

Analysis of Kinetic Langevin Monte Carlo Under The Stochastic Exponential Euler Discretization From Underdamped All The Way to Overdamped

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Abstract Simulating the kinetic Langevin dynamics is a popular approach for sampling from distributions, where only their unnormalized densities are available. Various discretizations of the kinetic Langevin dynamics have been considered, where the resulting algorithm is collectively referred to as the kinetic Langevin Monte Carlo (KLMC) or underdamped Langevin Monte Carlo. Specifically, the stochastic exponential Euler discretization, or exponential integrator for short, has previously been studied under strongly log-concave and log-Lipschitz smooth potentials via the synchronous Wasserstein coupling strategy. Existing analyses, however, impose restrictions on the parameters that do not explain the behavior of KLMC under various choices of parameters. In particular, all known results fail to hold in the overdamped regime, suggesting that the exponential integrator degenerates in the overdamped limit. In this work, we revisit the synchronous Wasserstein coupling analysis of KLMC with the exponential integrator. Our refined analysis results in Wasserstein contractions and bounds on the asymptotic bias that hold under weaker restrictions on the parameters, which assert that the exponential integrator is capable of stably simulating the kinetic Langevin dynamics in the overdamped regime, as long as proper time acceleration is applied.

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1 Introduction

Consider a differentiable potential function $U : \mathbb{R}^d \mapsto \mathbb{R}$. This work focuses on the kinetic Langevin dynamics $(Z_t = (X_t, V_t))_{t \geq 0}$ described by the system of equations, for each $t \geq 0$,

$$\begin{aligned} dX_t &= V_t dt \\ dV_t &= -\eta \nabla U(X_t) dt - \gamma V_t dt + \sqrt{2\gamma\eta} dB_t, \end{aligned} \tag{1}$$

where $(B_t)_{t \geq 0}$ is a standard d -dimensional brownian motion on the filtered probability space $(\Omega, \mathcal{F}, \mathbb{P}, (\mathcal{F}_t)_{t \geq 0})$ satisfying typical conditions, $\eta > 0$ is the inverse mass, $\gamma > 0$ is the friction coefficient, and X_t and V_t are respectively referred to as the position and the momentum. Numerically simulating Eq. (1) has been an important application in molecular dynamics for modeling interacting particles [LM15, Eqs. (6.30)–(6.31)].

In recent years, Eq. (1) has received massive interest from computational statistics and machine learning for the purpose of drawing samples from distributions with only unnormalized densities. Specifically, under mild assumptions, the process $(Z_t)_{t \geq 0}$ converges to its unique stationary measure [Pav14, Prop. 6.1] on $\mathbb{R}^{2d}$,

$$\pi(dx, dv) \triangleq \frac{1}{Z} \exp(-U(x)) dx \, N(dv; 0_d, \eta I_d), \quad \text{where } Z \triangleq \int_{\mathbb{R}^d} U(x) dx, \tag{2}$$

and $N(\cdot; 0_d, \eta I_d)$ is a d -dimensional multivariate Gaussian distribution with mean 0_d and covariance ηI_d . Therefore, even if we have only access to ∇U , Eq. (1) can be used to produce samples from π in Eq. (2) as long as Eq. (1) is accurately simulated. This scheme, known as kinetic Langevin Monte Carlo (KLMC), or underdamped Langevin Monte Carlo, has been used in various contexts from generative modeling [SS21; DVK21], producing unbiased estimators of expectations [CLP+24], multi-armed bandits [ZDM+24], simulating path measures [KXG+25; DGM+22; GD23; BBR+25] in sequential Monte Carlo [DMDJ06]

and annealed importance sampling [Nea01], marginal likelihood maximization [OA24], and many more.

For numerical simulation, however, a discretization scheme has to be involved. The Markov chain resulting from discretization $(Z_k = (X_k, V_k))_{k \geq 0}$ is often “asymptotically” biased in the sense that, for the discretization step size $h \geq 0$, the stationary distribution of $(Z_k)_{k \geq 0}$, π_h , will be different from π . Furthermore, different discretization schemes can behave differently in terms of speed of convergence to stationarity, computational efficiency, dependence on the properties of U , and the amount of asymptotic bias. As such, for the purpose of sampling from Eq. (2), various discretizations of Eq. (1) have been proposed [CCB+18; LM13; SZ21; FLO21; SL19; LFZ23] and analyzed [CDM+24; MS24; MCC+21; ACZ25; DR20; DEM+25; SW24; ZCL+23; JLS24; FW24; LPW24; Mon21; GBM+25; DKR22].

Among various discretization schemes, we focus on the stochastic exponential Euler scheme, which we will hereafter refer to as the exponential integrator. The use of this scheme for sampling was first proposed and analyzed by Cheng et al. [CCB+18], where they provide a mixing time guarantee under the assumption that U is α -strongly log-concave and β -log-Lipschitz smooth through a synchronous Wasserstein coupling analysis [Che24, §4.1]. Their analysis has since been refined multiple times [DR20; SZ21; LPW24], which we will formally introduce in the following paragraph. The exponential integrator has also been studied under the assumption that U is non-strongly log-concave [DKR22] and the framework of log-Sobolev and Poincaré functional inequalities [MCC+21; ZCL+23]. This work, however, focuses on the strongly log-concave setting.

To state formal results, consider the KLMC algorithm obtained via the exponential integrator with the initial state $(X_0, V_0) \sim \mu_0$ from some μ_0 . Denoting the Wasserstein-2 distance as $W_2(\cdot, \cdot)$, the marginal distribution at step $k \geq 0$ as μ_k such that $(X_k, V_k) \sim \mu_k$, for any $\epsilon > 0$, to guarantee that $W_2(\mu_k, \pi) \leq \alpha^{-1/2} \epsilon$ [SZ21; DR20], simulating the discretized kinetic Langevin dynamics for $O(\kappa^{3/2} d^{1/2} \epsilon \log \epsilon^{-1})$ steps is sufficient, where $\kappa = \beta/\alpha$ is the condition number. This number of steps has also been recently shown to be sufficient for bounding the Kullback-Leibler divergence [KL51] between μ_k and π [ACZ25] under the same conditions.

Unfortunately, the analysis by Sanz-Serna and Zygalkakis [SZ21] does not fully shed light on the effect of the parameters γ, η , and the integration step size h . That is, they only obtain a Wasserstein contraction for $\eta \in (0, 4/(\alpha + \beta))$, $\gamma = 2$ and when h is smaller than some unknown threshold [SZ21, Ex. 4.13]. While the remaining analyses [DR20; ACZ25] provide more general and concrete conditions on γ and h , they also have limitations. A well-known aspect of Eq. (1) is that, after rescaling the time as $t' = \gamma t$, setting $\eta = 1$, and taking the overdamped limit $\gamma \rightarrow \infty$, we obtain the overdamped Langevin dynamics [Pav14, §6.5]

$$dX_{t'} = -\nabla U(X_{t'}) dt' + \sqrt{2} dB_{t'} . \quad (3)$$

The results by Dalalyan and Riou-Durand [DR20, Thm. 2] and Altschuler, Chewi, and Zhang [ACZ25, Thm. 4.1] suggest that the exponential integrator is unable to simulate Eq. (1) in this regime. Specifically, they require that the discretization step size h satisfies $h = O(1/\gamma)$, which means that, as $\gamma \rightarrow \infty$, the step size has to degenerate as $h \rightarrow 0$. A similar conclusion is drawn by Leimkuhler, Paulin, and Whalley [LPW24], who conclude that the discretized dynamics require $h = O(1/\gamma)$ to form a Wasserstein contraction. This clearly cannot be the case since, for any $h_{\text{LMC}} > 0$, by setting $h = h_{\text{LMC}}\gamma$, $\eta = 1$, and taking

the limit $\gamma \rightarrow \infty$, the update rule for the KLMC with the exponential integrator exactly coincides with the Euler-Maruyama discretization of Eq. (3), widely known as Langevin Monte Carlo (LMC; [RDF78; Par81; GM94]). This suggests that there is still room for improvement for the synchronous Wasserstein coupling approach.

Furthermore, existing analyses of the asymptotic bias of KLMC with the exponential integrator become vacuous in the overdamped limit. More concretely, the asymptotic bias of KLMC with the exponential integrator in Wasserstein-2 distance $W_2(\pi_h, \pi)$ is well-known to scale as $O(h)$ [CCB+18, Thm. 9]. In the overdamped limit, however, as $\gamma \rightarrow \infty$, the time-accelerated step size diverges $h = h_{\text{LMC}}\gamma \rightarrow \infty$, making these bounds vacuous. Instead, one would expect a non-vacuous phase transition into a $O(h_{\text{LMC}}^{1/2})$ scaling, which is the asymptotic bias of LMC [DM19, Cor. 7]. Previously, no analysis has been able to identify this phase transition.

In this work, we refine the synchronous Wasserstein coupling analysis of KLMC with the exponential integrator when U is α -strongly log-concave and β -log smooth. Additional details on the setup and the assumptions are stated in Section 2. Our contributions are as follows:

- Section 3.1: We relax the assumptions on the parameters h, γ, η required to ensure that the discretized process converges to its (biased) stationary distribution. Under a general condition on h, η , and γ , Theorem 3.1 establishes a Wasserstein contraction with a rate that depends on these parameters. Corollary 3.2 states that this result implies a rate of convergence to stationarity of $O(h\eta\alpha/\gamma)$. In the underdamped regime, this matches previously known rates [LPW24, Thm. 6.1]. However, our result imposes weaker restrictions on the step size h , and can be satisfied even in the overdamped regime. Indeed, in the overdamped limit, the contraction rate of KLMC coincides with the corresponding contraction rate of the overdamped Langevin discretized with the Euler-Maruyama scheme (Corollary 3.3).
- Section 3.2: We provide a more general result on the asymptotic bias of the stationary distribution of the discretized process in Wasserstein-2 distance. Under conditions sufficient to ensure convergence to stationarity, Theorem 3.3 provides a bound on the asymptotic bias in Wasserstein-2 distance. Specifically, it shows that the asymptotic bias scales as $O(h^2\gamma + h)$ and $O(h^{1/2}\gamma^{-1/2} + h^{-1/2}\gamma^{-3/2})$ in the underdamped and overdamped regimes, respectively. For $h = h_{\text{LMC}}\gamma$, the bound on the overdamped regime remains non-vacuous even in the overdamped limit $\gamma \rightarrow \infty$. In fact, the asymptotic bias in the overdamped limit precisely matches known results for LMC obtained via synchronous Wasserstein coupling. Furthermore, numerically, the phase transition from underdamped to overdamped appears to happen around the point of $h\gamma = 1.69$.

In Section 3.3, we combine the convergence and the asymptotic bias analyses into a mixing time complexity guarantee. As a result, we obtain a sampling complexity guarantee that $O(\kappa^{3/2}d^{1/2}\epsilon^{-1}\log \epsilon^{-1})$ iterations are sufficient to achieve $W_2(\mu_k, \pi) \leq \alpha^{-1/2}\epsilon$, which matches previous results [SZ21; DR20; ACZ25]. We make some concluding remarks in Section 4, while the proofs are deferred to Section 5.

2 Preliminaries

Notation For some Euclidean space $\mathcal{X} \subseteq \mathbb{R}^d$, we denote its Borel-measurable subsets as $\mathcal{B}(\mathcal{X})$. $\mathcal{P}_2(\mathcal{X}) = \{\mu \mid \int_{\mathcal{X}} \|x\|^2 \mu(dx) < +\infty\}$ denotes the set of all distributions on $\mathcal{X}$ with a finite second moment. For vectors $x, y \in \mathbb{R}^d$, $\langle x, y \rangle = x^\top y$ and $\|x\| = \sqrt{\langle x, x \rangle}$ denote the Euclidean inner product and norms, respectively. Furthermore, for any random variable X , we denote the square root of its expectation as $\mathbb{E}^{1/2} X = \sqrt{\mathbb{E} X}$. For a Markov kernel $Q : \mathcal{X} \times \mathcal{B}(\mathcal{X}) \rightarrow \mathbb{R}_{\geq 0}$ and a probability measure $\mu : \mathcal{B}(\mathcal{X}) \rightarrow \mathbb{R}_{\geq 0}$, their composition is denoted as $\mu Q(dy) = \int_{\mathcal{X}} \mu(dx) Q(x, dy)$. For a diagonalizable matrix $A \in \mathbb{R}^{d \times d}$ and any $p \in \{1, \dots, d\}$, $\sigma_p(A)$ denotes its p th eigenvalue.

2.1 Stochastic Exponential Euler Discretization

We begin with a high-level derivation of the stochastic exponential Euler discretization. (Durmus et al. [DEM+25, Lem. 29] present a more rigorous derivation.) Consider the fact that the solution to Eq. (1) at time $t = T$ is given as the intractable expression

$$\begin{aligned} V_T &= e^{-\gamma T} v_0 - \eta \int_0^T e^{-\gamma(T-t)} \nabla U(X_t) dt + \sqrt{2\gamma\eta} \int_0^T e^{-\gamma(T-t)} dB_t \\ X_T &= X_0 + \int_0^T V_s ds. \end{aligned} \quad (4)$$

If we hold the drift ∇U constant, Eq. (4) reduces to an Ornstein-Uhlenbeck process, which has a known solution. The exponential integrator exploits this, for each $k \geq 0$, by integrating Eq. (4) over the interval $[hk, h(k+1)]$ and replacing the state-dependent drift $\nabla U(X_t)$ with the state-independent constant drift $\nabla U(X_{hk})$. Defining $\delta \triangleq e^{-\gamma h}$ for convenience, this yields the update rule for the discrete-time Markov chain $(Z_k = (X_k, V_k))_{k \geq 0}$,

$$\begin{aligned} X_{k+1} &= X_k + \frac{1-\delta}{\gamma} V_k - \eta \frac{\gamma h + \delta - 1}{\gamma^2} \nabla U(X_k) + \xi_{k+1}^X \\ V_{k+1} &= \delta V_k - \eta \frac{1-\delta}{\gamma} \nabla U(X_k) + \xi_{k+1}^V, \end{aligned} \quad (5)$$

where the sequence of noise variables $(\xi_k^X, \xi_k^V)_{k \geq 1}$ is given as

$$\xi_{k+1}^X \triangleq \sqrt{2\gamma\eta} \int_{hk}^{h(k+1)} \frac{1 - e^{-\gamma(h(k+1)-s)}}{\gamma} dB_s \text{ and } \xi_{k+1}^V \triangleq \sqrt{2\gamma\eta} \int_{hk}^{h(k+1)} e^{-\gamma(h(k+1)-s)} dB_s.$$

The noise sequence $(\xi_k^X, \xi_k^V)_{k \geq 1}$ can be simulated by drawing independent zero-mean $2d$ -dimensional Gaussian random vectors with covariance $\begin{bmatrix} \sigma_{XX}^2 & \sigma_{XV}^2 \\ \sigma_{XV}^2 & \sigma_{VV}^2 \end{bmatrix} \otimes \text{Id}$, where $\otimes$ denotes the Kronecker product, and

$$\sigma_{XX}^2 = \frac{2\eta}{\gamma} \left(h - 2\frac{1-\delta}{\gamma} + \frac{1-\delta^2}{2\gamma} \right), \quad \sigma_{XV}^2 = \frac{\eta}{\gamma} (1-\delta)^2, \quad \sigma_{VV}^2 = \eta (1-\delta^2).$$

Throughout the paper, we denote the corresponding Markov kernel as $K : \mathbb{R}^{2d} \times \mathcal{B}(\mathbb{R}^{2d}) \rightarrow \mathbb{R}_{\geq 0}$ such that the Markov chain $(Z_k)_{k \geq 0}$ is simulated as $Z_{k+1} \sim K(Z_k, \cdot)$ for each $k \geq 0$.

