Abstract. We study the problem of sampling from a distribution for which the negative logarithm of the target density is $L$-smooth everywhere and $m$-strongly convex outside a ball of radius $R$, but potentially nonconvex inside this ball. We study both overdamped and underdamped Langevin MCMC and establish upper bounds on the time required to obtain a sample from a distribution that is within $\varepsilon$ of the target distribution in 1-Wasserstein distance. For the first-order method (overdamped Langevin MCMC), the time complexity is $\tilde{O} \left( e^{cLR^2} \frac{d}{\varepsilon} \right)$, where $d$ is the dimension of the underlying space. For the second-order method (underdamped Langevin MCMC), the time complexity is $\tilde{O} \left( e^{cLR^2} \sqrt{\frac{d}{\varepsilon}} \right)$ for an explicit positive constant $c$. Surprisingly, the convergence rate is only polynomial in the dimension $d$ and the target accuracy $\varepsilon$. It is exponential, however, in the problem parameter $LR^2$, which is a measure of non-logconcavity of the target distribution.

1 Introduction

In this paper, we study the problem of sampling from a target distribution

$$p^*(x) \propto \exp \left( -U(x) \right),$$

where $x \in \mathbb{R}^d$, and the potential function $U : \mathbb{R}^d \mapsto \mathbb{R}$ is $L$-smooth everywhere and $m$-strongly convex outside a ball of radius $R$ (see detailed assumptions in Section 1.2.1).

Our focus is on theoretical rates of convergence of sampling algorithms, including analysis of the dependence of these rates on the dimension $d$. Much of the theory of convergence of sampling—for example, sampling based on Markov chain Monte Carlo (MCMC) algorithms—has focused on asymptotic convergence, and has stopped short of providing a detailed study of dimension dependence. In the allied field of optimization algorithms, a significant new literature has emerged in recent years on non-asymptotic rates, including tight characterizations of dimension dependence. The optimization literature, however, generally stops short of the kinds of inferential and decision-theoretic computations that are addressed by sampling, in domains such as Bayesian statistics (Robert and Casella, 2013), bandit algorithms (Cesa-Bianchi and Lugosi, 2006) and adversarial online learning (Bubeck, 2011, Abbasi et al., 2013).

In both optimization and sampling, the classical theory focused on convex problems, while recent work focuses on the more broadly useful setting of non-convex problems. While general non-convex problems are infeasible, it is possible to make reasonable assumptions that allow theory to proceed while still making contact with practice.
We will consider the class of MCMC algorithms that have access to the gradients of the potential, \( \nabla U(\cdot) \). A particular algorithm of this kind that has received significant recent attention from theoreticians is the over\-damped Langevin MCMC algorithm (Dalalyan, 2017, Durmus and Moulines, 2016, Dalalyan and Karagulyan, 2017). The underlying first-order stochastic differential equation (henceforth SDE) is given by:
\[
dx_t = -\nabla U(x_t)dt + \sqrt{2}dB_t,
\]
where \( B_t \) represents a standard Brownian motion in \( \mathbb{R}^d \). Overdamped Langevin MCMC (Algorithm 1) is a discretization of this SDE. It is possible to show that under mild assumptions on \( U \), the invariant distribution of the overdamped Langevin diffusion is given by \( p^* (x) \).

The second-order generalization of overdamped Langevin diffusion is under\-damped Langevin diffusion, which can be represented by the following SDE:
\[
dx_t = u_t dt ,
\]
\[
\dot{u}_t = -\lambda_1 u_t - \lambda_2 \nabla U(x_t)dt + \sqrt{2\lambda_1\lambda_2}dB_t,
\]
where \( \lambda_1, \lambda_2 > 0 \) are free parameters. This SDE can also be discretized appropriately to yield a corresponding MCMC algorithm (Algorithm 2). Second-order methods like underdamped Langevin MCMC are particularly interesting as it has been previously observed both empirically (Neal, 2011) and theoretically (Cheng et al., 2017, Mangoubi and Smith, 2017) that these methods can be faster than the more classical overdamped methods.

In this work, we show that it is possible to sample from \( p^* \) in time polynomial in the dimension \( d \) and the target accuracy \( \varepsilon \) (as measured in 1-Wasserstein distance). We also show that the convergence depends exponentially on the product \( LR^2 \). Intuitively, \( LR^2 \) is a measure of the non-convexity of \( U(x) \). Our results establish rigorously that as long as the problem is not “too badly non-convex,” sampling is provably tractable.

Our main results are presented in Theorem 2.1 and Theorem 3.1, and can be summarized informally as follows:

**Theorem 1.1** (informal). Given a potential \( U \) that is \( L \)-smooth everywhere and strongly-convex outside a ball of radius \( R \), we can output a sample from a distribution which is \( \varepsilon \) close in \( W_1 \) to \( p^* \propto \exp (-U) \) by running \( \tilde{O} \left( \frac{d}{\varepsilon^2} e^{cLR^2} \right) \) steps of overdamped Langevin MCMC (Algorithm 1), or \( \tilde{O} \left( \frac{\sqrt{d}}{\varepsilon} e^{cLR^2} \right) \) steps of under\-damped Langevin MCMC (Algorithm 2). Here, \( c \) is an explicit constant.

For the case of convex \( U \), it has been shown by Cheng et al. (2017) that the iteration complexity of Algorithm 2 is \( \tilde{O}(\sqrt{d}/\varepsilon) \), quadratically improving upon the best known iteration complexity of \( \tilde{O}(d/\varepsilon^2) \) for Algorithm 1, as shown by Durmus and Moulines (2016). We will find this quadratic speed-up in \( d \) and \( \varepsilon \) in our setting as well (see Theorem 2.1 versus Theorem 3.1).

The problem of sampling from non-logconcave distributions has been studied by Raginsky et al. (2017), but under weaker assumptions, with a worst-case convergence rate that is exponential in \( d \). On the other hand, Ge et al. (2017) established a \( \text{poly}(d, 1/\varepsilon) \) convergence rate for sampling from a distribution close to a mixture of Gaussians, where the mixture components have the same variance (which is subsumed by our assumptions).

### 1.1 Related Work

The convergence rate of overdamped Langevin diffusion, under assumptions (A1) - (A3) has been established by Eberle (2016), but the continuous-time diffusion studied in that paper is not implementable algorithmically. In a more algorithmic line of work, Dalalyan (2017) bounded the discretization error of overdamped Langevin MCMC, and provided the first non-asymptotic convergence rate of overdamped Langevin MCMC under log-concavity assumptions. This was followed
by a sequence of papers in the strongly log-concave setting (see, e.g., Durmus and Moulines, 2016, Cheng and Bartlett, 2017, Dalalyan and Karagulyan, 2017, Dwivedi et al., 2018).

Our result for overdamped Langevin MCMC is in line with this existing work; indeed, we combine the continuous-time convergence rate of Eberle (2016) with a variant of the discretization error analysis by Durmus and Moulines (2016). The final number of timesteps needed is $\tilde{O}(e^{LR^2 d^2/\varepsilon^2})$, which is expected, as the rate of Eberle (2016) is $O(e^{-L R^2})$ (for the continuous-time process) and the iteration complexity established by Durmus and Moulines (2016) is $\tilde{O}(d/\varepsilon^2)$.

On the other hand, convergence of underdamped Langevin MCMC under (strongly) log-concave assumptions was first established by Cheng et al. (2017). Also very relevant to this work is the paper by Eberle et al. (2017) that demonstrated a contraction property of the continuous-time process in (2). That result deals, however, with a much larger class of potential functions, and because of this the distance to the invariant distribution scales exponentially with dimension $d$. At a high level, our analysis in Section 3 yields a more favorable result by combining ideas from both Eberle et al. (2017) and Cheng et al. (2017), under new assumptions.

Also noteworthy is that the problem of sampling from non-log-concave distributions has been studied by Raginsky et al. (2017), but under weaker assumptions, with a worst-case convergence rate that is exponential in $d$. On the other hand, Ge et al. (2017) established a $\text{poly}(d, 1/\varepsilon)$ convergence rate for sampling from a distribution close to a mixture of Gaussians, where the mixture components have the same variance (which is subsumed by our assumptions).

Finally, there is a large class of sampling algorithms known as Hamiltonian Monte Carlo (HMC), which involve Hamiltonian dynamics in some form. We refer to Ma et al. (2015) for a survey of the results in this area. Among these, the variant studied in this paper (Algorithm 2), based on the discretization of (2), has a natural physical interpretation as the evolution of a particle’s dynamics under a viscous force field. This model was first studied by Kramers (1940) in the context of chemical reactions. The continuous-time process has been studied extensively (Hérau, 2002, Villani, 2009, Eberle et al., 2017, Gorham et al., 2016, Baudoin, 2016, Bolley et al., 2010, Calogero, 2012, Dolbeault et al., 2015, Mischler and Mouhot, 2014). Three recent papers—Mangoubi and Smith (2017), Lee and Vempala (2017) and Mangoubi and Vishnoi (2018)—study the convergence rate of HMC under log-concavity assumptions.

After the completion of this paper, Bou-Rabee et al. (2018) independently published a preprint on arXiv analyzing Hamiltonian Monte Carlo under similar assumptions as ours.

1.2 Notation, Definitions and Assumptions

In this section we present the basic definitions, notational conventions and assumptions used throughout the paper. For $q \in \mathbb{N}$ we let $\|v\|_q$ denote the $q$-norm of a vector $v \in \mathbb{R}^d$. Throughout the paper we use $B_t$ to denote standard Brownian motion (Mörters and Peres, 2010).

1.2.1 Assumptions on the potential $U$

We make the following assumption on the potential function $U(x)$:

(A1) The function $U(x)$ is continuously-differentiable on $\mathbb{R}^d$ and has Lipschitz continuous gradients; that is, there exists a positive constant $L > 0$ such that for all $x, y \in \mathbb{R}^d$,

$$\|\nabla U(x) - \nabla U(y)\|_2 \leq L\|x - y\|_2.$$ 

(A2) The function has a stationary point at zero:

$$\nabla U(0) = 0.$$
(A3) The function is strongly convex outside of a ball; that is, there exist constants $m, R > 0$ such that for all $x, y \in \mathbb{R}^d$ with $\|x - y\|_2 > R$, we have:
\[
\langle \nabla U(x) - \nabla U(y), x - y \rangle \geq m \|x - y\|_2^2.
\]

Finally we define the condition number as $\kappa := L/m$. Observe that Assumption (A2) is imposed without loss of generality, because we can always find a local minimum in polynomial time and shift the coordinate system so that the local minimum of $U$ is at zero. These conditions are similar to the assumptions made by Eberle (2016). Note that crucially Assumption (A3) is strictly stronger than the assumption made in recent papers by Raginsky et al. (2017) and Zhang et al. (2017). To see this observe that these papers only require Assumption (A3) to hold for a fixed $y = 0$, while we require this to hold for all $y \in \mathbb{R}^d$. One can also think of the difference between these two conditions as being analogous to the difference between strong convexity (outside a ball) and one-point strong convexity (outside a ball).

### 1.2.2 Coupling and Wasserstein Distance

Denote by $\mathcal{B}(\mathbb{R}^d)$ the Borel $\sigma$-field of $\mathbb{R}^d$. Given probability measures $\mu$ and $\nu$ on $(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d))$, we define a transference plan $\zeta$ between $\mu$ and $\nu$ as a probability measure on $(\mathbb{R}^d \times \mathbb{R}^d, \mathcal{B}(\mathbb{R}^d) \times \mathcal{B}(\mathbb{R}^d))$ such that for all sets $A \in \mathcal{B}(\mathbb{R}^d)$, $\zeta(A \times \mathbb{R}^d) = \mu(A)$ and $\zeta(\mathbb{R}^d \times A) = \nu(A)$. We denote $\Gamma(\mu, \nu)$ as the set of all transference plans. A pair of random variables $(X, Y)$ is called a coupling if there exists a $\zeta \in \Gamma(\mu, \nu)$ such that $(X, Y)$ are distributed according to $\zeta$. (With some abuse of notation, we will also refer to $\zeta$ as the coupling.)

Given a function $f : \mathbb{R} \to \mathbb{R}$, we define the $f$-Wasserstein distance between a pair of probability measures as follows:
\[
W_f(\mu, \nu) := \inf_{\zeta \in \Gamma(\mu, \nu)} \int f(\|x - y\|_2) d\zeta(x, y).
\]

Finally we denote by $\Gamma_{\text{opt}}(\mu, \nu)$ the set of transference plans that achieve the infimum in the definition of the Wasserstein distance between $\mu$ and $\nu$ (for more properties of $W_f(\cdot, \cdot)$, see Villani, 2008). For any $q \in \mathbb{N}$ we define the $q$-Wasserstein distance as
\[
W_q(\mu, \nu) := \left( \inf_{\zeta \in \Gamma(\mu, \nu)} \int \|x - y\|_2^q d\zeta(x, y) \right)^{1/q}.
\]

### 1.2.3 Defining $f$ and related inequalities

We follow Eberle (2016) in our specification of the distance function $f$ that is used in the definition of the Wasserstein distance. We let $\alpha_f > 0$ and $\mathcal{R}_f > 0$ be two arbitrary constants (these are parameters used in defining $f$). We begin by defining auxiliary functions $\psi(r)$, $\Psi(r)$ and $g(r)$, all from $\mathbb{R}^+$ to $\mathbb{R}$:
\[
\psi(r) := e^{-\alpha_f \min\{r^2, \mathcal{R}_f^2\}}, \quad \Psi(r) := \int_0^r \psi(s) ds, \quad g(r) := 1 - \frac{1}{2} \frac{\int_0^{\min\{r, \mathcal{R}_f\}} \psi(s) \psi(s) ds}{\int_0^{\mathcal{R}_f} \psi(s) \psi(s) ds}, \tag{3}
\]

Let us summarize some important properties of the functions $\psi$ and $g$:

- $\psi$ is decreasing, $\psi(0) = 1$, and $\psi(r) = \psi(\mathcal{R}_f)$ for any $r > \mathcal{R}_f$.

