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A four-state Markovian Mpemba effect in which every triplet test fails

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Abstract

Avitan, Factor and Gelbwaser-Klimovsky derived necessary conditions on the transition rates of a three-level system for the Markovian Mpemba effect, and proposed applying them to every triplet of levels of an N-level system. For a zero-temperature bath and non-degenerate spectrum they proved that a strong violation of the conditions in all triplets excludes the effect; for non-zero temperature they conjectured, on the basis of numerical sampling, that violation in all triplets excludes it. We give an explicit reversible four-state chain, with energies $U(0, 1, 2, 64)$ and a bath at inverse temperature $\ln 2/U$, in which all four triplet conditions fail strictly and yet a hotter thermal initial state has a strictly smaller slow-mode amplitude than a colder one. This is a direct Mpemba effect, so the finite-temperature conjecture fails for $N = 4$. The example is marginal: it uses Boltzmann weights of order 2^{-64}, initial temperatures of order $10^2\,U$, a relative amplitude gap of about 0.07%, and three of the four triplets fail by margins of order 10^{-6}. We then give a second, less marginal example with energies $(0, \frac{1}{30}, 0.434, 5)$, bath inverse temperature 3 and initial inverse temperatures 0.06 and $\frac{1}{6}$: every triplet fails by at least 1.08×10^{-3} relative to its largest rate, and the relative amplitude gap is 1.22%. A variant of the second example with rational Boltzmann factors has the same properties and is certified in exact rational arithmetic without exponential enclosures. All claims are reduced to finite exact rational or rational-interval computations, which we describe. In both examples the ground level escapes more slowly than the slowest mode relaxes; an exact elimination identity shows that the slow mode then sees effective couplings between the excited levels that depend on the slowest eigenvalue, and these are not visible to tests built from the original rates.

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1 Setting

Consider N levels with energies $E_1 < \cdots < E_N$ and a continuous-time Markov chain $\dot{p} = Mp$ on column probability vectors, with $M_{ij} = a_{ij} \geq 0$ the rate $j \to i$ for $i \neq j$ and $M_{jj} = -\sum_{i \neq j} a_{ij}$, as in [1, Eq. (1)]. The rates satisfy detailed balance with respect to the bath, $a_{ij} e^{-\beta_b E_j} = a_{ji} e^{-\beta_b E_i}$, so that $\pi(\beta_b)$ is stationary, where $\pi(\beta)_i = e^{-\beta E_i}/Z(\beta)$.

If the slowest nonzero eigenvalue λ_2 of M is simple, with right eigenvector V_2 and left eigenvector ℓ normalized by $\ell^{\mathsf{T}} V_2 = 1$, then for the initial state $p(0) = \pi(\beta)$,

$$p(t) - \pi(\beta_b) = b(\beta)\, e^{\lambda_2 t} V_2 + O\big(e^{\lambda_3 t}\big), \qquad b(\beta) = \ell^{\mathsf{T}} \pi(\beta),$$

where $\lambda_3 < \lambda_2$ is the next eigenvalue; b is the coefficient b_2 of [1, Eq. (2)], going back to [3]. For two initial temperatures above the bath temperature, $\beta_h < \beta_c < \beta_b$, a *direct Mpemba effect* occurs when $|b(\beta_h)| < |b(\beta_c)|$: the hotter state is asymptotically closer to equilibrium. This is the criterion of [3] and [4, Sec. II]; a *strong* effect in the sense of [4, Sec. III] would require in addition $b = 0$ at some initial temperature. For a review of the Mpemba effect and related anomalous relaxation phenomena see [5].

The triplet tests. For three levels $i < j < k$ write $- = i$, $0 = j$, $+ = k$, $\Delta_{0-} = E_j - E_i$, and $C_{+-} = 1 + \frac{1}{2}e^{-\beta_b(E_k - E_i)}$, $C_{+0} = 1 + \frac{1}{2}e^{-\beta_b(E_k - E_j)}$. With the original rates of M, set

$$\kappa = \frac{a_{-+} + a_{0+}}{a_{-0}\big(1 + e^{-\beta_b \Delta_{0-}}\big)}.$$

The necessary conditions of [1, Eq. (3)] are

$$\kappa \geq 1: \quad a_{-+}C_{+-} - a_{0+}C_{+0} > a_{-0}\big(1 - e^{-\beta_b \Delta_{0-}}\big), \tag{1}$$

$$\kappa \leq 1: \quad a_{-+}e^{-\beta_b \Delta_{0-}} > a_{0+}. \tag{2}$$

(The letter k is used for κ in [1].) A triplet *fails* the test if the inequality of its branch does not hold. In all triplets below $\kappa \neq 1$, so the convention at $\kappa = 1$ plays no role.

