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Block-Isospectral Invariance Obstructions, Multi-Subspace Dissipation, Product-Formula Stability Bifurcations, and Subset-Optimal Weight Duality for Excited-State Double-Bracket Flows

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Abstract

Aghaei Saem, Sahebi, Holmes, and Suzuki (`arXiv:2611.34871v1`) introduced a unified framework for simultaneously preparing the r lowest eigenstates of a d-dimensional Hamiltonian H via continuous-time, discretized, and product-formula double-bracket flows (DBFs) on rank-r density matrices $\rho_{\mathrm{ref}} = \sum_{i=1}^{r} p_i |\phi_i\rangle\langle\phi_i|$, establishing an overlap necessary condition $A_i = \langle\lambda_i|P_r|\lambda_i\rangle > 0$, a quadratic dissipation bound $\|[\rho, H]\|_{\mathrm{HS}}^2 \geq 2\Delta E(\gamma_{\min} - \Delta E)$, step-size guarantees $\bar{s} = 2/\gamma_{\max}$ and $\bar{s} = 12/(7\gamma_{\max})$, Chebyshev scheduling, and degenerate-weight single-excited-state preparation. Here we resolve four foundational structural, dynamical, stability, and optimization questions left open by their theory, with the underlying finite algebraic identities, rational witnesses, and Taylor brackets backed by 20 constructive Lean 4.36.0 theorems (zero external imports, zero `sorry`, zero `Classical.choice`, zero warnings), 16 AST-audited zero-float exact-rational SHA-256 certificates, and 60 adversarial tests:

1. **Exact Block-Isospectral Invariance, Strict Separation from Eq. (6), and Hyperbolic Morse-Index Classification (Theorem 1):** Any spectral projector Π_S commuting with ρ_{ref} commutes identically with ρ under all three DBFs and all step sizes $s_k > 0$, conserving all power traces $\mathrm{Tr}((\Pi_S \rho \Pi_S)^m)$. Convergence to ρ^* therefore requires multiset spectral compatibility $\mathrm{spec}(\Pi_{S_m} \rho_{\mathrm{ref}} \Pi_{S_m}) = \{p_a : a \in S_m\}$ on every connected component S_m of the eigenbasis support graph $G(\rho_{\mathrm{ref}})$. An explicit rational witness at $d = 3, r = 2$ satisfies $A_1 = 1/2 > 0$, $A_2 = 1 > 0$, and even $\mathrm{rank}(\Pi_2 P_2 \Pi_2) = 2$, yet remains permanently trapped at $\Delta E(\rho(t)) \geq \gamma_{1,2} = 1/3 > 0$. We further classify all $d!/(d-r)!$ fixed points ρ_σ as hyperbolic critical points with exact Jacobian eigenvalues $\mu_{ab}(\sigma) = -(q_a - q_b)(\lambda_b - \lambda_a)$, exact unstable real dimension $2\,\mathrm{inv}(q) \in [0, r(2d-r-1)]$, unique sink, exact r index-1 saddles, unique source, and multi-level excess bound $\Delta E(\rho_\sigma) \geq \sum_{j=1}^{r} \gamma_{j,j+1} k_j(\sigma)$.
2. **Exact Cross-Subspace Dissipation, Concentration-Ratio Sharpening Above $\gamma_{\min}$, Global Tightness, and Tighter Discrete Contraction (Theorem 2):** We prove the exact identity $\|[\rho, H]\|_{\mathrm{HS}}^2 = 2\sum_{j=1}^{r} (\delta p_j)^2 l_j + 4\sum_{1 \leq j < m \leq r} \delta p_j \delta p_m l_{j,m}$ and sharpen Lemma 1 via the subspace concentration ratio $\mathcal{C}(\rho) = \sum_j x_j^2/(\Delta E)^2 \in [1/r, 1]$ to $\|[\rho, H]\|_{\mathrm{HS}}^2 \geq 2\Delta E(\bar{\gamma}(\rho) - \mathcal{C}(\rho)\Delta E)$ with exact nonnegative surplus $2\sum_j (\gamma_{j,j+1} - \gamma_{\min}) x_j + 4\sum_{j<m} x_j x_m$, certifying strictly positive dissipation up to $r\gamma_{\min}$. Along the 2-level geodesic $|\lambda_{j^*}\rangle \leftrightarrow |\lambda_{j^*+1}\rangle$, Lemma 1, Lemma G.2, and Theorem G.1(1) are globally tight. In discrete time, we tighten Eq. (G5) to $y_{k+1} \leq y_k(1 - 2b_k\gamma_{\min}/(1 + 2b_k x_0)) < y_k/(1 + 2b_k\gamma_{\min})$ with exact gap $4b_k^2\gamma_{\min}(\gamma_{\min} - x_0)/((1 + 2b_k\gamma_{\min})(1 + 2b_k x_0)) > 0$, cutting step counts from $(1+\kappa)\ln(c_0/\varepsilon)$ and $(1+7\kappa/6)\ln(c_0/\varepsilon)$ to $(\kappa + x_0/\gamma_{\min})\ln(c_0/\varepsilon)$ and $(7\kappa/6 + x_0/\gamma_{\min})\ln(c_0/\varepsilon)$.

*Independent Researcher. ORCID: 0009-0006-7494-9040. Code and Lean 4 formalization: MIT License; manuscript: CC-BY-4.0. Repository: `https://github.com/lluiseriksson/paper145-double-bracket-flows` (`v1.0.3`).

3. **Discretized Period-Doubling Stall Bifurcation, Exact Product-Formula Complex Spectrum, and Unbalanced-Mode Chebyshev Instability (Theorem 3):** An exact 2-level reduction $\vartheta_{k+1} = \vartheta_k - s_k\gamma \sin\vartheta_k$ proves algebraic breakdown $\Delta E(\rho_k) \sim 3\gamma/(8k)$ at $u = 2$ (unimprovability of $\bar{s} = 2/\gamma_{\max}$) and a unique locally asymptotically stable symmetric period-2 stall orbit $\sin\vartheta^*/\vartheta^* = 2/u$ for all $u \in (2, \pi)$, explaining the stalled runs in Fig. 6(a) of `2611.34871v1`. For arbitrary (d, r), we derive the exact product-formula linearized complex multiplier $\mu_{ab}^{\mathrm{PF}} = 1 - 4e^{i(u_\rho - u_H)/2}\sin(u_H/2)\sin(u_\rho/2)$ and squared modulus $|\mu_{ab}^{\mathrm{PF}}|^2 = 1 - 8\sin(u_H/2)\sin(u_\rho/2)\cos((u_H + u_\rho)/2)$, show that the exact 2-level nonlinear step reproduces all three fourth-order constants $(1/6, 1/6, 1/4)$ of Theorem C.3, and prove AM–GM optimality of $\theta/\tau = \Omega/p_1$ yielding the sharp threshold $s_{\mathrm{crit}}^{\mathrm{PF}} = \pi^2/(4\gamma_{\max}) > 2/\gamma_{\max} > 12/(7\gamma_{\max})$. Finally, the exact unbalanced-mode Chebyshev expansion proves $m = 2$ is stable for all $\kappa \geq 1$ while $m = 4$ destabilizes at large κ ($\sum_{k=1}^{4} u_k \sin u_k < -1/2$ certified at $\kappa = 100$), explaining Fig. 15(b).
4. **Subset-Optimal Degenerate Weight Duality and Adaptive Untracked-Gap Asymmetry (Theorem 4):** For any target subset $T \subseteq \{1, \ldots, r\}$ with minimal boundary set $J(T)$—permitting exact Hamiltonian degeneracies $\delta\lambda_{j+1} = 0$ for $j \notin J(T)$—we establish the sharp dual bounds $\gamma_{\min}(p) \leq \gamma_{\min}^\star(T) = (\sum_{j\in J(T)} j/\delta\lambda_{j+1})^{-1}$ and $\kappa(p) \geq \kappa^\star(T) = \Omega\sum_{j\in J(T)} \delta\lambda_{j+1}^{-1}$. For single excited state $T = \{r\}$, this strictly outperforms Theorem EM1/Corollary H.2 whenever $\delta\lambda_r \neq \delta\lambda_{r+1}$, cutting κ by up to $2\times$ and expanding $\gamma_{\min}$ by up to $(2r-1)/(r-1) \in (2, 3]\times$. For estimated gaps $\hat{g}_j$, we prove $\kappa(\hat{p}) = \Omega(\sum_{j\in J}\hat{g}_j^{-1})(\max_{j\in J}\hat{g}_j/\delta\lambda_{j+1}) \leq (c_+/c_-)\kappa^\star(T)$ and uncover an exact $(r-1)$-to-1 untracked-gap asymmetry: overestimating $\hat{g}_r$ by $\alpha > 1$ incurs $(\alpha-1)\Omega\sum_{j=1}^{r-1}\delta\lambda_{j+1}^{-1}$ versus $(\alpha-1)\Omega/\delta\lambda_{r+1}$ for underestimation, explaining the empirical dominance of the min rule in Fig. 13.

1 Introduction and Setting

Computing multiple low-lying eigenstates of a Hermitian Hamiltonian H is a central bottleneck across quantum many-body physics, quantum chemistry, and fault-tolerant quantum algorithms [1, 2, 3]. Double-bracket flows (DBFs)—originally introduced in classical matrix analysis and continuous-time optimization by Brockett [4] and Helmke and Moore [5, 6], and independently in renormalization-group physics by Wegner [7] and Głazek and Wilson [8]—have recently emerged as a powerful quantum-compatible paradigm for both ground-state preparation ($r = 1$) [9, 10] and full diagonalization ($r = d$) [11, 12].

In a landmark recent contribution, Aghaei Saem, Sahebi, Holmes, and Suzuki [13] (see also the concurrent study [14]) systematically developed the intermediate-rank regime $1 < r < d$, evolving a rank-r reference mixture

$$\rho_{\mathrm{ref}} = \sum_{i=1}^{r} p_i|\phi_i\rangle\langle\phi_i|, \qquad p_1 \geq p_2 \geq \cdots \geq p_r > 0 = p_{r+1} = \cdots = p_d, \qquad \sum_{i=1}^{r} p_i = 1, \tag{1}$$

under three unitary-orbit flows minimizing the ensemble energy $E(\rho) = \mathrm{Tr}(\rho H)$ [15]:

$$\text{Continuous-time DBF:} \quad \partial_t\rho(t) = [W(t), \rho(t)], \qquad W(t) := [\rho(t), H], \tag{2}$$

$$\text{Discretized DBF:} \quad \rho_{k+1} = V_k\rho_k V_k^\dagger, \qquad V_k = e^{s_k W_k}, \quad W_k := [\rho_k, H], \tag{3}$$

$$\text{Product-formula DBF:} \quad \rho_{k+1} = V_k\rho_k V_k^\dagger, \qquad V_k = e^{i\tau_k H}e^{i\theta_k\rho_k}e^{-i\tau_k H}e^{-i\theta_k\rho_k}, \quad \tau_k\theta_k = s_k, \tag{4}$$

where $H = \sum_{a=1}^{d}\lambda_a|\lambda_a\rangle\langle\lambda_a|$ with ordered spectrum $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_d$ (strictly ordered $\lambda_1 < \cdots < \lambda_d$ in Theorems 1–3, and permitting exact degeneracies in Theorem 4), spectral width $\Omega := \lambda_d - \lambda_1$, and target global minimum $\rho^* := \sum_{i=1}^{r} p_i|\lambda_i\rangle\langle\lambda_i|$ with energy $E^* := \mathrm{Tr}(\rho^* H)$ and excess energy $\Delta E(\rho) := E(\rho) - E^*$.

