AIRR.SCIENCE · ARR-2026-3QE5CNAMRJ8TCSBT v1 [math.NA] 29 Nov 2026

Sharp Non-Asymptotic Shadow-Energy Geometry, Symmetric Splitting Metrics, Nonlinear Peano-Kernel Defects, and Conformal Dissipation for Symplectic Integrators

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November 29, 2026

Abstract

We establish four self-contained, sharp non-asymptotic structural theorems governing modified Hamiltonians, all-time energy envelopes, nonlinear shadow-energy defects, and conformal dissipation for symplectic integrators on separable Hamiltonian systems $H(q,p) = \frac{1}{2}p^\top M^{-1}p + V(q)$ ($M = M^\top \succ 0$ on $\mathbb{R}^d$). First, for coupled quadratic Hamiltonians $V(q) = \frac{1}{2}q^\top Kq$ ($K \succ 0$) with eigenfrequencies $0 < \omega_1 \le \cdots \le \omega_d$ and $\theta_j := \omega_j h$, we derive the exact invariant quadratic forms I_h^{KDK}, I_h^{DKD}, and I_h^{SE}, construct the exact closed-form modified Hamiltonian $\widetilde{H}_h^{\mathrm{KDK}} = \sum_{j=1}^d \frac{2\arcsin(\theta_j/2)}{\theta_j\sqrt{1-\theta_j^2/4}} I_{h,j}^{\mathrm{KDK}}$ (convergent as an h-power series on $|\theta_d| < 2$), prove the sharp all-time energy excursion hierarchy across Explicit Euler, Symplectic Euler ($2\theta_d/(2-\theta_d)$), Störmer–Verlet ($\theta_d^2/(4-\theta_d^2)$), and Implicit Midpoint (0), and establish sharp two-sided symplectic phase-velocity bracketing $2\arctan(\theta/2) < \theta < 2\arcsin(\theta/2)$. Second, for any palindromic s-stage symmetric symplectic splitting Φ_h of order $2p$, we prove that time-reversibility forces its 2×2 modal transfer matrix to have identical diagonal entries $P_s(\theta^2)$ (a polynomial in θ^2 of degree at most s) and admits an explicit purely diagonal positive-definite invariant metric $G_s(\theta)$ whenever $|P_s(\theta^2)| < 1$, yielding the exact all-time energy excursion ratio $\kappa_s(\theta) = \max\big((M_s)_{12}^2/(1-P_s^2), (1-P_s^2)/(M_s)_{12}^2\big) = 1 + O(\theta^{2p})$. Third, for general nonlinear potentials $V \in C^3(\mathbb{R}^d)$ and arbitrary $h > 0$, we prove exact Peano-kernel defect identities showing that the nonlinear Störmer–Verlet shadow energy $\mathcal{E}_h^{\mathrm{KDK}}(q,p) = H(q,p) - \frac{h^2}{8}\|M^{-1/2}\nabla V(q)\|_2^2$ and the Implicit Midpoint true energy H satisfy $|\Delta\mathcal{E}_h^{\mathrm{KDK}}| \le \frac{M_3}{12}\|\Delta q\|_2^3$ and $|\Delta H^{\mathrm{IM}}| \le \frac{M_3}{24}\|\Delta q\|_2^3$ (sharp for cubic potentials, opposite in sign, and strictly independent of linear stiffness K). Fourth, for symmetric conformal symplectic splitting $\Psi_h^{\mathrm{CS}} = D_{h/2}\circ\Phi_h^{\mathrm{KDK}}\circ D_{h/2}$ of damped Hamiltonian systems ($\gamma > 0$), we prove exact conformal symplecticity $(\Psi_h^{\mathrm{CS}})^*\omega = e^{-\gamma h}\omega$, an exact nonlinear shadow-energy dissipation identity, damping-invariant Schur stability ($0 < \theta_d < 2$ for every $\gamma > 0$), exact underdamped modulus $|\lambda_\pm| = e^{-\gamma h/2}$, and the unique closed-form optimal damping $\eta_*(\theta) = 2\,\mathrm{arccosh}(|1-\theta^2/2|^{-1})$ for all $\theta \in (0,2)\setminus\{\sqrt{2}\}$. All four theorems are verified across 255 randomized and structured benchmarks with zero bound violations.

Keywords: symplectic integrators, Störmer–Verlet, modified Hamiltonian, symmetric splitting methods, Peano kernel, shadow energy, conformal symplectic splitting, optimal damping.
MSC 2020: 65P10, 37M15, 70H05, 65L06, 34D20.

1 Introduction

Symplectic integrators preserve the canonical two-form $\omega = \sum_{i=1}^d dq_i \wedge dp_i$ on phase space $\mathbb{R}^{2d}$ and exhibit remarkable long-time energy fidelity on Hamiltonian systems [1, 4, 5, 6]. For a

separable Hamiltonian

$$H(q,p) := \frac{1}{2}p^\top M^{-1}p + V(q), \qquad (q,p) \in \mathbb{R}^d \times \mathbb{R}^d, \tag{1}$$

with symmetric positive definite mass matrix $M = M^\top \succ 0$ and smooth potential $V : \mathbb{R}^d \to \mathbb{R}$, the canonical equations $\dot{q} = M^{-1}p$, $\dot{p} = -\nabla V(q)$ are commonly integrated by kick–drift–kick (KDK) Störmer–Verlet Φ_h^{KDK},

$$p_{1/2} = p_0 - \frac{h}{2}\nabla V(q_0), \qquad q_1 = q_0 + hM^{-1}p_{1/2}, \qquad p_1 = p_{1/2} - \frac{h}{2}\nabla V(q_1), \tag{2}$$

higher-order palindromic compositions thereof [7, 8], or the implicit midpoint rule Φ_h^{IM} [1]. In dissipative mechanics $\dot{q} = M^{-1}p$, $\dot{p} = -\nabla V(q) - \gamma p$ ($\gamma > 0$), conformal symplectic splittings $\Psi_h^{\mathrm{CS}} = D_{h/2} \circ \Phi_h^{\mathrm{KDK}} \circ D_{h/2}$ preserve the exact exponential contraction of ω [9, 10].

Classical backward error analysis explains long-time near-conservation of energy via asymptotic Baker–Campbell–Hausdorff (BCH) series for a truncated modified Hamiltonian valid over exponentially long times for analytic potentials [2, 3, 1]. Yet four fundamental *non-asymptotic, exact* questions deserve a unified, elementary, closed-form treatment without asymptotic truncation:

1. *All-orders modified Hamiltonian, exact energy envelopes, and phase bracketing (Theorem 2.1):* For coupled quadratic Hamiltonians, what is the exact closed-form all-orders modified Hamiltonian $\widetilde{H}_h^{\mathrm{KDK}}$, what are the sharp all-time energy excursion constants across Explicit Euler, Symplectic Euler, Störmer–Verlet, and Implicit Midpoint, and how do Verlet and Implicit Midpoint bracket the exact phase velocity?

2. *Universal diagonal invariant metrics for arbitrary symmetric splittings (Theorem 3.1):* For any palindromic s-stage symmetric splitting of order $2p$ (including Yoshida and Suzuki schemes), how does time-reversibility produce an explicit purely diagonal positive-definite invariant metric $G_s(\theta)$ and exact $1 + O(\theta^{2p})$ all-time energy ratio?

3. *Exact nonlinear shadow-energy Peano-kernel defect laws (Theorem 4.1):* For arbitrary nonlinear $V \in C^3(\mathbb{R}^d)$ and *any* step size $h > 0$, what exact integral identities govern the one-step defect of the nonlinear KDK shadow energy $\mathcal{E}_h^{\mathrm{KDK}}(q,p) = H(q,p) - \frac{h^2}{8}\|M^{-1/2}\nabla V(q)\|_2^2$ and the Implicit Midpoint energy H, and why are both bounds completely independent of arbitrarily large linear stiffness K?

4. *Conformal symplectic stability, optimal damping, and nonlinear dissipation (Theorem 5.1):* For symmetric conformal splitting Ψ_h^{CS} under linear damping $\gamma > 0$, why is the asymptotic stability threshold $0 < \theta_d < 2$ strictly independent of γ, what unique closed-form damping $\eta_*(\theta)$ minimizes the spectral radius, and what exact nonlinear shadow-energy dissipation law governs damped anharmonic oscillators?