- $g$ is decreasing, $g(0) = 1$, and $g(r) = \frac{1}{2}$ for any $r > \mathcal{R}_f$. 


Finally we define $f$ as
\[
 f(r) := \int_0^r \psi(s)g(s)ds. \tag{4}
\]
We now state some useful properties of the distance function $f$.

**Lemma 1.2.** The function $f$ defined in Eq. (4) has the following properties.

1. **(F1)** $f(0) = 0$, $f'(0) = 1$.
2. **(F2)** $\frac{1}{2}e^{-\alpha f}R_j^2 \leq \frac{1}{2}\psi(r) \leq f'(r) \leq 1$.
3. **(F3)** $\frac{1}{2}e^{-\alpha f}R_j^2r \leq \frac{1}{2}\Psi(r) \leq f(r) \leq \Psi(r) \leq r$.
4. **(F4)** For all $0 \leq r \leq R_f$, $f''(r) + \alpha f f'(r) \leq -\frac{e^{-\alpha f}R_j^2}{R_j^2} f(r)$.
5. **(F5)** For all $r \geq 0$, $f''(r) \leq 0$, and $f''(r) = 0$ when $r > R_f$.
6. **(F6)** If $\alpha f R_j^2 \geq \ln 2$, for any $0 < c < 1$, $f(r) \leq e^{-\frac{\alpha f R_j^2}{4}}f((1+c)r)$.

These properties follow fairly easily from the definition of the function $f$ above. We present proofs in Appendix A.

## 2 Overdamped Langevin Diffusion

We first set up the notation specific to the continuous and discrete processes that we use to study overdamped Langevin diffusion:

1. Consider the exact overdamped Langevin diffusion defined by the SDE in Eq. (1), with an initial condition $x_0 \sim p^{(0)}$ for some distribution $p^{(0)}$ on $\mathbb{R}^d$. Let $p_t$ denote the distribution of $x_t$ and let $\Phi_t$ denote the operator that maps from $p^{(0)}$ to $p_t$:
   \[
   \Phi_t p^{(0)} = p_t. \tag{5}
   \]
2. One step of the overdamped Langevin MCMC is defined by the SDE:
   \[
   d\tilde{x}_t = -\nabla U(x_0)dt + \sqrt{2d}dB_t, \tag{6}
   \]
   with an initial condition $x_0 \sim p^{(0)}$. We define $\tilde{\Phi}_t$ analogously for the discrete process.

**Note 1:** The discrete update differs from Eq. (1) by using a fixed $x_0$ instead of $x_t$ in the drift.

**Note 2:** We will only be analyzing the solutions to Eq. (6) for small $t$. Think of an integral solution of Eq. (6) as a single step of the discrete Langevin MCMC.

**Algorithm 1: Overdamped Langevin MCMC**

\begin{algorithm}
\hspace{10pt}**Input**: Step size $\delta < 1$, number of iterations $n$, initial point $x^{(0)}$, and gradient oracle $\nabla U(\cdot)$
\hspace{10pt}1 for $i = 0, 1, \ldots, n - 1$ do
\hspace{10pt}2 \hspace{20pt}Sample $x^{(i+1)} \sim N(x^{(i)} - \delta \nabla U(x^{(i)}), 2\delta I_{d \times d})$
\hspace{10pt}end
\end{algorithm}

It can be easily verified that $x^{(1)}$ in Algorithm 1 has the same distribution as $\tilde{x}_\delta$ in Eq. (6). Throughout this section, we denote by $p^*$ the unique distribution which satisfies $p^*(x) \propto \exp(-U(x))$. It can be shown that $p^*$ is the unique invariant distribution of (1) (see, for example, Proposition 6.1 in Pavliotis, 2016). In the discussion that follows we will use $p^{(k)}$ to denote the distribution of $x^{(k)}$ as defined in Algorithm 1. The main result of this section is Theorem 2.1, which establishes a convergence rate for Algorithm 1.
Theorem 2.1. Let $p^{(0)}$ be the Dirac delta distribution at $x^{(0)}$ with $\|x^{(0)}\|_2 \leq R$. Define $\bar{R}^2 = \max\{R^2, \frac{8}{m}\}$. Let $p^{(n)}$ be the distribution of the $n^{th}$ iterate of Algorithm 1 with step size
\[
\delta \leq \min \left\{ \frac{\varepsilon^2 e^{-LR^2}}{64L^2R^4d}, \frac{\varepsilon e^{-LR^2/2}}{2L^2R^2 \sqrt{60R^2 + 6d/m}} \right\}.
\]
Let
\[
n \geq L^2 \max \left\{ \frac{64\varepsilon^2 e^{LR^2} R^6 d}{\varepsilon^2}, \frac{16\varepsilon^3 L R^2 R^2 \sqrt{R^2 + \frac{d}{m}}}{\varepsilon} \right\} \log \left( \frac{24\varepsilon L R^2/4 \sqrt{R^2 + \frac{d}{m}}}{\varepsilon} \right) = \tilde{\Omega}\left( e^{\frac{5}{4}LR^2 \bar{d}} \right).
\]
Then $W_1(p^{(n)}, p^*) \leq \varepsilon$.

Remark. Note that in most interesting cases, $\delta$ is constrained by the first term, which shows that it suffices to have
\[
n \geq \frac{64L^2R^6 d}{\varepsilon^2} e^{\frac{5}{4}LR^2} \log \left( \frac{24\varepsilon L R^2/4 \sqrt{R^2 + \frac{d}{m}}}{\varepsilon} \right) = \tilde{\Omega}\left( e^{\frac{5}{4}LR^2 \bar{d}} \right).
\]

Intuitively, $LR^2$ measures the extent of nonconvexity. When this quantity is large, it is possible for $U$ to contain numerous local minima that are very deep. It is reasonable that the runtime of the algorithm should be exponential in this quantity.

2.1 Convergence of Continuous-Time Process

We begin by establishing the convergence of the continuous-time process (1) to the invariant distribution. Following Eberle (2016), we construct a coupling between two processes evolving according to the SDE (1). We accordingly define the first process as:
\[
dx_t = -\nabla U(x_t)dt + \sqrt{2}dB_t,
\]
where $x_0 \sim p_0$, and the second process as:
\[
dy_t = -\nabla U(y_t)dt + \sqrt{2} \left( I_{d \times d} - 2\gamma_t \gamma_t^\top \right) dB_t,
\]
with $y_0 \sim p^*$, where
\[
\gamma_t := \frac{x_t - y_t}{\|x_t - y_t\|_2} : \mathbb{I} [x_t \neq y_t].
\]
($\mathbb{I} [x_t \neq y_t]$ is the indicator function, which is 1 if $x_t \neq y_t$ and 0 otherwise.)

Additionally we also couple the processes so that the initial joint distribution of $x_0$ and $y_0$ corresponds to the optimal coupling between the two processes under $W_f$. To simplify notation, we define the difference process as $z_t := x_t - y_t$ with
\[
\begin{align*}
    dz_t &= -\nabla U(x_t) - \nabla U(y_t) dt + 2\sqrt{2} \gamma_t \gamma_t^\top dB_t \\
    &= -\nabla_t dt + 2\sqrt{2} \gamma_t dB_t.
\end{align*}
\]

With this notation in place we now show the contraction of the continuous-time process (1) in $W_f$. 

Proposition 2.2. Let $f$ and $W_f$ be as defined in Section 1.2.3 with $\alpha_f = L/4$ and $\mathcal{R}_f = R$. Then for any $t > 0$, and any probability measure $p_0$,

$$W_f(\Phi_t p_0, p^*) \leq \exp\left(-e^{-LR^2/4} \min\left\{\frac{4}{R^2}, \frac{m}{2}\right\} \cdot t\right) W_f(p_0, p^*),$$

where $\Phi_t$ is as defined in Eq. (5) and $p^*$ is the invariant distribution of (1).

Proof We define $r_t := \|z_t\|_2$. By Itô’s Formula (see Theorem E.1, sufficient regularity is established in Lemma E.8),

$$d\|z_t\|_2 = dr_t = -\langle \gamma_t, \nabla_t \rangle dt + \frac{4}{r_t} \gamma_t^\top \left(I_{d \times d} - \gamma_t \gamma_t^\top\right) \gamma_t dt + 2\sqrt{2} \langle \gamma_t, \gamma_t \rangle dB_t^1$$

$$= -\langle \gamma_t, \nabla_t \rangle dt + 2\sqrt{2} dB_t^1,$$

where $dB_t^1$ is a one-dimensional Brownian motion. Applying Itô’s Formula once again to $f(r_t)$:

$$df(r_t) = -f'(r_t) \langle \gamma_t, \nabla_t \rangle dt + 4f''(r_t) dt + 2\sqrt{2} f'(r_t) dB_t^1.$$

Taking an expectation,

$$d\mathbb{E}[f(r_t)] \leq -\mathbb{E} \left[f'(r_t) \langle \gamma_t, \nabla_t \rangle\right] dt + 4\mathbb{E} \left[f''(r_t)\right] dt. \quad (8)$$

We now complete the argument by considering two cases:

**Case 1 ($r_t < R$):** In this case, we know that by the smoothness assumption on $U(x)$ (Assumption (A1)),

$$-\langle \gamma_t, \nabla_t \rangle = -\frac{1}{\|z_t\|_2} \langle x_t - y_t, \nabla U(x_t) - \nabla U(y_t) \rangle \leq L\|z_t\|_2 = LR_t.$$

Combining with Eq. (8),

$$d\mathbb{E}[f(r_t)] \leq LR \mathbb{E} \left[f'(r_t) r_t\right] dt + 4\mathbb{E} \left[f''(r_t)\right] dt \leq -\frac{4}{R} \exp\left(-\frac{LR^2}{4}\right) \mathbb{E} \left[f(r_t)\right] dt.$$

The second inequality follows from the choice of $\alpha_f = L/4$ and $\mathcal{R}_f = R$ given in the statement of Proposition 2.2 and (F4) in Lemma 1.2.

**Case 2 ($r_t \geq R$):** In this case, we know that for points that are far away, the potential satisfies a strong-convexity-like condition (Assumption (A3)). Also, by Lemma 1.2, for any $r_t > R$, $f''(r_t) = 0$ and $f'(r_t) \geq \frac{1}{2} e^{-LR^2/4}$. Thus

$$d\mathbb{E}[f(r_t)] \leq -\mathbb{E} \left[f'(r_t) \left(\frac{z_t}{\|z_t\|_2}, \nabla U(x_t) - \nabla U(y_t)\right)\right] dt \leq -\frac{m}{2} e^{-LR^2/4} \mathbb{E} [r_t] dt \leq -\frac{m}{2} e^{-LR^2/4} \mathbb{E} [f(r_t)] dt.$$

Combining the two cases we get that, for any $r_t > 0$,

$$d\mathbb{E}[f(r_t)] \leq -\exp(-LR^2/4) \min\left\{\frac{4}{R^2}, \frac{m}{2}\right\} \mathbb{E} [f(r_t)] dt.$$

The claimed result follows by Grönwall’s Inequality (see Corollary 3 in Dragomir, 2003) assuming that the initial distributions are optimally coupled under $W_f$.

\[\square\]
2.2 Convergence of the Discrete-Time Process

We control the discretization error between the continuous and discrete processes using standard arguments (see, for example, Durmus and Moulines, 2016). The main conclusion is that the discretization error in \( W_2 \) (and consequently in \( W_1 \)) essentially scales as \( \mathcal{O}(\sqrt{\delta d}) \).

**Proposition 2.3.** Let the initial distribution \( p^{(0)} \) be a Dirac-delta distribution at \( \|x^{(0)}\|_2 \leq R \). Let \( p^{(k)} \) be the distribution of \( x^{(k)} \). Then, for all \( k \in \mathbb{N} \), if \( \delta \in \left[ 0, \frac{m}{12R^2} \right] \),

\[
\mathbb{E}_{(\tilde{x},x) \sim (\tilde{\Phi}_{\delta} p^{(k)}, \Phi_{\delta} p^{(k)})} \left[ \|\tilde{x} - x\|_2^2 \right] \leq \frac{4}{3} \left[ L^4 \delta^4 \left( 59R^2 + \frac{6d}{m} \right) + \frac{3}{2} \delta^3 d \right].
\]

The proof of this proposition is in Appendix B.

2.3 Proof of Theorem 2.1

In this section we combine the continuous-time contraction result (Proposition 2.2) with the discretization error bound (Proposition 2.3) to prove Theorem 2.1.