2.2 Assumptions on the Potential

Our goal is to analyze the speed of approximately generating a sample from π , the stationary distribution of the continuous process (Eq. (1)), by simulating the Markov chain $(Z_k)_{k \geq 0}$ (Eq. (5)). This amounts to analyzing the speed in which $(Z_k)_{k \geq 0}$ converges to stationarity and the difference between π_h and π . These properties generally depend on the properties of the drift ∇U , and in turn the potential U . In this work, we consider the following assumption:

Assumption 2.1. The potential $U : \mathbb{R}^d \rightarrow \mathbb{R}$ is twice differentiable and there exist some $\alpha \in (0, +\infty)$ and $\beta \in [\alpha, +\infty)$ such that, for any $x \in \mathbb{R}^d$,

$$\alpha \text{Id} \preceq \nabla^2 U(x) \preceq \beta \text{Id}.$$

The existence of α, β is equivalent to the density $\exp(-U(x))/Z$ being α -strongly log-concave and β -log-smooth, and the ratio $\kappa \triangleq \beta/\alpha$ is referred to as the condition number. Assumption 2.1 has been widely used for analyzing the non-asymptotic complexity of approximate sampling schemes based on discretized kinetic Langevin diffusion [DR20; CCB+18; SZ21; LPW24; Mon21; FLO21; SL19; LFZ23; ACZ25]. In particular, it is known that Assumption 2.1 implies a contraction in Wasserstein distance for various discretizations of the kinetic/underdamped [LPW24; Mon21; SZ21] and overdamped [DM19] Langevin diffusions. We are, however, interested in how precisely and quantitatively the discretized diffusion depends on the properties of the drift represented by α and β .

2.3 Parametrization

Notice that, in Eq. (5), the Markov kernel K only interacts with the step size h through the product $\zeta \triangleq \gamma h$. Without loss of generality, it is possible to parametrize Eq. (5) with (ζ, γ, η) instead of the usual (h, γ, η) . Then δ becomes a monotonic transformation of ζ such that $\delta = \exp(-\zeta)$, while the update rule simplifies into

$$\begin{aligned} X_{k+1} &= X_k + (1 - \delta) \left(\frac{1}{\gamma} V_k \right) - (\zeta + \delta - 1) \left(\frac{\eta}{\gamma^2} \nabla U(X_k) \right) + \xi_{k+1}^X \\ V_{k+1} &= \delta V_k - (1 - \delta) \left(\frac{\eta}{\gamma} \nabla U(X_k) \right) + \xi_{k+1}^V. \end{aligned} \tag{6}$$

As a result, the analysis of the discretized algorithms is clearer and more natural in the (ζ, γ, η) parametrization. Therefore, our Wasserstein contraction analysis will operate under this parametrization. In the main text, however, we will present most results in the (h, γ, η) parametrization to be consistent with the literature.

Also, in the X_t update of Eq. (6), notice that the gradient ∇U is scaled as η/γ^2 . This scaling naturally appears in the analysis through

$$R(\lambda) \triangleq \frac{\eta \lambda}{\gamma^2},$$

where $\lambda \in [\alpha, \beta]$ represents any eigenvalue lying on the spectrum of $\nabla^2 U$. Then, under

Assumption 2.1, R is bounded as

$$\frac{\eta\alpha}{\gamma^2} \leq R(\lambda) \leq \frac{\eta\beta}{\gamma^2}.$$

The contraction of the discretized dynamics is directly dependent on the behavior of the scaled eigenvalues $R(\lambda)$. In fact, the scaling η/γ^2 partially hints at the fact that, for the discretized dynamics, keeping the ratio η/γ^2 constant results in similar behavior. For instance, the choices of $\eta \asymp 1/\beta$ and $\gamma \asymp 1$ [SZ21] and $\eta \asymp 1$ and $\gamma \asymp \sqrt{\beta}$ [DR20; ACZ25] have been used to obtain mixing time complexities that are comparable.

2.4 Weighted Norm and Wasserstein Distance

For obtaining a tight contraction for the kinetic Langevin dynamics, it is necessary to consider the Wasserstein-2 distance induced by an unconventional norm [DR20; MCC+21; Mon21]. Following previous works [Mon21; LPW24], we consider the following norm defined on the augmented state space $\mathbb{R}^{2d}$, where, for any $z = (x, v) \in \mathbb{R}^{2d}$,

$$\|z\|_{a,b}^2 = \|x\|^2 + 2b\langle x, v \rangle + a\|v\|^2,$$

and $a, b \in \mathbb{R}_{>0}$ satisfy $b^2 < a$. The last condition ensures that $\|z\|_{a,b}^2$ is a valid norm, which can be verified by using Young's inequality (for any $\epsilon > 0$, we have $2b\langle x, v \rangle \leq \epsilon\|x\|^2 + b^2\epsilon^{-1}\|v\|^2$). Furthermore, if we enforce the stronger condition $4b^2 \leq a$, we retrieve an explicit equivalence with the conventional Euclidean norm as

$$\frac{1}{2}\|z\|_{a,0}^2 \leq \|z\|_{a,b}^2 \leq \frac{3}{2}\|z\|_{a,0}^2. \quad (7)$$

For the values of the norm coefficients a and b , we will use the specific values of $a = 4/\gamma^2$ and $b = 1/\gamma$, which satisfy the condition for Eq. (7).

We denote Wasserstein-2 distance induced by the norm $\|\cdot\|_{a,b}$ as

$$W_{a,b}(\mu, \nu) \triangleq \inf_{\rho \in \Gamma(\mu, \nu)} \sqrt{\int_{\mathbb{R}^{2d} \times \mathbb{R}^{2d}} \|z - z'\|_{a,b}^2 d\rho(z, z')},$$

where $\Gamma(\mu, \nu)$ is the set of couplings between $\mu \in \mathcal{P}(\mathbb{R}^{2d})$ and $\nu \in \mathcal{P}(\mathbb{R}^{2d})$. The conventional Wasserstein-2 distance can be correspondingly defined as $W_2 \triangleq W_{1,0}$.

3 Main Results

3.1 Convergence to Stationarity

Firstly, we present a general Wasserstein contraction result for the Markov kernel K associated with the kinetic Langevin dynamics discretized via the exponential integrator. This will immediately imply that K admits a stationary distribution π_h and that it converges to π_h at a dimension-independent geometric rate. We follow the strategy [LPW24; SZ21] of reducing the problem to solving a special case of the discrete-time Lyapunov equation [AM06, §6.E]. Similarly to Leimkuhler, Paulin, and Whalley [LPW24], we directly solve the Lyapunov equation by analyzing the eigenvalues of a collection of matrices. However, our

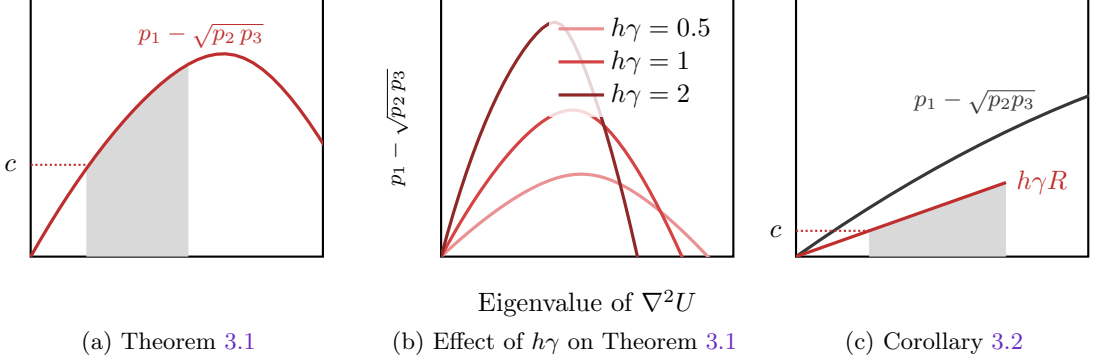


Figure 1: **Illustration of Theorem 3.1 and Corollary 3.2.** The grey region represents the spectrum of $\nabla^2 U$ under Assumption 2.1 for a certain choice of parameters. Intuitively, the grey region becomes wider as the problem becomes less well-conditioned (larger $\kappa = \beta/\alpha$). (a) Relationship between the function $p_1 - \sqrt{p_2 p_3}$, spectrum of $\nabla^2 U$, and the contraction coefficient. (b) Increasing $\zeta = h\gamma$ raises the peak value of $p_1 - \sqrt{p_2 p_3}$ but reduces the range of R where $p_1 - \sqrt{p_2 p_3}$ is positive. This results in a trade-off between the condition number $\kappa = \beta/\alpha$ and the resulting contraction coefficient. (c) Visualization of the linear under-approximation of $p_1 - \sqrt{p_2 p_3}$. Notice that the resulting contraction coefficient becomes worse.

analysis differs in that we first obtain the exact expression for the contraction rate. Under Assumption 2.1 and appropriate conditions on the parameters h, γ, η , K admits a contraction in Wasserstein distance induced by the weighted norm $\|\cdot\|_{a,b}$ (defined in Section 2.4) using $a = 4/\gamma^2$ and $b = 1/\gamma$.

Theorem 3.1. Suppose Assumption 2.1 holds and the parameters h, γ, η , where $\delta = \exp(-h\gamma)$, satisfy

$$\eta \left(\frac{2}{3} \frac{h}{\gamma(1-\delta^2)} + \frac{3}{2} \frac{1}{\gamma^2} \right) \leq \frac{1}{\beta}. \quad (8)$$

Then, for any $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^{2d})$ and all $n \geq 1$, we have

$$W_{a,b}(\mu K^n, \nu K^n)^2 \leq (1 - c(h, \gamma, \eta))^n W_{a,b}(\mu, \nu)^2$$

with the contraction coefficient

$$c(h, \gamma, \eta) = \inf_{\lambda \in [\alpha, \beta]} p_1(R(\lambda)) - \sqrt{p_2(R(\lambda)) p_3(R(\lambda))},$$

which is strictly positive, where

$$p_1(r) \triangleq -a_1 r^2 + b_1 r + e_1, \quad p_2(r) \triangleq a_1 r^2 + b_2 r + e_2, \quad p_3(r) \triangleq a_1 r^2 + b_3 r + e_3,$$

with the coefficients

$$\begin{aligned} a_1 &\triangleq \frac{2}{3}(h\gamma)^2 + 2(1-\delta)^2, & b_1 &\triangleq h\gamma - (\delta - \delta^2), & e_1 &\triangleq \frac{1}{2}(1-\delta^2), \\ b_2 &\triangleq -h\gamma(1+\delta) + (1-\delta^2), & e_2 &\triangleq \frac{1}{2}(1+\delta)^2, \end{aligned}$$

$$b_3 \triangleq -h\gamma(1-\delta) - (1-\delta)^2, \quad e_3 \triangleq \frac{1}{2}(1-\delta)^2.$$

Proof. The proof is deferred to Section 5.1. $\square$

This immediately implies the existence of a unique stationary distribution.

Corollary 3.1. *Suppose the conditions of Theorem 3.1 hold. Then K also admits a unique stationary distribution $\pi_h \in \mathcal{P}_2(\mathbb{R}^{2d})$.*

Proof. It is well known that $(\mathcal{P}_2(\mathbb{R}^{2d}), W_2)$ forms a Banach space metrized by W_2 [Wil09, Thm. 6.18]. The result then follows from Theorem 3.1, the equivalence between $\|\cdot\|_{a,b}$ and the Euclidean norm under $a = 4/\gamma^2$, $b = 1/\gamma$ and the Banach fixed point theorem. $\square$

For the special case of $\nu = \pi_h$, Theorem 3.1 immediately implies a geometric rate of convergence of $(Z_k)_{k \geq 0}$ to its stationary distribution π_h . The main contribution of Theorem 3.1, however, is the weaker restriction on the parameters stated in Eq. (8), where we notice an interplay between the parameters h, γ, η . In the overdamped regime,

$$\eta \left(\frac{2}{3} \frac{h}{\gamma(1-\delta^2)} + \frac{3}{2} \frac{1}{\gamma^2} \right) \stackrel{\gamma \rightarrow \infty}{\simeq} \frac{2}{3} \frac{\eta h}{\gamma}.$$

Therefore, the more we increase γ , the more we are free to increase either η or h . This contrasts with the result by Leimkuhler, Paulin, and Whalley [LPW24, Thm. 6.1], which strictly requires $h \leq 1/(2\gamma)$. In the underdamped regime, the inequality $\frac{\zeta}{1-e^{-\zeta}} \leq 1 + \frac{\zeta}{2} + \frac{\zeta^2}{6}$ yields

$$\eta \left(\frac{2}{3} \frac{h}{\gamma(1-\delta^2)} + \frac{3}{2} \frac{1}{\gamma^2} \right) \leq \eta \left(\frac{11}{6} \frac{1}{\gamma^2} + \frac{1}{3} \frac{h}{\gamma} + \frac{2}{9} h^2 \right).$$

That is, in the underdamped regime, $\gamma \geq \Omega(\sqrt{\beta})$ and $h \leq O(1/\sqrt{\beta})$, which is analogous to the constraint $h \leq O(1/\gamma)$. Thus, our restriction on the parameters does agree with that of Leimkuhler, Paulin, and Whalley [LPW24, Thm. 6.1] in the underdamped regime. Furthermore, for the fixed choices of $\gamma = 2$ and $\eta = 1/\beta$, as taken by Sanz-Serna and Zygalkakis [SZ21], Eq. (8) becomes

$$\frac{h}{1 - \exp(-4h)} \leq \frac{15}{8}$$

Numerically solving this inequality yields an approximate condition of $h \leq 1.87$, which is weaker than the $h \leq 1$ condition by Sanz-Serna and Zygalkakis [SZ21, Thm. 6.1].

Meanwhile, the contraction coefficient $c(h, \gamma, \eta)$ is determined by the function $p_1 - \sqrt{p_2 p_3}$. While $p_1 - \sqrt{p_2 p_3}$ is difficult to interpret, it is an exact expression for the contraction coefficient. The behavior of $c(h, \gamma, \eta)$ depending on the parameters is illustrated in Section 3. To obtain a more interpretable expression for the contraction coefficient, we can perform a linear under-approximation of $p_1 - \sqrt{p_2 p_3}$ (illustrated in Fig. 1c) with slightly stronger restrictions on the parameters:

Assumption 3.2. The parameters $h, \gamma, \eta > 0$ satisfy the inequality

$$\eta \left(2 \frac{h}{\gamma(1-\delta)} + \frac{6}{\gamma^2} \right) < \frac{1}{\beta}.$$

We will rely on this condition throughout the remainder of the article. It is apparent that Assumption 3.2 is very similar to Eq. (8). As such, in the overdamped regime, Assumption 3.2 also reduces to the condition $h\eta/\gamma \leq O(1/\beta)$. For the underdamped regime, by relying on the inequality $\frac{\zeta}{1-e^{-\zeta}} \leq 1 + \frac{\zeta}{2} + \frac{\zeta^2}{6}$ again, it can be simplified through

$$\begin{aligned} \frac{\eta}{\gamma^2} \left(2 \frac{h\gamma}{(1-\delta)} + 6 \right) \leq \frac{1}{\beta} &\Leftrightarrow \frac{\eta}{\gamma^2} \left(2 \left(1 + \frac{h\gamma}{2} + \frac{(h\gamma)^2}{6} \right) + 6 \right) \leq \frac{1}{\beta} \\ &\Leftrightarrow \gamma > \sqrt{9\beta\eta} \quad \text{and} \quad h \leq \sqrt{\frac{3}{4} \frac{1}{\beta\eta} - \frac{27}{4} \frac{1}{\gamma^2}}. \end{aligned}$$

For $\eta = 1$, this implies that γ must satisfy at least $\gamma \geq \sqrt{9\beta}$. Up to constants, this corresponds to the result by Leimkuhler, Paulin, and Whalley [LPW24, Thm. 6.1]. On the other hand, choosing $\eta = 1/(2\beta)$ and $\gamma = \sqrt{27/2}$ conveniently implies a condition of $h \leq 1$. This covers the choice of $\gamma \asymp 1$ and $\eta \asymp 1/\beta$ by Sanz-Serna and Zygalkakis [SZ21, Thm 4.9].