Notation and Modal Coordinates

Throughout, $d \geq 1$, $M = M^\top \succ 0$, and $\|\cdot\|_2$ denotes the Euclidean norm on $\mathbb{R}^d$. For a quadratic potential $V(q) = \frac{1}{2}q^\top Kq$ with $K = K^\top \succ 0$, the symmetrized stiffness matrix $W := M^{-1/2}KM^{-1/2} \succ 0$ admits an orthonormal spectral decomposition $W = U\Omega^2U^\top$ with $U^\top U = I_d$ and $\Omega = \mathrm{diag}(\omega_1, \ldots, \omega_d)$, $0 < \omega_1 \leq \cdots \leq \omega_d$. Introducing the canonical normal-mode coordinates

$$\hat{q} := \Omega^{1/2}U^\top M^{1/2}q, \qquad \hat{p} := \Omega^{-1/2}U^\top M^{-1/2}p, \tag{3}$$

we have $d\hat{q} \wedge d\hat{p} = dq \wedge dp$ (a linear symplectomorphism) and $H(q,p) = \sum_{j=1}^d H_j(\hat{q}_j, \hat{p}_j)$ with $H_j(\hat{q}_j, \hat{p}_j) := \frac{1}{2}\omega_j(\hat{q}_j^2 + \hat{p}_j^2)$. Every linear integrator decouples into d independent 2×2

blocks parameterized by the dimensionless frequencies $\theta_j := \omega_j h > 0$. For $V \in C^3(\mathbb{R}^d)$, we write $D^3V(q)[v,v,v] := \frac{d^3}{ds^3}\Big|_{s=0} V(q+sv)$ and define the symmetric trilinear operator norm $\|D^3V(q)\|_{\mathrm{op}} := \sup_{\|v\|_2=1} |D^3V(q)[v,v,v]|$.

2 Exact Modified Hamiltonian, All-Time Envelopes, and Phase Bracketing

On each normal mode $(\hat{q}_j, \hat{p}_j)$ with $\theta = \omega_j h$, KDK Störmer–Verlet (2) acts via the symplectic matrix

$$S(\theta) := \begin{pmatrix} 1-\theta^2/2 & \theta \\ -\theta(1-\theta^2/4) & 1-\theta^2/2 \end{pmatrix} \in \mathrm{SL}(2,\mathbb{R}). \tag{4}$$

Comparing KDK Verlet, drift–kick–drift (DKD) Verlet ($q_{1/2} = q_0 + \frac{h}{2}M^{-1}p_0$, $p_1 = p_0 - hKq_{1/2}$, $q_1 = q_{1/2} + \frac{h}{2}M^{-1}p_1$), Symplectic Euler ($p_1 = p_0 - hKq_0$, $q_1 = q_0 + hM^{-1}p_1$), Explicit Euler ($q_1 = q_0 + hM^{-1}p_0$, $p_1 = p_0 - hKq_0$), and Implicit Midpoint ($q_1 - q_0 = \frac{h}{2}M^{-1}(p_0+p_1)$, $p_1 - p_0 = -\frac{h}{2}K(q_0+q_1)$) yields the following exact structural hierarchy.

Theorem 2.1 (Exact All-Orders Modified Hamiltonian, Energy Hierarchy, and Phase Bracketing)**.** *Consider $H(q,p) = \frac{1}{2}p^\top M^{-1}p + \frac{1}{2}q^\top Kq$ with $M, K \succ 0$, eigenfrequencies $0 < \omega_1 \le \cdots \le \omega_d$, and $\theta_j := \omega_j h$.*

(a) ***Exact invariants, all-orders modified Hamiltonian, and sharp Verlet envelope.*** *For every $0 < h < 2/\omega_d$, KDK Störmer–Verlet preserves identically the positive-definite shadow energy*

$$I_h^{\mathrm{KDK}}(q,p) := H(q,p) - \frac{h^2}{8}\|M^{-1/2}Kq\|_2^2 = \frac{1}{2}p^\top M^{-1}p + \frac{1}{2}q^\top\left(K - \frac{h^2}{4}KM^{-1}K\right)q, \tag{5}$$

and coincides with the exact time-h canonical Hamiltonian flow $\Phi_h^{\mathrm{KDK}} = \exp(hX_{\widetilde{H}_h^{\mathrm{KDK}}})$ of the all-orders modified Hamiltonian

$$\widetilde{H}_h^{\mathrm{KDK}}(q,p) := \sum_{j=1}^{d} \frac{2\arcsin(\theta_j/2)}{\theta_j\sqrt{1-\theta_j^2/4}}\, I_{h,j}^{\mathrm{KDK}}(\hat{q}_j,\hat{p}_j), \tag{6}$$

where $I_{h,j}^{\mathrm{KDK}}(\hat{q}_j,\hat{p}_j) = \frac{1}{2}\omega_j\big((1-\theta_j^2/4)\hat{q}_j^2 + \hat{p}_j^2\big)$. Analogously, DKD Verlet preserves $I_h^{\mathrm{DKD}}(q,p) := H(q,p) - \frac{h^2}{8}\|K^{1/2}M^{-1}p\|_2^2$. For both KDK and DKD Verlet and every $z_0 = (q_0,p_0) \in \mathbb{R}^{2d}\setminus\{0\}$,

$$\left(1-\frac{\theta_d^2}{4}\right)H(z_0) \;\le\; H(z_n) \;\le\; \frac{1}{1-\theta_d^2/4}\,H(z_0) \qquad \forall n \in \mathbb{Z}, \tag{7}$$

yielding the sharp relative energy excursion $\sup_{n\in\mathbb{Z}} \frac{|H(z_n)-H(z_0)|}{H(z_0)} \le \frac{\theta_d^2}{4-\theta_d^2}$ (tight on mode d with $\hat{q}_{d,0} = 0, \hat{p}_{d,0} \neq 0$ and all other modes zero for KDK—or $\hat{p}_{d,0} = 0, \hat{q}_{d,0} \neq 0$ for DKD—where the supremum over $n \in \mathbb{Z}$ equals $\frac{\theta_d^2}{4-\theta_d^2}$ whenever $\frac{2}{\pi}\arcsin(\theta_d/2) \notin \mathbb{Q}$, and is attained at any finite integer n with $2n\arcsin(\theta_d/2) \equiv \frac{\pi}{2} \pmod{\pi}$).

(b) ***Exact four-method energy hierarchy.*** *For every $h > 0$ and $z_0 \in \mathbb{R}^{2d}\setminus\{0\}$:*

- Explicit Euler: $H(E_h^n z_0) = \sum_{j=1}^d (1+\theta_j^2)^n H_j(z_0) \ge (1+\theta_1^2)^n H(z_0)$ *for all $n \ge 0$ (unconditional exponential blow-up).*

- Symplectic Euler ($0 < \theta_d < 2$): *preserves* $I_h^{\mathrm{SE}}(q,p) := H(q,p) - \frac{h}{2} p^\top M^{-1} K q \succ 0$ *identically and satisfies*

$$\frac{2-\theta_d}{2+\theta_d}\, H(z_0) \;\le\; H(z_n) \;\le\; \frac{2+\theta_d}{2-\theta_d}\, H(z_0) \qquad \forall n \in \mathbb{Z}. \tag{8}$$

- Implicit Midpoint: *unconditionally preserves* $H((\Phi_h^{\mathrm{IM}})^n z_0) = H(z_0)$ *for all* $h > 0$ *and all* $n \in \mathbb{Z}$.

(c) ***Sharp symplectic phase-velocity bracketing.*** *On each mode* $\theta \in (0,2)$*, Implicit Midpoint and Störmer–Verlet have exact per-step rotation angles* $\phi_{\mathrm{IM}}(\theta) = 2\arctan(\theta/2)$ *and* $\phi_{\mathrm{SV}}(\theta) = 2\arcsin(\theta/2)$*, bracketing the exact flow angle* θ *strictly with non-asymptotic bounds (asymptotically sharp as* $\theta \to 0^+$*)*

$$\frac{\theta^3}{12(1+\theta^2/4)} < \theta - \phi_{\mathrm{IM}}(\theta) < \frac{\theta^3}{12}, \qquad \frac{\theta^3}{24} < \phi_{\mathrm{SV}}(\theta) - \theta < \frac{\theta^3}{12\sqrt{1-\theta^2/4}\big(1+\sqrt{1-\theta^2/4}\big)}. \tag{9}$$