**Proof** [Proof of Theorem 2.1] We know that for any measures \( p, q \),

\[
W_f(p, q) \leq W_1(p, q) \leq W_2(p, q),
\]

as \( f(r) \leq r \). We also have \( p^{(0)}(S) = \|x^{(0)} \in S \) with \( x^{(0)} \in B_2(R) \). Thus Proposition 2.3 implies that for any \( j \in \mathbb{N} \) for \( \delta \in \left[ 0, \frac{m}{12R^2} \right] \),

\[
W_f(\tilde{\Phi}_{\delta} p^{(j)}, \Phi_{\delta} p^{(j)}) \leq 2 \left[ L^2 \delta^2 \sqrt{60R^2 + \frac{6d}{m} + L\delta \sqrt{\delta d}} \right].
\]

By the triangle inequality and concavity of \( f \),

\[
W_f(\tilde{\Phi}_{\delta} p^{(j)}, p^*) \leq W_f(\tilde{\Phi}_{\delta} p^{(j)}, p^*) + W_f(\tilde{\Phi}_{\delta} p^{(j)}, \Phi_{\delta} p^{(j)})
\]

\[
\leq W_f(\Phi_{\delta} p^{(j)}, p^*) + 2 \left[ L^2 \delta^2 \sqrt{60R^2 + \frac{6d}{m} + L\delta \sqrt{\delta d}} \right].
\]

By Proposition 2.2, the continuous-time process contracts, so

\[
W_f(\tilde{\Phi}_{\delta} p^{(j)}, p^*) \leq \exp \left( -e^{-LR^2/4} \min \left\{ \frac{4}{R^2}, \frac{m}{2} \right\} \delta \right) W_f(p^{(j)}, p^*)
\]

\[
+ 2 \left[ L^2 \delta^2 \sqrt{60R^2 + \frac{6d}{m} + L\delta \sqrt{\delta d}} \right].
\]

Unrolling this inequality for \( k \) steps:

\[
W_f((\tilde{\Phi}_{\delta})^k p^{(0)}, p^*) \leq \exp \left( -e^{-LR^2/4} \min \left\{ \frac{4}{R^2}, \frac{m}{2} \right\} k\delta \right) W_f(p^{(0)}, p^*)
\]

\[
+ \frac{2 \left[ L^2 \delta^2 \sqrt{60R^2 + \frac{6d}{m} + L\delta \sqrt{\delta d}} \right]}{1 - \exp \left( -e^{-LR^2/4} \min \left\{ \frac{4}{R^2}, \frac{m}{2} \right\} \delta \right)}
\]

\[
\leq \exp \left( -e^{-LR^2/4} \min \left\{ \frac{4}{R^2}, \frac{m}{2} \right\} k\delta \right) W_f(p^{(0)}, p^*)
\]

\[
+ 4e^{LR^2/4} \max \left\{ \frac{R^2}{4}, \frac{m}{2} \right\} \left[ L^2 \delta \sqrt{60R^2 + \frac{6d}{m} + L\delta d} \right],
\]
where \((i)\) follows by the sum of the geometric series \(1 + z + z^2 + \ldots = 1/(1 - z)\) for any \(|z| < 1\) and \((ii)\) follows by the approximation \(e^{-z} \leq 1 - z/2\) for \(z \in [0, 1]\). Finally, for any two measures \(\mu_1\) and \(\mu_2\), we can upper bound \(W_1(\mu_1, \mu_2)\) by \(e^{-LR^2/4} W_1(p, q) \leq W_1(p, q)\) as \(e^{-LR^2/4} \leq 1\). Plugging this into the inequality above gives us the desired result:

\[
W_1((\tilde{\Phi}_\delta)^k p^{(0)}, p^*) \leq 2 \exp \left( LR^2/4 - e^{-LR^2/4} \min \left\{ \frac{4}{R^2}, \frac{m}{2} \right\} k\delta \right) W_1(p^{(0)}, p^*) + 8e^{LR^2/2} \max \left\{ \frac{R^2}{4}, \frac{2}{m} \right\} \left[ L^2 \delta \sqrt{60R^2 + \frac{6d}{m}} + L\sqrt{\delta d} \right].
\]

We choose

\[
\delta \leq \min \left\{ \frac{\varepsilon}{e}e^{-LR^2/2} \frac{1024L^2d}{\left(\max \left\{ \frac{R^2}{4}, \frac{2}{m} \right\}\right)^2}, \frac{\varepsilon e^{-LR^2/2}}{32L^2} \max \left\{ \frac{R^2}{4}, \frac{2}{m} \right\} \sqrt{60R^2 + 6d/m} \right\}
\]

to ensure that the second term corresponding to the discretization error is small,

\[
8e^{LR^2/2} \max \left\{ \frac{R^2}{4}, \frac{2}{m} \right\} \left[ L^2 \delta \sqrt{60R^2 + \frac{6d}{m}} + L\sqrt{\delta d} \right] \leq \frac{\varepsilon}{2},
\]

and we pick

\[
n \geq \frac{\varepsilon}{e}e^{LR^2/4} \log \left( \frac{4W_1(p^{(0)}, p^*)e^{LR^2/4}}{\varepsilon} \right) \max \left\{ \frac{R^2}{4}, \frac{2}{m} \right\}
\]

\[
= \min \left\{ \frac{\varepsilon^2 e^{-LR^2}}{1024L^2d \left(\max \left\{ \frac{R^2}{4}, \frac{2}{m} \right\}\right)^2}, \frac{\varepsilon e^{-LR^2/2}}{32L^2} \left(\max \left\{ \frac{R^2}{4}, \frac{2}{m} \right\}\right)^2 \sqrt{60R^2 + 6d/m} \right\}
\]

to ensure that the first step contracts sufficiently

\[
2 \exp \left( LR^2/4 - e^{-LR^2/4} \min \left\{ \frac{4}{R^2}, \frac{m}{2} \right\} n\delta \right) W_1(p^{(0)}, p^*) \leq \frac{\varepsilon}{2}.
\]

Finally, by our choice of \(p^{(0)}\), we can upper bound \(W_1(p^{(0)}, p^*)\) by

\[
W_1(p^{(0)}, p^*) \leq R + E_{p^*} [||x||^2] \leq R + \sqrt{E_{p^*} [||x||^2]} \leq 6\sqrt{(R^2 + d/m)},
\]

where the first inequality is by the triangle inequality and the last inequality follows from Lemma E.3. Combining the pieces and simplifying gives us the desired result.

\[
\]

3 Underdamped Langevin Diffusion

For the rest of this paper, we will define the absolute constant \(c := 1000\), which will help clarify presentation. In this section, we study underdamped Langevin diffusion, a second-order diffusion process given by the following SDE:

\[
dy_t = v_t dt,
\]
\[
dv_t = -2v_t - \frac{1}{ckL} \nabla U(y_t) dt + \sqrt{\frac{4}{ckL}} dB_t,
\]

\[
(9)
\]
\( \kappa := \frac{L}{m} \) is the condition number.

Similar to the case of overdamped Langevin diffusion, it can be readily verified that the invariant distribution of the SDE is \( p^\ast(y, v) \propto e^{-U(y) - \frac{\kappa}{2} \|v\|_2^2} \). This ensures that the marginal along \( y \) is the distribution that we are interested in. Based on Eq. (9), we can define the discretized underdamped Langevin diffusion as

\[
\begin{align*}
  dx_t &= u_t dt, \\
  du_t &= -2u_t - \frac{1}{c\kappa L} \nabla U(x_{\lfloor t/\delta \rfloor}) dt + \sqrt{\frac{4}{c\kappa L}} dB_t,
\end{align*}
\]

where \( \delta \) is the step size of the discretization. In Theorem 3.2, we establish the rate at which (10) converges to \( p^\ast \). The SDE in Eq. (10) is implementable as the following algorithm:

**Algorithm 2: Underdamped Langevin MCMC**

**Input**: Step size \( \delta < 1 \), number of iterations \( n \), initial point \((x^{(0)}, 0)\), smoothness parameter \( L \), condition number \( \kappa \) and gradient oracle \( \nabla U(\cdot) \)

1. for \( i = 0, 1, \ldots, n - 1 \) do
   2. Sample \((x^{(i+1)}, u^{(i+1)}) \sim Z^{i+1}(x^{(i)}, u^{(i)})\)
3. end

The random vector \( Z^{i+1}(x^{(i)}, u^{(i)}) \in \mathbb{R}^{2d} \), conditioned on \((x^{(i)}, u^{(i)})\), has a Gaussian distribution with conditional mean and covariance obtained from the following computations:

\[
\begin{align*}
  \mathbb{E} \left[ u^{(i+1)} \right] &= u^{(i)} e^{-2\delta} - \frac{1}{2c\kappa L} (1 - e^{-2\delta}) \nabla U(x^{(i)}), \\
  \mathbb{E} \left[ x^{(i+1)} \right] &= x^{(i)} + \frac{1}{2} (1 - e^{-2\delta}) u^{(i)} - \frac{1}{2c\kappa L} \left( \delta - \frac{1}{2} (1 - e^{-2\delta}) \right) \nabla U(x^{(i)}), \\
  \mathbb{E} \left[ \left( x^{(i+1)} - \mathbb{E} \left[ x^{(i+1)} \right] \right) \left( x^{(i+1)} - \mathbb{E} \left[ x^{(i+1)} \right] \right)^\top \right] &= \frac{1}{c\kappa L} \left[ \delta - \frac{1}{4} e^{-4\delta} - \frac{3}{4} + e^{-2\delta} \right] I_{d \times d}, \\
  \mathbb{E} \left[ \left( u^{(i+1)} - \mathbb{E} \left[ u^{(i+1)} \right] \right) \left( u^{(i+1)} - \mathbb{E} \left[ u^{(i+1)} \right] \right)^\top \right] &= \frac{1}{c\kappa L} \left( 1 - e^{-3\delta} \right) I_{d \times d}, \\
  \mathbb{E} \left[ \left( x^{(i)} - \mathbb{E} \left[ x^{(i)} \right] \right) \left( u^{(i)} - \mathbb{E} \left[ u^{(i)} \right] \right)^\top \right] &= \frac{1}{2c\kappa L} \left[ 1 + e^{-3\delta} - 2e^{-2\delta} \right] I_{d \times d}.
\end{align*}
\]

It can be verified that \((x^{(i)}, u^{(i)})\) from Algorithm 2 and \((x_{\delta}, u_{\delta})\) from Eq. (10) have the same distribution (see Lemma E.6 for a proof of this statement; this lemma is essentially extracted from the calculations of Cheng et al. (2017), and we include it in the appendix for completeness). In the discussion that follows we will use \( p^{(k)} \) to denote the distribution \((x^{(k)}, u^{(k)})\) as defined in Algorithm 2. The following theorem establishes the convergence rate of Algorithm 2.

**Theorem 3.1.** Let \( p^{(0)} \) be the Dirac delta distribution at \( [x^{(0)} \ 0] \) with \( \|x^{(0)}\|_2 \leq R \). Let \( p^{(n)} \) be the \( n \)th iterate of Algorithm 2 with step size

\[
\delta \leq e^{-11LR^2/4} \frac{\varepsilon}{10^8 \max \{\kappa, LR^2\} \sqrt{R^2 + \frac{d}{m}}},
\]

and let

\[
n \geq 10^{18} \cdot e^{11LR^2/2} \cdot \kappa \cdot \max \{\kappa, LR^2\}^2 \cdot \log \left( \frac{30e^{11LR^2/4} \sqrt{R^2 + \frac{d}{m}}}{\varepsilon} \right) \cdot \sqrt{R^2 + \frac{d}{m}} \cdot \frac{\varepsilon}{\varepsilon}.
\]
Then \( W_1(p^n, p^*) \leq \varepsilon \).

**Remark.** The final expression for \( n \) can be simplified to
\[
n = \tilde{\Omega} \left( e^{11LR^2/2 \sqrt{d}/\varepsilon} \right).
\]

The proof of this theorem relies on an intricate coupling argument. Similar to the overdamped case we begin by defining two processes, \((x_t, u_t)\) and \((y_t, v_t)\), and then couple them appropriately using both synchronous and reflection coupling. In the rest of this section we use the variables
\[
\begin{align*}
    &z_t := x_t - y_t; \quad w_t := u_t - v_t; \quad \phi_t := z_t + w_t; \quad \gamma_t := \frac{z_t + w_t}{\lVert z_t + w_t \rVert_2}; \\
    &\nabla_t := \nabla U(x_t) - \nabla U(y_t); \quad \tilde{\nabla}_t := \nabla U(x_t/\delta) - \nabla U(y_t).
\end{align*}
\]
(11)

Here \( z_t \) denotes the difference of the position variables, \( w_t \) is the difference of the velocity variables, \( \phi_t \) is the sum of \( z_t \) and \( w_t \), \( \gamma_t \) is the unit vector along \( \phi_t \). \( \nabla_t \) denotes the difference between the gradients at \( x_t \) and \( y_t \) while \( \tilde{\nabla}_t \) captures the difference between the gradients as \( x_t \) is discretized at a scale of \( \delta \).