Throughout this paper we use a single, consistent indexing convention:

$$\delta p_j := p_j - p_{j+1} \geq 0, \qquad \delta\lambda_{j+1} := \lambda_{j+1} - \lambda_j \geq 0, \qquad \gamma_{j,j+1} := \delta p_j\,\delta\lambda_{j+1}, \qquad j \in \{1, \ldots, r\}, \tag{5}$$

with $\gamma_{ab} := (p_a - p_b)(\lambda_b - \lambda_a)$ for $1 \le a < b \le d$, $\gamma_{\max} := \gamma_{1,d} = p_1\Omega$, $\gamma_{\min} := \min\{\gamma_{j,j+1} : 1 \le j \le r,\ \delta p_j > 0\}$, and condition number $\kappa := \gamma_{\max}/\gamma_{\min}$. (Note that Proposition I.3 of [13] temporarily wrote $\delta\lambda_j$ for $\lambda_{j+1} - \lambda_j$; keeping $\delta\lambda_{j+1} = \lambda_{j+1} - \lambda_j$ everywhere aligns Appendices D–I uniformly.)

Four open structural gaps in [13]. Although [13] established the core convergence guarantees and rich numerical diagnostics (including transverse-field Ising model [16] simulations in Figs. 5–16), four deep analytical gaps remained open:

1. *Invariance obstructions beyond Eq. (6):* Theorem E.1 of [13] proves that $A_i := \langle\lambda_i|P_r|\lambda_i\rangle > 0$ ($\forall i \le r$, where $P_r = \sum_{j=1}^{r} |\phi_j\rangle\langle\phi_j|$) is necessary for $\rho \to \rho^*$, leaving open whether $A_i > 0$ (or full target-subspace rank $\mathrm{rank}(\Pi_r P_r \Pi_r) = r$) captures all invariant-submanifold obstructions, and leaving the full Morse-index classification of the $d!/(d-r)!$ fixed points unproved.
2. *Dissipation above $\gamma_{\min}$ and discrete contraction slack:* Lemma 1 of [13] certifies positive dissipation only for $\Delta E(\rho) < \gamma_{\min}$ and drops all cross-subspace couplings in Eq. (F12), whereas Figs. 5(b) and 12 show rapid decay from cold starts far above $\gamma_{\min}$; furthermore, Eq. (G34) discards a strictly positive $O(b_k^2)$ term in discrete logistic contraction, inflating step-count guarantees.
3. *Exact nonlinear bifurcation, product-formula linear spectrum, and Chebyshev instability:* Fig. 6(a) of [13] exhibits stalled runs just above $\bar{s} = 2/\gamma_{\max}$; Theorem C.3 guarantees energy descent for the group-commutator product formula [17] only up to $\bar{s} = 12/(7\gamma_{\max})$, leaving its true linear stability threshold unknown; and Fig. 15(b) shows that a period-4 Chebyshev schedule [18, 19, 20] can destabilize under product-formula implementation even in the linear regime.
4. *General target subsets, degenerate spectra, and adaptive gap-estimation asymmetry:* Corollary H.2 (Theorem EM1) of [13] fixes equal weight gaps $\delta p_{r-1} = \delta p_r = 1/(2r-1)$ for preparing a single excited state $|\lambda_r\rangle$, which is suboptimal whenever $\delta\lambda_r \ne \delta\lambda_{r+1}$, and Fig. 13 empirically finds that estimating the untracked gap $\delta\lambda_{r+1}$ by the *min* rule strongly outperforms the *mean* rule without an analytical explanation.

The next four sections resolve all four problems via exact, self-contained theorems (Theorems 1–4), followed in Section 6 by a complete audit of our Lean 4 formalization and zero-float cryptographic verification pipeline.

2 Theorem 1: Block-Isospectral Invariance, Separation, and Morse-Index Classification

For any density matrix ρ expressed in the eigenbasis $\{|\lambda_a\rangle\}_{a=1}^{d}$ of H, define its *eigenbasis support graph* $G(\rho) = (V, E)$ with vertex set $V = \{1, \ldots, d\}$ and undirected edge $\{a, b\} \in E$ ($a \ne b$) if and only if $\langle\lambda_a|\rho|\lambda_b\rangle \ne 0$. For any $S \subseteq V$, let $\Pi_S := \sum_{a\in S} |\lambda_a\rangle\langle\lambda_a|$ denote the spectral projector onto $\mathrm{span}\{|\lambda_a\rangle : a \in S\}$, and let $\mathrm{spec}(\Pi_S\rho\Pi_S)$ denote the multiset of $|S|$ eigenvalues of the restriction of $\Pi_S\rho\Pi_S$ to $\mathrm{Ran}(\Pi_S)$.

Theorem 1 (Block-Isospectral Invariance, Strict Separation from Eq. (6), and Hyperbolic Morse Classification)**.** *Let $1 \le r < d$, let $H = \sum_{a=1}^{d} \lambda_a|\lambda_a\rangle\langle\lambda_a|$ have strictly ordered eigenvalues $\lambda_1 < \cdots < \lambda_d$, and let $\rho_{\mathrm{ref}} = \sum_{i=1}^{r} p_i|\phi_i\rangle\langle\phi_i|$ have distinct positive weights $p_1 > \cdots > p_r > 0$ (with $p_a := 0$ for $a > r$).*

(i) ***Exact block-isospectral conservation.*** *If $S \subseteq \{1, \ldots, d\}$ satisfies $[\rho_{\mathrm{ref}}, \Pi_S] = 0$, then under* all three *flows* (2)–(4) *(and any higher-order product formula generated by $e^{\pm i\tau H}$ and $e^{\pm i\theta\rho_k}$) and for* every *step-size sequence $s_k > 0$, one has $[\rho, \Pi_S] = 0$ at all times/iterations,*

the block restriction $\Pi_S\rho\Pi_S$ *evolves by unitary conjugation within* $\mathrm{Ran}(\Pi_S)$*, and all block Casimir invariants* $\mathrm{Tr}((\Pi_S\rho\Pi_S)^m)$ *(*$m \geq 1$*) and the multiset spectrum* $\mathrm{spec}(\Pi_S\rho\Pi_S)$ *are exactly conserved.*

(ii) ***Sharp block-compatibility obstruction and strict separation from Eq. (6).*** *Let* $S_1, \ldots, S_M$ *be the connected components of* $G(\rho_{\mathrm{ref}})$*. Convergence* $\rho \to \rho^*$ *under any of* (2)–(4) *and any* $s_k > 0$ *requires*

$$\mathrm{spec}(\Pi_{S_m}\rho_{\mathrm{ref}}\Pi_{S_m}) = \{p_a : a \in S_m\} \qquad \text{as multisets, for all } m \in \{1, \ldots, M\}. \tag{6}$$

Condition (6) *strictly generalizes Eq. (6) of [13] (*$A_i = \langle\lambda_i|P_r|\lambda_i\rangle > 0$ *for* $i \leq r$*). Specifically, for* $d = 3$*,* $r = 2$*,* $H = \mathrm{diag}(0, 1, 3)$*,* $p = (2/3, 1/3, 0)$*, and*

$$|\phi_1\rangle = |\lambda_2\rangle, \qquad |\phi_2\rangle = \frac{1}{\sqrt{2}}\big(|\lambda_1\rangle + |\lambda_3\rangle\big), \tag{7}$$

the reference state satisfies $A_1 = 1/2 > 0$*,* $A_2 = 1 > 0$*, and full target-subspace rank* $\mathrm{rank}(\Pi_2 P_2 \Pi_2) = 2$*, yet* $G(\rho_{\mathrm{ref}})$ *splits into* $S_1 = \{2\}$ *and* $S_2 = \{1, 3\}$ *with* $\mathrm{spec}(\Pi_{S_1}\rho_{\mathrm{ref}}\Pi_{S_1}) = \{2/3\} \neq \{1/3\}$*, trapping every trajectory of all three DBFs at*

$$\Delta E(\rho) \geq \gamma_{1,2} = \gamma_{\min} = \frac{1}{3} > 0 \qquad \text{for all } t \geq 0 \text{ (or } k \geq 0\text{).} \tag{8}$$

(iii) ***Complete hyperbolic Morse-index classification and multi-level excess bound.*** *Adapting the classical Hermitian isospectral Morse theory of Brockett [4] and Helmke–Moore [5] to the rank-r excited-state flag manifold* $\mathcal{O}_p = \{U\rho_{\mathrm{ref}}U^\dagger : U \in U(d)\}$ *of real dimension* $r(2d - r - 1)$*, every fixed point* $\rho_\sigma = \sum_{a=1}^d q_a|\lambda_a\rangle\langle\lambda_a|$ *(*$q_a := p_{\sigma(a)}$*) is* hyperbolic *under* (2)*: its Jacobian on* $T_{\rho_\sigma}\mathcal{O}_p$ *diagonalizes in the off-diagonal coordinates* $\{\delta\rho_{ab} : 1 \leq a < b \leq d,\ q_a \neq q_b\}$ *with exact real eigenvalues (each of real multiplicity* 2*)*

$$\mu_{ab}(\sigma) = -(q_a - q_b)(\lambda_b - \lambda_a) \neq 0. \tag{9}$$

Hence the unstable manifold of ρ_σ *has exact real dimension (real Morse index)* $2\,\mathrm{inv}(q)$*, where* $\mathrm{inv}(q) := |\{(a, b) : 1 \leq a < b \leq d,\ q_a < q_b\}| \in \big[0,\ r(2d-r-1)/2\big]$*. Among all* $d!/(d-r)!$ *fixed points, there is a* unique sink *(*$\mathrm{inv}(q) = 0$*, namely* ρ^**),* exact r minimal non-trivial saddles *(*$\mathrm{inv}(q) = 1$*, real Morse index* 2*, namely the adjacent swaps* $\rho_{\sigma_{j,j+1}}$ *for* $j = 1, \ldots, r$*), and a* unique source *(*$\mathrm{inv}(q) = r(2d - r - 1)/2$*, with* $q = (0, \ldots, 0, p_r, \ldots, p_1)$*). Moreover, letting* $k_j(\sigma) := j - \mathrm{Tr}(P_j(\rho_\sigma)\Pi_j) \in \{0, \ldots, \min(j, d-j)\}$ *be the subspace displacement count, every fixed point obeys*

$$\Delta E(\rho_\sigma) \geq \sum_{j=1}^{r} \gamma_{j,j+1}\, k_j(\sigma). \tag{10}$$

Proof. **(i)** Since Π_S is a spectral projector of H, $[H, \Pi_S] = 0$. Whenever $[\rho, \Pi_S] = 0$, the Jacobi identity gives

$$[W, \Pi_S] = [[\rho, H], \Pi_S] = -[[H, \Pi_S], \rho] - [[\Pi_S, \rho], H] = 0,$$

and repeating once more yields $[[W, \rho], \Pi_S] = 0$ (formalized universally for all dimensions n in Lean `thm01`). Thus the submanifold $\mathcal{M}_S = \{\rho : [\rho, \Pi_S] = 0\}$ is invariant under the smooth vector field $[[\rho, H], \rho]$ of (2); by Picard–Lindelöf uniqueness, $[\rho(t), \Pi_S] = 0$ for all $t \geq 0$, and the unitary propagator $U(t)$ solving $\partial_t U = W(t)U$ satisfies $[U(t), \Pi_S] = 0$. For (3), $[W_k, \Pi_S] = 0$ implies $[e^{s_k W_k}, \Pi_S] = 0$ by power-series convergence for *every* $s_k > 0$. For (4) (and any product of factors $e^{\pm i\tau H}, e^{\pm i\theta\rho_k}$), $[H, \Pi_S] = [\rho_k, \Pi_S] = 0$ implies every exponential factor commutes with Π_S, hence $[V_k, \Pi_S] = 0$ for all $\tau_k, \theta_k \in \mathbb{R}$. By induction, $[\rho_k, \Pi_S] = 0$ and $\Pi_S\rho_{k+1}\Pi_S = (\Pi_S V_k \Pi_S)(\Pi_S\rho_k\Pi_S)(\Pi_S V_k \Pi_S)^\dagger$, where $\Pi_S V_k \Pi_S$ is unitary on $\mathrm{Ran}(\Pi_S)$. Unitary similarity conserves $\mathrm{spec}(\Pi_S\rho\Pi_S)$ and $\mathrm{Tr}((\Pi_S\rho\Pi_S)^m)$ for all $m \geq 1$.