Proof. (a) In modal coordinates (3), $\|M^{-1/2}Kq\|_2^2 = \sum_{j=1}^d \omega_j^3 \hat{q}_j^2$, so $I_h^{\mathrm{KDK}}(q,p) = \sum_{j=1}^d I_{h,j}^{\mathrm{KDK}}(\hat{q}_j, \hat{p}_j)$ with quadratic form matrix $\frac{1}{2}\omega_j Q_{\theta_j}$, $Q_\theta := \mathrm{diag}(a,1)$ where $a := 1 - \theta^2/4 > 0$. Direct matrix multiplication using $(1-\theta^2/2)^2 + \theta^2 a = 1$ gives

$$S(\theta)^\top Q_\theta S(\theta) = \begin{pmatrix} a(1-\theta^2/2)^2 + \theta^2 a^2 & a(1-\theta^2/2)\theta - (1-\theta^2/2)\theta a \\ a(1-\theta^2/2)\theta - (1-\theta^2/2)\theta a & a\theta^2 + (1-\theta^2/2)^2 \end{pmatrix} = \begin{pmatrix} a & 0 \\ 0 & 1 \end{pmatrix} = Q_\theta,$$

proving exact invariance of I_h^{KDK} (and symmetrically I_h^{DKD} for DKD Verlet, whose modal matrix is $S_{\mathrm{DKD}}(\theta) = \begin{pmatrix} 1-\theta^2/2 & \theta(1-\theta^2/4) \\ -\theta & 1-\theta^2/2 \end{pmatrix} = S(-\theta)^\top = RS(\theta)^\top R$ with momentum-reversal matrix $R := \mathrm{diag}(1,-1)$, directly preserving $\mathrm{diag}(1,a)$ since $S_{\mathrm{DKD}}(\theta)^\top \mathrm{diag}(1,a) S_{\mathrm{DKD}}(\theta) = \mathrm{diag}(1,a)$). Next, define the canonical rescaling $x_j := a_j^{1/4}\hat{q}_j$, $y_j := a_j^{-1/4}\hat{p}_j$ ($dx_j \wedge dy_j = d\hat{q}_j \wedge d\hat{p}_j$). Conjugating $S(\theta_j)$ by $D_j := \mathrm{diag}(a_j^{1/4}, a_j^{-1/4})$ yields the exact planar rotation

$$D_j S(\theta_j) D_j^{-1} = \begin{pmatrix} 1-\theta_j^2/2 & \theta_j\sqrt{a_j} \\ -\theta_j\sqrt{a_j} & 1-\theta_j^2/2 \end{pmatrix} = \begin{pmatrix} \cos\phi_j & \sin\phi_j \\ -\sin\phi_j & \cos\phi_j \end{pmatrix}, \qquad \phi_j := 2\arcsin(\theta_j/2) \in (0,\pi),$$

since $\cos\phi_j = 1 - 2\sin^2(\phi_j/2) = 1 - \theta_j^2/2$ and $\sin\phi_j = 2\sin(\phi_j/2)\cos(\phi_j/2) = \theta_j\sqrt{1-\theta_j^2/4} > 0$. In canonical coordinates (x_j, y_j), $I_{h,j}^{\mathrm{KDK}} = \frac{1}{2}\omega_j\sqrt{a_j}(x_j^2 + y_j^2)$, so the Hamiltonian $\eta_j I_{h,j}^{\mathrm{KDK}} = \frac{\phi_j}{2h}(x_j^2 + y_j^2)$ with $\eta_j := \frac{\phi_j}{\theta_j\sqrt{a_j}}$ generates exact clockwise rotation by angle ϕ_j over time h, proving (6) (note that η_j is real-analytic in θ_j^2 for $|\theta_j| < 2$, so the h-power-series rearrangement of the modified Hamiltonian converges absolutely for all $|\theta_d| < 2$, in contrast to the formal double Lie series of BCH whose radius of convergence can be smaller [2, 1]). Because $(1-\theta_d^2/4)H(z) \le I_h^{\mathrm{KDK}}(z) \le H(z)$ for all $z \in \mathbb{R}^{2d}$ and $I_h^{\mathrm{KDK}}(z_n) = I_h^{\mathrm{KDK}}(z_0)$, we obtain $(1-\theta_d^2/4)H(z_0) \le I_h^{\mathrm{KDK}}(z_n) \le H(z_n) \le (1-\theta_d^2/4)^{-1} I_h^{\mathrm{KDK}}(z_n) \le (1-\theta_d^2/4)^{-1} H(z_0)$, establishing (7). On mode d with $\hat{q}_{d,0} = 0$, $\hat{p}_{d,0} \neq 0$, we have $I_{h,d}(z_0) = H_d(z_0)$ and $(x_{d,n}, y_{d,n}) = a_d^{-1/4}\hat{p}_{d,0}(\sin(n\phi_d), \cos(n\phi_d))$, so $H_d(z_n)/H_d(z_0) = a_d^{-1}\sin^2(n\phi_d) + \cos^2(n\phi_d) = 1 + \frac{\theta_d^2}{4-\theta_d^2}\sin^2(n\phi_d)$, attaining $\frac{\theta_d^2}{4-\theta_d^2}$ whenever $\sup_n \sin^2(n\phi_d) = 1$.

(b) In modal coordinates, Explicit Euler acts on mode j via $E(\theta_j) = \begin{pmatrix} 1 & \theta_j \\ -\theta_j & 1 \end{pmatrix}$, satisfying $E(\theta_j)^\top E(\theta_j) = (1+\theta_j^2) I_2$, so $H_j(E(\theta_j)^n z_{j,0}) = (1+\theta_j^2)^n H_j(z_{j,0})$. Symplectic Euler acts via $S_{\mathrm{SE}}(\theta) = \begin{pmatrix} 1-\theta^2 & \theta \\ -\theta & 1 \end{pmatrix}$, and direct verification shows $S_{\mathrm{SE}}(\theta)^\top Q_{\mathrm{SE}}(\theta) S_{\mathrm{SE}}(\theta) = Q_{\mathrm{SE}}(\theta)$ for

$Q_{\mathrm{SE}}(\theta) := \begin{pmatrix} 1 & -\theta/2 \\ -\theta/2 & 1 \end{pmatrix}$, proving exact invariance of I_h^{SE}. Since $Q_{\mathrm{SE}}(\theta)$ has eigenvalues $1 \pm \theta/2$ with orthogonal eigenvectors $v_\pm := \frac{1}{\sqrt{2}}(1, \mp 1)^\top$ ($Q_{\mathrm{SE}}(\theta)v_+ = (1+\theta/2)v_+$ and $Q_{\mathrm{SE}}(\theta)v_- = (1-\theta/2)v_-$), we have $(1-\theta_d/2)H \le I_h^{\mathrm{SE}} \le (1+\theta_d/2)H$, which immediately yields (8) (and relative excursion $\le \frac{2\theta_d}{2-\theta_d}$); moreover, conjugating $S_{\mathrm{SE}}(\theta_d)$ by $Q_{\mathrm{SE}}(\theta_d)^{1/2}$ produces an exact planar rotation by angle $\phi_d = 2\arcsin(\theta_d/2)$, so initializing mode d along v_+ (where $I_{h,d}^{\mathrm{SE}} = (1+\theta_d/2)H_d$) yields $H_d(z_n)/H_d(z_0) = 1 + \frac{2\theta_d}{2-\theta_d}\sin^2(n\phi_d)$, proving sharpness of (8) whenever $\sup_n \sin^2(n\phi_d) = 1$. Implicit Midpoint acts via the Cayley matrix $C(\theta) = \big(I_2 - \frac{\theta}{2}J_2\big)^{-1}\big(I_2 + \frac{\theta}{2}J_2\big) = \frac{1}{1+\theta^2/4}\begin{pmatrix} 1-\theta^2/4 & \theta \\ -\theta & 1-\theta^2/4 \end{pmatrix} \in \mathrm{SO}(2)$ (where $J_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$), which is orthogonal for every $\theta > 0$ and rotates by exact angle $\phi_{\mathrm{IM}}(\theta) = 2\arctan(\theta/2)$, conserving H identically.