Similar to Section 2, we initialize \((y_0, v_0)\) according to the invariant distribution \( p^*(y, v) \), and thus when \((y_t, v_t)\) evolves according to (9), it remains distributed according to the invariant distribution. The process \((x_t, u_t)\) will denote the path of the iterates of Algorithm 2 and we will use the difference between these processes to track the distance between the distributions. We define a stochastic process
\[
\theta_t = (x_t, u_t, y_t, v_t, \tau_t, \rho_t, \mu_t, \xi_t) : \mathbb{R}^+ \to \mathbb{R}^{4d+4}.
\]

The dynamics of \( \theta_t \) are defined as follows:
\[
\begin{align*}
    &d \begin{bmatrix} x_t \\ u_t \end{bmatrix} = \left[ -2u_t - \frac{u_t}{cKL} \nabla U(x_t) \right] dt + \left[ \frac{0}{2cKL} dB_t \right] \quad (12) \\
    &d \begin{bmatrix} y_t \\ v_t \end{bmatrix} = \left[ -2v_t - \frac{v_t}{cKL} \nabla U(y_t) \right] dt + \left[ \frac{0}{2cKL} dB_t \right] \cdot (1 - \mu_t) + \left[ \frac{0}{2cKL} (1 - 2\gamma_t \gamma_t^T) dB_t \right] \cdot \mu_t \quad (13) \\
    &d\tau_t = \Pi \left[ t \geq \tau_{t-} + T_{\text{sync}} \text{ AND } \sqrt{\lVert z_t \rVert_2^2 + \lVert z_t + w_t \rVert_2^2} \geq \sqrt{5R} \right] \cdot (t - \tau_{t-}) \quad (14) \\
    &\rho_t = \left( 1 + \frac{2}{cK} \right) \lVert z_{\tau_t} \rVert_2 + \lVert z_{\tau_t} + w_{\tau_t} \rVert_2 \quad (15) \\
    &\mu_t = \Pi \left[ t \geq \tau_t + T_{\text{sync}} \right] \quad (16) \\
    &\xi_t = \frac{4}{cKL} \int_{\tau_t}^t e^{(s-\tau_t)/(3cK)^2} \lVert \nabla_s - \tilde{\nabla}_s \rVert_2 ds, \quad (17)
\end{align*}
\]
where
\[
T_{\text{sync}} := 3(cK)^2 \cdot \log(10)
\]
and
\[
C_{\text{sync}}^u := \exp \left( -11LR^2/4 \right) / 200T_{\text{sync}} = \exp \left( -11LR^2/4 \right) / 600(cK)^2 \cdot \log 10.
\]

Note that \( z_t \) and \( w_t \) are continuous almost surely, so all occurrences of \( z_t \) and \( w_t \) can be replaced by \( z_{t-} \) and \( w_{t-} \). Thus \( \theta_t \) is left-continuous and adapted.

Some comments about each of the variables:
The marginal \((x_t, u_t)\) defined in Eq. (12) has exactly the same dynamics as Eq. (10) while the marginal \((y_t, v_t)\) defined in Eq. (13) has exactly the same dynamics as Eq. (9).

\(\mu_t\) acts as a binary variable that is either 0 or 1. The joint distribution of \((x_t, u_t, y_t, v_t)\) will evolve by synchronous coupling if \(\mu_t = 1\) and by reflection coupling along \(\gamma_t\)’s direction if \(\mu_t = 0\).

We use synchronous coupling when the two processes are separated by a distance greater than \(\sqrt{5}R\) because assumption (A3) guarantees contraction under synchronous coupling. We use reflection coupling when the two processes are closer than \(\sqrt{5}R\) as synchronous coupling cannot guarantee contraction in this regime.

The variable \(\xi_t\) accounts for the discretization error in the process \((x_t, u_t)\) as the dynamics of \((x_t, u_t)\) uses \(\nabla U(x_{\lfloor t/\delta \rfloor}\delta)\) instead of \(\nabla U(x_t)\).

Once we start running synchronous coupling, we stick to synchronous coupling for a time interval of at least \(T_{\text{sync}}\) to ensure adequate contraction between the two processes.

\(C_u\) denotes the contraction factor when we run synchronous coupling and will be used to define the Lyapunov function below.

The stochastic process \(\theta_t\) is initialized as follows:

\[
(x_0, u_0, y_0, v_0) \sim \Gamma_{\text{opt}}(p^{(0)}, p^*); \quad \xi_0 = 0;
\]

\[
\begin{bmatrix}
\tau_0 \\
\rho_0 \\
\mu_0
\end{bmatrix} = \begin{bmatrix}
\lfloor \sqrt{\|z_0\|_2 + \|z_0 + w_0\|_2} \geq \sqrt{5}R \rfloor \\
(1 + 2/(ck))\|z_0\|_2 + \|z_0 + w_0\|_2
\end{bmatrix} \cdot \begin{bmatrix}
0 \\
0
\end{bmatrix}
\]

\[
+ \begin{bmatrix}
\lfloor \sqrt{\|z_0\|_2 + \|z_0 + w_0\|_2} < \sqrt{5}R \rfloor \\
(1 + 2/(ck))\|z_0\|_2 + \|z_0 + w_0\|_2
\end{bmatrix} \cdot \begin{bmatrix}
-T_{\text{sync}} \\
1
\end{bmatrix},
\]

where \(\Gamma_{\text{opt}}\) is the optimal coupling between \(p^{(0)}(x, u)\) and \(p^*(y, v)\) under the \(W_1\) distance.

**Defining the Lyapunov Function**

Let the function \(f\) be as defined in Eq. (4), with parameters

\[
\mathcal{R}_f = \sqrt{11\alpha_f} = \frac{L}{4}, \quad \alpha_f = \frac{L}{4}
\]

Given such a \(f\), we define the Lyapunov function \(\mathcal{L}(\theta_t)\) as follows:

\[
\mathcal{L}(\theta_t) = \mu_t \cdot f\left(\left(1 + \frac{2}{ck}\right)\|z_t\|_2 + \|z_t + w_t\|_2\right)
\]

\[
+ (1 - \mu_t) \cdot \left(f(\mu_t) \cdot e^{-C_u T_{\text{sync}}(t - \tau_t)} + \xi_t\right). \tag{23}
\]

We show in Lemma E.7 that the expected value of this Lyapunov function, \(E[\mathcal{L}(\theta_t)]\), both upper and lower bounds \(W_1(p_t, p^*)\). Thus Theorem 3.1 follows almost immediately from the following proposition:
Proposition 3.2. Let \( p^{(0)} \) be the Dirac delta distribution at \((x^{(0)}, 0)\) for \( \|x^{(0)}\|_2 \leq R \). Let \( \theta_t \) be as defined above with step size
\[
\delta \leq e^{-11 LR^2/4} \frac{\varepsilon}{10^8 \max \{ \kappa, LR^2 \} \sqrt{R^2 + d/m}}
\]
if
\[
n \geq 10^{18} \cdot e^{11 LR^2/2} \cdot \kappa \cdot \max \{ \kappa, LR^2 \} \cdot \log \left( \frac{4E[L(\theta_0)]}{\varepsilon} \right) \cdot \sqrt{R^2 + d/m},
\]
then we are guaranteed to have \( E[L(\theta_n \delta)] \leq \varepsilon \).

Proof Sketch

For convenience in the proofs, we will assume in this section that
\[
e^{11 LR^2/4} \geq 2
\]
This assumption is not necessary but helps simplify the proof. This assumption is without loss of generality since we can always use a sufficiently large \( L \) in (A1).

The central ideas are contained in the proof of Proposition 3.2. Theorem 3.1 is a simple corollary of Proposition 3.2. The proof of Proposition 3.2 is roughly as follows:

- Outside the ball of radius \( \sqrt{5}R \), we use synchronous coupling. We can use the strong convexity of \( U(\cdot) \) when \( \|z_t\|_2 \geq R \) to obtain a contraction rate based on the drift of (10) alone, without needing Brownian motion.

- Within a ball of radius \( \sqrt{5}R \), we cannot rely on the convexity of \( U(\cdot) \) and the drift of (10) can actually increase the distance under coupling. However, \( f(\cdot) \) is designed so that it contracts under reflection coupling even without strong convexity. We pay the price of nonconvexity with a slow contraction rate of \( e^{-11 LR^2/4} \), where \( LR^2 \) roughly characterizes how badly nonconvex \( U(\cdot) \) is.

The dynamic of Eq. (12) - Eq. (17) switches between reflection and synchronous coupling depending on whether \( \left\| \begin{bmatrix} z_t \\ z_t + w_t \end{bmatrix} \right\|_2 \geq \sqrt{5}R \). One technical difficulty of the analysis is that synchronous coupling gives contraction in \( \sqrt{\|z_t\|^2 + \|z_t + w_t\|^2} \) whereas reflection coupling gives contraction in \( f((1 + 2/(c\kappa))\|z_t\|_2 + \|z_t + w_t\|_2) \). The Lyapunov function \( L(\cdot) \) is designed to stitch these two different contractions together.

Proof [Proof of Proposition 3.2] We study the evolution of \( L(\theta_t) \) by dividing it into four cases.

Case 1. \( \mu_{t-} = 1, \mu_t = 1 \) (reflection coupling)

Case 2. \( \mu_{t-} = 0, \mu_t = 0 \) (synchronous coupling)

Case 3. \( \mu_{t-} = 1, \mu_t = 0 \) (jump from reflection to synchronous)

Case 4. \( \mu_{t-} = 0, \mu_t = 1 \) (jump from synchronous to reflection)

The proof of convergence in each of these cases is fairly technical and we provide the proofs in Appendix C. Below, we gather the different results.

Case 1: We use Itô’s Lemma to study the evolution of \( E[L(\theta_t)] \). The technical proof (which relies on a reflection coupling argument) is provided in Lemma C.1, with the conclusion that,
\[
\frac{d}{dt} E[L(\theta_t)]|_{\mu_{t-} = \mu_t = 1} \leq -C_{\text{ref}}^u E[L(\theta_t)]|_{\mu_{t-} = \mu_t = 1} + \text{discretization error},
\]
where $C_{\text{ref}}^u := \min \left\{ \frac{e^{-11L^2/4}}{1375\kappa LR^2}, \frac{e^{-11L^2/4}}{4\kappa} \right\}$ as defined in Lemma C.1. We use the crucial fact that $\sqrt{\|z_t\|^2 + \|z_t + w_t\|^2} \leq \sqrt{5}R$, which implies $(1 + 2/(\kappa\varepsilon))\|z_t\|^2 + \|z_t + w_t\|^2 \leq \sqrt{11}R.$

**Case 2:** In this case there is no (explicit) Brownian motion added to the difference process, so we use basic calculus to study the dynamics of $E[L(\theta_t)]$. The technical proof is provided in Lemma C.2, with the conclusion that,

$$\frac{d}{dt}E[L(\theta_t)|\mu_t = 0] \leq - \min \left\{ C_{\text{sync}}^u, \frac{1}{3(\kappa\varepsilon)^2} \right\} E[L(\theta_t)|\mu_t = 0] + \text{discretization error},$$

where $C_{\text{sync}}^u := e^{-11L^2/4}/(600(\kappa\varepsilon)^2 \log(10))$ as defined in Eq. (19). In this case, we use the convexity of $U(\cdot)$ outside a ball of radius $R$ to get contraction of $\sqrt{\|z_t\|^2 + \|z_t + w_t\|^2}$ based on the drift alone.

**Case 3:** There is a jump in $\theta_t$, but by definition of $\rho_t$, there is no jump in $L(\theta_t)$, so the analysis is essentially the same as Case 1 and

$$\frac{d}{dt}E[L(\theta_t)|\mu_t = 1, \mu_t = 0] \leq - C_{\text{sync}}^u E[L(\theta_t)|\mu_t = 1, \mu_t = 0] + \text{discretization error}.$$ 

**Case 4:** There is a jump in $L(\theta_t)$ as we switch from $L(\theta_{t^-}) = f(\rho_{t^-}) \cdot e^{-C_{\text{sync}}^u (t^- - \tau_{t^-})} + \xi_{t^-}$ to $L(\theta_t) = f((1 + 2/(\kappa\varepsilon))\|z_t\|^2 + \|z_t + w_t\|^2)$, in addition to the contraction in Case 2 (when we just have pure synchronous coupling) in Proposition C.3. We show that the jump is almost surely negative, so by Itô’s Lemma (see Theorem E.1) and Lemma C.2 (contraction under synchronous coupling),

$$dE[L(\theta_t)|\mu_t = 0, \mu_t = 1] \leq - C_{\text{sync}}^u E[L(\theta_t)|\mu_t = 0, \mu_t = 1] dt + \text{discretization error}.$$ 

Putting the results of all the four cases together,

$$\frac{d}{dt}E[L(\theta_t)] \leq - \min \left\{ C_{\text{ref}}^u, C_{\text{sync}}^u, \frac{1}{3(\kappa\varepsilon)^2} \right\} E[L(\theta_t)] + \frac{4}{C_{\text{ref}}^u} \left\| \nabla U(x_t) - \nabla U(x_{t/\delta}) \right\|_2$$

$$\leq - \min \left\{ C_{\text{ref}}^u, C_{\text{sync}}^u, \frac{1}{3(\kappa\varepsilon)^2} \right\} E[L(\theta_t)] + \frac{200\delta}{\kappa} \sqrt{R^2 + d/m},$$

where the bound on the discretization error term follows from Proposition D.1 and Jensen’s inequality. By taking the step size small enough, specifically,

$$\delta \leq \frac{400\varepsilon\kappa \min \left\{ C_{\text{ref}}^u, C_{\text{sync}}^u, \frac{1}{3(\kappa\varepsilon)^2} \right\}}{\sqrt{R^2 + d/m}},$$

we ensure that the discretization error is less than $\min \left\{ C_{\text{ref}}^u, C_{\text{sync}}^u, \frac{1}{3(\kappa\varepsilon)^2} \right\} \cdot \varepsilon/2$, thus

$$d \left( E[L(\theta_t)] - \varepsilon/2 \right) \leq - \min \left\{ C_{\text{ref}}^u, C_{\text{sync}}^u, \frac{1}{3(\kappa\varepsilon)^2} \right\} \left( E[L(\theta_t)] - \frac{\varepsilon}{2} \right) dt.$$ 