Given Assumption 3.2, we obtain a simpler expression for the contraction coefficient.

Corollary 3.2. *Suppose Assumptions 2.1 and 3.2 hold. Then the contraction coefficient in Theorem 3.1 satisfies*

$$c(h, \gamma, \eta) \geq \tilde{c}(h, \gamma, \eta) \triangleq \frac{h\eta\alpha}{\gamma}.$$

Proof. The proof is deferred to Section 5.1.4. □

This implies a $O(h\eta\alpha/\gamma)$ contraction rate, which matches previous results [SZ21; LPW24]. However, our main contribution is the generality of the condition Assumption 3.2. Specifically, it allows for the contraction to hold even in the overdamped limit:

Corollary 3.3 (Overdamped Limit). *Suppose Assumption 2.1 holds and, for some $h_{\text{LMC}} > 0$ satisfying $h_{\text{LMC}} \leq 1/(2\beta)$, the parameters are set as $h = h_{\text{LMC}}\gamma$, $\eta = 1$, and $\gamma \rightarrow \infty$. Then Assumption 3.2 is satisfied while the overdamped limit of the contraction coefficient $c(h, \gamma, \eta)$ in Corollary 3.2 follows as*

$$\lim_{\gamma \rightarrow \infty} c(h, \gamma, \eta) = \lim_{\gamma \rightarrow \infty} c(h_{\text{LMC}}\gamma, \gamma, 1) = h_{\text{LMC}}\alpha.$$

This is equivalent to the Wasserstein contraction rate and step size limit of the Euler-Maruyama discretization of the overdamped Langevin dynamics [DM19, Prop 2.]. Therefore, under appropriate scaling of the step size ($h \propto \gamma$), the exponential integrator is able to non-degenerately simulate the kinetic Langevin dynamics in the overdamped regime. This puts the exponential integrator in the class of “ γ -limit convergent” integrators [LPW24], which includes the OBABO and BAOAB splitting schemes [LM13].

3.2 Asymptotic Bias

We now turn to analyzing the asymptotic bias $W_{a,b}(\pi_h, \pi)$ of the stationary distribution of K , π_h . Denote the Markov semigroup associated with Eq. (1) by $(P_t)_{t \geq 0}$, where we recall that $\pi P_t = \pi$ and $(Z_t^* \sim \pi P_t)_{t \geq 0}$ is the kinetic Langevin dynamics initialized from its stationary distribution π . Given a discretized process $(Z_k)_{k \geq 0}$, which need not be stationary,

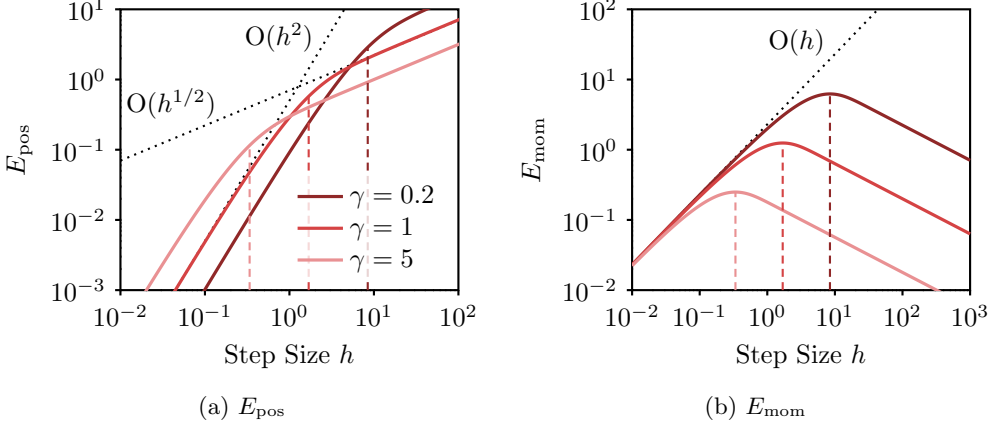


Figure 2: **Scaling of the asymptotic error bound with respect to the step size h .** The vertical dashed lines mark the point where $\zeta = h\gamma = 1.69$.

our goal is to bound the distance between $(Z_t^*)_{t \geq 0}$ and $(Z_k)_{k \geq 0}$ as $t = hk \rightarrow \infty$. The proof strategy follows Sanz-Serna and Zygalakis [SZ21], where we construct an auxiliary process $(Z')_{t \geq 0}$ that corresponds to the exponential integrator discretization of $(Z_t^*)_{t \geq 0}$. For each $k \geq 0$, consider the corresponding time step $(t_k = hk)_{k \geq 0}$. $(Z'_t)_{t \in [t_k, t_{k+1}]}$ is the linearly interpolation of $(Z_t^*)_{t \geq 0}$ over the interval $[t_k, t_{k+1}]$ with the associated Markov semigroup as $(\tilde{P}_t)_{t \in [t_k, t_{k+1}]}$. Specifically, for any $t \in [t_k, t_{k+1}]$,

$$\begin{aligned} V'_t &= e^{-\gamma t} V_{hk}^* - \eta \int_{hk}^t e^{-\gamma(s-hk)} \nabla U(X_{hk}^*) ds + \sqrt{2\gamma\eta} \int_{hk}^t e^{-\gamma(s-hk)} dB_s \\ X'_t &= X_{hk}^* + \int_{hk}^t V'_s ds. \end{aligned} \quad (9)$$

In essence, $(Z'_t)_{t \in [t_k, t_{k+1}]}$ is a kinetic Langevin diffusion process with the drift set to be the zeroth order interpolation of the drift of $(Z_t^*)_{t \geq 0}$. The resulting discrete-time operator is denoted by $\tilde{K}$ such that $\pi \tilde{P}_{t_k} = \pi \tilde{K}^k$. Given these, we can decompose the asymptotic error as

$$W_{a,b}(\pi_h, \pi) = \lim_{k \rightarrow \infty} W_{a,b}(\mu K^k, \pi P_{hk}) \leq \lim_{k \rightarrow \infty} \left\{ W_{a,b}(\mu K^k, \pi \tilde{K}^k) + W_{a,b}(\pi \tilde{P}_{t_k}, \pi P_{t_k}) \right\}.$$

To upper bound this, for all $k \geq 0$ and all $t \in [t_k, t_{k+1}]$, we will assume $(Z_k)_{k \geq 0}$, $(Z_t^*)_{t \geq 0}$, and $(Z'_t)_{t \geq 0}$ are synchronously coupled by sharing the same noise process $(B_t)_{t \geq 0}$. Then $W_{a,b}(\mu K^k, \pi \tilde{K}^k)$ can be bounded via the synchronous coupling established earlier in Corollary 3.2. The proof focuses on bounding the remaining $W_{a,b}(\pi \tilde{P}_{t_k}, \pi P_{t_k})$ by analyzing the local error committed at each time step.

Specifically, carefully quantifying the effect of the damping (terms involving $e^{-\gamma t}$) yields the following result.

Theorem 3.3. *Suppose Assumptions 2.1 and 3.2 hold. Then the stationary distribution of*

K, π_h , satisfies

$$W_{a,b}(\pi_h, \pi) \leq E_{\text{pos}} + E_{\text{mom}},$$

where

$$\begin{aligned} E_{\text{pos}} &\triangleq \left\{ \frac{1}{2} \frac{d\kappa^2\eta}{\gamma^2} \frac{1}{h\gamma} \left((h\gamma)^2 - 3 + \delta^2 \left(3 + 6h\gamma + 5(h\gamma)^2 + 2(h\gamma)^3 \right) \right) \right\}^{1/2} \\ E_{\text{mom}} &\triangleq \left\{ 4 \frac{d\kappa^2\eta}{\gamma^2} \frac{1}{h\gamma} \left(1 - \delta^2 \left(1 + 2h\gamma + 2(h\gamma)^2 \right) \right) \right\}^{1/2}. \end{aligned}$$

Proof. The proof is deferred to Section 5.2. $\square$

Notice that we decomposed the asymptotic error into the local error of the position E_{pos} and the momentum E_{mom} . Also, since we rely on Corollary 3.2, the restriction on the parameters is again given by Assumption 3.2. Although the bounds on E_{pos} and E_{mom} are highly non-linear in $\zeta = h\gamma$, making them difficult to interpret, we visualize the scaling with respect to h in Fig. 2 for different values of γ . In the underdamped regime, the error of the momentum E_{mom} , which scales as $O(h)$, dominates the error. On the other hand, in the overdamped regime, the error of the momentum E_{mom} decreases, while the error of the position E_{pos} dominates with a $O(h^{1/2})$ scaling. This $O(h^{1/2})$ scaling is typical of the Euler-Maruyama discretization of the overdamped Langevin [DM19, Cor. 7].

Notice in Fig. 2 that there is a phase transition from the underdamped to overdamped regime. We can locate the critical point of the phase transition by solving for the root of

$$\frac{dE_{\text{mom}}}{dh} = 0 \quad \Leftrightarrow \quad \frac{dE_{\text{mom}}}{d\zeta} = 0 \quad \Leftrightarrow \quad (2\zeta + 1)(2\zeta^2 + 1) = e^{2\zeta}.$$

Numerically solving this equation suggests that the critical point is $\zeta \approx 1.69$. Fig. 2 qualitatively shows that $\zeta = h\gamma = 1.69$ indeed accurately predicts the phase transition for both E_{pos} and E_{mom} .

By approximating the bounds with the series expansion at both extremes, $\gamma \rightarrow 0$ and $\gamma \rightarrow \infty$, we can formalize the scalings as follows:

Corollary 3.4. *Suppose Assumptions 2.1 and 3.2 hold. Then the following bounds hold simultaneously:*

(i) *Underdamped regime:*

$$E_{\text{pos}} \leq \frac{4}{15} d^{1/2} \kappa \eta^{1/2} \gamma h^2 \quad \text{and} \quad E_{\text{mom}} \leq \frac{4}{\sqrt{3}} d^{1/2} \kappa \eta^{1/2} h.$$

(ii) *Overdamped regime:*

$$E_{\text{pos}} \leq \frac{1}{\sqrt{2}} d^{1/2} \kappa \eta^{1/2} \frac{h^{1/2}}{\gamma^{1/2}} \quad \text{and} \quad E_{\text{mom}} \leq 4 d^{1/2} \kappa \eta^{1/2} \frac{1}{h^{1/2} \gamma^{3/2}}.$$

Proof. The proof is deferred to Section 5.2.4. $\square$

This means that, in the underdamped regime, the asymptotic bias $E_{\text{pos}} + E_{\text{mom}}$ can be bounded as $O(d^{1/2} \kappa \eta^{1/2} (h^2 \gamma + h))$, while in the overdamped regime, it can be bounded

as $O(d^{1/2}\kappa\eta^{1/2}h^{1/2}\gamma^{-1/2})$. While both bounds hold simultaneously, they are only tight (with regard to the general bound in Theorem 3.3) in their respective regime. What is worth noting is that, in the underdamped regime, the bias increases with γ , whereas in the overdamped regime, the bias decreases with γ . The fact that bias decreases with γ in the overdamped regime is unsurprising since lower friction results in stiffer dynamics. However, the fact that the bias in the position increases with γ in the underdamped regime is counterintuitive.

Compared to previous works, for the underdamped regime with the choice of $\eta = 1$ and $\gamma \asymp \sqrt{\beta}$, our bound is in agreement ([Che24, Thm. 5.3.9]; [DR20, Thm. 2]), as well as with $\gamma \asymp 1$ and $\eta \asymp 1/\beta$ [SZ21, Eq. 6.1]. Furthermore, notice that h and γ in the bound for the overdamped regime appear as a ratio $h^{1/2}\gamma^{-1/2}$. This immediately implies that this bound is non-vacuous in the overdamped limit $\gamma \rightarrow \infty$ under appropriate step size scaling ($h \propto \gamma$).

Corollary 3.5 (Overdamped Limit). *Suppose Assumption 2.1 holds and, for some $h_{\text{LMC}} > 0$ satisfying $h_{\text{LMC}} \leq 1/(2\beta)$, the parameters are set as $h = h_{\text{LMC}}\gamma$, $\eta = 1$, and $\gamma \rightarrow \infty$. Then the overdamped limits of E_{pos} and E_{mom} follow as*

$$\lim_{\gamma \rightarrow \infty} E_{\text{pos}} = (1/\sqrt{2})d^{1/2}\kappa h_{\text{LMC}}^{1/2} \quad \text{and} \quad \lim_{\gamma \rightarrow \infty} E_{\text{mom}} = 0.$$

This coincides with $O(d^{1/2}\kappa h_{\text{LMC}}^{1/2})$ scaling of the asymptotic bias of the Euler-Maruyama discretization of overdamped Langevin (LMC) under the synchronous Wasserstein coupling strategy [DM19, Cor. 7]. Under Assumption 2.1, however, the convex analysis strategy of Durmus, Majewski, and Miasojedow [DMM19] yields a bound of $O(d^{1/2}\kappa^{1/2}h_{\text{LMC}}^{1/2})$ for LMC. The dependence on κ in Corollary 3.5 is comparably suboptimal. The equivalence between overdamped KLMC and LMC thus only holds for results obtained under the synchronous Wasserstein coupling strategy. While it is probable that applying the convex analysis strategy to kinetic Langevin under the exponential integrator would bridge this gap by resulting in a better dependence on κ , no such result has been demonstrated so far.

Meanwhile, all previous strategies [SZ21; CCB+18; DR20] resulted in bounds on the asymptotic error that scale as $O(h)$ with respect to the step size h . In the overdamped regime, where applying time rescaling requires $h \propto \gamma$, these bounds are vacuous in the limit $\gamma \rightarrow \infty$. The main culprit is that previous analyses ignored the effect of stabilization due to high damping through the use of the bound $e^{-\gamma h} \leq 1$; as $\gamma \rightarrow \infty$, $e^{-\gamma h}$ becomes close 0, reducing the discretization error. The general strategy for bounding asymptotic bias by Durmus and Eberle [DE24] also suffers from a similar problem. For a free variable $n \geq 0$, their strategy unavoidably results in a bound that increases exponentially in time $t = hn$ with a factor of $\exp(t) = \exp(hn)$. (See the definition of $\epsilon(n)$ in Ex. 2; [DE24].) In the underdamped regime, the exponential term can be controlled by upper-bounding h . However, in the overdamped regime, time acceleration $t \rightarrow \infty$ makes the term uncontrollable, resulting in a vacuous bound. This also means that results based on the strategy of Durmus and Eberle [DE24], e.g., [Mon21; GBM+25; LPW24], will be ignorant of the precise dependence on γ . Thus, the asymptotic bias analysis of other discretizations, such as OBABO or BAOAB [LM13], has potential for improvement.