(c) Set $u := \theta/2 \in (0,1)$. For Implicit Midpoint,

$$\theta - \phi_{\mathrm{IM}}(\theta) = 2(u - \arctan u) = 2\int_0^u \frac{t^2}{1+t^2}\,dt.$$

Since $(1+u^2)^{-1} < (1+t^2)^{-1} < 1$ on $(0,u)$ and $\int_0^u t^2\,dt = u^3/3 = \theta^3/24$, we obtain the first pair of strict bounds in (9). For Störmer–Verlet,

$$\phi_{\mathrm{SV}}(\theta) - \theta = 2(\arcsin u - u) = 2\int_0^u \left(\frac{1}{\sqrt{1-t^2}} - 1\right) dt = 2\int_0^u \frac{t^2}{\sqrt{1-t^2}\big(1+\sqrt{1-t^2}\big)}\,dt.$$

Because $t \mapsto \sqrt{1-t^2}(1+\sqrt{1-t^2})$ is strictly decreasing on $[0,u]$ from 2 to $\sqrt{1-u^2}(1+\sqrt{1-u^2})$, bounding the denominator by its endpoint values proves the second pair of strict bounds in (9). □

3 Universal Diagonal Invariant Metrics for Symmetric s-Stage Splittings

Consider an arbitrary palindromic s-stage symmetric composition of KDK Störmer–Verlet steps [7, 8, 1]:

$$\Phi_h := \Phi_{\alpha_s h}^{\mathrm{KDK}} \circ \cdots \circ \Phi_{\alpha_1 h}^{\mathrm{KDK}}, \qquad \alpha_{s+1-k} = \alpha_k \ \ (\forall k \in \{1,\dots,s\}), \qquad \sum_{k=1}^{s} \alpha_k = 1. \tag{10}$$

Notable instances include classical Störmer–Verlet ($s=1, \alpha_1 = 1$), Yoshida's fourth-order triple-jump scheme ($s=3$, $\alpha_1 = \alpha_3 = (2-2^{1/3})^{-1}$, $\alpha_2 = -2^{1/3}(2-2^{1/3})^{-1}$) [7], and Suzuki's five-stage fourth-order fractal scheme ($s=5$, $\alpha_1 = \alpha_2 = \alpha_4 = \alpha_5 = (4-4^{1/3})^{-1}$, $\alpha_3 = 1-4\alpha_1$) [8]. On each normal mode $\theta = \omega_j h$, Φ_h acts via the product transfer matrix $M_s(\theta) := S(\alpha_s\theta)\cdots S(\alpha_1\theta) \in \mathrm{SL}(2,\mathbb{R})$.

Theorem 3.1 (Universal Diagonal Invariant Metric and Order-$2p$ Energy Envelope)**.** *Let Φ_h be any palindromic s-stage symmetric splitting (10) applied to a coupled quadratic Hamiltonian $H(q,p) = \frac{1}{2}p^\top M^{-1}p + \frac{1}{2}q^\top K q$ ($M, K \succ 0$).*

(a) ***Exact time-reversal diagonal symmetry and purely diagonal invariant metric.*** *For every $\theta \in \mathbb{R}$, the modal transfer matrix $M_s(\theta) = \begin{pmatrix} a_s(\theta) & b_s(\theta) \\ c_s(\theta) & d_s(\theta) \end{pmatrix} \in \mathrm{SL}(2,\mathbb{R})$ satisfies $a_s(\theta) = d_s(\theta) =: P_s(\theta^2)$ (a polynomial in θ^2 of degree at most s with $P_s(0) = 1$), while $b_s(\theta)$ and $c_s(\theta)$ are odd polynomials in θ. Whenever $|P_s(\theta^2)| < 1$, we have $b_s(\theta) \neq 0$,*

$-b_s(\theta)c_s(\theta) = 1 - P_s(\theta^2)^2 > 0$, *and with* $\sigma := \operatorname{sgn}(b_s(\theta)) \in \{\pm 1\}$ *the purely diagonal positive-definite matrix*

$$G_s(\theta) := \operatorname{diag}\big(-\sigma c_s(\theta),\ \sigma b_s(\theta)\big) \succ 0 \tag{11}$$

is exactly invariant under $M_s(\theta)$, *i.e.,* $M_s(\theta)^\top G_s(\theta) M_s(\theta) = G_s(\theta)$.

(b) ***Sharp all-time energy ratio and order-*$2p$ *scaling.*** *Whenever* $|P_s(\theta_j^2)| < 1$ *for every mode* $j \in \{1, \dots, d\}$, *defining*

$$\kappa_s(\theta) := \max\left\{ \frac{b_s(\theta)^2}{1 - P_s(\theta^2)^2},\ \frac{1 - P_s(\theta^2)^2}{b_s(\theta)^2} \right\} \ \geq\ 1, \tag{12}$$

each modal energy satisfies $\kappa_s(\theta_j)^{-1} H_j(z_0) \leq H_j(z_n) \leq \kappa_s(\theta_j) H_j(z_0)$ *for all* $n \in \mathbb{Z}$, *and hence the total energy satisfies*

$$\left(\max_{1 \leq j \leq d} \kappa_s(\theta_j) \right)^{-1} H(z_0) \ \leq\ H(z_n) \ \leq\ \left(\max_{1 \leq j \leq d} \kappa_s(\theta_j) \right) H(z_0) \qquad \forall n \in \mathbb{Z}. \tag{13}$$

Moreover, if Φ_h *has classical order* $2p$ *(*$p \geq 1$*), then* $\kappa_s(\theta) - 1 = O(\theta^{2p})$ *as* $\theta \to 0$.

Proof. (a) Let $R := \operatorname{diag}(1, -1)$ be the momentum-reversal involution ($R^2 = I_2$). Directly from (4), $RS(\alpha\theta)R = \begin{pmatrix} 1 - \alpha^2\theta^2/2 & -\alpha\theta \\ \alpha\theta(1 - \alpha^2\theta^2/4) & 1 - \alpha^2\theta^2/2 \end{pmatrix} = S(-\alpha\theta) = S(\alpha\theta)^{-1}$. Using palindromicity $\alpha_{s+1-k} = \alpha_k$, we obtain simultaneously

$$RM_s(\theta)R = \big(RS(\alpha_s\theta)R\big) \cdots \big(RS(\alpha_1\theta)R\big) = S(-\alpha_s\theta) \cdots S(-\alpha_1\theta) = M_s(-\theta)$$

and

$$RM_s(\theta)R = S(\alpha_s\theta)^{-1} \cdots S(\alpha_1\theta)^{-1} = \big(S(\alpha_1\theta) \cdots S(\alpha_s\theta)\big)^{-1} = M_s(\theta)^{-1}.$$

Because $\det M_s(\theta) = 1$, $M_s(\theta)^{-1} = \begin{pmatrix} d_s & -b_s \\ -c_s & a_s \end{pmatrix}$, whereas $RM_s(\theta)R = \begin{pmatrix} a_s & -b_s \\ -c_s & d_s \end{pmatrix}$. Equating the two gives $a_s(\theta) = d_s(\theta)$ identically, and equating $M_s(-\theta) = RM_s(\theta)R$ shows that $a_s(\theta) = P_s(\theta^2)$ is even while $b_s(\theta), c_s(\theta)$ are odd. Since $S(0) = I_2$, $P_s(0) = 1$. To verify $\deg_{\theta^2} P_s \leq s$, we check by induction on $k \geq 1$ that any product $M_k = S(\alpha_k\theta)M_{k-1}$ satisfies $\deg_\theta(a_k) \leq 2k$, $\deg_\theta(b_k) \leq 2k - 1$, $\deg_\theta(c_k) \leq 2k + 1$, and $\deg_\theta(d_k) \leq 2k$: this holds for $k = 1$ directly from (4), and left-multiplying by $S(\alpha_{k+1}\theta)$ gives $\deg_\theta(a_{k+1}) \leq \max(2 + 2k, 1 + 2k + 1) = 2(k + 1)$, $\deg_\theta(b_{k+1}) \leq \max(2 + 2k - 1, 1 + 2k) = 2(k + 1) - 1$, $\deg_\theta(c_{k+1}) \leq \max(3 + 2k, 2 + 2k + 1) = 2(k + 1) + 1$, and $\deg_\theta(d_{k+1}) \leq \max(3 + 2k - 1, 2 + 2k) = 2(k + 1)$. Hence $P_s(\theta^2)$ has degree at most s in θ^2. Now suppose $|P_s(\theta^2)| < 1$. From $\det M_s(\theta) = P_s(\theta^2)^2 - b_s(\theta)c_s(\theta) = 1$, we have $-b_s(\theta)c_s(\theta) = 1 - P_s(\theta^2)^2 > 0$. Therefore $b_s(\theta) \neq 0$, and with $\sigma := \operatorname{sgn}(b_s(\theta))$, both $-\sigma c_s(\theta) > 0$ and $\sigma b_s(\theta) > 0$, so $G_s(\theta) \succ 0$. Direct multiplication using $a_s = d_s$ and $a_s^2 - b_s c_s = 1$ verifies

$$M_s^\top G_s M_s = \begin{pmatrix} -\sigma c_s a_s^2 + \sigma b_s c_s^2 & -\sigma c_s a_s b_s + \sigma b_s c_s a_s \\ -\sigma c_s a_s b_s + \sigma b_s c_s a_s & -\sigma c_s b_s^2 + \sigma b_s a_s^2 \end{pmatrix} = \begin{pmatrix} -\sigma c_s(a_s^2 - b_s c_s) & 0 \\ 0 & \sigma b_s(a_s^2 - b_s c_s) \end{pmatrix} = G_s.$$