To get $E[L(\theta_t)] \leq \varepsilon$, it suffices to take total time ($t^*$) and total number of steps ($n$) to be

$$t^* = n\delta \geq \log \left( \frac{4E[L(\theta_0)]}{\varepsilon} \right) \min \left\{ C_{\text{ref}}^u, C_{\text{sync}}^u, \frac{1}{3(\kappa\varepsilon)^2} \right\}.$$
Recall that \( C_{\text{ref}}^u = \frac{\exp\left(-\frac{11L^2}{4}ight)}{1375\kappa LR^2} \) (Lemma C.1) and \( C_{\text{sync}}^u = \frac{\exp\left(-\frac{11LR^2}{4}\right)}{600(\kappa c)^2 \log 10} \) (19), so
\[
\min \left\{ C_{\text{ref}}^u, C_{\text{sync}}^u, \frac{1}{3(\kappa c)^2} \right\} \geq e^{-\frac{11LR^2}{4}} \frac{1}{10^{10} \kappa \max \{ \kappa, LR^2 \}}.
\]
It thus suffices to choose
\[
\delta \leq e^{-\frac{11LR^2}{4}} \frac{\varepsilon}{10^8 \max \{ \kappa, LR^2 \} \sqrt{R^2 + d/m}}
\]
and
\[
t^* \geq e^{\frac{11LR^2}{4}} \cdot 10^{10} \kappa \max \{ \kappa, LR^2 \} \cdot \log \left( \frac{4\mathbb{E}[\mathcal{L}(\theta_0)]}{\varepsilon} \right).
\]
The total number of steps then comes out to be
\[
n \geq \frac{t^*}{\delta} = 10^{18} \cdot e^{\frac{11LR^2}{2}} \cdot \kappa \cdot \max \{ \kappa, LR^2 \}^2 \cdot \log \left( \frac{4\mathbb{E}[\mathcal{L}(\theta_0)]}{\varepsilon} \right) \cdot \sqrt{R^2 + d/m} \varepsilon.
\]

The proof of Theorem 3.1 follows immediately from Theorem 3.2.

**Proof** [Proof of Theorem 3.1] By Lemma E.7,
\[
W_1(p^{(n)}, p^*) \leq e^{\frac{11LR^2}{4}} \frac{\mathbb{E}[\mathcal{L}(\theta_n)]}{\frac{5}{5}}.
\]
We can also upper bound \( \mathbb{E}[\mathcal{L}(\theta_0)] \) as
\[
\mathbb{E}[\mathcal{L}(\theta_0)] \leq W_1(p^{(0)}, p^*)
\]
\[
\leq \mathbb{E}_{p^{(0)}} \left[ \|x\|_2 + \|u\|_2 \right] + \mathbb{E}_{p^*} \left[ \|x\|_2 + \|u\|_2 \right]
\]
\[
\leq R + \mathbb{E}_{p^*} \left[ \|x\|_2 + \|u\|_2 \right]
\]
\[
\leq R + \sqrt{\mathbb{E}_{p^*} \left[ \|x\|_2^2 \right] + \mathbb{E}_{p^*} \left[ \|u\|_2^2 \right]}
\]
\[
\leq 6 \sqrt{R^2 + \frac{d}{m}},
\]
where the first inequality is by Lemma E.7, the second inequality is by the triangle inequality, the third inequality is by definition of \( p^{(0)} \), the fourth inequality is by Jensen’s inequality and the last inequality is by Lemma E.3.

Thus, in order to get \( W_1(p^{(n)}, p^*) \leq \varepsilon' \), we apply Proposition 3.2 with \( \varepsilon = \frac{\varepsilon'}{5e^{11LR^2/4}} \) and
\[
\mathbb{E}[\mathcal{L}(\theta_0)] \leq 6 \sqrt{R^2 + \frac{d}{m}}.
\]

### 4 Discussion

In this paper, we study algorithms for sampling from distributions which satisfy a more general structural assumption than log-concavity, in time polynomial in dimension and accuracy. We also demonstrate that using underdamped dynamics the run time can be improved, mirroring the strongly convex case.

There are a few natural questions that we hope to answer in order to continue this investigation of nonconvex sampling problems:
Structural Assumptions: It would be interesting to determine other structural assumptions that may be imposed on the target distribution that are more general than log-concavity but still admit tractable sampling guarantees, for example, additional assumptions that may alleviate the exponential dependence on $LR^2$. Conversely, existing guarantees may be extended to weaker assumptions, such as weak convexity outside a ball.

Algorithms: One might also wish to consider algorithms which have access to more than a gradient oracle, such as the Metropolis Hastings filter, or discretizations which use higher order information.

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## A Properties of the function $f$ and Proof of Lemma 1.2

**Proof** [Proof of Lemma 1.2] We refer to definitions of the functions $\psi$, $\Psi$, $g$ and $f$ in (3).

*(F1)* $f(0) = 0$ and $f'(0) = 1$ by the definition of $f$ and $\psi$.

*(F2)* and *(F3)* are verified from the definitions, noting that $\frac{1}{2} \leq g(r) \leq 1$ and $\frac{\psi(R_f)}{\psi(0)} \leq p^*(r) \leq \frac{\psi(R_f)}{\psi(0)}$. 

18
To prove this property first we observe that $f'(r) = \psi(r)g(r)$ so

$$f''(r) = \psi'(r)g(r) + \psi(r)g'(r).$$

By the definition of $\psi$, $\psi'(r) = -2\alpha_f r \psi(r)$ if $r < R_f$, thus

$$f''(r) + 2\alpha_f f'(r) = -2\alpha_f r \psi(r)g(r) + \psi(r)g'(r) + 2\alpha_f f'(r)$$

$$= \psi(r)g'(r)$$

$$= -\frac{1}{2} \frac{\Psi(r)}{\psi(r)} \int_{0}^{R_f} \frac{1}{\psi(s)} ds$$

$$\leq -\frac{1}{2} \frac{f(r)}{\psi(r)} \int_{0}^{R_f} \frac{\psi(s)}{\psi(r)} ds$$

$$(ii) \quad e^{-\alpha_f R_f^2} f(r),$$

where $(i)$ is because $f(r) \leq \Psi(r)$ and $(ii)$ is by $\psi(r) \leq 1$, $\Psi(r) \leq r$, and $\psi(r) := e^{-\alpha_f \min\{r^2, R_f^2\}} \geq e^{-\alpha_f R_f^2}$.

$f''(r) \leq 0$ follows from (F2), (F3) and (F4). For $r > R_f$, $\psi'(r) = g'(r) = 0$, so in that case $f''(r) = \psi(r)g(r) + \psi(r)g'(r) = 0$.

For any $0 < c < 1$,

$$f((1 + c)r) = f(r) + \int_{r}^{(1+c)r} f'(s) ds \geq f(r) + c r \cdot \frac{1}{2} e^{-\alpha_f R_f^2} \geq \left(1 + \frac{c}{2} e^{-\alpha_f R_f^2}\right) f(r),$$

where the first inequality follows from (F2), and the second inequality follows from (F3). Under the assumption that $e^{-\alpha_f R_f^2} \leq \frac{1}{2}$, and using the inequality $1 + x \geq e^{x/2}$ for all $x \in [0, 1/2]$, we get $1 + (c/2)e^{-\alpha_f R_f^2} \geq e^{(c/4)}e^{-\alpha_f R_f^2}$.

\[\blacksquare\]

\[\text{B} \quad \text{Discretization Analysis of Overdamped Langevin Diffusion}\]

All notation in this section is defined in Section 2. We will prove Proposition 2.3 in several steps. First, to obtain a bound on the discretization error, we will need to bound $E[\|x_t\|_2]$. As a first step to show this we show that the continuous-time process $x_t - y_t$ contracts exponentially fast to the invariant distribution outside a ball of radius $R$. This is not particularly surprising as we assume the potential to be strongly convex outside of a ball of radius $R$.

**Lemma B.1.** Let $x_t$ and $y_t$ be as defined in Section 2. Then for all $t > 0$,

$$E\left[\left(\|x_t - y_t\|_2 - R^2\right)_+\right] \leq E\left[\left(e^{-mt}\|x_0 - y_0\|_2 - R^2\right)_+\right].$$

**Proof** Under synchronous coupling (where we set $\gamma_t = 0$),

$$d\|x_t - y_t\|_2^2 = -2\langle x_t - y_t, \nabla U(x_t) - \nabla U(y_t) \rangle dt \leq -2m\|x_t - y_t\|_2^2 dt, \quad (25)$$

19
where (i) holds when \( \| x_t - y_t \|_2^2 \geq R^2 \). Thus,

\[
\mathbb{E} \left[ \left( \| x_t - y_t \|_2^2 - R^2 \right)_+ \right] = \mathbb{E} \left[ \left( \| x_t - y_t \|_2^2 - R^2 \right) \cdot I \left[ \| x_t - y_t \|_2^2 > R^2 \right] \right] \\
\leq \mathbb{E} \left[ \left( \| x_t - y_t \|_2^2 - R^2 \right) \cdot I \left[ \| x_s - y_s \|_2^2 > R^2 \right] \right] \\
\leq \mathbb{E} \left[ \left( e^{-mt} \| x_0 - y_0 \|_2^2 - R^2 \right) \cdot I \left[ \| x_s - y_s \|_2^2 > R^2 \right] \right] \\
\leq \mathbb{E} \left[ \left( e^{-mt} \| x_0 - y_0 \|_2^2 - R^2 \right)_+ \right],
\]

where (i) and (ii) both follow from Eq. (25).

As an immediate corollary, we can bound \( \mathbb{E} \left[ \| x_t \|_2^2 \right] \).

**Corollary B.2.** If \( \mathbb{E} \left[ \left( \| x_0 - y_0 \|_2^2 - R^2 \right)_+ \right] \leq \mathcal{E} \), then for all \( t > 0 \), \( \mathbb{E} \left[ \| x_t \|_2^2 \right] \leq 2\mathcal{E} + 38R^2 + \frac{4d}{m} \).

**Proof** By expanding using Young’s inequality,

\[
\mathbb{E} \left[ \| x_t \|_2^2 \right] \leq 2\mathbb{E} \left[ \| x_t - y_t \|_2^2 \right] + 2\mathbb{E} \left[ \| y_t \|_2^2 \right] \\
\leq 2\mathbb{E} \left[ \left( \| x_t - y_t \|_2^2 - R^2 \right)_+ \right] + 2R^2 + 2 \left( 18R^2 + \frac{2d}{m} \right) \\
\leq 2\mathbb{E} \left[ \left( e^{-mt} \| x_0 - y_0 \|_2^2 - R^2 \right)_+ \right] + 38R^2 + \frac{4d}{m} \leq 2\mathcal{E} + 38R^2 + \frac{4d}{m},
\]

where (i) follows from bound on \( \mathbb{E} \left[ \| y_t \|_2^2 \right] \) in Lemma E.3 and (ii) is by Lemma B.1.

Next, we will prove a bound on the discretization error assuming a bound on the second moment of the continuous time process \( x_t \) outside a ball of radius \( R \).

**Proposition B.3** (Discretization Error). If \( \mathbb{E} \left[ \left( \| x_0 - y_0 \|_2^2 - R^2 \right)_+ \right] \leq \mathcal{E} \), then for all \( t > 0 \)

\[
\mathbb{E} \left[ \| x_t - x'_t \|_2^2 \right] \leq \frac{4}{3} \left[ L^4 t^4 \left( \mathcal{E} + 19R^2 + \frac{2d}{m} \right) + \frac{3}{2} L^2 t^3 d \right].
\]
**Proof** We assume that $\tilde{x}_t$ and $x_t$ are synchronously coupled, so,

\[
\mathbb{E} \left[ \| \tilde{x}_t - x_t \|_2^2 \right] = \mathbb{E} \left[ \left\| \int_0^t \nabla U(x_0) - \nabla U(x_s) \, ds \right\|^2 \right] \\
\leq t \int_0^t \mathbb{E} \left[ \| \nabla U(x_0) - \nabla U(x_s) \|_2^2 \right] \, ds \\
\leq L^2 t \int_0^t \mathbb{E} \left[ \| x_0 - x_s \|_2^2 \right] \, ds \\
= L^2 t \int_0^t \mathbb{E} \left[ \left\| \int_0^s \nabla U(x_r) \, dr + \sqrt{2} \int_0^s dB_r \right\|_2^2 \right] \, ds \\
\leq 2L^2 t \int_0^t \left[ s \int_0^s \mathbb{E} \left[ \| \nabla U(x_r) \|_2^2 \right] \, dr + 2sd \right] \, ds \\
\leq 2L^2 t \int_0^t \left[ L^2 s \int_0^s \mathbb{E} \left[ \| x_r \|_2^2 \right] \, dr + 2sd \right] \, ds \\
\leq 2L^2 t \int_0^t \left[ L^4 t^4 \left( \mathcal{E} + 19R^2 + \frac{4d}{m} \right) + \frac{3}{2} L^2 t^3 d \right] \, ds \\
= \frac{4}{3} \left[ L^4 t^4 \left( \mathcal{E} + 19R^2 + \frac{2d}{m} \right) + \frac{3}{2} L^2 t^3 d \right],
\]

where (i) follows by Jensen’s inequality, (ii) is because the gradients of $U(\cdot)$ are Lipschitz smooth, (iii) is by the definition of $x_s$, (iv) is by Young’s inequality, (v) follows by Jensen’s inequality and a calculation of the variance of Brownian motion, (vi) is again by the smoothness of the gradients, and finally (vii) is by Corollary B.2. ■