What is proved in [1]. For N levels one applies (1)–(2) to every triplet with the original rates. For a zero-temperature bath (triangular M), with non-degenerate eigenvalues and the strong violation $a_{-0} > a_{-+} + a_{0+}$ in every triplet, [1] proves that the N-level system shows no Mpemba effect. For a non-zero-temperature bath, [1] conjectures that if all triplets violate (1)–(2) then there is no Mpemba effect, supported by random sampling of 4- to 7-level systems (section "Numerics for non-zero temperature baths"). For $N = 3$ the only triplet is the system itself and (1)–(2) are the three-level necessary conditions derived in [1], so the conjecture concerns $N \geq 4$. A protocol for producing the effect in N-level systems is developed in [2]; its Section II restates the triplet criterion, without the zero-temperature restriction, as a result of [1]: if no triplet satisfies the conditions, the N-level system shows no Markovian Mpemba effect. The examples below are counterexamples, with $N = 4$, to the finite-temperature conjecture and hence to this restatement; they are not in conflict with the zero-temperature theorem.

2 The example

Fix an energy unit $U > 0$, a time unit $\tau > 0$ and $0 < \varepsilon \leq 10^{-6}$. Let

$$E = U\,(0, 1, 2, 64), \qquad \beta_b = \frac{\ln 2}{U}, \qquad \delta = 2^{-64}, \qquad q = (1, \tfrac{1}{2}, \tfrac{1}{4}, \delta),$$

so $\pi(\beta_b) = q/(\frac{7}{4} + \delta)$. With the symmetric conductances

$$(d_{12}, d_{13}, d_{14}, d_{23}, d_{24}, d_{34}) = \big(1 + \varepsilon,\ \tfrac{5}{3},\ 2,\ 102,\ 3,\ 3 + \varepsilon\big),$$

set $a_{ij} = q_i d_{ij}/\tau$ for $i \neq j$. Then $a_{ij}q_j = q_i q_j d_{ij}/\tau = a_{ji}q_i$, which is detailed balance, and every rate is positive (the smallest is $a_{41} = 2\delta/\tau$). Explicitly,

$$\tau M_\varepsilon = \begin{pmatrix} -\frac{11}{12} - \frac{\varepsilon}{2} - 2\delta & 1 + \varepsilon & \frac{5}{3} & 2 \\ \frac{1+\varepsilon}{2} & -\frac{53}{2} - \varepsilon - 3\delta & 51 & \frac{3}{2} \\ \frac{5}{12} & \frac{51}{2} & -\frac{158}{3} - (3 + \varepsilon)\delta & \frac{3+\varepsilon}{4} \\ 2\delta & 3\delta & (3 + \varepsilon)\delta & -\frac{17}{4} - \frac{\varepsilon}{4} \end{pmatrix}.$$

The two initial inverse temperatures are

$$\beta_h = \frac{\ln(256/255)}{U} < \beta_c = \frac{\ln(128/127)}{U} < \beta_b,$$

which holds because $\frac{1}{2} < \frac{127}{128} < \frac{255}{256} < 1$. Writing $t = e^{-\beta U}$, one has $\pi(\beta) = (1, t, t^2, t^{64})/(1 + t + t^2 + t^{64})$, and $t_h = \frac{255}{256}$, $t_c = \frac{127}{128}$ are rational.

Theorem 1. *For every $U, \tau > 0$ and $0 < \varepsilon \leq 10^{-6}$:*

1. *all four triplets $\{1,2,3\}, \{1,2,4\}, \{1,3,4\}, \{2,3,4\}$ fail the tests (1)–(2), each with a strict inequality;*

2. the nonzero eigenvalues of M_ε are simple, and the slowest one is $\lambda_2 = \mu_2/\tau$ with

$$\mu_2 \in [-2.13661042001,\ -2.13660892000];$$

3. with the slow-mode amplitude b of Section 1,

$$0.398692971890 \le b(\beta_h) \le 0.398695686013,$$
$$0.398971230884 \le b(\beta_c) \le 0.398973922273,$$
$$0.000278140493 \le b(\beta_c) - b(\beta_h) \le 0.000278354761.$$

In particular $0 < b(\beta_h) < b(\beta_c)$, so $|b(\beta_h)| < |b(\beta_c)|$: the chain shows a direct Mpemba effect although every triplet fails the test.

Changing U rescales all energies and inverse temperatures together and leaves βE unchanged; changing τ multiplies all rates and eigenvalues by a common factor. Neither affects any statement, so below $U = \tau = 1$.

3 Proof

(i) Triplets. For the triplet $i < j < k$ one has $a_{-0} = q_i d_{ij}$, $a_{-+} = q_i d_{ik}$, $a_{0+} = q_j d_{jk}$ and $e^{-\beta_b \Delta_{0-}} = q_j/q_i$, $C_{+-} = 1 + q_k/(2q_i)$, $C_{+0} = 1 + q_k/(2q_j)$. Direct substitution gives the following, where "residual" is left side minus right side of the applicable inequality (1) or (2):

triplet	κ	branch	residual
123	$\dfrac{316}{9(1+\varepsilon)} > 1$	(1)	$-\dfrac{499}{8} - \dfrac{\varepsilon}{2}$
124	$\dfrac{7}{3(1+\varepsilon)} > 1$	(1)	$-\dfrac{\delta+\varepsilon}{2}$
134	$\dfrac{3(11+\varepsilon)}{25} > 1$	(1)	$-\dfrac{\delta}{2} - \Big(\dfrac{1}{4} + \dfrac{\delta}{2}\Big)\varepsilon$
234	$\dfrac{9+\varepsilon}{306} < 1$	(2)	$-\dfrac{\varepsilon}{4}$

For instance, for 234: $a_{-+}e^{-\beta_b\Delta_{0-}} - a_{0+} = \frac{1}{2}\cdot 3 \cdot \frac{1}{2} - \frac{1}{4}(3+\varepsilon) = -\frac{\varepsilon}{4}$. The κ values lie strictly on one side of 1 for all $0 \le \varepsilon \le 10^{-6}$, and every residual is strictly negative for $\varepsilon > 0$. Thus each triplet fails its test with a strict inequality.