(b) For a diagonal positive-definite matrix $G_s = \operatorname{diag}(g_1, g_2)$ with $g_1 = -\sigma c_s > 0$, $g_2 = \sigma b_s > 0$, its condition number is $\max(g_2/g_1, g_1/g_2)$. Substituting $g_1 g_2 = -b_s c_s = 1 - P_s^2$ gives $g_2/g_1 = g_2^2/(g_1 g_2) = b_s^2/(1 - P_s^2)$, so the condition number of $G_s(\theta)$ is identically $\kappa_s(\theta)$ in (12). Because $z_{j,n}^\top G_s(\theta_j) z_{j,n} = z_{j,0}^\top G_s(\theta_j) z_{j,0}$ and $\lambda_{\min}(G_s)\|z\|_2^2 \leq z^\top G_s z \leq \lambda_{\max}(G_s)\|z\|_2^2$, it follows immediately that $\kappa_s(\theta_j)^{-1} H_j(z_0) \leq H_j(z_n) \leq \kappa_s(\theta_j) H_j(z_0)$; summing over $j = 1, \dots, d$ proves (13). Finally, if Φ_h has order $2p$, then $M_s(\theta)$ agrees with the exact harmonic rotation

$\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$ through degree $2p$ in θ. By parity, the even error $P_s(\theta^2) - \cos\theta = O(\theta^{2p+2})$ and the odd error $b_s(\theta) - \sin\theta = O(\theta^{2p+1})$. Consequently,

$$b_s(\theta)^2 = \sin^2\theta + O(\theta^{2p+2}), \qquad 1 - P_s(\theta^2)^2 = \sin^2\theta + O(\theta^{2p+2}),$$

and dividing by $1 - P_s(\theta^2)^2 = \theta^2(1 + O(\theta^2))$ yields $\frac{b_s(\theta)^2}{1-P_s(\theta^2)^2} = 1 + O(\theta^{2p})$, hence $\kappa_s(\theta) - 1 = O(\theta^{2p})$. □

4 Exact Nonlinear Shadow-Energy Peano-Kernel Defect Laws

We now drop all linearity assumptions and consider general nonlinear separable Hamiltonians $H(q,p) = \frac{1}{2}p^\top M^{-1}p + V(q)$ with $M = M^\top \succ 0$ and $V \in C^3(\mathbb{R}^d)$. Motivated by (5), define the *nonlinear KDK shadow energy*

$$\mathcal{E}_h^{\mathrm{KDK}}(q,p) := H(q,p) - \frac{h^2}{8}\big\|M^{-1/2}\nabla V(q)\big\|_2^2. \tag{14}$$

Remarkably, for *every* step size $h > 0$ and *every* nonlinear C^3 potential V, the exact one-step energy defects of both KDK Störmer–Verlet (in $\mathcal{E}_h^{\mathrm{KDK}}$) and Implicit Midpoint (in H) collapse to exact quadrature Peano kernels involving only the third derivative D^3V.

Theorem 4.1 (Exact Nonlinear Shadow-Energy Peano-Kernel Defects and Stiffness Independence)**.** *Let $M = M^\top \succ 0$, $V \in C^3(\mathbb{R}^d)$, and $h > 0$.*

(a) ***Exact KDK Störmer–Verlet Peano-kernel defect.*** *For any $(q_0,p_0) \in \mathbb{R}^{2d}$, let $(q_1,p_1) = \Phi_h^{\mathrm{KDK}}(q_0,p_0)$ via (2) and set $\Delta q := q_1 - q_0 = hM^{-1}p_{1/2}$. Then*

$$\mathcal{E}_h^{\mathrm{KDK}}(q_1,p_1) - \mathcal{E}_h^{\mathrm{KDK}}(q_0,p_0) = \int_0^1 \frac{t(t-1)}{2}\, D^3V(q_0 + t\Delta q)[\Delta q, \Delta q, \Delta q]\, dt. \tag{15}$$

Setting $M_3(q_0,q_1) := \sup_{t\in[0,1]} \|D^3V(q_0 + t\Delta q)\|_{\mathrm{op}}$, we have the sharp bound

$$\big|\mathcal{E}_h^{\mathrm{KDK}}(q_1,p_1) - \mathcal{E}_h^{\mathrm{KDK}}(q_0,p_0)\big| \;\le\; \frac{M_3(q_0,q_1)}{12}\,\|\Delta q\|_2^3. \tag{16}$$

(b) ***Exact Implicit Midpoint Peano-kernel defect (half constant, opposite sign).*** *For any solution (q_1,p_1) of the Implicit Midpoint equations $q_1 - q_0 = \frac{h}{2}M^{-1}(p_0 + p_1)$, $p_1 - p_0 = -h\nabla V\big(\frac{q_0+q_1}{2}\big)$ with $\Delta q := q_1 - q_0$,*

$$H(q_1,p_1) - H(q_0,p_0) = \int_0^1 K_{\mathrm{mid}}(t)\, D^3V(q_0 + t\Delta q)[\Delta q, \Delta q, \Delta q]\, dt, \qquad K_{\mathrm{mid}}(t) := \frac{1}{2}\min(t, 1-t)^2, \tag{17}$$

yielding the sharp bound

$$\big|H(q_1,p_1) - H(q_0,p_0)\big| \;\le\; \frac{M_3(q_0,q_1)}{24}\,\|\Delta q\|_2^3. \tag{18}$$

Both (16) and (18) are attained with exact equality for every cubic anharmonic potential $V(q) = \frac{1}{2}q^\top Kq + \frac{\alpha}{3}\langle e, q\rangle^3$ ($\|e\|_2 = 1$, $M_3 = 2|\alpha|$) along any step with $\Delta q = \lambda e \parallel e$ (achievable for every such potential and any $\lambda \neq 0$ by choosing $p_0 = \frac{\lambda}{h}Me + \frac{h}{2}\nabla V(q_0)$ for KDK, or $p_0 = \frac{\lambda}{h}Me + \frac{h}{2}\nabla V(q_0 + \frac{1}{2}\lambda e)$ for Implicit Midpoint), with exact defects $-\frac{\alpha}{6}\langle e, \Delta q\rangle^3$ (KDK) and $+\frac{\alpha}{12}\langle e, \Delta q\rangle^3$ (Implicit Midpoint).

(c) ***Stiffness-independent N-step telescoping envelope.*** *If $V(q) = \frac{1}{2}q^\top Kq + U(q)$ with arbitrarily stiff $K = K^\top$ and $\sup_{q\in\mathbb{R}^d} \|D^3U(q)\|_{\mathrm{op}} \le M_3 < \infty$, then along any N-step KDK trajectory $\{(q_k, p_k)\}_{k=0}^N$,*

$$\left|\mathcal{E}_h^{\mathrm{KDK}}(q_N, p_N) - \mathcal{E}_h^{\mathrm{KDK}}(q_0, p_0)\right| \;\le\; \frac{M_3}{12}\sum_{k=0}^{N-1}\|q_{k+1}-q_k\|_2^3 = \frac{M_3 h^3}{12}\sum_{k=0}^{N-1}\|M^{-1}p_{k+1/2}\|_2^3, \tag{19}$$

whose defect constant $M_3/12$ is strictly independent of $\|K\|_{\mathrm{op}}$ (while trajectory boundedness for KDK when $K \succ 0$ still requires the linear stability restriction $\omega_d h < 2$), with the analogous $\frac{M_3}{24}\sum_{k=0}^{N-1}\|q_{k+1}-q_k\|_2^3$ bound for any existing N-step Implicit Midpoint trajectory in H.