Next, we want to bound the variance of $\tilde{x}_t$ (the discretized process) outside of a ball of radius $R$. To do this, we will study a single step of Algorithm 1:

**Lemma B.4.** If $\mathbb{E} \left[ \left( \| x_0 - y_0 \|_2^2 - R^2 \right)_+ \right] \leq \mathcal{E}$, then for any $t \in \left[ 0, \frac{m}{312L^2} \right]$,

\[
\mathbb{E} \left[ \left( \| \tilde{x}_t - y_t \|_2^2 - R^2 \right)_+ \right] \leq \max \left\{ \mathcal{E}, 2 \left( R^2 + \frac{d}{m} \right) \right\}.
\]

21
Proof By Young’s inequality, for any $\varepsilon > 0$,

$$
\mathbb{E}\left[ (\|\tilde{x}_t - y_t\|_2^2 - R^2)_+ \right] \\
\leq \mathbb{E}\left[ (1 + \varepsilon)\|x_t - y_t\|_2^2 + \left( 1 + \frac{1}{\varepsilon} \right)\|\tilde{x}_t - x_t\|_2^2 - R^2 \right]_+ \\
\overset{(i)}{=} \mathbb{E}\left[ (1 + \varepsilon)\|x_t - y_t\|_2^2 - R^2 \right]_+ + \left( 1 + \frac{1}{\varepsilon} \right) \mathbb{E}\left[ \|\tilde{x}_t - x_t\|_2^2 \right] \\
\overset{(ii)}{=} \mathbb{E}\left[ (e^{-mt} + \varepsilon)\|x_0 - y_0\|_2^2 - R^2 \right]_+ + \left( 1 + \frac{1}{\varepsilon} \right) \mathbb{E}\left[ \|\tilde{x}_t - x_t\|_2^2 \right] \\
\overset{(iii)}{=} \mathbb{E}\left[ (1 - \frac{mt}{4})\|x_0 - y_0\|_2^2 - R^2 \right]_+ + \left( 1 + \frac{2}{mt} \right) \mathbb{E}\left[ \|\tilde{x}_t - x_t\|_2^2 \right] \\
\overset{(iv)}{=} \left( 1 - \frac{mt}{8} \right) \mathbb{E} + \frac{16}{3mt} \left( L^4 t^4 \left( \mathcal{E} + 19R^2 + \frac{2d}{m} \right) + 2L^2 t^3 d \right) \\
\overset{(v)}{=} \left( 1 - \frac{mt}{8} \right) \mathbb{E} + \frac{16}{3mt} \left( L^4 t^4 \left( 19R^2 + \frac{2d}{m} \right) + 2L^2 t^3 d \right),
$$

(26)

where (i) is because $\max(a+b,0) \leq \max(a,0) + b$ if $b \geq 0$, (ii) is by Lemma B.1, (iii) is by setting $\varepsilon = \frac{mt}{4}$, (iv) is by the assumption that $t \leq m/(512L^2)$, which implies $mt/4 \leq 1/(2048\kappa^2) \leq 1/2$ since $\kappa \geq 1$, and (v) is by Proposition B.3 and the same assumption. Lastly, (vi) is because $t \leq m/(512L^2)$ implies $16L^4 t^4 \mathcal{E}/(mmt) \leq mt \mathcal{E}/8$. Now we consider two cases to finish the proof.

Case 1 $\mathcal{E} > R^2 + \frac{d}{m}$: By our assumption that $t \leq \frac{m}{512L^2}$,$$
\frac{mt}{8}\mathcal{E} \geq \frac{16}{3mt} \left( L^4 t^4 \left( 19R^2 + \frac{2d}{m} \right) + 2L^2 t^3 d \right)
$$
so together with Eq. (26) this gives \( \mathbb{E}\left[ (\|\tilde{x}_t - y_t\|_2^2 - R^2)_+ \right] \leq \mathcal{E} \).

Case 2 $\mathcal{E} \leq R^2 + \frac{d}{m}$: Together with our earlier assumptions on the upper bound of $t$, we get

$$
\frac{16L^4 t^4}{3mt} \left( 19R^2 + \frac{d}{m} \right) \leq \frac{1}{2} \left( R^2 + \frac{d}{m} \right) \quad \text{and,}
\frac{32L^2 t^3 d}{3mt} \leq \frac{d}{2m}.
$$

Combining this with Eq. (26) gives

$$
\mathbb{E}\left[ (\|\tilde{x}_t - y_t\|_2^2 - R^2)_+ \right] \leq 2 \left( R^2 + \frac{d}{m} \right).
$$

Combining the two cases completes the proof. 

With this result in place we can now bound the variance of the iterates of the Algorithm 1.

Lemma B.5. For $k \in \mathbb{N}$, let $x^{(k)}$ be iterates of the Algorithm 1 with step size $\delta \in \left[ 0, \frac{m}{512L^2} \right]$. Let the initial point $x^{(0)} \in \mathbb{B}_2(R)$. Let $y_0 \sim p^*$ (and evolved according to the exact flow) and let $(x^{(0)}, y_0)$ be coupled through the unique coupling (because $p^{(0)}$ is an atom). Then for all $k$,

$$
\mathbb{E}\left[ (\|x^{(k)} - y_0\|_2^2 - R^2)_+ \right] \leq 40R^2 + \frac{4d}{m}.
$$

22
Proof First, we show that the initial quantity is bounded.

\[
\mathbb{E} \left[ (\|x^{(0)} - y_0\|_2^2 - R^2)^+ \right] \leq 2\mathbb{E} \left[ \|x^{(0)}\|_2^2 \right] + 2\mathbb{E} \left[ \|y_0\|_2^2 - R^2 \right] \leq 2R^2 + 2 \left( 18R^2 + \frac{2d}{m} \right) \leq 40R^2 + \frac{4d}{m},
\]

where the first inequality is by Young’s inequality, and the second inequality is by Lemma E.3. We now use induction. Suppose the lemma holds for some \(i \in \mathbb{N}\), that is,

\[
\mathbb{E} \left[ (\|x^{(i)} - y_i\|_2^2 - R^2)^+ \right] \leq 40R^2 + \frac{4d}{m}.
\]

By recursively applying Lemma B.4, with \(x_0 = x^{(i)}\) and \(y_0 = y_i\), we get

\[
\mathbb{E} \left[ (\|x^{(i+1)} - y_{(i+1)}\|_2^2 - R^2)^+ \right] \leq \max \left\{ \mathcal{E}, 2 \left( R^2 + \frac{d}{m} \right) \right\} \leq 40R^2 + \frac{4d}{m}.
\]

Finally we put everything together and bound the discretization error of each iterate.

Proof [Proof of Proposition 2.3] From Lemma B.5, we show that for all \(k \in \mathbb{N}\),

\[
\mathbb{E}_{(x,y) \sim (p(k),p^{\star})} \left[ (\|x - y\|_2^2 - R^2)^+ \right] \leq 40R^2 + \frac{4d}{m}.
\]

This immediately allows us to apply Lemma B.3 with \(\mathcal{E} = 40R^2 + \frac{4d}{m}\) to get the conclusion.

C Contraction under Reflection and Synchronous Coupling of Underdamped Dynamics

Throughout this section we refer to notation introduced in Section 3, particularly in (11).

C.1 Reflection coupling contracts in \(\| \cdot \|_1\)

We consider the reflection coupling case: \(\mu_t = 1\) and \(\mu_t = 1\), and demonstrate that \(\mathbb{E} [\mathcal{L}(\theta_t)]\) (conditioned on \(\mu_t = 1\)) contracts with rate \(C_{\text{ref}}^u\).

Lemma C.1. Under reflection coupling (\(\mu_t = 1\)),

\[
\frac{d}{dt} \mathbb{E} [\mathcal{L}(\theta_t) | \mu_{t^-} = \mu_t = 1] \leq -C_{\text{ref}}^u \mathbb{E} [\mathcal{L}(\theta_t) | \mu_{t^-} = \mu_t = 1]
\]

\[
+ \frac{1}{c\kappa L} \mathbb{E} [\|\nabla U(x_t) - \nabla U(x_{\lfloor t/\delta \rfloor} \delta)\|_2 | \mu_{t^-} = \mu_t = 0]
\]

where

\[
C_{\text{ref}}^u := \min \left\{ \frac{e^{-11LR^2/4}}{1375\kappa LR^2}, \frac{e^{-11LR^2/4}}{4c\kappa} \right\}
\]

Remark: In most nontrivial cases, \(C_{\text{ref}}^u = e^{-11LR^2/4}/(11000\kappa LR^2)\).

Proof

In this proof, all expectations condition on \(\mu_{t^-} = \mu_t = 1\), but for clarity of notation, we do not explicitly write this in the remainder of this proof.
By Eq. (13), $\mu_t = 1$ implies that $(z_t, w_t)$ evolves under reflection coupling. We rely on Itô’s Lemma (for semi-martingales) to study the evolution of $L(\theta_t)$. We will consider a few cases as $\| \cdot \|_2$ is not differentiable at 0.

**Case 1**, $\|z_t\|_2 \neq 0$ and $\|\phi_t\|_2 \neq 0$: In this case, we apply Itô’s Lemma E.1 to get,

$$
dE \left[ L(z_t, \phi_t, \rho_t, \tau_t, \mu_t) \right] = \langle \nabla z_t L(\theta_t), w_t \rangle dt + \langle \nabla \phi_t L(\theta_t), -w_t - \frac{1}{cKL} \nabla L(\theta_t) \rangle dt + \frac{8}{cKL} \gamma_t^T \nabla^2 \phi_t L(\theta_t) dt
$$

$$
= \langle \nabla z_t L(\theta_t), w_t \rangle dt - \langle \nabla \phi_t L(\theta_t), w_t + \frac{1}{cKL} \nabla L(\theta_t) \rangle dt + \frac{8}{cKL} \gamma_t^T \nabla^2 \phi_t L(\theta_t) dt
$$

We start by analyzing the final term, which corresponds to the discretization error. Note that

$$
\nabla \phi_t L(\theta_t) = \frac{z_t + w_t}{\|z_t + w_t\|_2} f^\prime((1 + 2/(c\kappa))\|z_t\|_2 + \|\phi_t\|_2),
$$

so by Cauchy-Schwartz,

$$
\nabla \phi_t L(\theta_t) \leq \frac{1}{cKL} \|\nabla U(x_t) - \nabla U(x_{t\delta})\|_2 f^\prime((1 + 2/\kappa))\|z_t\|_2 + \|\phi_t\|_2).
$$

Considering the other terms in Eq. (27)

$$
\nabla \phi_t L(\theta_t) = f^\prime \left( \left(1 + \frac{2}{c\kappa}\right) \|z_t\|_2 + \|\phi_t\|_2 \right) \cdot \left(1 + \frac{2}{c\kappa}\right) \left( \frac{z_t}{\|z_t\|_2}, w_t \right) - \left( \frac{\phi_t}{\|\phi_t\|_2}, w_t + \frac{1}{cKL} \nabla L(\theta_t) \right)
$$

$$
+ \frac{8}{cKL} \cdot f^\prime \left( \left(1 + \frac{2}{c\kappa}\right) \|z_t\|_2 + \|\phi_t\|_2 \right) \cdot \nabla L(\theta_t) \cdot \gamma_t^T \phi_t \phi_t^T \gamma_t
$$

$$
+ \frac{8}{cKL} \cdot f^\prime \left( \left(1 + \frac{2}{c\kappa}\right) \|z_t\|_2 + \|\phi_t\|_2 \right) \cdot \frac{1}{\|\phi_t\|_2} \cdot \gamma_t^T \left( I_{d \times d} - \frac{\phi_t \phi_t^T}{\|\phi_t\|_2^2} \right) \gamma_t dt
$$

$$
= f^\prime \left( \left(1 + \frac{2}{c\kappa}\right) \|z_t\|_2 + \|\phi_t\|_2 \right) \cdot \left(1 + 2/(c\kappa)\right) \left( \frac{z_t}{\|z_t\|_2}, w_t \right) - \left( \frac{\phi_t}{\|\phi_t\|_2}, w_t + \frac{1}{cKL} \nabla L(\theta_t) \right)
$$

$$
+ \frac{8}{cKL} \cdot f^\prime \left( \left(1 + 2/(c\kappa)\right) \|z_t\|_2 + \|\phi_t\|_2 \right),
$$

where we used the definition of $\gamma_t := \frac{\phi_t}{\|\phi_t\|_2}$. Next, we study in detail the expression

$$
\left(1 + \frac{2}{c\kappa}\right) \left( \frac{z_t}{\|z_t\|_2}, w_t \right) - \left( \frac{\phi_t}{\|\phi_t\|_2}, w_t + \frac{1}{cKL} \nabla L(\theta_t) \right).
$$

By Cauchy Schwarz,

$$
\left(1 + \frac{2}{c\kappa}\right) \left( \frac{z_t}{\|z_t\|_2}, w_t \right) \leq \left(1 + \frac{2}{c\kappa}\right) \left( \frac{z_t}{\|z_t\|_2}, z_t + w_t - z_t \right)
$$

$$
\leq \left(1 + \frac{2}{c\kappa}\right) \left( \|z_t + w_t\|_2 - \|z_t\|_2 \right).
$$
On the other hand,
\[- \left\langle \frac{\phi_t}{\|\phi_t\|^2}, w_t + \frac{1}{cKL} \nabla_t \right\rangle = - \left\langle \frac{z_t + w_t}{\|z_t + w_t\|^2}, w_t + \frac{1}{cKL} \nabla_t \right\rangle \]
\[\leq - \|z_t + w_t\|_2 + \|z_t\|_2 + \left\langle \frac{z_t + w_t}{\|z_t + w_t\|^2}, \frac{1}{cKL} \nabla_t \right\rangle \]
\[\leq - \|z_t + w_t\|_2 + \|z_t\|_2 + \frac{1}{cKL} \|z_t\|_2. \]

where \((i)\) is by Cauchy-Schwartz and, \((ii)\) is by Assumption (A1). Putting the bounds on the two terms together, we get that (29) is bounded by

\[\left(1 + \frac{2}{c\kappa}\right) \left\langle \frac{z_t}{\|z_t\|^2}, w_t\right\rangle - \left\langle \frac{\phi_t}{\|\phi_t\|^2}, w_t + \frac{1}{cKL} \nabla_t \right\rangle \leq \frac{2}{c\kappa} \left(1 + \frac{2}{c\kappa}\right) \|z_t\|^2 + \|z_t + w_t\|^2. \]

Thus by combining the bound on (29) and plugging it into Eq. (28), we get

\[\star \leq \frac{2}{c\kappa} f' \left(\left(1 + \frac{2}{c\kappa}\right) \|z_t\|^2 + \|\phi_t\|^2\right) \cdot \left(1 + \frac{2}{c\kappa}\right) \|z_t\|^2 + \|\phi_t\|^2 \]
\[+ \frac{8}{c\kappa L} \cdot f'' \left(\left(1 + \frac{2}{c\kappa}\right) \|z_t\|^2 + \|\phi_t\|^2\right). \quad (30)\]

The inequality follows as \(1 \geq f' \geq 0\) by (F2) of Lemma 1.2.