(ii) Spectrum. At $\varepsilon = 0$, expanding the determinant gives $\det(zI - M_0) = z\, f(z)$ with

$$f(z) = z^3 + \frac{24\delta + 253}{3} z^2 + \frac{1008\delta^2 + 20380\delta + 24331}{48} z + \frac{(4\delta+7)(432\delta^2 + 11598\delta + 9707)}{96}.$$

Evaluating f exactly at rational endpoints shows sign changes on the disjoint intervals

$$[-2.13660892001, -2.13660892000], \qquad [-4.25000000001, -4.24999999999],$$
$$[-77.94672441334, -77.94672441332].$$

A cubic has at most three roots, so these contain all roots of f, each simple. For $\varepsilon > 0$ let $D = \mathrm{diag}(q)$ and $S_\varepsilon = D^{-1/2} M_\varepsilon D^{1/2}$, a real symmetric matrix with off-diagonal entries $\sqrt{q_i q_j}\, d_{ij}$ and the same spectrum as M_ε. Only d_{12} and d_{34} depend on ε, and

$$S_\varepsilon - S_0 = -\varepsilon\big(w_{12} w_{12}^{\mathsf T} + w_{34} w_{34}^{\mathsf T}\big), \qquad w_{ij} = \sqrt{q_j}\, e_i - \sqrt{q_i}\, e_j.$$

The vectors w_{12}, w_{34} have disjoint supports and squared norms $\frac{3}{2}$ and $\frac{1}{4} + \delta$, so $-\frac{3}{2}\varepsilon I \preceq S_\varepsilon - S_0 \preceq 0$. By Weyl's inequality each ordered eigenvalue moves down by at most 1.5×10^{-6}; zero remains an eigenvalue because $\pi(\beta_b)$ is stationary. The shifted intervals

$$\mu_2 \in [-2.13661042001, -2.13660892000], \qquad \mu_3 \in [-4.25000150001, -4.24999999999],$$
$$\mu_4 \in [-77.94672591334, -77.94672441332]$$

are disjoint and negative, which proves (ii).

(iii) Slow left eigenvector. Let $B = M_\varepsilon^{\mathsf{T}} - \mu_2 I$ and $J = \{1, 3, 4\}$. Fix $\ell_2 = 1$ and solve $B_{JJ}\ell_J = -B_{J2}$ by Cramer's rule in outward-rounded rational interval arithmetic, with μ_2 ranging over its enclosure and ε over $[0, 10^{-6}]$ independently. This gives $\det B_{JJ} \in [131.7448386,\ 131.7451652]$, so B_{JJ} is invertible, and

$$\ell_1 \in [-0.746173536399, -0.746170651756], \qquad \ell_3 \in [0.984686309510, 0.984691237270],$$
$$\ell_4 \in [0.353067360670, 0.353070507243].$$

The omitted equation (row 2) also holds: permuting index 2 last, $0 = \det B = \det B_{JJ}\left(B_{22} - B_{2J}B_{JJ}^{-1}B_{J2}\right)$, and the second factor is exactly row 2 evaluated at ℓ. Hence ℓ is a left eigenvector for λ_2. By reversibility $V_2 = \operatorname{diag}(\pi(\beta_b))\ell / (\ell^{\mathsf{T}} \operatorname{diag}(\pi(\beta_b))\ell)$ is a right eigenvector with $\ell^{\mathsf{T}} V_2 = 1$, so $b(\beta) = \ell^{\mathsf{T}}\pi(\beta)$ is the amplitude of Section 1.

(iv) Amplitudes. Since $\pi(\beta_h)$ and $\pi(\beta_c)$ have rational entries, evaluating $\ell^{\mathsf{T}}\pi(\beta_h)$, $\ell^{\mathsf{T}}\pi(\beta_c)$ and $\ell^{\mathsf{T}}(\pi(\beta_c) - \pi(\beta_h))$ in interval arithmetic with the enclosures of (iii) gives the bounds of (iii) in Theorem 1. The comparison $|b(\beta_h)| < |b(\beta_c)|$ does not depend on the normalization of ℓ, since both amplitudes use the same eigenvector. □

Remark 2 (Sign of b). The enclosures give $\ell_1 < 0 < \ell_4 < \ell_3 < \ell_2 = 1$. Hence $N(t) = \ell_1 + t + \ell_3 t^2 + \ell_4 t^{64}$ is strictly increasing for $t > 0$; since $b(\beta_b) = 0$, i.e. $N(\frac{1}{2}) = 0$, $b(\beta) > 0$ for all $0 \le \beta < \beta_b$. As $b(\beta_h) < b(\beta_c)$ and $b(\beta_b) = 0$, $|b|$ has an interior maximum on (β_h, β_b), which is the criterion for the effect quoted in [1]. Since b has no zero on $[0, \beta_b)$, the effect is not strong in the sense of [4] (its direct Mpemba index is zero). Note also that ℓ is not monotone in the energy ($\ell_4 < \ell_3$).