(ii) By definition of the connected components $S_1, \dots, S_M$ of $G(\rho_{\text{ref}})$, $\langle\lambda_a|\rho_{\text{ref}}|\lambda_b\rangle = 0$ whenever $a \in S_m$ and $b \notin S_m$, so $[\rho_{\text{ref}}, \Pi_{S_m}] = 0$ for each m. By part (i), $\text{spec}(\Pi_{S_m}\rho\Pi_{S_m})$ is constant along the flow; by continuity of eigenvalues, any limit point ρ^* must satisfy $\text{spec}(\Pi_{S_m}\rho^*\Pi_{S_m}) = \text{spec}(\Pi_{S_m}\rho_{\text{ref}}\Pi_{S_m})$, yielding (6). If $A_i = 0$ for some $i \le r$, then $\rho_{\text{ref}}|\lambda_i\rangle = 0$, so $\{i\}$ is an isolated component with $\text{spec}(\Pi_{\{i\}}\rho_{\text{ref}}\Pi_{\{i\}}) = \{0\} \neq \{p_i\}$ since $p_i > 0$; hence (6) strictly implies Eq. (6).

For the explicit witness (7), $\langle\phi_1|\phi_2\rangle = 0$, $\langle\phi_1|\phi_1\rangle = \langle\phi_2|\phi_2\rangle = 1$, and in the eigenbasis $\{|\lambda_1\rangle, |\lambda_2\rangle, |\lambda_3\rangle\}$:

$$P_2 = \begin{pmatrix} 1/2 & 0 & 1/2 \\ 0 & 1 & 0 \\ 1/2 & 0 & 1/2 \end{pmatrix}, \qquad \rho_{\text{ref}} = \begin{pmatrix} 1/6 & 0 & 1/6 \\ 0 & 2/3 & 0 \\ 1/6 & 0 & 1/6 \end{pmatrix}.$$

Thus $A_1 = 1/2 > 0$, $A_2 = 1 > 0$, and $\Pi_2 P_2 \Pi_2 = \text{diag}(1/2, 1, 0)$ has $\text{rank}(\Pi_2 P_2 \Pi_2) = 2$. Yet $G(\rho_{\text{ref}})$ has components $S_1 = \{2\}$ and $S_2 = \{1, 3\}$, with $\Pi_{S_1}\rho_{\text{ref}}\Pi_{S_1} = \frac{2}{3}|\lambda_2\rangle\langle\lambda_2|$ and $\text{spec}(\Pi_{S_2}\rho_{\text{ref}}\Pi_{S_2}) = \{1/3, 0\}$. By part (i), along any trajectory of (2)–(4), the S_1-block stays frozen with energy $\frac{2}{3}\lambda_2 = \frac{2}{3}$, while the S_2-block has diagonal entries $d_1, d_3 \ge 0$ summing to $1/3$, so $d_1\lambda_1 + d_3\lambda_3 = 3d_3 \ge 0$ (Lean `thm02`, `thm05`; Cert. `C02`). Since $E^* = \frac{2}{3}(0) + \frac{1}{3}(1) = \frac{1}{3}$ and $\gamma_{1,2} = (\frac{2}{3} - \frac{1}{3})(1 - 0) = \frac{1}{3} < \gamma_{2,3} = \frac{2}{3}$, we obtain $\Delta E(\rho) \ge \frac{2}{3} - \frac{1}{3} = \gamma_{1,2} = \gamma_{\min} > 0$ for all t or k, while $\Delta E(\rho_{\text{ref}}) = \frac{7}{6} - \frac{1}{3} = \frac{5}{6}$ decays strictly to the trapped saddle $\rho_{\sigma_{1,2}}$ (Figure 1(a)).

(iii) Any fixed point $\rho \in \mathcal{O}_p$ of (2) satisfies $0 = \text{Tr}(H[[\rho, H], \rho]) = -\|[\rho, H]\|_{\text{HS}}^2$, hence $[\rho, H] = 0$; because H has simple spectrum $\lambda_1 < \cdots < \lambda_d$, ρ is diagonal in $\{|\lambda_a\rangle\}$ with eigenvalues $(q_1, \dots, q_d)$ obtained by placing the r distinct positive weights $(p_1, \dots, p_r)$ at r distinct slots and 0 at the remaining $d - r$ slots (indexed by cosets $\sigma \in S_d/S_{d-r}$, giving exactly $d!/(d-r)!$ fixed points ρ_σ). Writing a nearby point on $\mathcal{O}_p$ as $\rho = e^K \rho_\sigma e^{-K} = \rho_\sigma + \delta\rho + O(K^2)$ with $K^\dagger = -K$ and $K_{ab} = 0$ whenever $q_a = q_b$, the tangent space $T_{\rho_\sigma}\mathcal{O}_p$ is parametrized by the complex entries $\delta\rho_{ab} = (q_b - q_a)K_{ab}$ for $1 \le a < b \le d$ with $q_a \neq q_b$. There are $\binom{r}{2}$ pairs among the r distinct positive weights and $r(d-r)$ pairs between a positive weight and a zero weight, giving complex dimension $\binom{r}{2} + r(d-r) = r(2d-r-1)/2$ and real dimension $r(2d-r-1)$ (Lean `thm03`). Linearizing (2) at ρ_σ (using $[\rho_\sigma, H] = 0$) gives $W = [\delta\rho, H] + O(\delta\rho^2)$ with $W_{ab} = (\lambda_b - \lambda_a)\delta\rho_{ab}$, and hence

$$\partial_t(\delta\rho)_{ab} = [W, \rho_\sigma]_{ab} + O(\delta\rho^2) = (q_b - q_a)(\lambda_b - \lambda_a)\delta\rho_{ab} + O(\delta\rho^2) = \mu_{ab}(\sigma)\,\delta\rho_{ab} + O(\delta\rho^2),$$

establishing (9). Since $\lambda_b - \lambda_a > 0$ and $q_a \neq q_b$, every $\mu_{ab}(\sigma) \neq 0$ (hyperbolicity), with $\mu_{ab}(\sigma) > 0 \iff q_a < q_b$. Each unstable complex mode contributes real dimension 2, so the Morse index is $2\,\text{inv}(q)$. Clearly $\text{inv}(q) = 0 \iff q_1 \ge \cdots \ge q_d \iff \rho_\sigma = \rho^*$; $\text{inv}(q) = r(2d-r-1)/2 \iff q_1 \le \cdots \le q_d$ (unique source); and $\text{inv}(q) = 1$ requires an adjacent inversion $q_j < q_{j+1}$ whose swap eliminates the sole inversion and recovers $q = (p_1, \dots, p_r, 0, \dots, 0)$, yielding precisely the r adjacent swaps $\rho_{\sigma_{j,j+1}}$ $(j = 1, \dots, r)$. Finally, combining Eq. (D7) ($\Delta E(\rho_\sigma) = \sum_{j=1}^r \delta p_j \varepsilon_j(\rho_\sigma)$) with Lemma D.1 ($\varepsilon_j(\rho_\sigma) \ge \delta\lambda_{j+1}[j - \text{Tr}(P_j(\rho_\sigma)\Pi_j)] = \delta\lambda_{j+1}k_j(\sigma)$) of [13] immediately yields (10) (Lean `thm04b`, Cert. `C04`). □

3 Theorem 2: Cross-Subspace Dissipation, Sharpening, Tightness, and Discrete Contraction

Following Appendices D and F of [13], let $V_j := \text{span}\{|\phi_1\rangle, \dots, |\phi_j\rangle\}$ $(1 \le j \le r)$ with projector P_j, subspace energy excess $\varepsilon_j := \text{Tr}(P_j H) - \sum_{i=1}^j \lambda_i \ge 0$, weighted subspace excess $x_j := \delta p_j \varepsilon_j \ge 0$ (so $\Delta E(\rho) = \sum_{j=1}^r x_j$), and single-subspace leakage $l_j := \|(I - P_j)HP_j\|_{\text{HS}}^2 = \sum_{i=1}^j \sum_{k=j+1}^d |H_{ik}|^2$, where $H_{ik} := \langle\phi_i|H|\phi_k\rangle$ in an eigenbasis $\{|\phi_i\rangle\}_{i=1}^d$ of ρ. For every $1 \le j <$

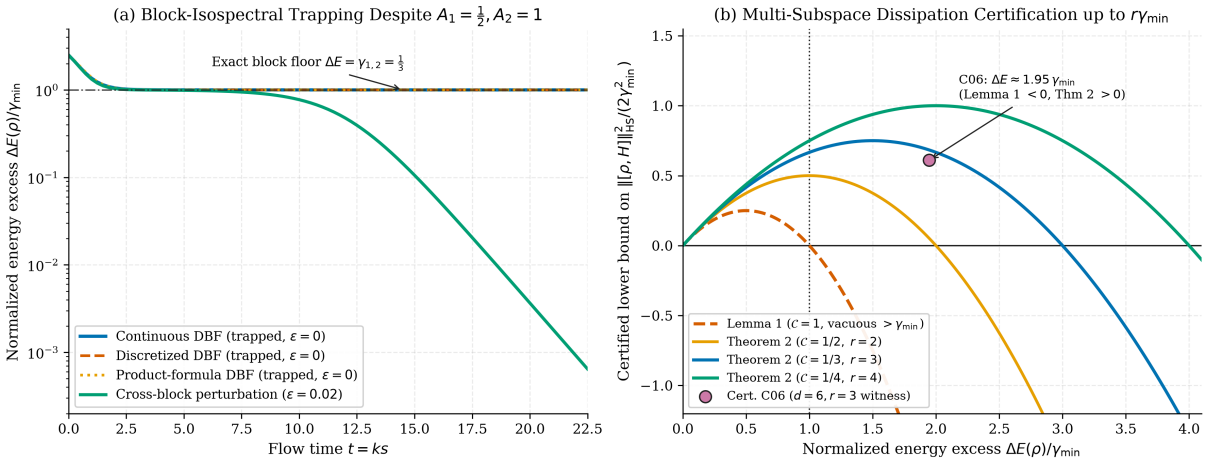


Figure 1: **Theorems 1 and 2.** (a) Exact block-isospectral trapping of the $d = 3, r = 2$ separation witness (7) ($A_1 = 1/2, A_2 = 1, \mathrm{rank}(\Pi_2 P_2 \Pi_2) = 2$) at $\Delta E = \gamma_{1,2} = 1/3$ across all three DBFs ($s = 0.25$), contrasted with escape to ρ^* under a cross-block perturbation $\epsilon = 0.02$. (b) Concentration-ratio dissipation lower bound (14) versus Lemma 1 of [13] ($\mathcal{C} = 1$), certifying strictly positive dissipation up to $r\gamma_{\min}$ and verified by the exact rational witness of Certificate `C06` at $\Delta E \approx 1.95\,\gamma_{\min}$.