We can upper bound the value of \(\left(1 + \frac{2}{c\kappa}\right) \|z_t\|^2 + \|\phi_t\|^2\) by

\[\left(1 + \frac{2}{c\kappa}\right) \|z_t\|^2 + \|\phi_t\|^2 \leq 1.002 \sqrt{2} \sqrt{\|z_t\|^2 + \|z_t + w_t\|^2} \leq \sqrt{11} R. \]

The first inequality is by Young’s inequality. The second inequality is by our assumption that \(\mu = 1\) and Lemma E.9, which states that \(\sqrt{\|z_t\|^2 + \|z_t + w_t\|^2} \leq \sqrt{5} R. \)

We apply (F4) of Lemma 1.2 with \(\alpha f = L/4\) and radius \(R = \sqrt{11} R\) as defined in Eq. (21) to get

\[f''(r) + \frac{L}{4} f'(r) \leq - \frac{e^{-11LR^2/4}}{11R^2} f(r) \]

for \(r \leq R f = \sqrt{11} R. \)

Combined with our bound above on \(\star\) by (27) we get

\[dE[\mathcal{L}(\theta_t)] \leq - \frac{e^{-11LR^2/4}}{1370\kappa LR^2} E[\mathcal{L}(\theta_t, t)] dt + \frac{1}{cKL} E \left[\|\nabla U(x_t) - \nabla U(x_{t|\delta})\|_2\right]. \quad (31)\]

Case 2, \(\|z_t\|^2 = 0\) and \(\|\phi_t\|^2 \neq 0\):

In this case, \(\phi_t = w_t\) and \(\nabla_t = 0\). We perform a similar decomposition as done in Eq. (27) to obtain:

\[\star \leq f' \left(\left(1 + \frac{2}{c\kappa}\right) \|z_t\|^2 + \|\phi_t\|^2\right) \cdot \left(1 + \frac{2}{c\kappa}\right) \|w_t\|^2 - \left\langle \frac{\phi_t}{\|\phi_t\|^2}, w_t + \frac{1}{cKL} \nabla_t \right\rangle \]
\[+ \frac{8}{c\kappa L} \cdot f'' \left(\left(1 + \frac{2}{c\kappa}\right) \|z_t\|^2 + \|\phi_t\|^2\right) \]
\[= f' \left(\left(1 + \frac{2}{c\kappa}\right) \|z_t\|^2 + \|\phi_t\|^2\right) \cdot \left(1 + \frac{2}{c\kappa}\right) \|w_t\|^2 - \|w_t\|^2 \]
\[+ \frac{8}{c\kappa L} \cdot f'' \left(\left(1 + \frac{2}{c\kappa}\right) \|z_t\|^2 + \|\phi_t\|^2\right) \]
\[\leq \frac{2}{c\kappa} f' \left((1 + 2/\kappa) \|z_t\|^2 + \|\phi_t\|^2\right) \cdot \left(1 + \frac{2}{c\kappa}\right) \|z_t\|^2 + \|\phi_t\|^2 \]
\[+ \frac{8}{c\kappa L} \cdot f'' \left(\left(1 + \frac{2}{c\kappa}\right) \|z_t\|^2 + \|\phi_t\|^2\right) \]
where the last line follows as \( \phi_t = w_t \). The bound now follows by a similar argument as in Case 1 above.

**Case 3, \( \|z_t\|_2 \neq 0 \) and \( \|\phi_t\|_2 = 0 \):** In this case, \( \gamma_t = 0 \) and \( z_t = -w_t \). When \( \gamma_t = 0 \), \((z_t, w_t)\) evolves as synchronous coupling, so

\[
\sum \leq f' \left( \left( 1 + \frac{2}{c_k} \right) \|z_t\|_2 + \|\phi_t\|_2 \right) \cdot \left( \left( 1 + \frac{2}{c_k} \right) \|z_t\|_2 + \|z_t - \frac{1}{c_k L} \nabla_t\|_2 \right)
\]

\[
\leq f' \left( \left( 1 + \frac{2}{c_k} \right) \|z_t\|_2 + \|\phi_t\|_2 \right) \cdot \left( \left( 1 + \frac{2}{c_k} \right) \|z_t\|_2 + \|z_t\|_2 + \frac{1}{c_k} \|z_t\|_2 \right)
\]

\[
= -f' \left( \left( 1 + \frac{2}{c_k} \right) \|z_t\|_2 + \|\phi_t\|_2 \right) \cdot \frac{1}{c_k} \|z_t\|_2
\]

\[
\leq -\frac{1}{4c_k} \cdot e^{-11L^2R^2/4} \cdot \left( \left( 1 + \frac{2}{c_k} \right) \|z_t\|_2 + \|\phi_t\|_2 \right)
\]

where the second inequality uses the triangle inequality and the fact that \( \|\nabla_t\|_2 \leq L \|z_t\|_2 \). The last inequality uses the fact that \( \phi_t = 0 \) and \( \kappa \geq 1 \), and the fact that \( r \geq f(r) \) from (F3) in Lemma 1.2, so \( \|z_t\|_2 \geq \frac{1}{2} \left( 1 + \frac{2}{c_k} \right) \|z_t\|_2 + \|\phi_t\|_2 \) \( \geq \frac{1}{2} f \left( \left( 1 + \frac{2}{c_k} \right) \|z_t\|_2 + \|\phi_t\|_2 \right) \). We also use the fact that \( f'(r) \geq \frac{1}{e} e^{-11L^2R^2/4} \) from (F2) in Lemma 1.2.

**Case 4, \( \|z_t\|_2 = 0 \) and \( \|z_t + w_t\|_2 = 0 \):** In this case, there is no drift and no Brownian motion term (\( \gamma_t = 0 \) implies synchronous coupling), so we are done.

Combining the four cases, we get

\[
d \mathbb{E} [\mathcal{L}(\theta_t)] \leq -C_{\text{ref}}^u \mathbb{E} [\mathcal{L}(\theta_t, t)] + \frac{1}{c_k L} \mathbb{E} [\|\nabla U(x_t) - \nabla U(x_{\tau_{t/\delta}})\|_2],
\]

where \( C_{\text{ref}}^u := \min \left\{ \frac{e^{-11L^2R^2/4}}{1.375kL^2}, \frac{e^{-11L^2R^2/4}}{4c_k} \right\} \). \( \square \)

### C.2 Contraction under synchronous coupling

In this section we demonstrate that our Lyapunov function contracts under synchronous coupling \((\mu_t = 0)\). It will be useful to keep in mind the definitions for \( C_{\text{sync}}^u = \frac{\exp(-11L^2R^2/4)}{600(c_k)^2 \cdot \log 10} \) and \( T_{\text{sync}} = 3(c_k)^2 \cdot \log(10) \) in Eq. (21). We first examine the easy case that \( \mu_{t^-} = \mu_t = 0 \):

**Lemma C.2.** Under synchronous coupling \((\mu_{t^-} = \mu_t = 0)\), we have

\[
\frac{d}{dt} \mathbb{E} [\mathcal{L}(\theta_t) | \mu_{t^-} = \mu_t = 0] \leq -\min \left\{ C_{\text{sync}}^u \frac{1}{3(c_k)^2} \right\} \mathbb{E} [\mathcal{L}(\theta_t) | \mu_{t^-} = \mu_t = 0]
\]

\[
+ \frac{1}{200 \kappa L} \mathbb{E} [\|\nabla U(x_t) - \nabla U(x_{\tau_{t/\delta}})\|_2 | \mu_{t^-} = \mu_t = 0].
\]

**Proof** [Proof of Lemma C.2] In this proof, all expectations condition on \( \mu_{t^-} = \mu_t = 0 \), but for clarity of notation, we do not explicitly write this in the remainder of this proof.

By definition of \( \mathcal{L} \), when \( \mu_{t^-} = \mu_t = 0 
\]

\[
d \mathcal{L}(\theta_t) = d \left( f(\rho_t) e^{-C_{\text{sync}}^u(t-\tau_t)} + \xi_t \right)
\]

\[
\leq -\min \left\{ C_{\text{sync}}^u \frac{1}{3(c_k)^2} \right\} \mathbb{E} [\left( f(\rho_t) e^{-C_{\text{sync}}^u(t-\tau_t)} + \xi_t \right) dt + \frac{1}{200 \kappa L} \mathbb{E} [\|\nabla_t - \nabla_t\|_2] dt
\]

\[
= -C_{\text{sync}}^u \mathbb{E} \left[ \left( f(\rho_t) e^{-C_{\text{sync}}^u(t-\tau_t)} + \xi_t \right) dt
\]

\[
+ \frac{1}{200 \kappa L} \mathbb{E} [\|\nabla U(x_t) - \nabla U(x_{\tau_{t/\delta}})\|_2] dt,
\]
where the inequality follows by the definition of $\xi_t$. 

Next, we demonstrate that the discontinuous jumps in the Lyapunov function value are strictly nonpositive when $\mu_{t-} = 0, \mu_t = 1$ (which is an equivalent condition to $t = \tau_t + T_{\text{sync}}$).

**Proposition C.3.** For all $t \geq 0$, the inequality

$$f \left( \left( 1 + \frac{2}{Ck} \right) \|z_{\tau_t + T_{\text{sync}}} \|_2 + \|z_{\tau_t + T_{\text{sync}}} + w_{\tau_t + T_{\text{sync}}} \|_2 \right) \leq f(\rho_t) - e^{-C_{\text{sync}} T_{\text{sync}}} + \xi_{\tau_t + T_{\text{sync}}}$$

holds almost surely.

This result ensures that the Lyapunov function ($L(\theta_t)$) will not suddenly increase in value. We will prove this in a series of steps. We begin by first showing that the gradient points in a direction that reduces the function value.