4 How marginal the first example is

The example of Theorem 1 is a counterexample, not a typical case.

- *Extreme weights.* Level 4 sits at $64U$ with $\beta_b U = \ln 2$, so its bath weight is $\delta/(\frac{7}{4} + \delta) \approx 3 \times 10^{-20}$ and all rates into it are of order $\delta = 2^{-64}$. At the initial temperatures, by contrast, level 4 is well populated: $t_h^{64} \approx 0.78$.
- *Near-infinite initial temperatures.* $k_B T_h = U/\ln(256/255) \approx 255.5\,U$ and $k_B T_c \approx 127.5\,U$, compared with $k_B T_b \approx 1.44\,U$.
- *Small gap.* $b(\beta_c) - b(\beta_h) \approx 2.78 \times 10^{-4}$, about 0.07% of $b(\beta_h) \approx 0.3987$.
- *Nearly passing triplets.* Triplet 123 fails by a wide margin, but the residuals of 124, 134, 234 are $-(\delta + \varepsilon)/2$, $-\delta/2 - (\frac{1}{4} + \frac{\delta}{2})\varepsilon$ and $-\varepsilon/4$, i.e. of order $\varepsilon \le 10^{-6}$ in units of $1/\tau$. At $\varepsilon = 0$ the triplet 234 meets (2) with equality, which is still a failure of the strict test.

Since for $\varepsilon > 0$ every inequality in Theorem 1 is strict and every quantity is continuous in the rates, small perturbations of the rates (keeping detailed balance) and of the energies preserve the conclusions; the example is therefore not an isolated point. Section 5 gives an example with much larger margins.

5 A robust example

For a triplet that fails its test, define the *relative margin* as $-(\text{residual})/\max(a_{-0}, a_{-+}, a_{0+})$, with the residual of Section 3(i); it is invariant under rescaling all rates. Take $U = \tau = 1$ and

$$E = \left(0, \tfrac{1}{30}, \tfrac{217}{500}, 5\right), \qquad \beta_b = 3, \qquad \beta_h = \tfrac{3}{50}, \qquad \beta_c = \tfrac{1}{6},$$

$$(d_{12}, d_{13}, d_{14}, d_{23}, d_{24}, d_{34}) = (0.01646,\ 2.504,\ 2.648,\ 29.12,\ 2.928,\ 3.044),$$

and $a_{ij} = e^{-\beta_b E_i} d_{ij}$ for $i \ne j$, so detailed balance holds exactly. The bath weights relative to the ground level are 1, $e^{-0.1} \approx 0.905$, $e^{-1.302} \approx 0.272$ and $e^{-15} \approx 3.1 \times 10^{-7}$.

Theorem 3. *For this chain M:*

1. all four triplets fail the tests (1)–(2)*, with* κ*, branch and relative margin*

triplet	κ	*branch*	*relative margin*
123	$920.240\ldots$	(1)	≥ 1.0423
124	$168.955\ldots$	(1)	$\geq 1.1060 \times 10^{-3}$
134	$1.0913\ldots$	(1)	$\geq 1.0850 \times 10^{-3}$
234	$0.10147\ldots$	(2)	$\geq 1.1974 \times 10^{-3}$

2. the nonzero eigenvalues $\lambda_2 > \lambda_3 > \lambda_4$ *of* M *are simple, with*

$$\lambda_2 \in [-1.218899696, -1.218899693], \qquad \lambda_3 \in [-6.125294088, -6.125294085],$$
$$\lambda_4 \in [-36.266646875, -36.266646872];$$

3. with the left eigenvector normalized by $\ell_1 = 1$*,*

$$\ell_2 \in [-0.8801465839, -0.8801465701], \qquad \ell_3 \in [-0.7486027690, -0.7486027569],$$
$$\ell_4 \in [-0.0618822687, -0.0618822652],$$
$$b(\beta_h) \in [-0.1760225842, -0.1760225766], \qquad b(\beta_c) \in [-0.1781722318, -0.1781722239],$$
$$|b(\beta_c)| - |b(\beta_h)| \in [0.0021496470, 0.0021496478], \qquad \frac{|b(\beta_c)| - |b(\beta_h)|}{|b(\beta_h)|} \in [0.0122123, 0.0122124].$$

In particular $|b(\beta_h)| < |b(\beta_c)|$ *with* $\beta_h < \beta_c < \beta_b$*: a direct Mpemba effect with a relative amplitude gap of* 1.22%*, while every triplet fails its test by a relative margin of at least* 1.08×10^{-3}*.*