3.3 Sampling Complexity

Lastly, we present a non-asymptotic sampling complexity guarantee. Since the scaling of the asymptotic bias of KLMC in the overdamped regime is strictly worse than in the underdamped regime, we restrict our interest to the latter. The proof is a straightforward combination of the results in Sections 3.1 and 3.2. For any $\mu \in \mathcal{P}_2(\mathbb{R}^{2d})$, any $n \geq 0$, and the choice of $a = 4/\gamma^2$ and $b = 1/\gamma$, we have the decomposition

$$W_{a,b}(\mu K^n, \pi) \leq \underbrace{W_{a,b}(\mu K^n, \pi_h)}_{\text{non-stationarity error}} + \underbrace{W_{a,b}(\pi_h, \pi)}_{\text{asymptotic bias error}}.$$

Each term is bounded by invoking Corollary 3.2 and Corollary 3.4, respectively. For any given $\epsilon > 0$, solving for the smallest n that ensures both terms are bounded by $\epsilon/2$ yields a sampling complexity result.

Theorem 3.4. *Suppose Assumption 2.1 holds and suppose there exists some γ, η, h_0 such that Assumption 3.2 is satisfied for all $h \in (0, h_0]$. Then, for any $\epsilon > 0$,*

$$h = \min \left\{ \sqrt{\frac{5}{4}} \frac{\epsilon^{1/2}}{d^{1/4} \kappa^{1/2} \eta^{1/4} \gamma^{1/2}}, \frac{1}{4\sqrt{3}} \frac{\epsilon}{d^{1/2} \kappa \eta^{1/2}}, h_0 \right\}$$

and any number of iterations of at least

$$n \geq \max \left\{ \sqrt{5} \frac{\gamma^{3/2}}{\eta^{3/4}} \frac{d^{1/4} \kappa^{1/2}}{\alpha} \frac{1}{\epsilon^{1/2}}, 8\sqrt{3} \frac{\gamma}{\eta^{1/2}} \frac{d^{1/2} \kappa}{\alpha} \frac{1}{\epsilon}, h_0 \gamma \right\} \log \left(3W_{a,b}(\mu, \pi_h) \frac{1}{\epsilon} \right)$$

guarantees that $W_{a,b}(\mu K^n, \pi) \leq \epsilon$.

Proof. The proof is deferred to Section 5.3. □

Substituting γ, η , and h_0 with values that satisfy Assumption 3.2 yields a more concrete complexity guarantee. In particular, we retrieve previous sampling complexity guarantees for the KLMC in the underdamped regime.

Corollary 3.6. *For any $\epsilon > 0$ and the parameters h, γ, η satisfying any of the following choices:*

1. $\gamma = \sqrt{27\beta}, \eta = 1, h = O(\epsilon / (d^{1/2} \kappa \eta^{1/2}))$
2. $\gamma = \sqrt{27/2}, \eta = 1/(2\beta), h = O(\alpha^{1/2} \epsilon / (d^{1/2} \kappa^{1/2}))$

and a number of iterations of at least

$$n \geq O \left(d^{1/2} \kappa^{3/2} \frac{1}{\alpha^{1/2} \epsilon} \log \frac{1}{\alpha^{1/2} \epsilon} \right),$$

we have that $W_{a,b}(\mu K^n, \pi) \leq \epsilon$.

For the dimensionless target condition $W_{a,b}(\mu K^n, \pi) \leq \alpha^{-1/2} \epsilon$, Corollary 3.6 provides an iteration complexity of $O(d^{1/2} \kappa^{3/2} \epsilon^{-1} \log \epsilon^{-1})$, which matches known results [SZ21; DR20; ACZ25].

4 Discussions

In this work, we have presented new results on the Wasserstein contraction (Section 3.1) and asymptotic bias (Section 3.2) of kinetic Langevin dynamics discretized via the stochastic exponential Euler scheme. Our results are in accordance with past results [SZ21; DR20; ACZ25] in the underdamped regime, but are general enough to accommodate all of the different parameter choices in past works, for example, large friction $\gamma \asymp \sqrt{\beta}$ and fixed inverse mass $\eta \asymp 1$ [DR20; ACZ25] versus fixed friction $\gamma \asymp 1$ versus small inverse mass $\eta \asymp 1/\beta$ [SZ21]. Furthermore, we have extended the convergence guarantees of KLMC to the overdamped regime ($\gamma \rightarrow \infty$). This demonstrates that the exponential integrator does *not* degenerate in the overdamped limit as long as proper time scaling $h \propto \gamma$ is applied. This contrasts with the conclusion of Leimkuhler, Paulin, and Whalley [LPW24], as their analysis required stronger constraints on the parameters, which prevented time acceleration.

Now that we know the fact that the exponential integrator does not degenerate as long as proper time acceleration is applied, it is rather surprising that the OBABO and BAOAB discretization of the kinetic Langevin diffusion reduces to LMC *without* any sort of explicit time scaling of the parameters [LPW24]. This suggests that, somehow, splitting schemes implicitly experience automatic time acceleration, which would be interesting to identify in their respective analysis.

Furthermore, our bounds on asymptotic bias revealed a more precise dependence on the friction γ . In particular, the bias increases with γ in the underdamped regime, whereas it decreases with γ in the overdamped regime. It would be interesting to see if a similar dependence on γ exhibits in the asymptotic bias of alternative discretization schemes. Furthermore, our bounds on the asymptotic bias exhibit a clear phase transition from the overdamped regime to the underdamped regime. Numerically solving the critical point suggests that the transition happens around $h\gamma = 1.69$. It would be curious to see if this phase transition also consistently happens at $h\gamma \approx 1.69$ for other discretizations as well.

5 Proofs

5.1 Wasserstein Contraction Analysis

This section will present the proof for Theorem 3.1 as well as the necessary components for the proof. The proof follows a synchronous Wasserstein coupling strategy similarly to that of Leimkuhler, Paulin, and Whalley [LPW24], and can thus be viewed as a refinement of their strategy. Consider two discrete-time Markov chains $(Z_k = (X_k, V_k))_{k \geq 0}$ and $(Z'_k = (X'_k, V'_k))_{k \geq 0}$ following the update rule in Eq. (6) with a shared noise process $(\xi_k^X, \xi_k^V)_{k \geq 1}$. That is, for each $k \geq 0$,

$$\begin{cases} X_{k+1} &= X_k + (1 - \delta) \left(\frac{1}{\gamma} V_k \right) - (\zeta + \delta - 1) \left(\frac{\eta}{\gamma^2} \nabla U(X_k) \right) + \xi_{k+1}^X \\ V_{k+1} &= \delta V_k - (1 - \delta) \left(\frac{\eta}{\gamma} \nabla U(X_k) \right) + \xi_{k+1}^V \\ X'_{k+1} &= X'_k + (1 - \delta) \left(\frac{1}{\gamma} V'_k \right) - (\zeta + \delta - 1) \left(\frac{\eta}{\gamma^2} \nabla U(X'_k) \right) + \xi_{k+1}^X \\ V'_{k+1} &= \delta V'_k - (1 - \delta) \left(\frac{\eta}{\gamma} \nabla U(X'_k) \right) + \xi_{k+1}^V \end{cases}$$

Since the two processes $(Z_k)_{k \geq 0}$ and $(Z'_k)_{k \geq 0}$ are sharing the same noise process $(\xi_k^X, \xi_k^V)_{k \geq 1}$, they are *synchronously coupled*. The proof is dedicated to establishing that, for all $k \geq 0$, a contraction holds for some fixed $c > 0$ holds for the norm $\|\cdot\|_{a,b}$ introduced in Section 2.4 as

$$\|Z_{k+1} - Z'_{k+1}\|_{a,b}^2 \leq (1 - c) \|Z_k - Z'_k\|_{a,b}^2. \quad (10)$$

As the two Markov chains $(Z_k)_{k \geq 0}$ and $(Z'_k)_{k \geq 0}$ are synchronously coupled, conditional on the noise sequence $(B_k)_{k \geq 0}$ and a corresponding linear operator S_k , the difference sequence $(\bar{Z}_k = Z_k - Z'_k)_{k \geq 0}$ is a deterministic time-variant linear dynamical system

$$\bar{Z}_{k+1} = S_k \bar{Z}_k.$$

Note that S_k is dependent on the states Z_k and Z'_k , and the parameters h , η , and γ . The contraction in Eq. (10) follows from a Lyapunov analysis of the operator S_k . Consider the quadratic Lyapunov function

$$z \mapsto \|z\|_{a,b}^2 = z^\top G z, \quad \text{where} \quad G \triangleq \begin{bmatrix} 1 & b \\ b & a \end{bmatrix}.$$

Due to the relationship

$$\|\bar{Z}_{k+1}\|_{a,b}^2 = \|S_k \bar{Z}_k\|_{a,b}^2 = \bar{Z}_k^\top S_k^\top G S_k \bar{Z}_k,$$

the existence of $c > 0$ such that Eq. (10) holds can be reduced to solving a special case of the “discrete-time Lyapunov equation” [AM06, §6.E]

$$S_k^\top G S_k - G \preceq -cG. \quad (11)$$

In particular, the feasibility of this matrix inequality implies a strong form of Lyapunov stability known as exponential stability. (See also Exercise 6.10 by Antsaklis and Michel [AM06], which presents the continuous-time analog of this statement.) This is also the

condition identified by Sanz-Serna and Zygalakis [SZ21, Prop. 4.6], although they didn't draw connections with Lyapunov analysis of linear systems.

In our case, establishing Eq. (11) corresponds to checking the positive-definiteness of a 2×2 block matrix comprised of the blocks $A_k, B_k, C_k \in \mathbb{R}^{d \times d}$,

$$(1 - c)G - S_k^\top G S_k^\top \triangleq \begin{bmatrix} A_k & B_k \\ B_k & C_k \end{bmatrix}. \quad (12)$$

While Sanz-Serna and Zygalakis [SZ21] avoided directly analyzing the spectrum of this matrix, Leimkuhler, Paulin, and Whalley [LPW24] relied on the following lemma to enable a direct analysis:

Lemma 5.1. *Suppose the block matrices in Eq. (12) are symmetric and commutative. Then, there exists a constant $c > 0$ satisfying Eq. (11) for all $k \geq 0$ if and only if $A_k \succ 0$ and $A_k C_k - B_k^2 \succeq 0$ for all $k \geq 0$.*

Proof. Any block matrix of the form of Eq. (12) is positive semidefinite if and only if $A_k \succ 0$ and its Schur complement is positive semidefinite such that $C_k - B_k^\top A_k^{-1} B_k \succeq 0$ [BV04, §A.5.5]. Since the blocks A_k, B_k, C_k are symmetric and commutative,

$$C_k - B_k^\top A_k^{-1} B_k \succeq 0 \quad \Leftrightarrow \quad C_k - A_k^{-1} B_k^\top B_k \succeq 0.$$

Multiplying $A \succ 0$ on the left of both hand sides,

$$C_k - A_k^{-1} B_k^\top B_k \succeq 0 \quad \Leftrightarrow \quad A_k C_k - B_k^2 \succeq 0,$$

which is the stated result. $\square$

Therefore, it is sufficient to show that, for any $k \geq 0$ and some $h, \eta, \gamma, c > 0$, the conditions

$$A_k \succ 0 \quad \text{and} \quad A_k C_k - B_k^2 \succeq 0 \quad (13)$$

hold. The derivation of the blocks is presented in Section 5.1.1, where the proof of Theorem 3.1, which consists of establishing Eq. (13), proceeds in Section 5.1.2.

5.1.1 Derivation of A_k, B_k , and C_k

In this section, we compute the blocks A_k, B_k , and C_k . Since U is twice differentiable under Assumption 2.1, we can invoke the fundamental theorem of calculus, which, for all $x, x' \in \mathbb{R}^d$, yields the identity

$$\nabla U(x) - \nabla U(x') = H(x - x') \quad \text{with} \quad H(x, x') \triangleq \int_0^1 \nabla^2 U(x + t(x' - x)) dt.$$

Define $H_k \triangleq H(X_k, X'_k)$. Then the difference sequence satisfies

$$\begin{aligned} \bar{Z}_{k+1} &= \begin{bmatrix} (X_k - X'_k) + \frac{1-\delta}{\gamma} (V_k - V'_k) - \eta \frac{\zeta+\delta-1}{\gamma^2} (\nabla U(X_k) - \nabla U(X'_k)) \\ \delta (V_k - V'_k) - \eta \frac{1-\delta}{\gamma} (\nabla U(X_k) - \nabla U(X'_k)) \end{bmatrix} \\ &= \begin{bmatrix} (X_k - X'_k) + \frac{1-\delta}{\gamma} (V_k - V'_k) - \eta \frac{\zeta+\delta-1}{\gamma^2} H_k (X_k - X'_k) \\ \delta (V_k - V'_k) - \eta \frac{1-\delta}{\gamma} H_k (X_k - X'_k) \end{bmatrix} \end{aligned}$$

$$= \begin{bmatrix} \mathbf{I}_d - \eta \frac{\zeta + \delta - 1}{\gamma^2} H_k & \frac{1 - \delta}{\gamma} \mathbf{I}_d \\ -\eta \frac{1 - \delta}{\gamma} H_k & \delta \mathbf{I}_d \end{bmatrix} \bar{Z}_k.$$

Therefore, the time-variant transition operator of the difference sequence is

$$S_k = \begin{bmatrix} \mathbf{I}_d - \eta \frac{\zeta + \delta - 1}{\gamma^2} H_k & \frac{1 - \delta}{\gamma} \mathbf{I}_d \\ -\eta \frac{1 - \delta}{\gamma} H_k & \delta \mathbf{I}_d \end{bmatrix}.$$

Since H_k is symmetric, it is diagonalizable for all $k \geq 0$. Furthermore, all blocks in S_k only involve H_k and $\mathbf{I}_d$, meaning that they are all diagonalizable with the same eigenvectors, which also implies that the blocks commute. Using this fact and substituting $a = 4/\gamma^2$ and $b = 1/\gamma$ in G , symbolic computation shows that the matrices A_k , B_k , and C_k are symmetric and follow as

$$\begin{aligned} A_k &= \left(-\zeta^2 - 3(\delta - 1)^2 \right) \left(\frac{\eta}{\gamma^2} H_k \right)^2 + 2\gamma h \left(\frac{\eta}{\gamma^2} H_k \right) - c \mathbf{I}_d \\ B_k &= \frac{1}{\gamma} (\zeta - 3\delta^2 + 3\delta) \left(\frac{\eta}{\gamma^2} H_k \right) - \frac{1}{\gamma} c \mathbf{I}_d \\ C_k &= -\frac{1}{\gamma^2} (4c - 3(1 - \delta^2)) \mathbf{I}_d. \end{aligned}$$

(The material for replicating the symbolic computation results is available as supplementary material. See ?? for details.)

Furthermore, again from symbolic computation, $A_k C_k - B_k^2$ follows as

$$\begin{aligned} A_k C_k - B_k^2 &= \frac{1}{\gamma^2} \left\{ \left(12c(1 - \delta)^2 - 4\zeta^2(1 - c) + 3\zeta^2\delta^2 - 6\zeta(\delta - \delta^2) - 9(1 - \delta)^2 \right) \left(\frac{\eta}{\gamma^2} H_k \right)^2 \right. \\ &\quad \left. + 6(c(\delta - \delta^2) + \zeta(1 - c) - \zeta\delta^2) \left(\frac{\eta}{\gamma^2} H_k \right) + (3c^2 - 3c(1 - \delta^2)) \mathbf{I}_d \right\}. \end{aligned}$$

We will now proceed to establish the positive-definiteness of A_k and $A_k C_k - B_k^2$.