$m \le r$, define the *cross-subspace leakage*

$$l_{j,m} := \|(I - P_m) H P_j\|^2_{\mathrm{HS}} = \sum_{i=1}^{j} \sum_{k=m+1}^{d} |H_{ik}|^2 \ge 0. \tag{11}$$

For $\Delta E(\rho) > 0$, define the excess-weighted effective rate and *subspace concentration ratio*

$$\bar{\gamma}(\rho) := \frac{\sum_{j=1}^{r} \gamma_{j,j+1} x_j}{\Delta E(\rho)} \ge \gamma_{\min}, \qquad \mathcal{C}(\rho) := \frac{\sum_{j=1}^{r} x_j^2}{(\Delta E(\rho))^2} \in \left[\frac{1}{r},\, 1\right]. \tag{12}$$

Theorem 2 (Cross-Subspace Dissipation, Sharpening, Tightness, and Contraction)**.** *Let $1 \le r < d$, let H have strictly ordered eigenvalues $\lambda_1 < \cdots < \lambda_d$, and let $\rho = \sum_{i=1}^{r} p_i |\phi_i\rangle\langle\phi_i|$ have $p_1 > \cdots > p_r > 0$.*

(i) ***Exact cross-subspace dissipation identity.*** *The energy dissipation rate satisfies the exact decomposition*

$$\|[\rho, H]\|^2_{\mathrm{HS}} = 2 \sum_{j=1}^{r} (\delta p_j)^2 l_j + 4 \sum_{1 \le j < m \le r} \delta p_j\, \delta p_m\, l_{j,m}. \tag{13}$$

(ii) ***Concentration-ratio sharpening above*** $\gamma_{\min}$**.** *Whenever $\Delta E(\rho) > 0$,*

$$\|[\rho, H]\|^2_{\mathrm{HS}} \ge 2\Delta E(\rho)\big(\bar{\gamma}(\rho) - \mathcal{C}(\rho)\Delta E(\rho)\big) \ge 2\Delta E(\rho)\big(\gamma_{\min} - \Delta E(\rho)\big), \tag{14}$$

with exact nonnegative surplus between the middle and right-hand expressions

$$\begin{aligned} &2\Delta E(\rho)\big(\bar{\gamma}(\rho) - \mathcal{C}(\rho)\Delta E(\rho)\big) - 2\Delta E(\rho)\big(\gamma_{\min} - \Delta E(\rho)\big) \\ &\quad = 2 \sum_{j=1}^{r} (\gamma_{j,j+1} - \gamma_{\min}) x_j + 4 \sum_{1 \le j < m \le r} x_j x_m \ge 0. \end{aligned} \tag{15}$$

Consequently, $\|[\rho, H]\|^2_{\mathrm{HS}} > 0$ is certified throughout the region $\Delta E(\rho) < \bar{\gamma}(\rho)/\mathcal{C}(\rho)$, reaching up to $r\gamma_{\min}$ for balanced multi-subspace excitations ($\mathcal{C}(\rho) = 1/r$).

(iii) ***Exact global tightness along the*** 2***-level geodesic.*** *Choose* $j^* \in \{1,\dots,r\}$ *attaining* $\gamma_{j^*,j^*+1} = \gamma_{\min}$*, and define the* 1*-parameter geodesic* $\rho(\vartheta)$ *(*$\vartheta \in [0,\pi]$*) rotating only* $\mathrm{span}\{|\lambda_{j^*}\rangle, |\lambda_{j^*+1}\rangle\}$ *via*

$$|\phi_{j^*}(\vartheta)\rangle = \cos\frac{\vartheta}{2}|\lambda_{j^*}\rangle + \sin\frac{\vartheta}{2}|\lambda_{j^*+1}\rangle,$$

with $|\phi_{j^*+1}(\vartheta)\rangle = -\sin\frac{\vartheta}{2}|\lambda_{j^*}\rangle + \cos\frac{\vartheta}{2}|\lambda_{j^*+1}\rangle$ *when* $j^* < r$ *and* $|\phi_i\rangle = |\lambda_i\rangle$ *otherwise. Writing* $f_i(|\phi_i\rangle) := |\langle\lambda_i|\phi_i\rangle|^2$ *for the* i*-th eigenstate fidelity (*$F_i(k) := |\langle\lambda_i|\phi_i(k)\rangle|^2$ *at discrete step* k*), along* $\rho(\vartheta)$ *Lemma 1, Lemma G.2, and the continuous-time bound of Theorem G.1(1) in [13] all hold with* exact global equality*:*

$$1 - f_{j^*}(|\phi_{j^*}(\vartheta)\rangle) = \frac{\Delta E(\rho(\vartheta))}{\gamma_{\min}}, \qquad \|[\rho(\vartheta), H]\|_{\mathrm{HS}}^2 = 2\Delta E(\rho(\vartheta))\big(\gamma_{\min} - \Delta E(\rho(\vartheta))\big),$$
$$\frac{\Delta E(\rho(t))}{\gamma_{\min} - \Delta E(\rho(t))} = c_0 e^{-2\gamma_{\min} t}. \tag{16}$$

(iv) ***Strictly tighter discrete logistic contraction and reduced step complexity.*** *Under the discretized DBF* (3) *(*$\bar{s} = 2/\gamma_{\max}$*) or product-formula DBF* (4) *(*$\bar{s} = 12/(7\gamma_{\max})$ *with* $\theta_k/\tau_k = \Omega/p_1$*), if* $x_0 := \Delta E(\rho_{\mathrm{ref}}) < \gamma_{\min}$ *and* $0 < s_k < \bar{s}$*, let* $x_k := \Delta E(\rho_k)$*,* $y_k := x_k/(\gamma_{\min} - x_k)$*,* $c_0 := y_0$*, and* $b_k := s_k(1 - s_k/\bar{s})$*. Then at every step* $k \geq 0$ *with* $y_k > 0$*,*

$$y_{k+1} \leq y_k\left(1 - \frac{2b_k\gamma_{\min}}{1 + 2b_k x_0}\right) < \frac{y_k}{1 + 2b_k\gamma_{\min}}, \tag{17}$$

(and $y_{k+1} = 0$ *whenever* $y_k = 0$*), with exact positive contraction-factor gap*

$$\frac{1}{1 + 2b_k\gamma_{\min}} - \left(1 - \frac{2b_k\gamma_{\min}}{1 + 2b_k x_0}\right) = \frac{4b_k^2\gamma_{\min}(\gamma_{\min} - x_0)}{(1 + 2b_k\gamma_{\min})(1 + 2b_k x_0)} > 0. \tag{18}$$

At constant step $s = \bar{s}/2$*, achieving* $1 - F_i(K) \leq \varepsilon$ *for all* $i \in \{1,\dots,r\}$ *requires at most* $\lceil K_{\mathrm{disc}}\rceil$ *(respectively* $\lceil K_{\mathrm{PF}}\rceil$*) iterations, where the continuous iteration thresholds satisfy*

$$K_{\mathrm{disc}} = \left(\kappa + \frac{x_0}{\gamma_{\min}}\right)\ln\frac{c_0}{\varepsilon} < (1+\kappa)\ln\frac{c_0}{\varepsilon},$$
$$K_{\mathrm{PF}} = \left(\frac{7\kappa}{6} + \frac{x_0}{\gamma_{\min}}\right)\ln\frac{c_0}{\varepsilon} < \left(1 + \frac{7\kappa}{6}\right)\ln\frac{c_0}{\varepsilon}, \tag{19}$$

strictly improving the continuous prefactors of Eqs. (G49)–(G50) in [13] uniformly for every $x_0 \in (0, \gamma_{\min})$*.*

Proof. **(i)** From Eq. (F8) of [13], $\|[\rho, H]\|_{\mathrm{HS}}^2 = 2\sum_{1\leq i<k\leq d}(p_i - p_k)^2|H_{ik}|^2$. Substituting the telescoping sum $p_i - p_k = \sum_{j=1}^{r}\delta p_j\,\mathbf{1}_{i\leq j<k}$ into *both* factors of $(p_i - p_k)^2$ gives

$$(p_i - p_k)^2 = \sum_{j=1}^{r}(\delta p_j)^2\,\mathbf{1}_{i\leq j<k} + 2\sum_{1\leq j<m\leq r}\delta p_j\,\delta p_m\,\mathbf{1}_{i\leq j<m<k}$$

(Lean `thm06`). Multiplying by $2|H_{ik}|^2$, summing over $1 \leq i < k \leq d$, and exchanging summation order yields (13) directly via (11).

(ii) Dropping the nonnegative cross-subspace term in (13) and applying Lemma F.2 of [13] ($l_j \geq \varepsilon_j(\delta\lambda_{j+1} - \varepsilon_j)$) to each term gives

$$\|[\rho, H]\|_{\mathrm{HS}}^2 \geq 2\sum_{j=1}^{r}(\delta p_j)^2 l_j \geq 2\sum_{j=1}^{r}\delta p_j\varepsilon_j\big(\delta p_j\delta\lambda_{j+1} - \delta p_j\varepsilon_j\big) = 2\sum_{j=1}^{r}x_j(\gamma_{j,j+1} - x_j).$$

Using (12), $\sum_j \gamma_{j,j+1} x_j = \bar{\gamma}(\rho)\Delta E(\rho)$ and $\sum_j x_j^2 = \mathcal{C}(\rho)(\Delta E(\rho))^2$, which gives the first inequality in (14). By Cauchy–Schwarz and nonnegativity of x_j, $(\Delta E)^2 \le r\sum_{j=1}^r x_j^2 \le r(\Delta E)^2$, so $\mathcal{C}(\rho) \in [1/r, 1]$ (Lean `thm08`). Subtracting $2\Delta E(\gamma_{\min} - \Delta E)$ and applying $(\sum_j x_j)^2 - \sum_j x_j^2 = 2\sum_{j<m} x_j x_m$ yields (15) identically (Lean `thm07`). Explicit rational witness `C06` ($d = 6, r = 3$, $H = \mathrm{diag}(0, 10, 20, 30, 40, 50)$, $p = (1/2, 1/3, 1/6, 0, 0, 0)$ with Pythagorean rotations $(12/13, 5/13)$, $(24/25, 7/25)$, $(40/41, 9/41)$ on pairs $(1, 4), (2, 5), (3, 6)$) achieves $\Delta E/\gamma_{\min} \approx 1.946 > 1$, where Lemma 1 is strictly negative while (14) certifies positive dissipation (Figure 1(b)).