Proof. The argument is that of Section 3, with exact rationals replaced by rational intervals because the Boltzmann factors are irrational. Each e^{-y} with rational $y \geq 0$ is enclosed by writing $y = 2^k z$ with $0 \leq z \leq \frac{1}{8}$, bracketing e^{-z} between two consecutive partial sums of its alternating Taylor series (the terms decrease), and squaring k times; all endpoints are rounded outward to multiples of 2^{-320}. This gives interval enclosures of all rates, of the diagonal of M, of κ and of both residuals of every triplet, and (i) follows because the computed κ intervals exclude 1 and the relevant residual intervals are negative. Since the columns of M sum to zero, $\det(zI - M) = z\,f(z)$ with f a monic cubic; expanding the determinant over the 24 permutations in interval arithmetic encloses the coefficients of f, and evaluating f at the six rational bracket endpoints gives strict sign changes. The three brackets are disjoint, so they contain all roots of f, each simple, which is (ii). For (iii), solve $(M^{\mathsf{T}} - \mu I)\ell = 0$ with $\ell_1 = 1$ by Cramer's rule on the rows and columns $\{2, 3, 4\}$, with μ ranging over the bracket of λ_2; the denominator lies in $[113.0915273, 113.0915291]$, so it is nonzero, and the omitted row holds by the Schur determinant argument of Section 3(iii). The amplitudes are then evaluated with interval enclosures of $\pi(\beta_h)$ and $\pi(\beta_c)$; their signs agree, so $|b(\beta_c)| - |b(\beta_h)| = -\big(b(\beta_c) - b(\beta_h)\big)$, which is evaluated as $-\ell^{\mathsf{T}}(\pi(\beta_c) - \pi(\beta_h))$. □

What is and is not robust. Every residual in (1)–(2) is a combination of the three rates with coefficients of absolute value at most $\frac{3}{2}$, so multiplying each d_{ij} by a factor in $[1 - \eta, 1 + \eta]$ with $\eta \leq 2.5 \times 10^{-4}$ keeps all four failures (and all branches) of Theorem 3(i); the Mpemba inequality is an open condition, but we have not quantified its neighbourhood. The energies lie in $[0, 5]$ and the bath weight of the top level is e^{-15} instead of 2^{-64}. Three features remain special: the ground pair is close in energy ($\beta_b(E_2 - E_1) = 0.1$) and weakly coupled directly (d_{12} is the smallest conductance); the rates span about seven orders of magnitude because of the Boltzmann factor e^{-15}; and the initial temperatures, $k_B T_h = \frac{50}{3} \approx 16.7$ and $k_B T_c = 6$, are moderate compared with $E_4 = 5$ but large compared with $k_B T_b = \frac{1}{3}$. The numerical search behind this example is summarized in Appendix A; in it we found no example meeting the same margins with $\beta_h > 0.1\,\beta_b$.

An exactly rational version. The proof of Theorem 3 needs interval enclosures of exponentials only because its Boltzmann factors are irrational. As in Section 2, this can be avoided by taking integer energies and rational values of $e^{-\beta U}$.

Proposition 4. *Let $U > 0$ and $\tau = 1$, and define $\beta_b, \beta_h, \beta_c$ by $e^{-\beta_b U} = \frac{19}{21}$, $e^{-\beta_h U} = \frac{499}{500}$, $e^{-\beta_c U} = \frac{179}{180}$, so that $\beta_h < \beta_c < \beta_b$. Let $E = U(0, 1, 13, 150)$, let d be the conductances of Theorem 3, and $a_{ij} = (\frac{19}{21})^{n_i} d_{ij}$ for $i \neq j$, where $n = (0, 1, 13, 150)$. Then:*

1. *all four triplets fail the tests (1)–(2), on the same branches as in Theorem 3, with relative margins at least 1.0425 (123), 1.0231×10^{-3} (124), 1.1358×10^{-3} (134) and 1.1986×10^{-3} (234);*

2. *the nonzero eigenvalues of M are simple, with*

$$\lambda_2 \in [-1.2199282300, -1.2199282299], \qquad \lambda_3 \in [-6.1258309069, -6.1258309068],$$
$$\lambda_4 \in [-36.2712922746, -36.2712922745];$$

3. *with the left eigenvector normalized by $\ell_1 = 1$,*

$$b(\beta_h) \in [-0.1759821412, -0.1759821409], \qquad b(\beta_c) \in [-0.1781358067, -0.1781358064],$$
$$\frac{|b(\beta_c)| - |b(\beta_h)|}{|b(\beta_h)|} \in [0.0122379, 0.0122380].$$

In units of $k_B T_b$ the energies are $\beta_b E = \ln \frac{21}{19}\,(0, 1, 13, 150) \approx (0, 0.1001, 1.3011, 15.013)$, and $\beta_h/\beta_b \approx 0.0200$, $\beta_c/\beta_b \approx 0.0557$; all of these are within 0.2% of the corresponding values $(0, 0.1, 1.302, 15)$, 0.02, 0.0556 of Theorem 3.