5.1.2 Proof of Theorem 3.1

Under Assumption 2.1, all of the eigenvalues of H_k are strictly positive. This implies that the p th eigenvalue of A_k and $A_k C_k - B_k^2$ follow as

$$\begin{aligned} \sigma_p(A_k) &= \left(-\zeta^2 - 3(\delta - 1)^2 \right) \left(\frac{\eta \sigma_p(H_k)}{\gamma^2} \right)^2 + 2\zeta \left(\frac{\eta \sigma_p(H_k)}{\gamma^2} \right) - c \\ \sigma_p(A_k C_k - B_k^2) &= \\ &\quad \frac{1}{\gamma^2} \left\{ \left(12c(1 - \delta)^2 - 4\zeta^2(1 - c) + 3\zeta^2\delta^2 - 6\zeta(\delta - \delta^2) - 9(1 - \delta)^2 \right) \left(\frac{\eta \sigma_p(H_k)}{\gamma^2} \right)^2 \right. \\ &\quad \left. + 6(c(\delta - \delta^2) + \zeta(1 - c) - \zeta\delta^2) \left(\frac{\eta \sigma_p(H_k)}{\gamma^2} \right) + 3c^2 - 3c(1 - \delta^2) \right\}. \end{aligned}$$

For notational convenience, consider the functions

$$\begin{aligned}\chi_A(r, \zeta, \gamma, c) &\triangleq \left(-\zeta^2 - 3(1-\delta)^2\right) r^2 + 2\zeta r - c \\ \chi_{AC-B^2}(r, \zeta, \gamma, c) &\triangleq \frac{1}{\gamma^2} \left\{ \left(12c(1-\delta)^2 - 4\zeta^2(1-c) + 3\zeta^2\delta^2 - 6\zeta(\delta-\delta^2) - 9(1-\delta)^2\right) r^2 \right. \\ &\quad \left. + 6(c(\delta-\delta^2) + \zeta(1-c) - \zeta\delta^2) r + 3c^2 - 3c(1-\delta^2) \right\}.\end{aligned}$$

These functions characterize the spectrum of A_k and $A_k C_k - B_k^2$ via the relationship

$$\begin{aligned}\chi_A(R(\sigma_p(H_k)), \zeta, \gamma, c) &= \sigma_p(A_k), \\ \chi_{AC-B^2}(R(\sigma_p(H_k)), \zeta, \gamma, c) &= \sigma_p(A_k C_k - B_k^2).\end{aligned}\tag{14}$$

Therefore, analyzing χ_A and χ_{AC-B^2} sufficiently characterizes the spectrum of A_k and $A_k C_k - B_k^2$, respectively. Specifically, we are interested in the conditions on h, γ, r, c that guarantees $\chi_A > 0$ and $\chi_{AC-B^2} \geq 0$. For this, we need to analyze χ_A and χ_{AC-B^2} in detail.

Let's begin with χ_{AC-B^2} . Notice that it can be rewritten as

$$\begin{aligned}\chi_{AC-B^2}(r, \zeta, \gamma, c) &\triangleq \frac{1}{\gamma^2} \left\{ 3c^2 + \left(4\left(3(1-\delta)^2 + \zeta^2\right) r^2 + 6\left((\delta-\delta^2) - \zeta\right) r - 3(1-\delta^2)\right) c \right. \\ &\quad \left. + \left(-9(1-\delta)^2 + \zeta^2(3\delta^2 - 4) - 6\zeta(\delta-\delta^2)\right) r^2 + 6\zeta(1-\delta^2) r \right\}.\end{aligned}$$

It is apparent that this is a quadratic function with respect to c . Furthermore, this quadratic always has two distinct real roots:

Lemma 5.2. *For any $r, \zeta, \gamma > 0$, the equation $\chi_{AC-B^2}(r, \zeta, \gamma, c) = 0$ has two distinct real roots with respect to $c \in \mathbb{R}$.*

Proof. The proof is deferred to Section 5.1.3. □

By the quadratic formula, the roots can be found via symbolic computation as

$$c^\pm(r, \zeta) = p_1(r) \pm \sqrt{p_2(r)p_3(r)}$$

with the quadratics p_1 , p_2 , and p_3 defined in the proof statement. For convenience, let us restate the constants in the ζ parametrization:

$$\begin{aligned}a_1 &= \frac{2}{3}\zeta^2 + 2(1-\delta)^2, & b_1 &= \zeta - (\delta - \delta^2), & e_1 &= \frac{1}{2}(1 - \delta^2), \\ b_2 &= -\zeta(1 + \delta) + (1 - \delta^2), & e_2 &= \frac{1}{2}(1 + \delta)^2, \\ b_3 &= -\zeta(1 - \delta) - (1 - \delta^2)^2, & e_3 &= \frac{1}{2}(1 - \delta)^2.\end{aligned}$$

Since the leading coefficient of $c \mapsto \chi_{AC-B^2}(r, \zeta, \gamma, c)$ is positive, $c \mapsto \chi_{AC-B^2}(r, \zeta, \gamma, c)$

is a convex quadratic. Therefore, its left root

$$c^-(r, \zeta) = p_1(r) - \sqrt{p_2(r)p_3(r)} \quad (15)$$

identifies the region where χ_{AC-B^2} is positive.

Lemma 5.3. *For any $r, \zeta, \gamma > 0$ and all $c \in (-\infty, c^-(r, \zeta)]$, $\chi_{AC-B^2}(r, \zeta, \gamma, c) \geq 0$.*

Proof. The result follows from the fact that c^- is the left root of the equation $\chi_{AC-B^2}(r, \zeta, \gamma, c) = 0$ with respect to c and that χ_{AC-B^2} is a convex quadratic with respect to c . $\square$

However, recall that the argument c must satisfy $c > 0$ to be a valid contraction coefficient. Therefore, we must identify the conditions on $r, \zeta > 0$ that leads to $c^- > 0$ such that the range $(0, c^-)$ is non-empty. Define

$$r_{\max}(\zeta) \triangleq \frac{2\zeta(1-\delta^2)}{(4/3-\delta^2)\zeta^2 + 2\delta(1-\delta)\zeta + 3(1-\delta)^2}. \quad (16)$$

In the next lemma, we show that, for any fixed $\zeta > 0$, we have $c^-(r, \zeta) > 0$ for all $r \in (0, r_{\max})$.

Lemma 5.4. *For any $\zeta, \gamma > 0$ and all $r \in (0, r_{\max})$, we have $c^-(r, \zeta) > 0$.*

Proof. Consider the equivalence relations

$$\begin{aligned} & c^-(r, \zeta) = p_1(r) - \sqrt{p_2(r)p_3(r)} > 0 \\ \Leftrightarrow & p_1(r)^2 - p_2(r)p_3(r) > 0 \\ \Leftrightarrow & \left(-\left(\frac{4}{3} - \delta^2\right)\zeta^2 - 2\delta(1-\delta)\zeta - 3(1-\delta)^2 \right) r^2 + 2\zeta(1-\delta^2)r > 0. \end{aligned}$$

The last equivalence was derived using symbolic computation. Since $\delta \in (0, 1)$ and $\zeta > 0$, all of the coefficients on the left-hand side of the last line are non-zero. Also, it is a quadratic function with two roots: $r = 0$ and $r = r_{\max}$, and its leading coefficient is negative, implying that it is a concave quadratic. Therefore, it is strictly positive in between the two roots, which turns out to be the open interval $(0, r_{\max})$. The equivalence with the condition $c^- > 0$ implies the result. $\square$

The remaining condition $\chi_A > 0$ automatically follows by choosing $c = c^-(r, \zeta)$.

Lemma 5.5. *For any $\zeta, \gamma, r > 0$, if $c^-(r, \zeta) > 0$ then $\chi_A(r, \zeta, \gamma, c^-(r, \zeta)) > 0$.*

Proof. First, notice that

$$\chi_A(r, \zeta, \gamma, c) > 0 \Leftrightarrow \left(-\zeta^2 - 3(1-\delta)^2 \right) r^2 + 2\zeta r > c.$$

Denote the left-hand side as a polynomial in r as

$$\left(-\zeta^2 - 3(1-\delta)^2 \right) r^2 + 2\zeta r \triangleq p_4(r)$$

and pick $c = c^-(r, \zeta)$. Then

$$\begin{aligned}
& 0 < \chi_A(r, \zeta, \gamma, c^-(r, \zeta)) \\
\Leftrightarrow & p_1(r) - \sqrt{p_2(r)p_3(r)} < p_4(r) \\
\Leftrightarrow & (p_1(r) - p_4(r))^2 < p_2(r)p_3(r) \\
\Leftrightarrow & (p_1(r) - p_4(r))^2 - p_2(r)p_3(r) < 0
\end{aligned}$$

The left-hand side forms a polynomial, which follows from symbolic computation,

$$(p_1(r) - p_4(r))^2 - p_2(r)p_3(r) = p_5(r)r^2 = (a_5r^2 + b_5r + e_5)r^2$$

with the coefficients

$$\begin{aligned}
a_5 &\triangleq 3\delta(2-\delta)\left((1-\delta)^2 + 1\right) - \frac{1}{3}\zeta^4 - 2\zeta^2(1-\delta)^2 - 3 \\
b_5 &\triangleq -6\delta(1-\delta)^3 + \frac{2}{3}\zeta^3 - 2\zeta^2\delta(1-\delta) + 2\zeta(1-\delta)^2 \\
e_5 &\triangleq -3\delta^2(1-\delta)^2 - \frac{1}{3}\zeta^2 + 2\zeta\delta(1-\delta).
\end{aligned}$$

Analyzing the coefficient a_5 reveals that p_5 is a concave quadratic. Specifically, $a_5|_{\zeta=0} = 0$, and a_5 is monotonically decreasing with respect to ζ since, for all $\zeta > 0$,

$$\begin{aligned}
\frac{da_5}{d\zeta} &= \frac{d}{d\zeta} \left\{ 3\delta \left(1 + (1-\delta) + (1-\delta)^2 + (1-\delta)^3 \right) - \frac{1}{3}\zeta^4 - 2\zeta^2(1-\delta)^2 - 3 \right\} \\
&= -12\delta(1-\delta)^3 - \frac{4}{3}\zeta^3 - 4\zeta(1-\delta)^2 - 4\zeta^2(1-\delta)\delta < 0.
\end{aligned}$$

That is, $a_5 < 0$. Furthermore, using symbolic computation, the discriminant of p_5 follows as $\text{disc}(p_5) = b_5^2 - 4a_5e_5 = 0$, meaning that p_5 has a unique root. Said differently, for all $r \in \mathbb{R}$, $p_5(r) < 0$, meaning that, for any $\zeta > 0$ and all $r > 0$, $c^-(r, \zeta) = p_1(r) - \sqrt{p_2(r)p_3(r)} < p_4(r)$ holds. $\square$

Therefore, ensuring that χ_{AC-B^2} is non-negative also results in χ_A being positive. As such, we have characterized the conditions under which χ_A and χ_{AB-C^2} are positive. We are now ready to formally prove Theorem 3.1.

Proof of Theorem 3.1. Recall $r_{\max}$ in Eq. (16). Lemma 5.4 implies

$$r \in (0, r_{\max}) \quad \Rightarrow \quad c^-(r, \zeta) > 0.$$

Furthermore, as long as $c^-(r, \zeta) > 0$ can be ensured,

$$\begin{aligned}
c \in (0, c^-(r, \zeta)] &\quad \Rightarrow \quad \chi_{AC-B^2}(r, \zeta, \gamma, c) \geq 0 \quad \text{and} \quad (\text{Lemma 5.3}) \\
c \in (0, c^-(r, \zeta)] &\quad \Rightarrow \quad \chi_A(r, \zeta, \gamma, c) > 0. \quad (\text{Lemma 5.5})
\end{aligned}$$

Recall the equivalence in Eq. (14) that χ_A and χ_{AC-B^2} can be related to the spectrum of

$A_k, A_k C_k - B_k^2$ through the choice of $r = R(\sigma(H_k))$. Furthermore, under Assumption 2.1,

$$0 < \frac{\alpha\eta}{\gamma^2} \leq R(\sigma_p(H_k)) \leq \frac{\beta\eta}{\gamma^2}.$$

Therefore, the choice of contraction coefficient c in the proof statement satisfies

$$c = \inf_{\lambda \in [\alpha, \beta]} c^-(R(\lambda), \zeta) \quad \Rightarrow \quad \forall k \geq 0, \quad c \in (0, c^-(R(\sigma_p(H_k)), \zeta))$$

On the other hand, the boundedness of $r = R(\sigma(H_k))$ can be ensured through

$$\frac{\beta\eta}{\gamma^2} < r_{\max} \quad \Rightarrow \quad \forall k \geq 0, \quad 0 < R(\sigma_p(H_k)) < r_{\max} \quad \Rightarrow \quad \forall k \geq 0, \quad r \in (0, r_{\max})$$

Since the expression for $r_{\max}$ is rather complex, the condition in Eq. (8) serves as a simpler sufficient condition. This follows from the implications

$$\begin{aligned} & \frac{\beta\eta}{\gamma^2} < r_{\max} \\ \Leftrightarrow & \frac{\beta\eta}{\gamma^2} < \frac{2\zeta(1-\delta^2)}{\left(\frac{4}{3}-\delta^2\right)\zeta^2 + 2\delta(1-\delta)\zeta + 3(1-\delta)^2} \\ \Leftrightarrow & \frac{1}{\beta} > \frac{\eta}{\gamma^2} \frac{\left(\frac{4}{3}-\delta^2\right)\zeta^2 + 2\delta(1-\delta)\zeta + 3(1-\delta)^2}{2\zeta(1-\delta^2)} \\ \Leftrightarrow & \frac{1}{\beta} > \frac{\eta}{\gamma^2} \frac{\left(\frac{4}{3}-\delta^2\right)\zeta + 2\delta(1-\delta) + 3(1-\delta)^2/\zeta}{2(1-\delta^2)} \\ \Leftarrow & \frac{1}{\beta} \geq \frac{\eta}{\gamma^2} \frac{\left(\frac{4}{3}-\delta^2\right)\zeta + 3\delta(1-\delta) + 3(1-\delta)}{2(1-\delta^2)} & (1-\delta \leq \zeta, 2\delta < 3\delta) \\ \Leftrightarrow & \frac{1}{\beta} \geq \frac{\eta}{\gamma^2} \frac{\left(\frac{4}{3}-\delta^2\right)\zeta + 3(1-\delta^2)}{2(1-\delta^2)} \\ \Leftarrow & \frac{1}{\beta} \geq \frac{\eta}{\gamma^2} \frac{\frac{4}{3}\zeta + 3(1-\delta^2)}{2(1-\delta^2)} & (-\delta^2 < 0) \\ \Leftrightarrow & \text{Eq. (8)}. \end{aligned}$$

Therefore, under the choices of $r = R(\sigma_p(H_k))$, $c = \inf_{\lambda \in [\alpha, \beta]} c^-(R(\lambda), \zeta)$,

$$\text{Eq. (8)} \quad \Rightarrow \quad \forall k \geq 0, \quad A_k \succ 0 \quad \text{and} \quad A_k C_k - B_k^2 \succeq 0.$$

Finally, by invoking Lemma 5.1, we can conclude that, as long as Eq. (8) is ensured, Eq. (10) holds with $c = \inf_{\lambda \in [\alpha, \beta]} c^-(r, \zeta) > 0$ for all $k \geq 0$.