(iii) Along $\rho(\vartheta)$, only the 2×2 block $\{j^*, j^*+1\}$ is rotated, giving $\Delta E(\rho(\vartheta)) = \gamma_{\min}\sin^2(\vartheta/2)$, $1 - f_{j^*}(|\phi_{j^*}(\vartheta)\rangle) = \sin^2(\vartheta/2) = \Delta E/\gamma_{\min}$, and $|[\rho(\vartheta), H]_{j^*,j^*+1}| = \frac{1}{2}\gamma_{\min}\sin\vartheta$, so $\|[\rho(\vartheta), H]\|_{\mathrm{HS}}^2 = \frac{1}{2}\gamma_{\min}^2\sin^2\vartheta = 2\Delta E(\gamma_{\min} - \Delta E)$ (Lean `thm09`, Cert. `C07`). By Theorem 1(i), the block $\{j^*, j^*+1\}$ is invariant under (2), so $\rho(t) = \rho(\vartheta(t))$ solves $\partial_t \Delta E = -2\Delta E(\gamma_{\min} - \Delta E)$ exactly, integrating to $\Delta E(\rho(t))/(\gamma_{\min} - \Delta E(\rho(t))) = c_0 e^{-2\gamma_{\min} t}$ for all $t \ge 0$.

(iv) By Eq. (G33) of [13], every step obeys

$$y_{k+1} \le y_k \frac{1 - 2b_k(\gamma_{\min} - x_k)}{1 + 2b_k x_k} = y_k\left(1 - \frac{2b_k\gamma_{\min}}{1 + 2b_k x_k}\right).$$

Since $0 \le x_k \le x_0 < \gamma_{\min}$ by monotonic energy decrease (Eq. (G30)), we have $1 + 2b_k x_k \le 1 + 2b_k x_0 < 1 + 2b_k\gamma_{\min}$, proving (17). Combining fractions over the common positive denominator $(1 + 2b_k\gamma_{\min})(1 + 2b_k x_0)$ gives

$$(1 + 2b_k x_0) - (1 + 2b_k\gamma_{\min})(1 + 2b_k x_0 - 2b_k\gamma_{\min}) = 4b_k^2\gamma_{\min}(\gamma_{\min} - x_0) > 0,$$

proving (18) (Lean `thm10`, Cert. `C08`). Setting $u_k := 2b_k\gamma_{\min}/(1 + 2b_k x_0) \in (0, 1)$ (as $2b_k\gamma_{\min} \le \gamma_{\min}/\gamma_{\max} \le 1$) and using $1 - u_k \le e^{-u_k}$ yields $y_K \le c_0 \exp(-\sum_{k=0}^{K-1} u_k)$. For constant step $s = \bar{s}/2$, $b_k = \bar{s}/4$, so $u_k^{-1} = \frac{2}{\bar{s}\gamma_{\min}} + \frac{x_0}{\gamma_{\min}}$; substituting $\bar{s} = 2/\gamma_{\max}$ and $\bar{s} = 12/(7\gamma_{\max})$ gives (19). □

4 Theorem 3: Discretized Stall Bifurcation, Product-Formula Complex Spectrum, and Unbalanced Chebyshev Instability

We now establish the exact nonlinear and spectral stability boundaries of both discrete implementations (3) and (4), resolving the empirical instabilities observed in Figs. 6(a) and 15(b) of [13].

Theorem 3 (Discretized Bifurcation, PF Spectrum, and Chebyshev Instability)**.**

(i) ***Exact** 2**-level discretized reduction and period-**2** **stall bifurcation.** On any invariant 2-level block $\{a, b\}$ with $\gamma = \gamma_{ab} = (p_a - p_b)(\lambda_b - \lambda_a) > 0$ (in particular $\{1, d\}$ with $\gamma = \gamma_{\max}$), writing*

$$\rho(\vartheta) = \frac{p_a + p_b}{2} I + \frac{p_a - p_b}{2}(\cos\vartheta\,\sigma_z + \sin\vartheta\,\sigma_x)$$

reduces the discretized DBF (3) exactly to the 1-dimensional map

$$\vartheta_{k+1} = F_{u_k}(\vartheta_k) := \vartheta_k - u_k\sin\vartheta_k, \qquad u_k := s_k\gamma, \qquad \Delta E(\rho(\vartheta)) = \gamma\sin^2(\vartheta/2). \tag{20}$$

For constant $u = s\gamma$:

- *At $u = 2$ ($s = \bar{s} = 2/\gamma_{\max}$), $F_2(\vartheta) = -\vartheta + \frac{1}{3}\vartheta^3 + O(\vartheta^5)$, and F_2 has a unique positive zero $\tilde{\vartheta} \approx 1.89549 \in (\pi/2, \pi)$ solving $\tilde{\vartheta} = 2\sin\tilde{\vartheta}$; for every nonzero initial angle $\vartheta_0 \in (-\tilde{\vartheta}, \tilde{\vartheta}) \setminus \{0\}$ (and more generally every $\vartheta_0 \in (-\pi, \pi)$ outside the countable zero-orbit preimage set $\bigcup_{k\ge0} F_2^{-k}(0)$), the iterates decay only algebraically as $\vartheta_k^2 \sim \frac{3}{2k}$ and $\Delta E(\rho_k) \sim \frac{3\gamma}{8k}$, proving that $\bar{s} = 2/\gamma_{\max}$ is unimprovable for exponential convergence.*

- *For* every $u \in (2,\pi)$*, there exists a unique symmetric period-2 stall orbit* $\{\pm\vartheta^*(u)\}$ *with* $\vartheta^*(u) \in (0,\pi/2)$ *solving*

$$\frac{\sin\vartheta^*}{\vartheta^*} = \frac{2}{u}. \tag{21}$$

Its 2-step Floquet multiplier satisfies $(F_u \circ F_u)'(\vartheta^*) = (1-u\cos\vartheta^*)^2 = (1-2\vartheta^*\cot\vartheta^*)^2 \in [0,1)$ *(vanishing at the superstable parameter* $u_0 = 2\vartheta_0^*/\sin\vartheta_0^* \approx 2.5366$ *where* $\tan\vartheta_0^* = 2\vartheta_0^*$*), certifying local asymptotic stability throughout* $u \in (2,\pi)$ *(and instability for* $u > \pi$*). Along* $\{\pm\vartheta^*(u)\}$*,* $\Delta E(\rho_{k+1}) = \Delta E(\rho_k) = \gamma\sin^2(\vartheta^*/2) > 0$ *is strictly constant, causing energy-stagnation stopping rules to terminate prematurely away from* ρ^**.*

(ii) ***Exact product-formula complex spectrum, exact 2-level nonlinear step, and sharp threshold*** $s_{\mathrm{crit}}^{\mathrm{PF}} = \pi^2/(4\gamma_{\max})$***.*** *For arbitrary* (d,r)*, linearizing the group-commutator product-formula DBF* (4) *at* ρ^* *yields, for every off-diagonal mode* (a,b) *(*$a < b, p_a > p_b$*) with* $u_H := \tau(\lambda_b - \lambda_a)$ *and* $u_\rho := \theta(p_a - p_b)$*, the exact complex multiplier and squared modulus*

$$\begin{aligned}\mu_{ab}^{\mathrm{PF}}(\tau,\theta) &= 1 - 4e^{i(u_\rho - u_H)/2}\sin\frac{u_H}{2}\sin\frac{u_\rho}{2},\\ |\mu_{ab}^{\mathrm{PF}}(\tau,\theta)|^2 &= 1 - 8\sin\frac{u_H}{2}\sin\frac{u_\rho}{2}\cos\frac{u_H+u_\rho}{2}.\end{aligned} \tag{22}$$

On the 2-level block $\{a,b\}$*, the* exact *nonlinear one-step energy change is*

$$E(\rho_1) - E(\rho_0) = -\frac{\|W_0\|_{\mathrm{HS}}^2}{\gamma}\Big[\sin u_H \sin u_\rho - \cos\vartheta\,(1-\cos u_H)(1-\cos u_\rho)\Big], \tag{23}$$

whose fourth-order expansion at $\vartheta \to 0^+$ *is* $-s\|W_0\|_{\mathrm{HS}}^2(1 - \frac{1}{6}u_H^2 - \frac{1}{6}u_\rho^2 - \frac{1}{4}u_H u_\rho + O(u^4))$*, proving that all three error constants* $(1/6, 1/6, 1/4)$ *in Theorem C.3 of [13] are exact at fourth order. Moreover, by AM–GM* ($u_H + u_\rho \ge 2\sqrt{s\gamma_{\max}}$)*, the angle ratio* $\theta/\tau = \Omega/p_1$ *uniquely maximizes the primary linear stability boundary* $u_H + u_\rho < \pi$*, yielding the exact sharp threshold*

$$s_{\mathrm{crit}}^{\mathrm{PF}} = \frac{\pi^2}{4\gamma_{\max}} > \frac{2}{\gamma_{\max}} > \frac{12}{7\gamma_{\max}}. \tag{24}$$

(iii) ***Unbalanced-mode Chebyshev instability dichotomy.*** *Under an* m*-periodic Chebyshev schedule* $s_k^{-1} = \frac{\gamma_{\max}+\gamma_{\min}}{2} + \frac{\gamma_{\max}-\gamma_{\min}}{2}\cos\frac{(2k-1)\pi}{2m}$ *(*$k = 1,\dots,m$*) with* $\theta_k/\tau_k = \Omega/p_1$*, any unbalanced mode* (a,b) *with relative energy gap* $\eta := (\lambda_b - \lambda_a)/\Omega \in (0,1]$ *and vanishing weight gap* $\epsilon := p_a - p_b \to 0^+$ *(e.g.,* $a \ge 2, b = d$ *with* $p_a \ll p_1$ *and* $\lambda_a - \lambda_1 \ll \Omega$*, so* $(a,b) \ne (1,d)$ *and* $u_\rho = \epsilon\theta_k \to 0^+$*) has per-cycle squared amplification*

$$\prod_{k=1}^{m}|\mu_{ab}^{\mathrm{PF}}(\tau_k,\theta_k)|^2 = 1 - \frac{2\epsilon}{p_1}S_m(\kappa;\eta) + O(\epsilon^2), \qquad S_m(\kappa;\eta) := \sum_{k=1}^{m} u_k\sin(\eta u_k), \tag{25}$$

where $u_k := \tau_k\Omega = \sqrt{s_k\gamma_{\max}}$ *and* $S_m(\kappa) := S_m(\kappa;1)$ *is the near-maximal-gap limit* $\eta \to 1^-$*:*