Proof. All Boltzmann weights $(\frac{19}{21})^{n_i}$, $(\frac{499}{500})^{n_i}$, $(\frac{179}{180})^{n_i}$ are rational, hence so are all entries of M, of $\pi(\beta_h)$ and $\pi(\beta_c)$, every κ, every residual and every relative margin; (i) is an exact rational computation. As in Section 3(ii), $\det(zI - M) = z\,f(z)$ with f a cubic with rational coefficients and $f(0) \neq 0$; f has strict sign changes at the rational endpoints of the three disjoint brackets, which gives (ii). For (iii), solve $(M^{\mathsf{T}} - \mu I)\ell = 0$ with $\ell_1 = 1$ by Cramer's rule on the rows and columns $\{2, 3, 4\}$, with μ ranging over the bracket of λ_2, in rational interval arithmetic with exact endpoints; the denominator lies in $[113.1948667, 113.1948669]$, and the omitted row holds by the Schur determinant argument of Section 3(iii). The amplitudes are then evaluated in the same arithmetic; both are negative, and $|b(\beta_c)| - |b(\beta_h)| = -\ell^{\mathsf{T}}(\pi(\beta_c) - \pi(\beta_h)) \in [0.0021536654, 0.0021536656]$. No exponential is enclosed and no endpoint is rounded. □

6 Why the triplet tests do not see the effect

The following two facts are elementary and hold for any reversible N-level chain with λ_2 simple; we include their proofs.

Lemma 5. *If ℓ is monotone in the energy ($\ell_1 \leq \cdots \leq \ell_N$ or $\ell_1 \geq \cdots \geq \ell_N$), then $|b|$ is strictly decreasing on $[0, \beta_b]$; in particular there is no direct Mpemba effect.*

Proof. $\frac{d}{d\beta}\pi(\beta)_i = \pi(\beta)_i(\langle E\rangle_\beta - E_i)$, so $b'(\beta) = -\mathrm{Cov}_\beta(\ell, E) = -\frac{1}{2}\sum_{i,j} \pi(\beta)_i \pi(\beta)_j (\ell_i - \ell_j)(E_i - E_j)$. All terms have the same sign, and not all vanish because ℓ is not constant ($\ell^{\mathsf{T}}\pi(\beta_b) = 0$ and $\ell \neq 0$). So b is strictly monotone, and $b(\beta_b) = 0$ gives the claim. □

Lemma 5 is the discrete-state form of an argument already used for overdamped Langevin dynamics. There the derivative of the slow-mode overlap with respect to the initial temperature is an equilibrium covariance of the slow left eigenfunction with the potential [6, Eq. (7)], [7, Eq. (15)], and [7, Sec. III.D] applies the Fortuin–Kasteleyn–Ginibre inequality to a monotone slow eigenfunction and a monotone potential to exclude the effect in symmetric single wells. A decomposition of the effect into contributions of pairs of states, with factors given by differences of the second eigenfunction and of the energy, appears in the Supplemental Material of [8]. We did not find the statement of Lemma 5 for finite-state chains in these works.

Both examples have non-monotone ℓ: $\ell_1 < 0 < \ell_4 < \ell_3 < \ell_2$ in Theorem 1 and $\ell_2 < \ell_3 < \ell_4 < 0 < \ell_1$ in Theorem 3. The ordering of ℓ is a property of the slow eigenvector of the whole chain. The next identity shows how it depends on rates outside a given triplet. Write $\gamma_m = \sum_{j \neq m} a_{jm}$ for the escape rate of level m.

Lemma 6. *Let $M^{\mathsf{T}}\ell = \lambda\ell$ and let m be a level with $\gamma_m + \lambda \neq 0$. Then for every $i \neq m$,*

$$\sum_{j\neq i,m} \tilde{a}_{ji}(\ell_j - \ell_i) = \lambda\Big(1 + \frac{a_{mi}}{\gamma_m + \lambda}\Big)\ell_i, \qquad \tilde{a}_{ji} = a_{ji} + \frac{a_{jm}a_{mi}}{\gamma_m + \lambda}.$$

The $\tilde{a}$ satisfy detailed balance with respect to $\pi(\beta_b)$ restricted to the levels $\neq m$.

Proof. Row i of $M^{\mathsf{T}}\ell = \lambda\ell$ reads $\sum_{j\neq i} a_{ji}(\ell_j - \ell_i) = \lambda\ell_i$. Row m gives $(\gamma_m + \lambda)\ell_m = \sum_{j\neq m} a_{jm}\ell_j$, hence $\ell_m - \ell_i = \big(\sum_{j\neq m} a_{jm}(\ell_j - \ell_i) - \lambda\ell_i\big)/(\gamma_m + \lambda)$. Substituting this into row i gives the identity. Detailed balance follows from $a_{jm}a_{mi}\pi_i = a_{jm}a_{im}\pi_m = a_{mj}a_{im}\pi_j$. □

For a 4-level chain and m the level outside a triplet, Lemma 6 is a three-level eigen-equation for ℓ on the triplet, but with the couplings $\tilde{a}$ and a level-dependent weight on the right-hand side. The tests (1)–(2) are applied to the original rates a, i.e. they ignore the correction $a_{jm}a_{mi}/(\gamma_m + \lambda_2)$. This correction depends on the slowest eigenvalue λ_2 of the whole chain. It is large when γ_m is close to $|\lambda_2|$, and it is negative when $\gamma_m < |\lambda_2|$, in which case some $\tilde{a}$ can be negative and the effective three-level problem need not come from a Markov generator (in Theorem 3, with $m = 1$ and $\lambda = \lambda_2$, $\tilde{a}_{34} \approx -2.62$ and $\tilde{a}_{43} \approx -2.9 \times 10^{-6}$; in Theorem 1 all six $\tilde{a}$ remain positive, floating-point evaluation). At $\lambda = 0$ the $\tilde{a}$ are the rates of the chain observed only on the levels $\neq m$, which is again an ordinary reversible chain.