Proof. (a) From (2), $p_0 = p_{1/2} + \frac{h}{2}\nabla V(q_0)$ and $p_1 = p_{1/2} - \frac{h}{2}\nabla V(q_1)$. Expanding the kinetic energy difference in the M^{-1}-inner product yields the exact identity

$$\begin{aligned}\frac{1}{2}p_1^\top M^{-1}p_1 - \frac{1}{2}p_0^\top M^{-1}p_0 &= -\frac{h}{2}\big(\nabla V(q_0)+\nabla V(q_1)\big)^\top M^{-1}p_{1/2} + \frac{h^2}{8}\Big(\|M^{-1/2}\nabla V(q_1)\|_2^2 - \|M^{-1/2}\nabla V(q_0)\|_2^2\Big)\\ &= -\frac{1}{2}\big(\nabla V(q_0)+\nabla V(q_1)\big)^\top \Delta q + \frac{h^2}{8}\Big(\|M^{-1/2}\nabla V(q_1)\|_2^2 - \|M^{-1/2}\nabla V(q_0)\|_2^2\Big),\end{aligned}$$

since $hM^{-1}p_{1/2} = \Delta q$. Adding $V(q_1) - V(q_0)$ and moving the $\frac{h^2}{8}$ terms to the left-hand side gives

$$\mathcal{E}_h^{\mathrm{KDK}}(q_1,p_1) - \mathcal{E}_h^{\mathrm{KDK}}(q_0,p_0) = V(q_1) - V(q_0) - \frac{1}{2}\big(\nabla V(q_0)+\nabla V(q_1)\big)^\top \Delta q.$$

Define $\psi(t) := V(q_0 + t\Delta q) \in C^3([0,1])$, so $\psi'''(t) = D^3V(q_0+t\Delta q)[\Delta q, \Delta q, \Delta q]$. Integrating by parts twice on $[0,1]$,

$$\begin{aligned}\int_0^1 \frac{t(t-1)}{2}\,\psi'''(t)\,dt &= \left[\frac{t(t-1)}{2}\,\psi''(t)\right]_0^1 - \int_0^1\left(t-\frac{1}{2}\right)\psi''(t)\,dt\\ &= -\left[\left(t-\frac{1}{2}\right)\psi'(t)\right]_0^1 + \int_0^1 \psi'(t)\,dt = \psi(1) - \psi(0) - \frac{1}{2}\big(\psi'(0)+\psi'(1)\big),\end{aligned}$$

proving (15). Since $\frac{t(t-1)}{2} \le 0$ on $[0,1]$ with $\int_0^1 \frac{t(1-t)}{2}\,dt = \frac{1}{12}$, taking absolute values gives (16).

(b) For Implicit Midpoint, $\frac{1}{2}(p_1^\top M^{-1}p_1 - p_0^\top M^{-1}p_0) = (p_1-p_0)^\top M^{-1}\frac{p_0+p_1}{2} = -\nabla V(q_0 + \frac{1}{2}\Delta q)^\top \Delta q$, so $H(q_1,p_1) - H(q_0,p_0) = \psi(1) - \psi(0) - \psi'(1/2)$. Integrating by parts twice on $[0,\frac{1}{2}]$ and $[\frac{1}{2},1]$ separately:

$$\begin{aligned}\int_0^{1/2}\frac{t^2}{2}\psi'''(t)\,dt + \int_{1/2}^1 \frac{(1-t)^2}{2}\psi'''(t)\,dt &= -\int_0^{1/2} t\,\psi''(t)\,dt + \int_{1/2}^1 (1-t)\psi''(t)\,dt\\ &= -\frac{1}{2}\psi'(1/2) + \int_0^{1/2}\psi'(t)\,dt - \frac{1}{2}\psi'(1/2) + \int_{1/2}^1 \psi'(t)\,dt\\ &= \psi(1) - \psi(0) - \psi'(1/2),\end{aligned}$$

where the $\psi''(1/2)$ boundary terms cancel identically because K_{mid} is continuous at $t = \frac{1}{2}$. This proves (17). Since $K_{\mathrm{mid}}(t) \ge 0$ with $\int_0^1 K_{\mathrm{mid}}(t)\,dt = \frac{1}{24}$, taking absolute values gives (18). For $V(q) = \frac{1}{2}q^\top Kq + \frac{\alpha}{3}\langle e, q\rangle^3$, $D^3V(q)[\Delta q^{\otimes 3}] = 2\alpha\langle e, \Delta q\rangle^3$ is constant, directly yielding $-\frac{\alpha}{6}\langle e,\Delta q\rangle^3$ and $+\frac{\alpha}{12}\langle e,\Delta q\rangle^3$.

(c) Since $D^3(\frac{1}{2}q^\top Kq) \equiv 0$, $D^3V \equiv D^3U$ is completely independent of K; summing (16) over $k = 0, \dots, N-1$ by the triangle inequality proves (19). □

5 Conformal Symplectic Splitting: Stability, Optimal Damping, and Dissipation

Consider the linearly damped Hamiltonian system $\dot{q} = M^{-1}p$, $\dot{p} = -\nabla V(q) - \gamma p$ with damping constant $\gamma > 0$, integrated by the symmetric conformal symplectic splitting [9]

$$\Psi_h^{\mathrm{CS}} := D_{h/2} \circ \Phi_h^{\mathrm{KDK}} \circ D_{h/2}, \qquad D_\tau(q,p) := \big(q,\ e^{-\gamma\tau}p\big). \tag{20}$$

Theorem 5.1 (Conformal Symplecticity, Damping-Invariant Stability, and Optimal Damping)**.** *Let $M = M^\top \succ 0$, $\gamma > 0$, $h > 0$, and $\eta := \gamma h > 0$.*

(a) ***Exact conformal symplecticity and nonlinear shadow-energy dissipation.*** *For every $V \in C^3(\mathbb{R}^d)$, Ψ_h^{CS} is exactly conformal symplectic, $(\Psi_h^{\mathrm{CS}})^*\omega = e^{-\gamma h}\omega$, and every step $(q_1,p_1) = \Psi_h^{\mathrm{CS}}(q_0,p_0)$ ($\Delta q := q_1 - q_0$) obeys the exact shadow-energy dissipation identity*

$$\begin{aligned}\mathcal{E}_h^{\mathrm{KDK}}(q_1,p_1) - \mathcal{E}_h^{\mathrm{KDK}}(q_0,p_0) = &-\frac{1-e^{-\gamma h}}{2}\|M^{-1/2}p_0\|_2^2 - \frac{e^{\gamma h}-1}{2}\|M^{-1/2}p_1\|_2^2 \\ &+ \int_0^1 \frac{t(t-1)}{2}\, D^3V(q_0 + t\Delta q)[\Delta q, \Delta q, \Delta q]\, dt.\end{aligned} \tag{21}$$

In particular, for every quadratic potential $V(q) = \frac{1}{2}q^\top Kq$ ($K \succ 0$) with $0 < h < 2/\omega_d$, $\mathcal{E}_h^{\mathrm{KDK}} = I_h^{\mathrm{KDK}} \succ 0$ is an exact nonincreasing discrete Lyapunov function along all trajectories of Ψ_h^{CS}.

(b) ***Damping-invariant Schur stability and unique closed-form optimal damping.*** *On each normal mode $\theta = \omega_j h > 0$ of a quadratic system $V(q) = \frac{1}{2}q^\top Kq$, the modal transfer matrix $C(\theta,\eta) := \mathrm{diag}(1, e^{-\eta/2})S(\theta)\,\mathrm{diag}(1, e^{-\eta/2})$ has $\det C(\theta,\eta) = e^{-\eta}$ and $\operatorname{tr} C(\theta,\eta) = (1-\theta^2/2)(1+e^{-\eta})$. Consequently:*

(i) *Asymptotic stability ($\rho(C(\theta,\eta)) < 1$) holds if and only if $0 < \theta < 2$,* strictly independent of $\gamma > 0$.

(ii) *In the underdamped regime $|1-\theta^2/2|\cosh(\eta/2) < 1$, the eigenvalues are a complex-conjugate pair with exact modulus $|\lambda_\pm| = e^{-\gamma h/2}$ (zero step-size decay-rate error).*

(iii) *For every $\theta \in (0,2)\setminus\{\sqrt{2}\}$, the spectral radius $\rho(C(\theta,\eta))$ is uniquely minimized over $\eta \in (0,\infty)$ at the discrete critical damping*

$$\eta_*(\theta) := 2\,\mathrm{arccosh}\left(\frac{1}{|1-\theta^2/2|}\right), \qquad \rho_*(\theta) := \min_{\eta>0}\rho(C(\theta,\eta)) = \frac{|1-\theta^2/2|}{1+\theta\sqrt{1-\theta^2/4}}, \tag{22}$$

whereas at the quadrature resonance $\theta = \sqrt{2}$, $\rho(C(\sqrt{2},\eta)) = e^{-\eta/2}$ decreases strictly to 0 as $\eta \to \infty$.