We now know that, under Eq. (8), the one-step contraction in Eq. (10) holds with the coefficient $c = \inf_{\lambda \in [\alpha, \beta]} c^-(r, \zeta)$. This implies that, for any $n \geq 1$, unrolling the recursion over $k = 1, \dots, n$ yields that

$$\|Z_n - Z'_n\|_{a,b}^2 \leq (1-c)^n \|Z_0 - Z'_0\|_{a,b}^2$$

holds almost surely. Now, for any $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^{2d})$, we know that there exists an optimal

coupling ρ^* between the two [Vil09, Cor. 5.22]. By initializing $(Z_0, Z'_0) \sim \rho^*$ and taking expectation over the noise sequence $(\xi_k^X, \xi_k^V)_{k \geq 1}$, for any $n \geq 1$, we obtain

$$W_{a,b}(\mu K^n, \nu K^n)^2 \leq \mathbb{E} \|Z_n - Z'_n\|_{a,b}^2 \leq (1-c)^n \mathbb{E} \|Z_0 - Z'_0\|_{a,b}^2 = (1-c)^n W_{a,b}(\mu, \nu) .$$

□

5.1.3 Proof of Lemma 5.2

Lemma 5.2. *For any $r, \zeta, \gamma > 0$, the equation $\chi_{AC-B^2}(r, \zeta, \gamma, c) = 0$ has two distinct real roots with respect to $c \in \mathbb{R}$.*

Proof. The discriminant of $c \mapsto \chi_{AC-B^2}(r, \zeta, \gamma, c)$ is given as

$$\text{disc}(c \mapsto \chi_{AC-B^2}(r, \zeta, \gamma, c)) = p_2(r) p_3(r),$$

where both p_2 and p_3 are quadratics in r . Since the leading coefficient of p_2 and p_3 are $a_1 > 0$, both are convex. Now, if a convex quadratic in $r \in \mathbb{R}$ has a strictly negative discriminant, it is strictly positive for all values of $r \in \mathbb{R}$.

The discriminant of p_2 can be shown to be strictly negative since

$$\begin{aligned} \text{disc}(p_2) &= b_2^2 - 4a_1e_2 \\ &= (\zeta(1+\delta) - (1-\delta^2))^2 - 4\left(\frac{2}{3}\zeta^2 + 2(1-\delta)^2\right)\left(\frac{1}{2}(1+\delta)^2\right) \\ &= (1-\delta)^2 \left\{ \left(\zeta \frac{1+\delta}{1-\delta} - (1+\delta)\right)^2 - 2\left(\frac{2}{3}\zeta^2 + 2(1-\delta)^2\right)\left(\frac{1+\delta}{1-\delta}\right)^2 \right\} \\ &= (1-\delta)^2 \left\{ \zeta^2 \left(\frac{1+\delta}{1-\delta}\right)^2 - 2\zeta \frac{(1+\delta)^2}{1-\delta} + (1+\delta)^2 - \frac{4}{3}\zeta^2 \left(\frac{1+\delta}{1-\delta}\right)^2 - 4(1+\delta)^2 \right\} \\ &= (1-\delta)^2 \left\{ -\frac{1}{3}\zeta^2 \left(\frac{1+\delta}{1-\delta}\right)^2 - 2\zeta \frac{(1+\delta)^2}{1-\delta} - 3(1+\delta)^2 \right\} \\ &< 0, \end{aligned}$$

while that of p_3 also turns out to be strictly negative since

$$\begin{aligned} \text{disc}(p_3) &= b_3^2 - 4a_1e_3 \\ &= (\zeta(1-\delta) + (1-\delta)^2)^2 - 4\left(\frac{2}{3}\zeta^2 + 2(1-\delta)^2\right)\left(\frac{1}{2}(1-\delta)^2\right) \\ &= (1-\delta)^2 \left\{ (\zeta + (1-\delta))^2 - 2\left(\frac{2}{3}\zeta^2 + 2(1-\delta)^2\right) \right\} \\ &= (1-\delta)^2 \left\{ \zeta^2 + 2\zeta(1-\delta) + (1-\delta)^2 - \frac{4}{3}\zeta^2 - 4(1-\delta)^2 \right\} \\ &= (1-\delta)^2 \left\{ -\frac{1}{3}\zeta^2 + 2\zeta(1-\delta) - 3(1-\delta)^2 \right\} \\ &= (1-\delta)^2 \left\{ -\left(\frac{1}{\sqrt{3}}\zeta - \sqrt{3}(1-\delta)\right)^2 \right\} \\ &< 0. \end{aligned}$$

Therefore, $p_1 > 0$ and $p_3 > 0$. Evidently, this implies that $\text{disc}(c \mapsto \chi_{AC-B^2}(r, \zeta, \gamma, c))$ is always strictly positive and that $c \mapsto \chi_{AC-B^2}(r, \zeta, \gamma, c)$ always has two distinct roots. $\square$

5.1.4 Proof of Corollary 3.2

Recall $c^-(r, \zeta)$ in Eq. (15). Define

$$r_{\text{lin}} \triangleq \frac{\zeta(1-\delta)}{2\zeta^2 + 6(1-\delta)^2}. \quad (17)$$

We establish that, for any $\zeta > 0$ and all $r \in (0, r_{\text{lin}}]$, the inequality $c^-(r, \zeta) \geq \zeta r$ holds. This is equivalent to establishing, for all $r \in (0, r_{\text{lin}}]$, the inequality

$$p_1(r) - \sqrt{p_2(r)p_3(r)} \geq \zeta r. \quad (18)$$

To proceed, we will use the following fact:

Lemma 5.6. *For all $r \in (0, r_{\text{lin}}]$, $p_1(r) \geq \zeta r$ holds.*

Proof. Consider the equivalence relations

$$\begin{aligned} p_1(r) &> \zeta r \\ \Leftrightarrow p_1(r) - \zeta r &> 0 \\ \Leftrightarrow -a_1 r^2 + (b_1 - \zeta)r + e_1 &> 0. \end{aligned} \quad (19)$$

The left-hand side forms a concave quadratic. Thus, if we find two points where this quadratic is strictly positive, all points in between satisfy Eq. (19). Since $e_1 > 0$, $r = 0$ trivially satisfies Eq. (19). On the other hand, since

$$r_{\text{lin}} < \frac{\zeta(1-\delta)}{\frac{2}{3}\zeta^2 + 2(1-\delta)^2} = \frac{\zeta(1-\delta)}{a_1}, \quad (20)$$

for $r = r_{\text{lin}}$, we have

$$\begin{aligned} &-a_1 r^2 + (b_1 - \zeta)r_{\text{lin}} + e_1 \\ &> -a_1 \frac{\zeta(1-\delta)}{a_1} r_{\text{lin}} - \delta(1-\delta)r_{\text{lin}} + \frac{1}{2}(1-\delta^2) \quad (\text{Eq. (20)}) \\ &= -(\zeta + \delta)(1-\delta)r_{\text{lin}} + \frac{1}{2}(1-\delta^2) \\ &= (1-\delta) \left\{ -(\zeta + \delta)r_{\text{lin}} + \frac{1}{2}(1+\delta) \right\} \\ &= (1-\delta) \left\{ -(\zeta + \delta) \frac{\zeta(1-\delta)}{2\zeta^2 + 6(1-\delta)^2} + \frac{1}{2}(1+\delta) \right\} \\ &= (1-\delta) \left\{ -\frac{\zeta^2(1-\delta)}{2\zeta^2 + 6(1-\delta)^2} + \frac{\delta\zeta(1-\delta)}{2\zeta^2 + 6(1-\delta)^2} + \frac{1}{2}(1+\delta) \right\} \\ &> (1-\delta) \left\{ -\frac{\zeta^2(1-\delta)}{2\zeta^2} + \frac{\delta\zeta(1-\delta)}{6(1-\delta)^2} + \frac{1}{2}(1+\delta) \right\} \quad (\zeta > 0, (1-\delta) > 0) \\ &= (1-\delta) \left\{ -\frac{1}{2}(1-\delta) + \frac{1}{6} \frac{\delta\zeta}{1-\delta} + \frac{1}{2}(1+\delta) \right\} \end{aligned}$$

$$\begin{aligned}
&= (1 - \delta) \left(\delta + \frac{1}{6} \frac{\delta \zeta}{1 - \delta} \right) \\
&> 0 .
\end{aligned} \tag{0 < \delta < 1}$$

Therefore, all points $r \in (0, r_{\text{lin}}]$ satisfy $p_1(r) > \zeta r$. □

Then, for all $r \in (0, r_{\text{lin}}]$, Eq. (18) can be developed as follows:

$$\begin{aligned}
& p_1(r) - \zeta r \geq \sqrt{p_2(r) p_3(r)} \\
\Leftrightarrow & (p_1(r) - \zeta r)^2 \geq p_2(r) p_3(r) \quad (p_1(r) > \zeta r) \\
\Leftrightarrow & (p_1(r) - \zeta r)^2 - p_2(r) p_3(r) \geq 0 .
\end{aligned} \tag{21}$$

Denote the left-hand side, which follows from symbolic computation, as

$$(p_1(r) - \zeta r)^2 - p_2(r) p_3(r) \triangleq p_6(r) r = (a_6 r^2 - b_6 r + e_6) r$$

with the coefficients

$$\begin{aligned}
a_6 &= \frac{4}{3} \zeta^3 + 4\zeta(1 - \delta)^2 \\
b_6 &= 3(1 - \delta)^2 + \zeta^2 \left(\frac{7}{3} - \delta^2 \right) \\
e_6 &= \zeta(1 - \delta^2) .
\end{aligned}$$

Under the conditions on the parameters, p_6 can be shown to be non-negative.

Lemma 5.7. *For all $r \in (0, r_{\text{lin}}]$, $p_6(r) \geq 0$ holds.*

Proof. Since p_6 is a convex quadratic, it suffices to verify that

$$\frac{dp_6}{dr}(r_{\text{lin}}) \leq 0 \quad \text{and} \quad p_6(r_{\text{lin}}) \geq 0 . \tag{22}$$

Then, by the monotonicity of the derivative of convex functions, all $r \in (0, r_{\text{lin}})$ satisfy $p_6(r) > 0$. First, notice that

$$\begin{aligned}
r_{\text{lin}} &= \frac{2}{3} \frac{\zeta^2(1 - \delta)}{(4/3)\zeta^3 + 4\zeta(1 - \delta)^2} \\
&= \frac{2}{3} \frac{\zeta^2(1 - \delta)}{a_6}
\end{aligned} \tag{23}$$

$$\begin{aligned}
&= \frac{2}{7} \frac{\zeta^2(\frac{7}{3} - \frac{7}{3}\delta)}{a_6} \\
&< \frac{2}{7} \frac{\zeta^2(\frac{7}{3} - \delta^2)}{a_6} \quad (- (7/3)\delta < -\delta < -\delta^2) \\
&< \frac{2}{7} \frac{3(1 - \delta)^2 + \zeta^2(\frac{7}{3} - \delta^2)}{a_6} \quad (0 < 3(1 - \delta)^2) \\
&= \frac{2}{7} \frac{b_6}{a_6} .
\end{aligned} \tag{24}$$

Then Eq. (24) implies

$$\frac{dp_6}{dr}(r_{\text{lin}}) = 2a_6 r_{\text{lin}} - b_6 < -\frac{3}{7}b_6 < 0.$$

Furthermore, using Eq. (23) and symbolic computation,

$$p_6(r_{\text{lin}}) = a_6 r_{\text{lin}}^2 - b_6 r_{\text{lin}} + e_6 = \frac{\frac{4}{9}\zeta^4(1-\delta)^2 - \frac{2}{3}\zeta^2(1-\delta)b_6 + a_6 e_6}{a_6}.$$

The denominator a_6 satisfies $a_6 > 0$. Therefore, we only need to analyze the sign of the numerator. Denote the numerator as a function of ζ , which follows from symbolic computation, as

$$\frac{4}{9}\zeta^4(1-\delta)^2 - \frac{2}{3}\zeta^2(1-\delta)b_6 + a_6 e_6 \triangleq p_7(\zeta)\zeta^2 = a_7\zeta^4 + b_7\zeta^2$$

with the coefficients

$$\begin{aligned} a_7 &\triangleq \frac{2}{9}(1+3\delta)(1-\delta)(1+\delta) \\ b_7 &\triangleq 2(1-\delta)^3(1+2\delta). \end{aligned}$$

By inspection, it is clear that $a_7, b_7 > 0$ for all $\delta \in (0, 1)$. Therefore, $p_7 > 0$ for all $\zeta > 0$. We can then conclude that $p_6(r) > 0$ for all $r \in (0, r_{\text{lin}}]$. $\square$

Thus, the inequality in Eq. (21) holds. We are now ready to prove Corollary 3.2.

Proof of Corollary 3.2. Recall r_{lin} in Eq. (17). For all $r \in (0, r_{\text{lin}}]$, we have the following equivalences:

$$\begin{aligned} &c^-(r, \zeta) \geq \zeta r \\ \Leftrightarrow &p_1(r) - \sqrt{p_2(r)p_3(r)} \geq \zeta r \\ \Leftrightarrow &(p_1(r) - \zeta r)^2 \geq p_2(r)p_3(r) \quad (\text{Lemma 5.6}) \\ \Leftrightarrow &p_6(r)r \geq 0 \quad (\text{Lemma 5.7}). \end{aligned}$$

This implies that, for the choice $r = R(\lambda)$, where $\lambda \in [\alpha, \beta]$, if $R(\lambda) \leq r_{\text{lin}}$ can be ensured, the contraction coefficient in Theorem 3.1 is lower bounded as

$$\inf_{\lambda \in [\alpha, \beta]} c^-(R(\lambda), \zeta) \geq \inf_{\lambda \in [\alpha, \beta]} \zeta R(\lambda) = \zeta \frac{\eta\alpha}{\gamma^2}.$$

Since $\lambda \in [\alpha, \beta]$, the condition $R(\lambda) \leq r_{\text{lin}}$ is sufficiently ensured by Assumption 3.2 due to the implications

$$\begin{aligned} R(\lambda) &\leq r_{\text{lin}} = \frac{\zeta(1-\delta)}{2\zeta^2 + 6(1-\delta)^2} \\ \Leftrightarrow \frac{\beta\eta}{\gamma^2} &\leq \frac{\zeta(1-\delta)}{2\zeta^2 + 6(1-\delta)^2} \end{aligned}$$

$$\begin{aligned}
\Leftrightarrow \quad \frac{1}{\beta} &\geq \frac{\eta}{\gamma^2} \frac{2\zeta^2 + 6(1-\delta)^2}{\zeta(1-\delta)} \\
\Leftrightarrow \quad \frac{1}{\beta} &\geq \frac{\eta}{\gamma^2} \left(2\frac{\zeta}{(1-\delta)} + 6\frac{1-\delta}{\zeta} \right) \\
\Leftrightarrow \quad \frac{1}{\beta} &\geq \frac{\eta}{\gamma^2} \left(2\frac{\zeta}{(1-\delta)} + 6 \right) \quad (1-\delta < \zeta) .
\end{aligned}$$

□

5.2 Asymptotic Bias Analysis

For the analysis of the asymptotic bias, we will define the following:

- $(Z_k)_{k \geq 0}$ is a Markov chain following the kinetic Langevin diffusion discretized with the stochastic exponential integrator (Eq. (5)), where, for some arbitrary distribution $\mu \in \mathcal{P}(\mathbb{R}^{2d})$, it is initialized as $Z_0 \sim \mu$.
- $(Z_t^*)_{t \geq 0}$ is the kinetic Langevin dynamics (Eq. (1)) initialized from its stationary distribution π .
- $(Z'_t)_{t \in [hk, h(k+1)]}$ is, for each $k \geq 0$, the stochastic exponential integration of $(Z_t^*)_{t \geq 0}$ linearly interpolated over the interval $[hk, h(k+1)]$. Specifically, for any $k \geq 0$ and any $t \in [hk, h(k+1)]$,

$$\begin{aligned} V'_t &= e^{-\gamma t} V_{hk}^* - \eta \int_{hk}^t e^{-\gamma(s-hk)} \nabla U(X_{hk}^*) ds + \sqrt{2\gamma\eta} \int_{hk}^t e^{-\gamma(s-hk)} dB_s \\ X'_t &= X_{hk}^* + \int_{hk}^t V'_s ds. \end{aligned} \quad (25)$$

In essence, $(Z'_t)_{t \in [hk, h(k+1)]}$ is a kinetic Langevin diffusion process with the drift set to be the zeroth order interpolation of the drift of $(Z_{hk}^*)_{k \geq 0}$.