- *For* $m = 2$*,* $0 < u_1 < u_2 < \sqrt{4+2\sqrt{2}} < 3 < \pi$ *for* all $\kappa \ge 1$*, so* $S_2(\kappa;\eta) > 0$ *unconditionally for every* $\eta \in (0,1]$ *and every* $\kappa \ge 1$*.*
- *For* $m = 4$*,* $u_4 \to 1/\sin(\pi/16) \approx 5.126 \in (\pi, 2\pi)$ *as* $\kappa \to \infty$*, destabilizing near-maximal-gap unbalanced modes for large* κ*; in particular, at* $\kappa = 100$*, exact rational Taylor brackets certify* $S_4(100) < -1/2 < 0$*, and Lipschitz continuity* $|S_4(100;\eta) - S_4(100)| \le (1-\eta)\sum_{k=1}^4 u_k^2 < 27(1-\eta)$ *guarantees* $S_4(100;\eta) < 0$ *(hence per-cycle amplification* > 1 *for all sufficiently small* $\epsilon > 0$*) for every unbalanced mode with* $\eta \in [\frac{53}{54}, 1)$*.*

Proof. **(i)** In the $\{a,b\}$ block with $H = \frac{\lambda_a+\lambda_b}{2}I - \frac{\lambda_b-\lambda_a}{2}\sigma_z$, direct Pauli algebra yields $W = [\rho(\vartheta), H] = \frac{i\gamma\sin\vartheta}{2}\sigma_y$, so $V_k = e^{s_k W} = e^{i\frac{u_k\sin\vartheta}{2}\sigma_y}$ rotates the Bloch vector $(\sin\vartheta, 0, \cos\vartheta)$ in the (x,z)-plane by $-u_k\sin\vartheta$, giving (20) exactly. At $u = 2$, for every $\vartheta \in (0,\pi)$ we have $0 < \sin\vartheta < \vartheta$, hence $-\vartheta < F_2(\vartheta) < \vartheta$ and $|F_2(\vartheta)| < |\vartheta|$ with no nonzero fixed point of $|F_2|$ on $(0,\pi)$; moreover, $F_2(\vartheta) = \vartheta - 2\sin\vartheta$ is strictly negative on $(0,\tilde{\vartheta})$ (where $\tilde{\vartheta} \approx 1.89549 \in (\pi/2,\pi)$ is its unique positive zero) and strictly positive on $(\tilde{\vartheta},\pi)$. By odd symmetry, for every $\vartheta_0 \in (-\tilde{\vartheta},\tilde{\vartheta}) \setminus \{0\}$ (and more generally every $\vartheta_0 \in (-\pi,\pi) \setminus \bigcup_{k\geq 0} F_2^{-k}(0)$: on $(\tilde{\vartheta},\pi)$, $0 < F_2(\vartheta) < \vartheta$ with no fixed point of F_2 on $(0,\pi)$, so iterates decrease strictly and cross below $\tilde{\vartheta}$ in finitely many steps), no iterate vanishes and $|\vartheta_k| \downarrow 0$ strictly, entering $[-1,1] \setminus \{0\}$ in finitely many steps. Once $0 < |\vartheta_k| \leq 1$, the alternating Taylor bracket $\vartheta - \vartheta^3/6 \leq \sin\vartheta \leq \vartheta - \vartheta^3/6 + \vartheta^5/120$ gives $\vartheta - \vartheta^3/3 \leq -F_2(\vartheta) \leq \vartheta - \vartheta^3/3 + \vartheta^5/60 < \vartheta$ (Lean `thm11`, Cert. `C09`). Hence $|\vartheta_k| \downarrow 0$ monotonically and $\vartheta_{k+1}^{-2} - \vartheta_k^{-2} = \frac{2}{3} + O(\vartheta_k^2)$; Cesàro averaging yields $\vartheta_k^2 \sim \frac{3}{2k}$ and $\Delta E(\rho_k) = \gamma\sin^2(\vartheta_k/2) \sim \frac{\gamma}{4}\vartheta_k^2 \sim \frac{3\gamma}{8k}$.

For $u > 2$, a symmetric period-2 orbit satisfies $F_u(\vartheta^*) = -\vartheta^* \iff \sin\vartheta^*/\vartheta^* = 2/u$. Since $g(\vartheta) = \sin\vartheta/\vartheta$ is continuous and strictly decreasing on $(0,\pi)$ with $g(0^+) = 1$ and $g(\pi^-) = 0$, a unique root $\vartheta^*(u) \in (0,\pi)$ exists for every $u > 2$, with $\vartheta^*(u) \in (0,\pi/2) \iff 2/u > g(\pi/2) = 2/\pi \iff u \in (2,\pi)$. By odd symmetry $F_u(-\vartheta) = -F_u(\vartheta)$, $(F_u \circ F_u)'(\vartheta^*) = (F_u'(\vartheta^*))^2 = (1-u\cos\vartheta^*)^2 = (1-2\vartheta^*\cot\vartheta^*)^2$. For all $\vartheta^* \in (0,\pi/2)$, $0 < \vartheta^* < \tan\vartheta^*$ implies $0 < \vartheta^*\cot\vartheta^* < 1$, hence $-1 < 1 - 2\vartheta^*\cot\vartheta^* < 1$ and $(F_u \circ F_u)'(\vartheta^*) \in [0,1)$ (Lean `thm12`, Cert. `C10`), with superstable vanishing at the unique root $\tan\vartheta_0^* = 2\vartheta_0^*$ in $(0,\pi/2)$. For $u > \pi$, $\vartheta^* \in (\pi/2,\pi)$ gives $\cos\vartheta^* < 0$ so $1 - u\cos\vartheta^* > 1$ (unstable). Finally, $\Delta E(\rho(-\vartheta^*)) = \gamma\sin^2(-\vartheta^*/2) = \Delta E(\rho(\vartheta^*)) > 0$.

(ii) Since $e^{-i\theta\rho}\rho e^{i\theta\rho} = \rho$, Eq. (4) simplifies to $V\rho V^\dagger = e^{i\tau H}e^{i\theta\rho}Xe^{-i\theta\rho}e^{-i\tau H}$, where $X := e^{-i\tau H}\rho e^{i\tau H} = \rho^* + \delta X$ and $\delta X_{ab} = e^{iu_H}\delta\rho_{ab}$ for $\rho = \rho^* + \delta\rho$. By Duhamel's formula, $e^{i\theta(\rho^*+\delta\rho)} = e^{i\theta\rho^*}(I + \Phi(\delta\rho) + O(\delta\rho^2))$ with $\Phi(\delta\rho)_{ab} = \delta\rho_{ab}(1 - e^{-iu_\rho})/(p_a - p_b)$, hence $[\Phi(\delta\rho),\rho^*]_{ab} = (e^{-iu_\rho} - 1)\delta\rho_{ab}$. Conjugating $\rho^* + [\Phi(\delta\rho),\rho^*] + \delta X$ by $e^{i\theta\rho^*}$ (factor e^{iu_ρ}) and $e^{i\tau H}$ (factor e^{-iu_H}) yields

$$\mu_{ab}^{\mathrm{PF}}(\tau,\theta) = e^{-iu_H}\big(1 - e^{iu_\rho} + e^{i(u_\rho+u_H)}\big) = 1 - (1-e^{-iu_H})(1-e^{iu_\rho}) = 1 - 4e^{i(u_\rho-u_H)/2}\sin\frac{u_H}{2}\sin\frac{u_\rho}{2}.$$

Taking the squared modulus and applying the identity $\cos((u_\rho - u_H)/2) - 2\sin(u_H/2)\sin(u_\rho/2) = \cos((u_H+u_\rho)/2)$ yields (22) (verified algebraically in Lean `thm13`). For the 2-level nonlinear step, Eq. (C28) of [13] gives $E(\rho_1) = \mathrm{Tr}(A(\tau)B(\theta))$ with $A(\tau) = e^{-i\tau H}\rho_0 e^{i\tau H}$ and $B(\theta) = e^{-i\theta\rho_0}He^{i\theta\rho_0}$. On the Bloch sphere, $A(\tau)$ rotates $\hat{n} = (\sin\vartheta, 0, \cos\vartheta)$ around $\hat{z}$ by $-u_H$ to $\hat{n}_A = (\sin\vartheta\cos u_H, -\sin\vartheta\sin u_H, \cos\vartheta)$, while $B(\theta)$ rotates $\hat{z}$ around $\hat{n}$ by $+u_\rho$ to

$$\hat{z}_B = \big(\sin\vartheta\cos\vartheta(1-\cos u_\rho),\ -\sin\vartheta\sin u_\rho,\ 1 - \sin^2\vartheta(1-\cos u_\rho)\big).$$

Computing $\hat{n}_A \cdot \hat{z}_B$ and using $\|W_0\|_{\mathrm{HS}}^2 = \frac{1}{2}\gamma^2\sin^2\vartheta$ gives (23), whose Taylor expansion at $\cos\vartheta = 1$ matches $(1/6, 1/6, 1/4)$ identically (Lean `thm14`, Cert. `C11`). For stability $|\mu_{ab}^{\mathrm{PF}}|^2 < 1$ on the primary lobe $u_H, u_\rho > 0$, we require $u_H + u_\rho < \pi$. On the maximal mode $(1,d)$ where $u_H u_\rho = s\gamma_{\max}$, AM–GM yields $u_H + u_\rho \geq 2\sqrt{s\gamma_{\max}}$ with equality iff $\theta/\tau = \Omega/p_1$, giving $2\sqrt{s\gamma_{\max}} < \pi \iff s < \pi^2/(4\gamma_{\max})$. At this ratio, every other mode obeys $u_H(a,b) \leq u_H(1,d) < \pi/2$ and $u_\rho(a,b) \leq u_\rho(1,d) < \pi/2$, so $u_H(a,b) + u_\rho(a,b) < \pi$ simultaneously; above $\pi^2/(4\gamma_{\max})$, $\cos((u_H+u_\rho)/2) < 0$ makes $|\mu_{1,d}^{\mathrm{PF}}|^2 > 1$.