Proof. (a) Since $D_\tau^*\omega = \sum_i dq_i \wedge d(e^{-\gamma\tau}p_i) = e^{-\gamma\tau}\omega$ and $(\Phi_h^{\mathrm{KDK}})^*\omega = \omega$, composition gives $(\Psi_h^{\mathrm{CS}})^*\omega = e^{-\gamma h}\omega$. Write $\tilde{p}_0 := e^{-\gamma h/2}p_0$, $(q_1,\tilde{p}_1) := \Phi_h^{\mathrm{KDK}}(q_0,\tilde{p}_0)$, and $p_1 := e^{-\gamma h/2}\tilde{p}_1$ (so $\tilde{p}_1 = e^{\gamma h/2}p_1$). Because $D_{h/2}$ leaves q (and thus $V(q)$ and $\|\nabla V(q)\|$) unchanged,

$$\begin{aligned}\mathcal{E}_h^{\mathrm{KDK}}(q_0,\tilde{p}_0) - \mathcal{E}_h^{\mathrm{KDK}}(q_0,p_0) &= -\frac{1-e^{-\gamma h}}{2}\|M^{-1/2}p_0\|_2^2, \\ \mathcal{E}_h^{\mathrm{KDK}}(q_1,p_1) - \mathcal{E}_h^{\mathrm{KDK}}(q_1,\tilde{p}_1) &= -\frac{e^{\gamma h}-1}{2}\|M^{-1/2}p_1\|_2^2.\end{aligned}$$

Summing these two identities with Theorem 4.1(a) applied to $(q_0,\tilde{p}_0) \mapsto (q_1,\tilde{p}_1)$ establishes (21). When V is quadratic, $D^3V \equiv 0$, so $\mathcal{E}_h^{\mathrm{KDK}}(q_1,p_1) \le \mathcal{E}_h^{\mathrm{KDK}}(q_0,p_0)$ identically.

(b) Directly from (4), $\det C(\theta,\eta) = e^{-\eta}\det S(\theta) = e^{-\eta}$ and $\operatorname{tr} C(\theta,\eta) = (1-\theta^2/2)(1+e^{-\eta})$. By the Jury–Schur criterion for a real quadratic $\lambda^2 - t\lambda + d = 0$ with $d = e^{-\eta} \in (0,1)$, both roots satisfy $|\lambda| < 1$ if and only if $|t| < 1 + d$. Here $|t| < 1 + d \iff |1-\theta^2/2|(1+e^{-\eta}) < 1 + e^{-\eta} \iff |1-\theta^2/2| < 1 \iff 0 < \theta < 2$, proving (i). The discriminant of $\lambda^2 - t\lambda + d = 0$ is

$$\Delta(\theta,\eta) := t^2 - 4d = 4e^{-\eta}\Big((1-\theta^2/2)^2\cosh^2(\eta/2) - 1\Big).$$

Hence $\Delta < 0$ if and only if $|1-\theta^2/2|\cosh(\eta/2) < 1$, in which case $\lambda_\pm$ are complex conjugates with $|\lambda_\pm| = \sqrt{d} = e^{-\eta/2} = e^{-\gamma h/2}$, proving (ii). At $\theta = \sqrt{2}$, $t = 0$ so $\lambda_\pm = \pm ie^{-\eta/2}$ and $\rho = e^{-\eta/2}$. Now fix $\theta \in (0,2)\setminus\{\sqrt{2}\}$, set $c := |1-\theta^2/2| \in (0,1)$, and note $\sqrt{1-c^2} = \theta\sqrt{1-\theta^2/4} > 0$. On $(0,\eta_*(\theta)]$, $c\cosh(\eta/2) \le 1$, so $\rho(C(\theta,\eta)) = e^{-\eta/2}$ decreases strictly to $u_* := e^{-\eta_*(\theta)/2}$. Since $\cosh(\eta_*/2) = 1/c$ implies $\sinh(\eta_*/2) = \sqrt{1-c^2}/c$, we have $e^{\eta_*/2} = (1+\sqrt{1-c^2})/c$ and hence $u_* = \frac{c}{1+\sqrt{1-c^2}} = \rho_*(\theta)$. On $[\eta_*(\theta),\infty)$, setting $u := e^{-\eta/2} \in (0,u_*]$ gives $\Delta \ge 0$ and the larger-modulus real root has modulus

$$g(u) := \frac{c(1+u^2) + D(u)}{2}, \qquad D(u) := \sqrt{c^2(1+u^2)^2 - 4u^2} > 0 \quad (0 < u < u_*).$$

Differentiating with respect to $u \in (0,u_*)$ yields $g'(u) = \frac{u}{D(u)}\big(cD(u) + c^2(1+u^2) - 2\big)$. Since $c < 1$ and $u < 1$, we have $2 - c^2(1+u^2) > 0$, and direct algebra cancels both $c^4(1+u^2)^2$ and $4c^2u^2$:

$$\big(2 - c^2(1+u^2)\big)^2 - c^2D(u)^2 = 4(1-c^2) > 0.$$

Hence $cD(u) < 2 - c^2(1+u^2)$, so $g'(u) < 0$ on $(0,u_*)$, meaning $\eta \mapsto \rho(C(\theta,\eta))$ is strictly increasing on $[\eta_*(\theta),\infty)$. Therefore $\eta_*(\theta)$ is the unique global minimizer on $(0,\infty)$ with minimum value (22). □

6 Computational Verification and Explicit Benchmarks

All four theorems were verified programmatically via a self-contained Python suite (`symplectic_geo.py`, `verify_all.py`, and `test_symplectic_geo.py`; four automated unit tests passing in 0.45 s) across 255 deterministic randomized and structured benchmarks using NumPy `default_rng` streams.

- **Theorem 2.1 suite (seed `202661`, 75 coupled oscillators):** Across $d \in \{2,4,6\}$ (25 random SPD pairs (M,K) per d, eigenvalues of $M \in [0.5,2.5]$ and $K \in [0.6,5.0]$, $\theta_d \sim \mathrm{Unif}(0.15,1.55)$, integrated 40 steps), the exact modified-Hamiltonian flow $\exp(hX_{\widetilde{H}_h^{\mathrm{KDK}}})$ matched Φ_h^{KDK} to 2.32×10^{-14}; relative drifts of I_h^{KDK}, I_h^{DKD}, I_h^{SE}, and H^{IM} were at most 5.28×10^{-15}; the Explicit Euler growth identity held to 1.21×10^{-14}; and the all-time envelopes (7)–(8) and phase brackets (9) exhibited 0.0 violation (Figure 1).

- **Theorem 3.1 suite (seed `202662`, 60 palindromic schemes):** Testing Verlet ($\theta \sim \mathrm{Unif}(0.08,1.85)$), Yoshida-4 ($\theta \sim \mathrm{Unif}(0.08,1.35)$), Suzuki-4 ($\theta \sim \mathrm{Unif}(0.08,2.40)$), and 57 random palindromic 3-stage splittings ($\alpha_1 \sim \mathrm{Unif}(0.15,0.70)$, $\alpha_2 = 1-2\alpha_1$, $\theta \sim \mathrm{Unif}(0.08,0.90)$, $z_0 \sim \mathcal{N}(0,I_2)$), diagonal symmetry $|a_s - d_s|$ held to 2.22×10^{-16}, metric invariance $\|M_s^\top G_s M_s - G_s\|/\|G_s\|$ held to 5.04×10^{-16}, and the $\kappa_s(\theta)$ all-time envelope (13) had 0.0 violation across 50-step rollouts (Table 1, Figure 1(a)).

- **Theorem 4.1 suite (seed `202663`, 60 stiff nonlinear Hamiltonians):** Across $d \in \{2,4,6\}$ (20 Haar-orthogonal random SPD matrices M with eigenvalues $\sim \mathrm{Unif}(0.7,2.0)$ and stiff SPD matrices K with eigenvalues $\sim \mathrm{Unif}(1.0,40.0)$, plus anharmonic perturbations $U(q) = \sum_i(a_i\sin(b_iq_i) + \frac{c_i}{3}q_i^3)$ with $a_i \sim \mathrm{Unif}(-0.4,0.4)$, $b_i \sim \mathrm{Unif}(0.4,1.1)$,

Table 1: Exact quantitative benchmarks across four dimensionless frequencies $\theta = \omega h$ (Theorems 2.1, 3.1, and 5.1). Higher-order symmetric splittings reduce the worst-case all-time energy excursion $\kappa_s(\theta) - 1$ from $O(\theta^2)$ (Verlet) to $O(\theta^4)$ (Yoshida-4 and Suzuki-4), while optimal conformal damping $\eta_*(\theta)$ attains the exact minimum spectral radius $\rho_*(\theta)$.