Throughout the proof, we will assume that for any $k \geq 0$ and any $t \in [hk, h(k+1)]$, $(Z_k)_{k \geq 0}$, $(Z_t^*)_{t \geq 0}$, and $(Z'_t)_{t \geq 0}$ are synchronously coupled by sharing the same noise process $(B_t)_{t \geq 0}$.

5.2.1 Proof of Theorem 3.3

Under Assumption 3.2, Corollary 3.2 asserts that $(Z_k)_{k \geq 0}$ converges to the unique stationary distribution of K , π_h , such that $\lim_{k \rightarrow \infty} \mu K^k = \lim_{k \rightarrow \infty} \text{Law}(Z_k) = \pi_h$. Also, since (Z_t^*) is initialized from its stationary distribution π , for all $t \geq 0$, its law is $\text{Law}(Z_t^*) = \pi$. Notice

$$W_{a,b}(\pi_h, \pi) = \lim_{k \rightarrow \infty} W_{a,b}(\mu K^k, \pi P_{hk}) = \lim_{k \rightarrow \infty} W_{a,b}(\text{Law}(Z_k), \text{Law}(Z_{hk}^*)) . \quad (26)$$

Since $W_{a,b}$ is a proper distance metric under $a = 4/\gamma^2$ and $b = 1/\gamma$. Then, for any $k \geq 0$, we have the decomposition

$$\begin{aligned} &W_{a,b}(\text{Law}(Z_{k+1}), \text{Law}(Z_{h(k+1)}^*)) \\ &\leq W_{a,b}(\text{Law}(Z_{k+1}), \text{Law}(Z'_{h(k+1)})) + W_{a,b}(\text{Law}(Z'_{h(k+1)}), \text{Law}(Z_{h(k+1)}^*)) . \end{aligned}$$

Furthermore, Corollary 3.2 asserts that a contraction holds as

$$\begin{aligned} &W_{a,b}(\text{Law}(Z_{k+1}), \text{Law}(Z_{h(k+1)}^*)) \\ &\leq (1 - \tilde{c})^{1/2} W_{a,b}(\text{Law}(Z_k), \text{Law}(Z'_{hk})) + \underbrace{W_{a,b}(\text{Law}(Z'_{h(k+1)}), \text{Law}(Z_{h(k+1)}^*))}_{\triangleq E_{\text{disc}}} \end{aligned} \quad (27)$$

By bounding the one-step local discretization error E_{disc} and iterating the recursion, we obtain a bound on the asymptotic bias.

The following lemma relates the total local error to the local error of the momentum

alone:

Lemma 5.8. *Suppose $b^2 \leq a$ holds. Then, for any $k \geq 0$,*

$$W_{a,b}(\text{Law}(Z'_{hk}), \text{Law}(Z^*_{hk})) \leq \tilde{E}_{\text{pos}} + \tilde{E}_{\text{mom}},$$

where

$$\tilde{E}_{\text{pos}} \triangleq \left\{ h \int_{hk}^{h(k+1)} \mathbb{E} \|V_t^* - V_t'\|^2 dt \right\}^{1/2} \quad \text{and} \quad \tilde{E}_{\text{mom}} \triangleq \left\{ a \mathbb{E} \|V_{h(k+1)}^* - V'_{h(k+1)}\|^2 \right\}^{1/2}.$$

Proof. The proof is deferred to Section 5.2.2. $\square$

Here, $\tilde{E}_{\text{pos}}$ is the local error of the position $(X_k)_{k \geq 0}$, while $\tilde{E}_{\text{mom}}$ is that of the momentum $(V_k)_{k \geq 0}$. The second-order behavior of KLMC can be seen by the fact that $\tilde{E}_{\text{pos}}$ has an extra integral with a factor of h .

Using the fact that $(Z_t')_{t \geq 0}$ is the zeroth-order interpolation of $(Z_t^*)_{t \geq 0}$ and that $(Z_t^*)_{t \geq 0}$ is stationary, the local error of the momentum can be bounded as follows:

Lemma 5.9. *Suppose, Assumption 2.1 holds. Then, for any $k \geq 0$,*

$$\begin{aligned} \mathbb{E} \|V_{h(k+1)}^* - V'_{h(k+1)}\|^2 &\leq \frac{1}{4} d \beta^2 \eta^3 \left\{ \frac{h}{\gamma^3} - e^{-2h\gamma} \left(\frac{h}{\gamma^3} + 2 \frac{h^2}{\gamma^2} + 2 \frac{h^3}{\gamma} \right) \right\} \\ \int_{hk}^{h(k+1)} \mathbb{E} \|V_t^* - V_t'\|^2 dt &\leq \frac{1}{8} d \beta^2 \eta^3 \left\{ \frac{h^2}{\gamma^3} - 3 \frac{1}{\gamma^5} + e^{-2h\gamma} \left(3 \frac{1}{\gamma^5} + 6 \frac{h}{\gamma^4} + 5 \frac{h^2}{\gamma^3} + 2 \frac{h^3}{\gamma^2} \right) \right\}. \end{aligned}$$

Proof. The proof is deferred to Section 5.2.3. $\square$

Using these supporting results, we are now ready to prove Theorem 3.3.

Proof of Theorem 3.3. Under the stated assumptions, we can invoke Lemmas 5.8 and 5.9, which yield a bound on the total local error:

$$W_{a,b}(\text{Law}(Z'_{h(k+1)}), \text{Law}(Z^*_{h(k+1)})) \leq \left(\mathbb{E} \|Z'_{h(k+1)} - Z^*_{h(k+1)}\|_{a,b}^2 \right)^{1/2} \leq \tilde{E}_{\text{pos}} + \tilde{E}_{\text{mom}},$$

where

$$\begin{aligned} \tilde{E}_{\text{pos}}^2 &\leq \frac{1}{8} h d \beta^2 \eta^3 \left\{ \frac{h^2}{\gamma^3} - 3 \frac{1}{\gamma^5} + e^{-2h\gamma} \left(3 \frac{1}{\gamma^5} + 6 \frac{h}{\gamma^4} + 5 \frac{h^2}{\gamma^3} + 2 \frac{h^3}{\gamma^2} \right) \right\} \\ &= \frac{1}{8} d \beta^2 \eta^3 \left\{ \frac{h^3}{\gamma^3} - 3 \frac{h}{\gamma^5} + e^{-2h\gamma} \left(3 \frac{h}{\gamma^5} + 6 \frac{h^2}{\gamma^4} + 5 \frac{h^3}{\gamma^3} + 2 \frac{h^4}{\gamma^2} \right) \right\} \\ &= \frac{1}{8} d \beta^2 \eta^3 \frac{\zeta}{\gamma^6} \left\{ \zeta^2 - 3 + e^{-2\zeta} (3 + 6\zeta + 5\zeta^2 + 2\zeta^3) \right\} \\ \tilde{E}_{\text{mom}}^2 &\leq \frac{1}{4} a d \beta^2 \eta^3 \left\{ \frac{h}{\gamma^3} - e^{-2h\gamma} \left(\frac{h}{\gamma^3} + 2 \frac{h^2}{\gamma^2} + 2 \frac{h^3}{\gamma} \right) \right\} \end{aligned}$$

$$\begin{aligned}
&= d\beta^2\eta^3 \frac{h}{\gamma^5} (1 - e^{-2h\gamma} (1 + 2h\gamma + 2h^2\gamma^2)) \quad (a = 4/\gamma^2) \\
&= d\beta^2\eta^3 \frac{\zeta}{\gamma^6} (1 - e^{-2\zeta} (1 + 2\zeta + 2\zeta^2)) .
\end{aligned}$$

Denote $\Delta_k \triangleq W_{a,b}(\text{Law}(Z_{k+1}), \text{Law}(Z_{h(k+1)}^*))$. Then Eq. (27) yields

$$\Delta_{k+1} \leq (1 - \tilde{c})^{1/2} \Delta_k + \tilde{E}_{\text{pos}} + \tilde{E}_{\text{mom}} .$$

Unrolling the recursion,

$$\Delta_{k+1} \leq (1 - \tilde{c})^{k/2} \Delta_0 + \left(\tilde{E}_{\text{pos}} + \tilde{E}_{\text{mom}} \right) \sum_{i=0}^k (1 - \tilde{c})^{i/2} .$$

By taking the limit $k \rightarrow \infty$, and given the fact that $\lim_{k \rightarrow \infty} \text{Law}(Z_k) = \pi_h$ due to Corollary 3.2, and that (Z_t^*) is stationary for all $t \geq 0$,

$$W_{a,b}(\pi_h, \pi) = \Delta_\infty \leq \left(\tilde{E}_{\text{pos}} + \tilde{E}_{\text{mom}} \right) \sum_{i=0}^{\infty} (1 - \tilde{c})^{i/2} .$$

Using the bound

$$\sum_{i=0}^{\infty} (1 - \tilde{c})^{i/2} \leq \frac{1}{1 - \sqrt{1 - \tilde{c}}} \leq \frac{2}{\tilde{c}} = \frac{2\gamma^2}{\eta\zeta\alpha} ,$$

we finally conclude that

$$W_{a,b}(\pi_h, \pi) \leq \frac{2\gamma^2}{\eta\zeta\alpha} \tilde{E}_{\text{pos}} + \frac{2\gamma^2}{\eta\zeta\alpha} \tilde{E}_{\text{mom}} = E_{\text{pos}} + E_{\text{mom}} .$$

□

5.2.2 Proof of Lemma 5.8

For the proof of Lemma 5.8, we will use the following Minkowski-type inequality that holds for the norm $\|\cdot\|_{a,b}$:

Lemma 5.10. *Suppose $b^2 \leq a$ holds. Then, for any pair of random variables $Z = (X, V)$, the norm $\|\cdot\|_{a,b}$ satisfies*

$$\mathbb{E}^{1/2} \|Z\|_{a,b}^2 \leq \mathbb{E}^{1/2} \|X\|^2 + \sqrt{a} \mathbb{E}^{1/2} \|V\|^2.$$

Proof.

$$\begin{aligned} \mathbb{E}^{1/2} \|Z\|_{a,b}^2 &= \sqrt{\mathbb{E} \|X\|^2 + 2b \mathbb{E} \langle X, V \rangle + a \mathbb{E} \|V\|^2} \\ &\leq \sqrt{\mathbb{E} \|X\|^2 + 2b \left(\mathbb{E} \|X\|^2 \right)^{1/2} \left(\mathbb{E} \|V\|^2 \right)^{1/2} + a \mathbb{E} \|V\|^2} \quad (\text{Cauchy-Schwarz}) \\ &\leq \sqrt{\mathbb{E} \|X\|^2 + 2 \left(\mathbb{E} \|X\|^2 \right)^{1/2} \sqrt{a} \left(\mathbb{E} \|V\|^2 \right)^{1/2} + a \mathbb{E} \|V\|^2} \quad (b^2 \leq a) \\ &= \mathbb{E}^{1/2} \|X\|^2 + \sqrt{a} \mathbb{E}^{1/2} \|V\|^2. \end{aligned}$$

□

Proof of Lemma 5.8. For each $k \geq 0$, (Z_t^*) over the time interval $[hk, h(k+1)]$,

$$\begin{aligned} W_{a,b} \left(\text{Law} \left(Z'_{h(k+1)} \right), \text{Law} \left(Z_{h(k+1)}^* \right) \right) \\ \leq \mathbb{E}^{1/2} \|Z_{h(k+1)}^* - Z'_{h(k+1)}\|_{a,b}^2. \end{aligned}$$

Applying Lemma 5.10,

$$\begin{aligned} &\leq \mathbb{E}^{1/2} \|X_{h(k+1)}^* - X'_{h(k+1)}\|^2 + \sqrt{a} \mathbb{E}^{1/2} \|V_{h(k+1)}^* - V'_{h(k+1)}\|^2 \\ &= \mathbb{E}^{1/2} \left\| \int_{hk}^{h(k+1)} (V_t^* - V_t') dt + (X_{hk}^* - X'_{hk}) \right\|^2 + \sqrt{a} \mathbb{E}^{1/2} \|V_{h(k+1)}^* - V'_{h(k+1)}\|^2 \end{aligned}$$

and the fact that $(Z_t')_{t \geq 0}$ and $(Z_t^*)_{t \geq 0}$ are synchronously coupled,

$$= \mathbb{E}^{1/2} \left\| \int_{hk}^{h(k+1)} (V_t^* - V_t') dt \right\|^2 + \sqrt{a} \mathbb{E}^{1/2} \|V_{h(k+1)}^* - V'_{h(k+1)}\|_2^2.$$

The result follows by applying Jensen's inequality.

$$\leq \left(h \int_{hk}^{h(k+1)} \mathbb{E} \|V_t^* - V_t'\|^2 dt \right)^{1/2} + \sqrt{a} \mathbb{E}^{1/2} \|V_{h(k+1)}^* - V'_{h(k+1)}\|^2. \quad (28)$$

□

5.2.3 Proof of Lemma 5.9

In the proof, we will use the function

$$I_p(t) \triangleq \int_{hk}^t (s - hk)^p e^{-2\gamma(s-hk)} ds.$$

For any $p \geq 2$, integration by part yields the recursive definition

$$\begin{aligned} I_1(t) &= \frac{1}{4\gamma^2} - \frac{1}{4\gamma^2} e^{-2\gamma(t-hk)} - \frac{1}{2\gamma} e^{-2\gamma(t-hk)} (t - hk) \\ I_p(t) &= -\frac{1}{2\gamma} (t - hk)^p e^{-2\gamma(t-hk)} + \frac{p}{2\gamma} I_{p-1}(t) \quad (\text{for } p > 1). \end{aligned}$$

The exact form of I_p for any order $p > 1$ can then be conveniently computed via symbolic computation.