(iii) Substituting $u_\rho = \epsilon\theta_k$ and $u_H = \tau_k(\lambda_b - \lambda_a) = \eta u_k$ into (22) as $\epsilon \to 0^+$ (with $\theta_k = u_k/p_1$ under $\theta_k/\tau_k = \Omega/p_1$) yields

$$|\mu_{ab}^{\mathrm{PF}}(\tau_k,\theta_k)|^2 = 1 - 4\epsilon\theta_k\sin\frac{\eta u_k}{2}\cos\frac{\eta u_k}{2} + O(\epsilon^2) = 1 - \frac{2\epsilon}{p_1}u_k\sin(\eta u_k) + O(\epsilon^2);$$

multiplying over $k = 1,\ldots,m$ yields (25). When $m = 2$, $\cos(\pi/4) = \sqrt{2}/2$, so for all $\kappa \geq 1$, $u_2^{-2} = \frac{1+\kappa^{-1}}{2} - \frac{1-\kappa^{-1}}{2}\frac{\sqrt{2}}{2} > \frac{2-\sqrt{2}}{4} > \frac{1}{8} > \frac{1}{9} > \frac{1}{\pi^2}$, forcing $0 < \eta u_1 < \eta u_2 < 3 < \pi$ and $S_2(\kappa;\eta) > 0$

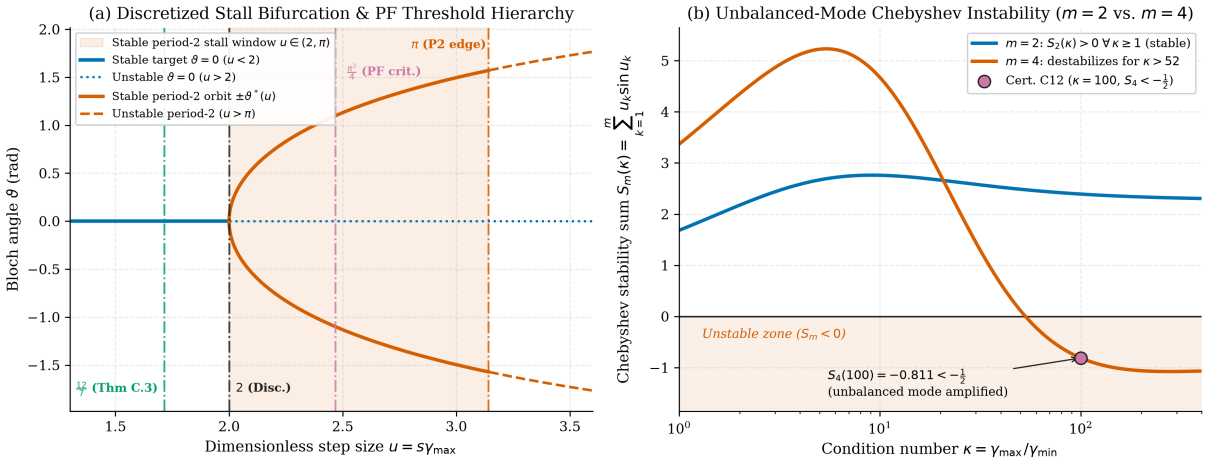


Figure 2: **Theorem 3.** (a) Exact 2-level discretized DBF bifurcation diagram showing the critical algebraic breakdown at $u = 2$, the unique locally asymptotically stable symmetric period-2 stall orbit $\pm\vartheta^*(u)$ on $u \in (2, \pi)$ (shaded), and the exact threshold hierarchy $12/7 < 2 < \pi^2/4 < \pi$. (b) Unbalanced-mode Chebyshev stability sum $S_m(\kappa) = \sum_{k=1}^{m} u_k \sin u_k$: $m = 2$ remains strictly positive for all $\kappa \geq 1$, whereas $m = 4$ crosses zero near $\kappa \approx 52$ and is certified below $-1/2$ at $\kappa = 100$ (Certificate `C12`).

for every $\eta \in (0, 1]$. When $m = 4$ at $\kappa = 100$, the roots $c_1 = \cos(\pi/8)$ and $c_2 = \cos(3\pi/8)$ of $8c^4 - 8c^2 + 1 = 0$ are bracketed by $c_1 \in (\frac{9238}{10000}, \frac{9239}{10000})$ and $c_2 \in (\frac{3826}{10000}, \frac{3827}{10000})$, giving $u_1 \leq 1.02$, $u_2 \leq 1.21$, $u_3 \leq 1.79$, and $4.57 \leq u_4 \leq 4.59$. Applying $\sin x \leq x - x^3/6 + x^5/120$ to u_1, u_2, $\sin u_3 \leq 1$, and $-\sin u_4 = \sin(u_4 - \pi) \geq w - w^3/6$ at $w = 1.42 \leq u_4 - \pi$ yields the exact rational bound

$$S_4(100) \leq -\frac{61939305404015}{120000000000000} \approx -0.5162 < -\frac{1}{2} < 0$$

(Lean `thm15`, Cert. `C12`; Figure 2(b)). Moreover, since $|\sin(\eta u_k) - \sin u_k| \leq (1 - \eta)u_k$ and $\sum_{k=1}^{4} u_k^2 \leq 1.02^2 + 1.21^2 + 1.79^2 + 4.59^2 = 26.7767 < 27$, every near-maximal-gap unbalanced mode with $\eta \in [\frac{53}{54}, 1)$ obeys $S_4(100; \eta) < -\frac{1}{2} + 27(1-\eta) \leq 0$ (strictly negative because $S_4(100) < -\frac{1}{2}$ and $\sum u_k^2 < 27$), proving per-cycle amplification for all sufficiently small $\epsilon > 0$. Note that the maximal mode $(1, d)$ itself has $\epsilon = p_1$ (not small) and is not governed by (25); the instability specifically targets unbalanced near-maximal-gap modes such as $(2, d)$ with $p_2 \ll p_1$ and $\lambda_2 - \lambda_1 \leq \frac{1}{54}\Omega$. □

5 Theorem 4: Subset-Optimal Degenerate Weight Duality and Adaptive Untracked-Gap Asymmetry

Suppose an application requires preparing only a non-empty subset $T \subseteq \{1, \ldots, r\}$ of eigenstates (with $r = \max T < d$). By Theorem H.1(4) of [13], isolating every $|\lambda_i\rangle$ ($i \in T$) requires positive weight gaps $\delta p_j > 0$ precisely on the minimal boundary index set

$$J(T) := \bigcup_{i \in T} \big(\{i - 1, i\} \cap \{1, \ldots, r\}\big) \subseteq \{1, \ldots, r\}. \tag{26}$$

Crucially, because terms with $\delta p_j = 0$ drop out of $\Delta E(\rho) = \sum_{j \in J(T)} \delta p_j \varepsilon_j$ and $\gamma_{\min}$, the Hamiltonian H need only be nondegenerate across $J(T)$: we allow exact spectral degeneracies $\delta\lambda_{j+1} = 0$ for any $j \notin J(T)$!

Theorem 4 (Subset-Optimal Degenerate Weight Duality and Exact Adaptive Untracked-Gap Asymmetry)**.** *Let $1 \le r < d$, let $T \subseteq \{1, \dots, r\}$ be non-empty with minimal boundary set $J(T)$ ($r = \max T$), and let H satisfy $\delta\lambda_{j+1} > 0$ for all $j \in J(T)$ (permitting $\delta\lambda_{j+1} = 0$ for $j \notin J(T)$).*

(i) ***Subset-optimal weight duality.*** *For every valid weight vector $p_1 \ge \cdots \ge p_r > 0$ ($\sum_{i=1}^{r} p_i = 1$) with $\delta p_j > 0$ for all $j \in J(T)$ and $\delta p_j = 0$ whenever $\delta\lambda_{j+1} = 0$ (which guarantees $\gamma_{\min}(p) > 0$; by convention $\kappa(p) := +\infty$ if $\gamma_{\min}(p) = 0$),*

$$\gamma_{\min}(p) \le \gamma^\star_{\min}(T) := \left(\sum_{j \in J(T)} \frac{j}{\delta\lambda_{j+1}} \right)^{-1}, \qquad \kappa(p) \ge \kappa^\star(T) := \Omega \sum_{j \in J(T)} \frac{1}{\delta\lambda_{j+1}}. \tag{27}$$

Both bounds are attained simultaneously and uniquely by the degenerate inverse-gap weights $\delta p^\star_j = \gamma^\star_{\min}(T)/\delta\lambda_{j+1}$ for $j \in J(T)$ and $\delta p^\star_j = 0$ for $j \notin J(T)$.

(ii) ***Strict improvement over Theorem EM1 / Corollary H.2 for single excited state $T = \{r\}$ ($r \ge 2$).*** *Writing $g_- := \delta\lambda_r$, $g_+ := \delta\lambda_{r+1}$, $\delta\lambda_{\min} := \min(g_-, g_+)$, and $\delta\lambda_{\max} := \max(g_-, g_+)$, the subset-optimal weights for $T = \{r\}$ ($J(\{r\}) = \{r-1, r\}$) are*

$$p^\star_1 = \cdots = p^\star_{r-1} = \frac{g_- + g_+}{(r-1)g_+ + r g_-}, \qquad p^\star_r = \frac{g_-}{(r-1)g_+ + r g_-}, \tag{28}$$

giving $\gamma^\star_{\min}(\{r\}) = \frac{g_- g_+}{(r-1)g_+ + r g_-}$ and $\kappa^\star(\{r\}) = \Omega(g_-^{-1} + g_+^{-1})$. Compared against Theorem EM1 ($\gamma^{\mathrm{EM1}}_{\min} = \delta\lambda_{\min}/(2r-1)$, $\kappa^{\mathrm{EM1}} = 2\Omega/\delta\lambda_{\min}$), whenever $g_- \ne g_+$ we obtain strict simultaneous improvements:

$$\begin{aligned} \frac{\kappa^{\mathrm{EM1}}}{\kappa^\star(\{r\})} &= \frac{2}{1 + \delta\lambda_{\min}/\delta\lambda_{\max}} \in (1, 2), \\ \frac{\gamma^\star_{\min}(\{r\})}{\gamma^{\mathrm{EM1}}_{\min}} &= \frac{2r-1}{(r-1)(\delta\lambda_{\min}/g_-) + r(\delta\lambda_{\min}/g_+)} \in \left(1,\ \frac{2r-1}{r-1}\right), \end{aligned} \tag{29}$$

achieving up to a $2\times$ reduction in κ and up to a $\frac{2r-1}{r-1} \in (2, 3]\times$ expansion of the convergence basin $\gamma_{\min}$ (reaching $3\times$ at $r = 2$).

(iii) ***Exact perturbation formula and adaptive untracked-gap asymmetry.*** *Suppose inverse-gap weights $\hat{p}$ are constructed from positive gap estimates $\{\hat{g}_j\}_{j \in J(T)}$ via $\delta\hat{p}_j \propto \hat{g}_j^{-1}$ ($j \in J(T)$) and $\delta\hat{p}_j = 0$ ($j \notin J(T)$). Then*

$$\kappa(\hat{p}) = \Omega \left(\sum_{j \in J(T)} \frac{1}{\hat{g}_j} \right) \left(\max_{j \in J(T)} \frac{\hat{g}_j}{\delta\lambda_{j+1}} \right) \le \frac{c_+}{c_-}\, \kappa^\star(T) \tag{30}$$

whenever $c_- \delta\lambda_{j+1} \le \hat{g}_j \le c_+ \delta\lambda_{j+1}$ ($0 < c_- \le c_+$). In full tracking $J = \{1, \dots, r\}$ where $\hat{g}_j = \delta\lambda_{j+1}$ for $j = 1, \dots, r-1$ and only the untracked gap $\hat{g}_r$ is misestimated by a factor $\alpha > 1$, overestimation ($\hat{g}_r = \alpha\delta\lambda_{r+1}$) versus underestimation ($\hat{g}_r = \delta\lambda_{r+1}/\alpha$) obey

$$\kappa_{\mathrm{over}}(\alpha) - \kappa^\star = (\alpha - 1)\Omega \sum_{j=1}^{r-1} \frac{1}{\delta\lambda_{j+1}}, \qquad \kappa_{\mathrm{under}}(\alpha) - \kappa^\star = (\alpha - 1)\frac{\Omega}{\delta\lambda_{r+1}}. \tag{31}$$

Hence overestimation incurs an $(r-1)$-term global penalty whereas underestimation incurs only a single-term local penalty, with exact gap $\kappa_{\mathrm{over}}(\alpha) - \kappa_{\mathrm{under}}(\alpha) = (\alpha - 1)\Omega(\sum_{j=1}^{r-1} \delta\lambda_{j+1}^{-1} - \delta\lambda_{r+1}^{-1})$ (strictly positive whenever $\sum_{j=1}^{r-1} \delta\lambda_{j+1}^{-1} > \delta\lambda_{r+1}^{-1}$, and reversing otherwise).