Observation (both examples). In both examples the ground level is a bottleneck: its escape rate is below the spectral gap. The test function $\mathbf{1}_{\{1\}}$ in the Rayleigh quotient of the reversible generator gives $|\lambda_2| \leq \gamma_1/(1 - \pi(\beta_b)_1)$, and

- in Theorem 1: $\gamma_1 = \frac{11}{12} + \frac{\varepsilon}{2} + 2\delta < 0.92 < 2.13 \leq |\lambda_2| \leq \gamma_1/(1 - \pi(\beta_b)_1) \approx 2.139$;
- in Theorem 3: $\gamma_1 \in [0.6959505683, 0.6959505684]$, $\gamma_1 + \lambda_2 \in [-0.5229491277, -0.5229491246]$ (certified), and $\gamma_1/(1 - \pi(\beta_b)_1) \approx 1.287$.

So λ_2 nearly saturates the bound, and the slow mode is close to the mode that changes only the ground-state population: ℓ is nearly constant on the excited levels. Whether $|b|$ rises at high temperature is then decided by the small variation of ℓ over $\{2, 3, 4\}$, which by Lemma 6 with $m = 1$ is governed by the couplings $\tilde{a}$ with $\gamma_1 + \lambda_2 < 0$. Consistently, the triplet $\{2, 3, 4\}$ fails its test (2) with the original rates and also with the $\lambda = 0$ rates $\tilde{a}$ (floating-point evaluation), but satisfies (2) when the rates $\tilde{a}$ at $\lambda = \lambda_2$ are inserted: for Theorem 3 the formal κ is $-0.00137\ldots < 1$ and the residual of (2) lies in $[3.39436930, 3.39436933] > 0$ (certified); for Theorem 1 the residual is about $+5.4 \times 10^{-3}$ relative to the largest rate (floating-point only).

This is a heuristic explanation, not a theorem: the tests of [1] are derived for genuine three-level generators, and we do not claim that the tests applied to $\tilde{a}$ are necessary or sufficient for anything. What the identity does show is the quantity the triplet tests miss: the slowest eigenvalue λ_2 of the full chain, through the factor $1/(\gamma_m + \lambda_2)$, which compares it with the escape rate of the level outside the triplet.

7 Verification procedure

For Theorem 1, every step above is a finite exact computation over $\mathbb{Q}$; no floating-point value is used in any decision.

1. Build τM_ε with $\delta = 2^{-64}$ as an exact rational matrix at $\varepsilon = 0$ and $\varepsilon = 10^{-6}$. Check column sums zero, $M\,q = 0$, detailed balance $M_{ij}q_j = M_{ji}q_i$ and positivity of off-diagonal entries.
2. For each triplet compute κ and both residuals exactly at the two endpoints; they are affine in ε, so endpoint signs cover $[0, 10^{-6}]$. Require that no branch passes, with strict failure at $\varepsilon = 10^{-6}$.
3. Expand $\det(zI - \tau M_0)$ over the 24 permutations and compare with $zf(z)$ at the actual δ; also compare at $\delta = 0, 1, 2, 3, 4$, which proves the identity as polynomials in δ (each coefficient has degree at most 4 in δ).

4. Evaluate f at the six rational interval endpoints and require sign changes; shift the intervals by $-\frac{3}{2}\cdot 10^{-6}$ and require disjointness.

5. With μ_2 and ε as rational intervals, compute $\det B_{JJ}$ and the Cramer quotients by outward interval arithmetic; require $0 \notin \det B_{JJ}$ and the sign pattern of ℓ.

6. Form π at $t = \frac{255}{256}$ and $t = \frac{127}{128}$ exactly; require $b(\beta_h) > 0$, $b(\beta_c) > 0$ and $b(\beta_c) - b(\beta_h) > 0$ for the interval lower bounds.

The ancillary file `check_four_state.py` (Python standard library only, `fractions.Fraction`) performs steps 1–6 and writes all rational endpoints to a JSON file; its checks raise exceptions and remain active under `python -O`. A run with Python 3.14 returned `PASS` in under 0.01 s of arithmetic time and reproduced every interval stated above. The script certifies the finite arithmetic; the use of Weyl's inequality, Cramer's rule, the Schur determinant identity and the spectral expansion is the mathematical argument given in Section 3.