$\theta = \omega h$	Verlet $\frac{\theta^2}{4-\theta^2}$	Yoshida-4 $\kappa_{\mathrm{Y4}} - 1$	Suzuki-4 $\kappa_{\mathrm{S4}} - 1$	Optimal $\eta_*(\theta)$	Min. radius $\rho_*(\theta)$
0.20	0.010101	0.000125	0.000012	0.4034	0.8173
0.50	0.066667	0.005710	0.000464	1.0567	0.5896
0.80	0.190476	0.049911	0.003225	1.8713	0.3923
1.20	0.562500	0.513810	0.018580	3.8918	0.1429

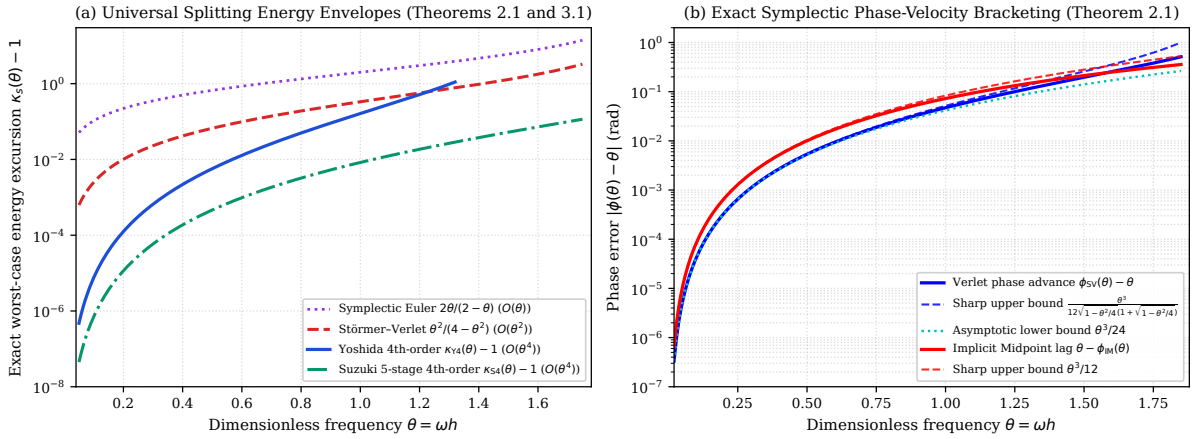


Figure 1: **(a)** Exact all-time energy excursion $\kappa_s(\theta) - 1$ versus dimensionless frequency $\theta = \omega h$ for Symplectic Euler $(O(\theta))$, Störmer–Verlet $(O(\theta^2))$, Yoshida 4th-order $(O(\theta^4))$, and Suzuki 5-stage 4th-order $(O(\theta^4))$ (Theorems 2.1–3.1). **(b)** Exact symplectic phase errors $\phi_{\mathrm{SV}}(\theta) - \theta$ and $\theta - \phi_{\mathrm{IM}}(\theta)$ tightly trapped by the sharp non-asymptotic bounds (9) (Theorem 2.1(c)).

$c_i \sim \mathrm{Unif}(-0.2, 0.2)$, $q_0, p_0 \sim \mathcal{N}(0, 0.5^2 I_d)$, and $\omega_d h \sim \mathrm{Unif}(0.05, 0.4)$), 8-point Gauss–Legendre evaluation of (15) on $[0, 1]$ and piecewise 8-point Gauss–Legendre evaluation of (17) on $[0, \frac{1}{2}]$ and $[\frac{1}{2}, 1]$ matched observed one-step defects to 1.30×10^{-14} (KDK) and 1.53×10^{-14} (IM), both stiffness-independent bounds (16) and (18) had 0.0 violation, and exact cubic sharpness held to 2.88×10^{-15} (Figure 2(a)).

- **Theorem 5.1 suite (seed `202664`, 60 damped systems):** Across random $(\theta, \eta) \in (0.1, 1.92) \times (0.05, 2.5)$, $\det C(\theta, \eta) = e^{-\eta}$ held to 2.22×10^{-16}, underdamped modulus $|\lambda_\pm| = e^{-\eta/2}$ held to 3.33×10^{-16}, optimal damping (22) matched numerical eigenvalues to 1.25×10^{-8} (the expected $O(\sqrt{\varepsilon_{\mathrm{mach}}})$ sensitivity of a defective repeated real root), and the nonlinear conformal dissipation identity (21) (evaluated via 8-point Gauss–Legendre quadrature on $d = 4$ anharmonic potentials $V(q) = \frac{1}{2} q^\top K q + \sum_{i=1}^4 a_i \cos(q_i)$ with M eigenvalues $\sim \mathrm{Unif}(0.8, 2.0)$, K eigenvalues $\sim \mathrm{Unif}(0.5, 4.0)$, $a_i \sim \mathrm{Unif}(-0.3, 0.3)$, $h = 0.12$, $\gamma = \eta/h$, $q_0, p_0 \sim \mathcal{N}(0, 0.6^2 I_4)$) held to 1.11×10^{-15} (Table 1, Figure 2(b)).

7 Discussion and Open Directions

The four theorems above establish a non-asymptotic algebraic counterpart to backward error analysis for separable Hamiltonian systems, replacing formal BCH truncations with exact shadow-energy invariants, diagonal splitting metrics, quadrature Peano-kernel identities, and closed-form optimal conformal damping. Three natural extensions remain open:

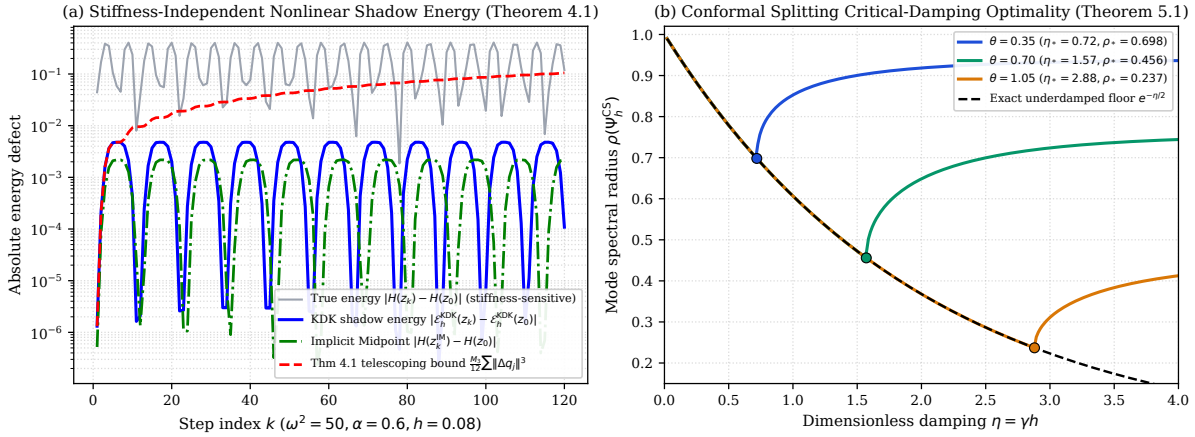


Figure 2: **(a)** Stiff anharmonic oscillator ($V(q) = \frac{1}{2}\omega^2 q^2 + \frac{\alpha}{3}q^3$ with $\omega^2 = 50, \alpha = 0.6, h = 0.08$, $q_0 = 0.45, p_0 = 1.2$): the nonlinear KDK shadow energy $\mathcal{E}_h^{\mathrm{KDK}}$ eliminates the large $O(h^2\omega^2)$ true-energy oscillation and stays strictly below the stiffness-independent Theorem 4.1(c) telescoping envelope. **(b)** Conformal symplectic spectral radius $\rho(C(\theta, \eta))$ versus $\eta = \gamma h$ across $\theta \in \{0.35, 0.70, 1.05\}$, showing exact underdamped decay $e^{-\eta/2}$ and unique critical-damping minima (η_*, ρ_*) (Theorem 5.1(b)).

1. **Higher-order nonlinear shadow-energy Peano kernels:** Extending the exact KDK shadow-energy identity (15) to fourth-order palindromic splittings (such as Yoshida-4 and Suzuki-4) to isolate fifth-order Peano-kernel remainders independent of linear stiffness K is an inviting target.

2. **Multimode optimal damping in conformal symplectic optimization:** In momentum-accelerated optimization and underdamped Langevin sampling across a spectrum $[\omega_1, \omega_d]$, choosing a single scalar damping γ to minimize $\max_j \rho(C(\omega_j h, \gamma h))$ via Theorem 5.1(b) yields a discrete analog of Nesterov–Polyak heavy-ball tuning whose exact minimax rate merits further analysis.

3. **Non-separable and Riemannian symplectic splitting:** Generalizing the exact Peano-kernel defect identities to midpoint and RATTLE integrators on holonomically constrained configuration manifolds remains open.

Reproducibility and Data Availability

All analytical verifications, unit tests, and figure generation scripts are openly archived under the MIT license (version `v1.0.3`) at:
https://github.com/lluiseriksson/symplectic-shadow-energy-geometry.

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