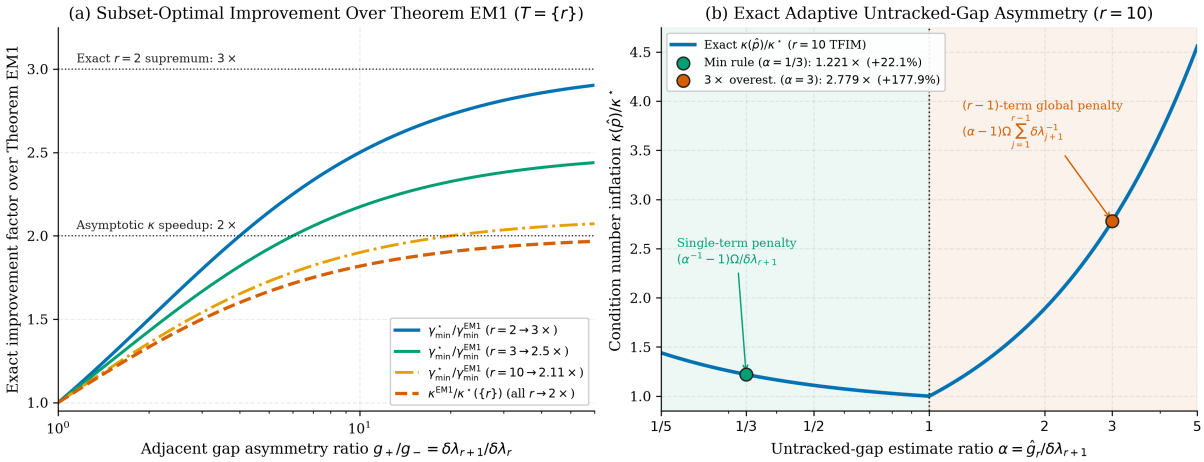


Figure 3: **Theorem 4.** (a) Exact condition-number speedup $\kappa^{\mathrm{EM1}}/\kappa^\star(\{r\}) \to 2\times$ and convergence-basin expansion $\gamma^\star_{\min}(\{r\})/\gamma^{\mathrm{EM1}}_{\min} \to (2r-1)/(r-1) \in (2,3]\times$ over Theorem EM1 for single excited state $T = \{r\}$. (b) Exact adaptive untracked-gap asymmetry (31) for the $r = 10$ TFIM spectrum of Fig. 13 in [13]: underestimating by $3\times$ (min rule) incurs only a $+22.1\%$ single-term penalty, while overestimating by $3\times$ incurs a $+177.9\%$ global penalty.

Proof. **(i)** By telescoping summation $p_i = \sum_{j=i}^r \delta p_j$, normalization and top weight obey $1 = \sum_{i=1}^r p_i = \sum_{j=1}^r j\,\delta p_j \geq \sum_{j\in J(T)} j\,\delta p_j$ and $p_1 = \sum_{j=1}^r \delta p_j \geq \sum_{j\in J(T)} \delta p_j$. Since $\gamma_{\min}(p) \leq \delta p_j \delta\lambda_{j+1}$ for every $j \in J(T)$, we have $\delta p_j \geq \gamma_{\min}(p)/\delta\lambda_{j+1}$, yielding

$$1 \geq \gamma_{\min}(p) \sum_{j\in J(T)} \frac{j}{\delta\lambda_{j+1}}, \qquad p_1 \geq \gamma_{\min}(p) \sum_{j\in J(T)} \frac{1}{\delta\lambda_{j+1}},$$

which establish both inequalities in (27) (Lean `thm16`, Cert. `C13`). Equality holds in both iff $\delta p_j = 0$ for all $j \notin J(T)$ and $\delta p_j \delta\lambda_{j+1} = \gamma^\star_{\min}(T)$ for all $j \in J(T)$.

(ii) Specializing part (i) to $J(\{r\}) = \{r-1, r\}$ directly yields (28) and the ratios (29). When $g_- \neq g_+$, $\delta\lambda_{\min}/\delta\lambda_{\max} < 1$ gives $\kappa^{\mathrm{EM1}}/\kappa^\star(\{r\}) \in (1,2)$, while at least one of $\delta\lambda_{\min}/g_-$, $\delta\lambda_{\min}/g_+$ is strictly below 1, making $(r-1)(\delta\lambda_{\min}/g_-) + r(\delta\lambda_{\min}/g_+) < 2r-1$; as $g_+/g_- \to \infty$, the denominator approaches $r-1$, giving the sharp supremum $(2r-1)/(r-1) \in (2,3]$ (Lean `thm17`, Cert. `C14`; Figure 3(a)).

(iii) Let $\delta\hat{p}_j = c/\hat{g}_j$ for $j \in J(T)$ where $c = (\sum_{j\in J(T)} j/\hat{g}_j)^{-1}$. Then $\hat{p}_1 = c\sum_{j\in J(T)} \hat{g}_j^{-1}$ and $\gamma_{\min}(\hat{p}) = c\min_{j\in J(T)}(\delta\lambda_{j+1}/\hat{g}_j) = c(\max_{j\in J(T)} \hat{g}_j/\delta\lambda_{j+1})^{-1}$. The normalization factor c cancels identically in $\kappa(\hat{p}) = \hat{p}_1\Omega/\gamma_{\min}(\hat{p})$, proving the equality in (30); substituting $\hat{g}_j^{-1} \leq (c_-\delta\lambda_{j+1})^{-1}$ and $\hat{g}_j/\delta\lambda_{j+1} \leq c_+$ yields the upper bound (Lean `thm18`, Cert. `C15`). Finally, setting $S_{r-1} := \sum_{j=1}^{r-1} \delta\lambda_{j+1}^{-1}$ and $s_r := \delta\lambda_{r+1}^{-1}$ in (30): for $\hat{g}_r = \alpha\delta\lambda_{r+1}$ ($\alpha > 1$), $\max_j(\hat{g}_j/\delta\lambda_{j+1}) = \alpha$ gives $\kappa_{\mathrm{over}}(\alpha) = \Omega(S_{r-1} + s_r/\alpha)\alpha = \Omega(\alpha S_{r-1} + s_r)$; for $\hat{g}_r = \delta\lambda_{r+1}/\alpha$, $\max_j(\hat{g}_j/\delta\lambda_{j+1}) = 1$ gives $\kappa_{\mathrm{under}}(\alpha) = \Omega(S_{r-1} + \alpha s_r)$, yielding (31) (Lean `thm19`). In the Fig. 13 TFIM regime of [13] ($r = 10$, $\Omega = 2$, $\delta\lambda_{\min} = 0.0042$, $\delta\lambda_{11} = 0.0126 = 3\delta\lambda_{\min}$, $S_9 = 640$), the min rule underestimates by $\alpha = 3$ and inflates κ by only $+22.1\%$ ($\kappa_{\mathrm{under}}/\kappa^* < 5/4$), whereas a symmetric $3\times$ overestimation inflates κ by $+177.9\%$ ($> 11/4$; Lean `thm20`, Cert. `C16`; Figure 3(b)). □

6 Formal Verification and Cryptographic Certificate Audit

The finite algebraic identities, universal polynomial/rational inequalities, exact separation witnesses, and rational Taylor brackets underlying Theorems 1–4 (complementing the continuous-time ODE, matrix-exponential, and analytic proofs in Sections 2–5) are machine-checked across three independent layers (archived at tag `v1.0.3`):

Table 1: Traceability matrix linking Theorems 1–4 to Lean 4.36.0 constructive theorems (`thm01`–`thm20`, 0 `Classical.choice`) and exact-rational SHA-256 certificates (`C01`–`C16`, 8-hex prefixes).

Result	Lean 4	Certs	SHA-256 Prefixes
Thm. 1 (Invariance & Morse)	`thm01`–`thm05`	`C01`–`C04`	`54dad7c3`, `9f9474d5`, `a8f01b17`, `1fd33fc9`
Thm. 2 (Dissipation & Logistic)	`thm06`–`thm10`	`C05`–`C08`	`643bee85`, `90e12979`, `e16e5c6a`, `4f24ec04`
Thm. 3 (Bifurcations & PF/Cheb.)	`thm11`–`thm15`	`C09`–`C12`	`ac300956`, `157e59de`, `40898db1`, `d7c18832`
Thm. 4 (Weight Duality & Asym.)	`thm16`–`thm20`	`C13`–`C16`	`e9d5a5b8`, `53ff8bd4`, `6085a6c0`, `50bc989c`

1. **Constructive Lean 4.36.0 Formalization:** Twenty constructive theorems (`thm01`–`thm20`) in `lean/DoubleBracketFlowBarriers.lean` (pure Lean 4 core, *zero external imports*) compile cleanly under `lean -DwarningAsError=true` (exit code 0, zero warnings, zero `sorry`, zero `grind`). Running `#print axioms` on all 20 theorems confirms *zero* occurrences of `Classical.choice` or `sorryAx` (using only constructive `propext` and `Quot.sound`, with `thm04`, `thm15`, `thm20` depending on no axioms at all).

2. **AST-Audited Zero-Float Exact-Rational Verifier:** Our pure Python standard-library verifier (`verification/verify_double_bracket_flows.py`) uses only `int` and exact rational `Fraction` arithmetic. Its built-in AST self-auditor verifies **0 float/complex/math violations** and emits 16 canonical SHA-256 certificates (`C01`–`C16`) aggregated into the deterministic manifest digest:

   `MANIFEST SHA-256: 94fb63331545e03fce19c45b2838227491d7f329ba304ab199d5fcf46b048010`

3. **Adversarial Test Suite (`tests/test_adversarial.py`):** 60 automated `pytest` checks (60/60 passing in 1.02 s) testing every positive certificate, negative counterexample (non-block perturbations, degenerate-Hamiltonian hyperbolicity failure, $x_0 > \gamma_{\min}$ logistic reversal, $u > \pi$ period-2 instability, $s_r > S_{r-1}$ asymmetry reversal), boundary equality, AST tamper injection, and SHA-256 tamper detection.

7 Conclusion

We have established a complete structural, dynamical, stability, and optimization theory extending the excited-state double-bracket flow framework of [13]. Practically, our results deliver four immediate algorithmic prescriptions: (i) verify eigenbasis-graph connectivity and block-spectral compatibility (6) rather than merely subspace overlap $A_i > 0$; (ii) spread initial excitations across subspaces (minimizing $\mathcal{C}(\rho)$) to retain certified positive dissipation up to $r\gamma_{\min}$; (iii) respect the exact step-size boundaries $s < 2/\gamma_{\max}$ (discretized) and $s < \pi^2/(4\gamma_{\max})$ (group-commutator PF at $\theta/\tau = \Omega/p_1$), while limiting first-order PF Chebyshev cycles to $m = 2$ or deploying higher-order commutator formulas when $\kappa \gtrsim 50$; and (iv) use subset-optimal degenerate inverse-gap weights (27)–(28) together with conservative (underestimating) untracked-gap rules such as the min rule to avoid $(r-1)$-fold condition-number inflation.

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