Proof of Lemma 5.9. Since $(V_t^*)_{t \geq 0}$ and $(V_t')_{t \geq 0}$ are synchronously coupled and $V_{hk}^* = V_{hk}'$ for all $t \in [hk, h(k+1)]$,

$$\begin{aligned} &\mathbb{E} \|V_t^* - V_t'\|^2 \\ &= \mathbb{E} \|V_t^* - V_{hk}^* + V_{hk}' - V_t'\|^2 \quad (V_{hk}' = V_{hk}^*) \\ &= \mathbb{E} \left\| e^{-\gamma t} V_{hk}^* + \eta \int_{hk}^t e^{-\gamma(s-hk)} \nabla U(X_s^*) ds \right. \\ &\quad \left. - e^{-\gamma t} V_{hk}^* + \eta \int_{hk}^t e^{-\gamma(s-hk)} \nabla U(X_{hk}^*) ds \right\|^2 \\ &= \mathbb{E} \left\| \eta \int_{hk}^t e^{-\gamma(s-hk)} (\nabla U(X_s^*) - \nabla U(X_{hk}^*)) ds \right\|^2 \\ &\leq \eta^2 (t - hk) \int_{hk}^t e^{-2\gamma(s-hk)} \mathbb{E} \|\nabla U(X_s^*) - \nabla U(X_{hk}^*)\|^2 ds \quad (\text{Jensen's inequality}) \\ &\leq \beta^2 \eta^2 (t - hk) \int_{hk}^t e^{-2\gamma(s-hk)} \mathbb{E} \|X_s^* - X_{hk}^*\|^2 ds \quad (\text{Assumption 2.1}) \\ &= \beta^2 \eta^2 (t - hk) \int_{hk}^t e^{-2\gamma(s-hk)} \mathbb{E} \left\| \int_{hk}^s V_u^* du \right\|^2 ds \\ &\leq \beta^2 \eta^2 (t - hk) \int_{hk}^t e^{-2\gamma(s-hk)} (s - hk) \int_{hk}^s \mathbb{E} \|V_u^*\|^2 du ds. \quad (\text{Jensen's inequality}) \end{aligned}$$

Since $(V_t^*)_{t \geq 0}$ is stationary with the stationary distribution $N(0_d, \eta I_d)$,

$$\begin{aligned} \mathbb{E} \|V_t^* - V_t'\|^2 &\leq d\beta^2 \eta^3 (t - hk) \int_{hk}^t e^{-2\gamma(s-hk)} (s - hk) \int_{hk}^s du ds \\ &= d\beta^2 \eta^3 (t - hk) \int_{hk}^t e^{-2\gamma(s-hk)} (s - hk)^2 ds. \end{aligned} \quad (29)$$

Using the function $I_p(t)$, Eq. (29) becomes

$$\begin{aligned}
& \mathbb{E} \|V_t^* - V_t'\|^2 \\
& \leq d\beta^2\eta^3 (t - hk) I_2(t) \\
& = d\beta^2\eta^3 (t - hk) \left\{ \frac{1}{4\gamma^3} - \frac{1}{4\gamma^3} e^{-2\gamma(t-hk)} - \frac{(t-hk)}{2\gamma^2} e^{-2\gamma(t-hk)} - \frac{(t-hk)^2}{2\gamma} e^{-2\gamma(t-hk)} \right\} \\
& = d\beta^2\eta^3 \left\{ \frac{(t-hk)}{4\gamma^3} - \frac{(t-hk)}{4\gamma^3} e^{-2\gamma(t-hk)} - \frac{(t-hk)^2}{2\gamma^2} e^{-2\gamma(t-hk)} - \frac{(t-hk)^3}{2\gamma} e^{-2\gamma(t-hk)} \right\}.
\end{aligned} \tag{30}$$

The first inequality in the statement follows by substituting $t = h(k+1)$.

The second inequality follows by integrating Eq. (30) again. Then

$$\begin{aligned}
& \int_{hk}^t \mathbb{E} \|V_s^* - V_s'\|^2 ds \\
& \leq d\beta^2\eta^3 \left\{ \frac{(t-hk)^2}{8\gamma^3} - \frac{1}{4\gamma^3} I_1(t) - \frac{1}{2\gamma^2} I_2(t) - \frac{1}{2\gamma} I_3(t) \right\} \\
& = d\beta^2\eta^3 \left\{ \frac{(t-hk)^2}{8\gamma^3} - \frac{3}{8} \frac{1}{\gamma^5} \right. \\
& \quad \left. + e^{-2\gamma(t-hk)} \left(\frac{3}{8} \frac{1}{\gamma^5} + \frac{3}{4} \frac{1}{\gamma^4} (t-hk) + \frac{5}{8} \frac{1}{\gamma^3} (t-hk)^2 + \frac{1}{4} \frac{1}{\gamma^2} (t-hk)^3 \right) \right\}.
\end{aligned}$$

Substituting $t = h(k+1)$ yields the statement.

□

5.2.4 Proof of Corollary 3.4

Recall E_{pos} and E_{mom} in Theorem 3.3. The result follows by upper-bounding the terms depending on ζ , f_{pos} for E_{pos} and f_{mom} for E_{mom} as

$$\begin{aligned} f_{\text{pos}}(\zeta) &\triangleq \zeta^2 - 3 + \exp(-2\zeta) (3 + 6\zeta + 5\zeta^2 + 2\zeta^3) \\ f_{\text{mom}}(\zeta) &\triangleq 1 - \exp(-2\zeta) (1 + 2\zeta + 2\zeta^2) . \end{aligned}$$

The upper bound for the underdamped and overdamped regimes corresponds to upper bounding f_{pos} and f_{mom} with their asymptotes in the direction of $\zeta \rightarrow 0$ and $\zeta \rightarrow \infty$, respectively.

For obtaining the upper bound, we will use the fact that, for two differentiable functions $f, g : \mathbb{R} \rightarrow \mathbb{R}$, suppose $f' \leq g'$ and there exists some $\zeta_0 \in \mathbb{R}$ such that $f(\zeta_0) \leq g(\zeta_0)$. Then the fundamental theorem of calculus yields $f \leq g$. This strategy can be applied recursively such that, for any $n \geq 2$, if the n th derivative satisfies $f^{(n)} \leq g^{(n)}$ and there exists a collection of points $(\zeta_0^{(k)})_{k=1, \dots, n-1}$ such that, for all $k = 1, \dots, n-1$, the bounds $f^{(k)}(\zeta_0^{(k)}) \leq g^{(k)}(\zeta_0^{(k)})$ hold, then $f \leq g$. Therefore, analyzing the derivatives of f_{pos} and f_{mom} will yield our bounds.

The derivatives of f_{pos} follow as

$$\frac{df_{\text{pos}}}{d\zeta}(\zeta) = 2\zeta \left(1 - e^{-2\zeta} (\zeta^2 + (1 + \zeta)^2) \right) \quad (31)$$

$$\frac{d^2 f_{\text{pos}}}{d\zeta^2}(\zeta) = 2e^{-2\zeta} (8\zeta^3 - 4\zeta^2 - 4\zeta) + 2 - 4e^{-2\zeta} \quad (32)$$

$$\frac{d^3 f_{\text{pos}}}{d\zeta^3}(\zeta) = -16e^{-2\zeta} (\zeta - 2) \zeta^2 , \quad (33)$$

while the derivative of f_{mom} follows as

$$\frac{df_{\text{mom}}}{d\zeta}(\zeta) = 4e^{-2\zeta} \zeta^2 . \quad (34)$$

Proof of Corollary 3.4. We will begin with (i). For E_{pos} , we will prove that that, for any $\zeta > 0$, the bound

$$f_{\text{pos}}(\zeta) \leq \frac{8}{15} \zeta^5$$

holds. Denote the right-hand side as $g_{\text{pos}}^{(i)}(\zeta) \triangleq \frac{8}{15} \zeta^5$. Recall the derivatives of f_{pos} in Eqs. (31) to (33). Then the bound on E_{pos} follow from the facts that

$$\frac{d^3 f_{\text{pos}}}{d\zeta^3}(\zeta) < 32\zeta^2 = \frac{d^3 g_{\text{pos}}^{(i)}}{d\zeta^3}(\zeta) , \quad \frac{d^2 f_{\text{pos}}}{d\zeta^2}(0) \leq \frac{d^2 g_{\text{pos}}^{(i)}}{d\zeta^2}(0) , \quad \frac{df_{\text{pos}}}{d\zeta}(0) = \frac{dg_{\text{pos}}^{(i)}}{d\zeta}(0) .$$

That is, $f_{\text{pos}}(\zeta) < g_{\text{pos}}^{(i)}(\zeta)$ for all $\zeta > 0$.

For E_{mom} , we will prove that, for any $\zeta > 0$, the bound

$$f_{\text{mom}}(\zeta) \leq \frac{4}{3} \zeta^3$$

holds. Denote the right-hand side as $g_{\text{mom}}^{(i)}(\zeta) \triangleq \frac{4}{3}\zeta^3$. Clearly, for all $\zeta > 0$ and Eq. (34),

$$\frac{df_{\text{mom}}}{d\zeta} < \frac{dg_{\text{mom}}^{(i)}}{d\zeta} \quad \text{and} \quad f_{\text{mom}}(0) = g_{\text{mom}}^{(i)}(0) .$$

Therefore, for all $\zeta > 0$, $f_{\text{mom}}(\zeta) < g_{\text{mom}}^{(i)}(\zeta)$. This implies the bound on E_{mom} .

Let's turn to (ii). The bound on E_{pos} is equivalent to

$$f_{\text{pos}}(\zeta) \leq \zeta^2 .$$

Denote the right-hand side as $g^{(ii)}(\zeta) = \zeta^2$ and recall Eq. (31). The bound immediately follows from the fact that

$$\frac{df_{\text{pos}}}{d\zeta}(\zeta) \leq 2\zeta = \frac{dg^{(ii)}}{d\zeta}(\zeta) \quad \text{and} \quad f(0) = g^{(ii)}(0) .$$

Finally, the bound on E_{mom} follows by using the fact that $f_{\text{mom}} < 1$. □

5.3 Complexity Analysis (Proof of Theorem 3.4)

From our choice of a and b , $\|\cdot\|_{a,b}$ is a valid norm meaning that we have

$$W_{a,b}(\mu K^n, \pi) \leq W_{a,b}(\mu K^n, \pi_h) + W_{a,b}(\pi_h, \pi) .$$

Thus, for any given $\epsilon > 0$, the result follows by solving for the smallest $n \geq 0$ ensuring

$$W_{a,b}(\mu K^n, \pi_h) + W_{a,b}(\pi_h, \pi) \leq \epsilon \Rightarrow W_{a,b}(\mu K^n, \pi) \leq \epsilon . \quad (35)$$

Denote the non-stationarity error as $E_{\text{stat}} \triangleq W_{a,b}(\mu K^n, \pi_h)$ and recall E_{mom} and E_{pos} in Theorem 3.3. Then the condition in Eq. (35) can be ensured by

$$E_{\text{stat}} \leq \frac{\epsilon}{3} \quad \wedge \quad E_{\text{pos}} \leq \frac{\epsilon}{3} \quad \wedge \quad E_{\text{mom}} \leq \frac{\epsilon}{3} . \quad (36)$$

E_{stat} is bounded by Corollary 3.2, while E_{stat} and E_{pos} is bounded by Corollary 3.4.

Let's first solve for the number of steps that guarantees E_{pos} is small.

Lemma 5.11. *Suppose Assumption 2.1 and Assumption 3.2 hold, and n denotes the number of KLMC steps. Then, for any $\epsilon > 0$,*

$$n \geq \frac{2\gamma^2}{\zeta\eta\alpha} \log \left(W_{a,b}(\mu, \pi_h) \frac{1}{\epsilon} \right) \Rightarrow E_{\text{stat}} \leq \epsilon .$$

Proof. The result follows as a corollary of Corollary 3.2, which implies

$$E_{\text{stat}} \leq \left(1 - \frac{\zeta\eta\alpha}{\gamma^2} \right)^{n/2} W_{a,b}(\mu, \pi_h) \leq \exp \left(-\frac{\zeta\eta\alpha}{2\gamma^2} n \right) W_{a,b}(\mu, \pi_h) . \quad (37)$$

This yields the necessary number of iterations through the implications

$$\begin{aligned} E_{\text{stat}} \leq \epsilon &\Leftrightarrow \exp \left(-\frac{\zeta\alpha}{2\gamma^2} n \right) W_{a,b}(\mu, \pi_h) \leq \epsilon \\ &\Leftrightarrow \exp \left(\frac{\zeta\alpha}{2\gamma^2} k \right) \geq W_{a,b}(\mu, \pi_h) \frac{1}{\epsilon} \\ &\Leftrightarrow \frac{\zeta\alpha}{2\gamma^2} n \geq \log \left(W_{a,b}(\mu, \pi_h) \frac{1}{\epsilon} \right) \\ &\Leftrightarrow n \geq \frac{2\gamma^2}{\zeta\alpha} \log \left(W_{a,b}(\mu, \pi_h) \frac{1}{\epsilon} \right) . \end{aligned}$$

□

The condition on the discretization error can be ensured by making ζ small enough.

Lemma 5.12. *Suppose Assumption 2.1 and Assumption 3.2 hold. Then, for any $\epsilon > 0$,*

$$\zeta \leq \min \left\{ \sqrt{\frac{15}{4}} \frac{\epsilon^{1/2} \gamma^{1/2}}{d^{1/4} \kappa^{1/2} \eta^{1/4}}, \frac{\sqrt{3}}{4} \frac{\epsilon \gamma}{d^{1/2} \kappa \eta^{1/2}} \right\} \Rightarrow E_{\text{pos}} \leq \epsilon \quad \wedge \quad E_{\text{mom}} \leq \epsilon .$$

Proof. Under the stated conditions, we can invoke Corollary 3.4, which implies

$$E_{\text{pos}} \leq \frac{4}{15} \frac{d^{1/2} \kappa \eta^{1/2}}{\gamma} \zeta^2 \quad \text{and} \quad E_{\text{mom}} \leq \frac{4}{\sqrt{3}} \frac{d^{1/2} \kappa \eta^{1/2}}{\gamma} \zeta.$$

We can solve for the conditions $E_{\text{pos}} \leq \epsilon$ and $E_{\text{mom}} \leq \epsilon$:

$$\begin{aligned} E_{\text{pos}} \leq \epsilon &\Leftrightarrow \frac{4}{15} \frac{d^{1/2} \kappa \eta^{1/2}}{\gamma} \zeta^2 \leq \epsilon \\ &\Leftrightarrow \frac{15}{4} \frac{\epsilon \gamma}{d^{1/2} \kappa \eta^{1/2}} \geq \zeta^2 \\ &\Leftrightarrow \sqrt{\frac{15}{4}} \frac{\epsilon^{1/2} \gamma^{1/2}}{d^{1/4} \kappa^{1/2} \eta^{1/4}} \geq \zeta \\ E_{\text{mom}} \leq \epsilon &\Leftrightarrow \frac{4}{\sqrt{3}} \frac{d^{1/2} \kappa \eta^{1/2}}{\gamma} \zeta \leq \epsilon \\ &\Leftrightarrow \frac{\sqrt{3}}{4} \frac{\epsilon \gamma}{d^{1/2} \kappa \eta^{1/2}} \geq \zeta. \end{aligned}$$

Taking the minimum over the two upper bounds on ζ ensures that both $E_{\text{pos}} \leq \epsilon$ and $E_{\text{mom}} \leq \epsilon$ are satisfied simultaneously. $\square$

Proof of Theorem 3.4. Assuming there exists some ζ such that all $\zeta \leq \zeta_0$ satisfies Assumption 3.2, according to Lemma 5.12, the choice

$$\zeta = \min \left\{ \sqrt{\frac{5}{4}} \frac{\epsilon^{1/2} \gamma^{1/2}}{d^{1/4} \kappa^{1/2} \eta^{1/4}}, \frac{1}{4\sqrt{3}} \frac{\epsilon \gamma}{d^{1/2} \kappa \eta^{1/2}}, \zeta_0 \right\}.$$

ensure $E_{\text{pos}} \leq \frac{\epsilon}{3} \wedge E_{\text{mom}} \leq \frac{\epsilon}{3}$. For the number of steps n guaranteeing $E_{\text{stat}} \leq \frac{\epsilon}{3}$, it suffices to substitute our choice of ζ in Lemma 5.11. This yields

$$n \geq \max \left\{ \sqrt{5} \frac{\gamma^{3/2}}{\eta^{3/4}} \frac{d^{1/4} \kappa^{1/2}}{\alpha} \frac{1}{\epsilon^{1/2}}, 8\sqrt{3} \frac{\gamma}{\eta^{1/2}} \frac{d^{1/2} \kappa}{\alpha} \frac{1}{\epsilon}, \zeta_0 \right\} \log \left(3W_{a,b}(\mu, \pi_h) \frac{1}{\epsilon} \right).$$

$\square$

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Supplementary Material The code for replicating our symbolic computation results is available online¹, along the instructions for executing the code².

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¹URL: <https://gist.github.com/Red-Portal/d157fd23cf254b61dd36379920abd7d3>

²URL: <https://gist.github.com/Red-Portal/98835096ca82203231e046bffc980ebf>

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