\ln 10$	10	110/111	110/111	$w = -1$	1
1/4	$\ln 4$	4	20/21	20/21	$w = -1$	1
1/3	$\ln 3$	3	12/13	12/13	$w = -1$	1
1/2	$\ln 2$	2	6/7	6/7	$w = -1$	1
2/3	$\ln(3/2)$	3/2	15/19	15/19	$w = -1$	1
3/4	$\ln(4/3)$	4/3	28/37	28/37	$w = -1$	1
1	0	1	2/3	2/3	$w = \pm 1$	1
4/3	$-\ln(4/3)$	4/3	28/37	28/37	$w = +1$	1
3/2	$-\ln(3/2)$	3/2	15/19	15/19	$w = +1$	1
2	$-\ln 2$	2	6/7	6/7	$w = +1$	1
3	$-\ln 3$	3	12/13	12/13	$w = +1$	1

q	$\beta = \ln(1/q)$	$r = \max(q, 1/q)$	$f(r)$	$\max_w \Delta(w) $	attained at	$\max V$
10	$-\ln 10$	10	110/111	110/111	$w = +1$	1
7/5	$-\ln(7/5)$	7/5	84/109	84/109	$w = +1$	1

The value $\frac{6}{7}$ appears at $q = \frac{1}{2}$ and at $q = 2$ and nowhere else, since $7r(1+r) - 6(1+r+r^2) = r^2 + r - 6 = (r-2)(r+3)$ has the single positive root $r = 2$. The maximum is strictly larger than $\frac{6}{7}$ whenever $r > 2$ and strictly smaller whenever $1 \leq r < 2$, and $1 - f(r) = 1/(1+r+r^2)$ is positive at every finite temperature, so the supremum one is attained at none.

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