For Theorem 3, the ancillary file `check_robust_four_state.py` (Python standard library only) reads the data from `robust_witness.json` and performs the interval computation described in the proof: the exponential enclosures, the triplet tests with certified relative margins, the interval characteristic polynomial and the sign changes at the given brackets, the interval Cramer solve, and the amplitudes. It also certifies the two diagnostics of Section 6 ($\gamma_1 + \lambda_2 < 0$ and the sign of the residual of (2) for the triplet $\{2, 3, 4\}$ with the rates $\tilde{a}$ at $\lambda = \lambda_2$). All decisions raise exceptions and remain active under `python -O`. A run with Python 3.14 returned `PASS` in under 0.1 s and reproduced every interval stated in Theorem 3. As an independent check, a 50-digit floating-point computation with `mpmath` gave values inside all these intervals; it is not part of the proof.

For Proposition 4, the ancillary file `check_rational_four_state.py` (Python standard library only, `fractions.Fraction`, no rounding) reads the integers n_i, the three rational Boltzmann factors, the conductances and the eigenvalue brackets from `rational_witness.json`. It checks the generator (column sums, stationarity of $\pi(\beta_b)$, detailed balance, positivity), computes every κ, residual and relative margin exactly, expands $\det(zI - M)$ over the 24 permutations and checks the sign changes of f, and performs the interval Cramer solve and the amplitude evaluation of the proof. All decisions raise exceptions and remain active under `python -O`. A run with Python 3.14 returned `PASS` in under 0.1 s and reproduced every number stated in Proposition 4; a 60-digit `mpmath` computation gave values inside these intervals (not part of the proof). The same script, given the data of Theorem 1 at $\varepsilon = 10^{-6}$ with the brackets of Section 3(ii), also returns `PASS`; this checks a single value of ε only.

AI assistance disclosure

OpenAI GPT-5.6 Sol, accessed through ChatGPT and Codex, was used to find and audit the first counterexample and its exact verification, and for drafting. Anthropic Claude Opus 5.5, used through Claude Code, was used to write the note, find and certify the robust witness of Theorem 3, and for the mechanism section. Anthropic Claude Opus 5.5 (Claude Code) produced the exact rational variant of Proposition 4 and its checker `check_rational_four_state.py`. The author reviewed and takes responsibility for every statement and proof. AI systems are not authors of this work, and the work has not been peer reviewed.

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A The numerical search (numerical evidence only)

Nothing in this appendix is proved; it records how the example of Theorem 3 was found and what the search did not find. Units are $\beta_b = 1$, so energies are measured in units of $k_B T_b$; write $\varrho = \beta_h/\beta_b$ and $s = \beta_b(E_2 - E_1)$. The score was the minimum of (relative margin of the worst triplet)$/10^{-3}$ and (relative amplitude gap)$/10^{-2}$, where the gap is $\max_{\varrho\beta_b \le \beta_h < \beta_c \le \beta_b} (|b(\beta_c)| - |b(\beta_h)|)/|b(\beta_c)|$ on a grid; a branch with κ within the margin of 1 was required to fail in both lines. Eigenvectors were computed in double precision from the symmetrized generator.

- *Global search.* Differential evolution over $E \in [0,5]^4$ with spacings ≥ 0.05, $\beta_b \in (0.1, 6]$, $\beta_h \ge 0.1$, $|\ln d_{ij}| \le 8$ and smallest bath weight $\ge 10^{-6}$, several seeds: no point was found with all four triplets failing and any Mpemba gap. Without the triplet constraints, gaps of 100% (a sign change of b) were found at once.

- *Continuation* from the example of Theorem 1 (Nelder–Mead, step-wise tightening of $\beta_b E_4$, ϱ and s). Best scores found, as (worst relative triplet margin, relative gap):

$\beta_b E_4 \le$	ϱ	s	margin	gap
6	0	3×10^{-4}	9.3×10^{-4}	0.93%
6	0	0.03	3.8×10^{-5}	0.04%
10	0	0.07	1.1×10^{-3}	1.1%
10	0.02	0.02	1.4×10^{-3}	1.4%
15	0.02	0.1	1.2×10^{-3}	1.2%
20	0.02	0.2	8.7×10^{-4}	0.87%
20	0.05	0.003	1.3×10^{-3}	1.3%
20	0.05	0.1	1.3×10^{-4}	0.13%
30	0.07	0.001	3.7×10^{-4}	0.37%
30	0.1	0.001	none found	

  All 62 optimized continuation points with worst relative margin $\ge 10^{-4}$ have a ground pair that is close in energy and weakly coupled directly (d_{12} at most 0.05 times every other conductance), triplets 124, 134, 234 failing by margins within a factor 2 of each other, and $\gamma_1 < |\lambda_2|$, the structure discussed in Section 6. Theorem 3 is the $\beta_b E_4 \le 15$, $\varrho = 0.02$, $s = 0.1$ point with rounded data, rescaled to $E_4 = 5$.

The search is local and not exhaustive. It suggests a trade-off between the margins, the size of $\beta_b E_4$, the closeness of the ground pair and the hot temperature, and in particular that examples with $\beta_b E_{\max} \lesssim 6$ or $\beta_h \gtrsim 0.1\,\beta_b$ that meet the margins of Theorem 3 are rare or absent; we have not proved either statement.