**Lemma C.4.** If $\|z_t\|_2^2 + \|z_t + w_t\|_2^2 \geq 2.2R^2$, then

$$\left\langle \left[ \begin{array}{c} z_t \\ z_t + w_t \end{array} \right], \left[ \begin{array}{c} -w_t - \frac{1}{CkL} \nabla_{\xi_t} \end{array} \right] \right\rangle \leq -\frac{1}{3(Ck)^2}(\|z_t\|_2^2 + \|z_t + w_t\|_2^2)$$

**Proof** Expanding the term on the left-hand side,

$$2 \left\langle \left[ \begin{array}{c} z_t \\ z_t + w_t \end{array} \right], \left[ \begin{array}{c} -w_t - \frac{1}{CkL} \nabla_{\xi_t} \end{array} \right] \right\rangle$$

$$= 2 \langle z_t, w_t \rangle + 2 \left\langle z_t + w_t, -w_t - \frac{1}{CkL} \nabla_{\xi_t} \right\rangle$$

$$= -2\|w_t\|_2^2 - 2 \left\langle z_t, \frac{1}{CkL} \nabla_{\xi_t} \right\rangle - 2 \left\langle w_t, \frac{1}{CkL} \nabla_{\xi_t} \right\rangle$$

$$= -2\|w_t\|_2^2 - 2 \left\langle z_t, \frac{1}{CkL} \nabla_{\xi_t} \right\rangle + \|w_t\|_2^2 + \frac{1}{(Ck)^2 L^2} \|\nabla_{\xi_t}\|_2^2 - \|w_t + \frac{1}{CkL} \nabla_{\xi_t}\|_2^2$$

$$\leq -\|w_t\|_2^2 - 2 \left\langle z_t, \frac{1}{CkL} \nabla_{\xi_t} \right\rangle + \frac{1}{(Ck)^2 L^2} \|\nabla_{\xi_t}\|_2^2$$

$$\leq -\|w_t\|_2^2 - 2 \left\langle z_t, \frac{1}{CkL} \nabla_{\xi_t} \right\rangle + \frac{1}{(Ck)^2} \|z_t\|_2^2,$$  \hspace{1cm} (33)

where the third equality is by a simple quadratic expansion of $\|w_t + \frac{1}{CkL} \nabla_{\xi_t}\|_2^2$. Now, we consider two cases:

**Case 1:** $\|z_t\|_2 \leq R$. We first lower bound $\|w_t\|_2^2$ by $\|z_t\|_2^2$. By Young’s inequality,

$$\|z_t + w_t\|_2^2 \leq (1 + 1/\varepsilon)\|w_t\|_2^2 + (1 + \varepsilon)\|z_t\|_2.$$  

Choosing $\varepsilon = 0.1$ gives

$$11\|w_t\|_2^2 + 1.1\|z_t\|_2^2 \geq \|z_t + w_t\|_2.$$ 

Combining with the assumption that $\|z_t\|_2^2 \leq R^2$ and $\|z_t\|_2^2 + \|z_t + w_t\|_2^2 \geq 2.3R^2$,

$$11\|w_t\|_2 \geq 2.2R^2 - 2.1\|z_t\|_2^2 \geq 0.1R^2 \geq 0.1\|z_t\|_2^2,$$ 

so

$$\|w_t\|_2 \geq \frac{9}{c} R^2 \geq \frac{9}{c} \|z_t\|_2^2.$$
We now upper bound the term in Eq. (33) by

\[
\left(-\|w_t\|_2^2 + 2\left\langle z_t, -\frac{1}{c\kappa L}\nabla_t\right\rangle + \frac{1}{(c\kappa)^2}\|z_t\|_2^2\right) \leq \left(-\|w_t\|_2^2 + \frac{2}{c\kappa}\|z_t\|_2^2 + \frac{1}{(c\kappa)^2}\|z_t\|_2^2\right)
\]

\[
\leq \left(-\|w_t\|_2^2 + \frac{3}{c}\|z_t\|_2^2\right)
\]

\[
\leq -\frac{6}{c}\|w_t\|_2^2
\]

\[
\leq -\frac{6}{c \cdot 400} (\|z_t\|_2^2 + \|z_t + w_t\|_2^2),
\]

where (i) is by Cauchy-Schwartz and smoothness, (ii) is because \(\kappa \geq 1\), (iii) is by our earlier bound that \(\|w_t\|_2^2 \geq 0.009R^2 \geq 0.009\|z_t\|_2^2\) and finally (iv) is by the fact that \(\|z_t\|_2^2 + \|z_t + w_t\|_2^2 \leq 3\|z_t\|_2^2 + 2\|w_t\|_2^2 \leq \frac{3}{4}\|w_t\|_2 + 2\|w_t\|_2 \leq 400\|w_t\|_2^2\).

**Case 2:** \(\|z_t\|_2 \geq R\). Then by Assumption (A3) (strong convexity outside a ball), \(\left\langle z_t, -\frac{1}{c\kappa L}\nabla_t\right\rangle \leq -\frac{1}{(c\kappa)^2}\|z_t\|_2^2\). Thus (33) can be upper bounded by

\[
\left(-\|w_t\|_2^2 - 2\left\langle z_t, \frac{1}{c\kappa L}\nabla_t\right\rangle + \frac{1}{(c\kappa)^2}\|z_t\|_2^2\right) \leq \left(-\|w_t\|_2^2 - \frac{1}{(c\kappa)^2}\|z_t\|_2^2\right)
\]

\[
\leq -\frac{1}{(c\kappa)^2} (\|w_t\|_2^2 + \|z_t\|_2^2) dt
\]

\[
\leq -\frac{1}{3(c\kappa)^2} (\|z_t\|_2^2 + \|z_t + w_t\|_2^2).
\]

Putting the two cases together, and using the fact that \(\kappa \geq 1\), gives the desired result.

From Lemma C.4, we derive the following corollary which ensures contraction when the norm of the difference process is outside of a ball of radius \(\sqrt{2.2}R\).

**Corollary C.5.** If \(\mu_t = 0\), then

\[
\frac{d}{dt} \left(\sqrt{\|z_t\|_2^2 + \|z_t + w_t\|_2^2} - \sqrt{2.2}R\right) + \frac{1}{c\kappa L} \|\nabla U(x_t) - \nabla U(x_{\lfloor t/\delta \rfloor})\|_2
\]

\[
\leq -\frac{1}{3(c\kappa)^2} \left(\sqrt{\|z_t\|_2^2 + \|z_t + w_t\|_2^2} - \sqrt{2.2}R\right) + \frac{1}{c\kappa L} \|\nabla U(x_t) - \nabla U(x_{\lfloor t/\delta \rfloor})\|_2.
\]
Proof Expanding,
\[
d (\sqrt{\|z_t\|_2^2 + \|z_t + w_t\|_2^2 - \sqrt{2.2}R}) +
\]
\[
\geq \frac{1}{3(cK)^2} \left( \sqrt{\|z_t\|_2^2 + \|z_t + w_t\|_2^2 - \sqrt{2.2}R} \right) + \frac{1}{cKL} \left\| \nabla U(x_t) - \nabla U(x_{(t/\delta)\hat{\beta}}) \right\|_2 dt
\]
where the first inequality is by Lemma C.4.

Finally, we show that when \( \mu_t = 0 \), \( \|z_t\|_2 + \|z_t + w_t\|_2 \) contracts over \( T_{sync} \) time by a factor of \( \sqrt{\frac{2.3}{cK}} \), plus some discretization error.

Lemma C.6. For any \( t > 0 \),
\[
\sqrt{\|z_t + T_{sync}\|_2^2 + \|z_t + T_{sync} + w_t + T_{sync}\|_2^2}
\]
\[
\leq \sqrt{\frac{2.3}{5}} \left( \sqrt{\|z_t\|_2^2 + \|z_t + w_t\|_2^2} \right) + \frac{1}{cKL} \int_{\tau_t}^{\tau_t + T_{sync}} e^{(r - \tau_t - T_{sync})/(3(cK)^2)} \|\nabla U(x_t) - \nabla U(x_{(t/\delta)\hat{\beta}})\|_2 dr,
\]
holds almost surely.

Proof We consider an arbitrary fixed \( t \). The following statements can be readily verified:

(C1) For all \( s \in [t, \tau_t + T_{sync}] \), \( \tau_s = \tau_t \) and \( \mu_s = 0 \) (see Eq. (14));

(C2) for \( s \in [t, \tau_t + T_{sync}] \), \( \begin{bmatrix} z_s \\ w_s + z_s \end{bmatrix} \) is evolved through synchronous coupling (see (C1));

(C3) \( \sqrt{\|z_t\|_2^2 + \|z_t + w_t\|_2^2} \geq \sqrt{5}R \) (see Eq. (14));

(C4) \( e^{-T_{sync}/(3(cK)^2)} \leq \frac{1}{10} \) (see Eq. (18)).

For any \( s \in [t, \tau_t + T_{sync}] \), by the statement of Corollary C.5 and (C2) above, and by Grönwall’s Lemma,
\[
\left( \sqrt{\|z_s\|_2^2 + \|z_s + w_s\|_2^2 - \sqrt{2.2}R} \right) +
\]
\[
\leq e^{-(s - \tau_t)/(3(cK)^2)} \left( \sqrt{\|z_t\|_2^2 + \|z_t + w_t\|_2^2 - \sqrt{2.2}R} \right) +
\]
\[
+ \frac{1}{cKL} \int_{\tau_t}^{s} e^{-(s - r)/(3(cK)^2)} \|\nabla U(x_t) - \nabla U(x_{(t/\delta)\hat{\beta}})\|_2 dr.
\]
Taking $s = \tau_t + T_{sync}$, we have that by (C4):
\[
\left( \sqrt{\|z_{\tau_t+T_{sync}}\|^2 + \|z_{\tau_t+T_{sync}} + w_{\tau_t+T_{sync}}\|^2} - \sqrt{2.2R} \right) \leq \frac{1}{10} \left( \sqrt{\|z_s\|^2 + \|z_s + w_s\|^2} - \sqrt{2.2R} \right) + \\
+ \frac{1}{ckL} \int_{\tau_t}^{\tau_t+T_{sync}} e^{(r-\tau_t-T_{sync})/(3ck)^2} \left\| \nabla U(x_t) - \nabla U(x_{[t/\delta]}) \right\|_2 \, dr.
\]
This yields:
\[
\sqrt{\|z_{\tau_t+T_{sync}}\|^2 + \|z_{\tau_t+T_{sync}} + w_{\tau_t+T_{sync}}\|^2} \leq \sqrt{2.2R} + \left( \sqrt{\|z_{\tau_t+T_{sync}}\|^2 + \|z_{\tau_t+T_{sync}} + w_{\tau_t+T_{sync}}\|^2} - \sqrt{2.2R} \right) + \\
\leq \sqrt{2.2R} + \frac{1}{10} \sqrt{\|z_{\tau_t}\|^2 + \|z_{\tau_t} + w_{\tau_t}\|^2} \\
+ \frac{1}{ckL} \int_{\tau_t}^{\tau_t+T_{sync}} e^{(r-\tau_t-T_{sync})/(3ck)^2} \left\| \nabla U(x_t) - \nabla U(x_{[t/\delta]}) \right\|_2 \, dr \\
\leq \sqrt{\frac{2.2R}{5}} \sqrt{\|z_{\tau_t}\|^2 + \|z_{\tau_t} + w_{\tau_t}\|^2} \\
+ \frac{1}{ckL} \int_{\tau_t}^{\tau_t+T_{sync}} e^{(r-\tau_t-T_{sync})/(3ck)^2} \left\| \nabla U(x_t) - \nabla U(x_{[t/\delta]}) \right\|_2 \, dr,
\]
where the second inequality is by the immediately preceding inequality, and the third inequality is by (C3).

With these pieces in place we are ready to prove Proposition C.3 by combining the claim of Lemma C.6 with the properties of $f(\cdot)$.

**Proof [Proof of Proposition C.3]** The following statements can be verified:

(C1) $\rho_t = (1 + 2/(ck))\|z_{\tau_t}\|_2 + \|z_{\tau_t} + w_{\tau_t}\|_2$ (by definition of $\rho_t$ in Eq. (15));

(C2) $e^{-C^u_{sync}T_{sync}} = \exp \left( - \exp \left( - \frac{11LR^2/4}{200} \right) \right)$, (by definition of $T_{sync}$ and $C^u_{sync}$ in Eq. (19)).

By Lemma C.6,
\[
\sqrt{\|z_{\tau_t+T_{sync}}\|^2 + \|z_{\tau_t+T_{sync}} + w_{\tau_t+T_{sync}}\|^2} \leq \sqrt{\frac{2.2R}{5}} \sqrt{\|z_{\tau_t}\|^2 + \|z_{\tau_t} + w_{\tau_t}\|^2} \\
+ \frac{1}{ckL} \int_{\tau_t}^{\tau_t+T_{sync}} e^{(r-\tau_t-T_{sync})/(3ck)^2} \left\| \nabla U(x_t) - \nabla U(x_{[t/\delta]}) \right\|_2 \, dr.
\]
As $\sqrt{a^2 + b^2} \leq a + b \leq \sqrt{2}\sqrt{a^2 + b^2}$, and because $(1 + 2/(ck)) \leq 1.002$, we have
\[
(1 + 2/(ck))\|z_{\tau_t+T_{sync}}\|_2 + \|z_{\tau_t+T_{sync}} + w_{\tau_t+T_{sync}}\|_2 \\
\leq 1.002\sqrt{2} \sqrt{\|z_{\tau_t+T_{sync}}\|^2 + \|z_{\tau_t+Tsync} + w_{\tau_t+T_{sync}}\|^2} \\
\leq \frac{4.7}{5} \sqrt{\|z_{\tau_t}\|^2 + \|z_{\tau_t} + w_{\tau_t}\|^2} \\
+ \frac{4}{ckL} \int_{\tau_t}^{\tau_t+T_{sync}} e^{(r-\tau_t-T_{sync})/(3ck)^2} \left\| \nabla U(x_t) - \nabla U(x_{[t/\delta]}) \right\|_2 \, dr \\
\leq 0.98 ((1 + 2/(ck))\|z_{\tau_t}\|_2 + \|z_{\tau_t} + w_{\tau_t}\|_2 + \xi_{\tau_t+T_{sync}}).
\]
where the last inequality is by definition of $\xi_t$. We have thus shown that under synchronous coupling for time $T_{sync}$, the quantity $(1 + 2/(c\kappa))\|z_t\|_2 + \|z_t + w_t\|_2$ contracts by a factor of 0.98 along with some discretization error. We will now use this fact to also demonstrate a contraction in $f(r_t)$.

Recall our definition of $\alpha_f = L/4$ and $R_f = \sqrt{11}R$ in (21). By (F6) of Lemma 1.2 and assumption in (24), we know that $f(r) \leq \exp\left(-\frac{\exp(-11LR^2/4)}{200}\right) f(f_{0.98}(r))$, thus

$$
\begin{align*}
    f \left( (1 + \frac{2}{c\kappa}) \|z_t + T_{sync}\|_2 + \|z_t + T_{sync} + w_t\|_2 \right) \\
    \leq \exp\left(-\frac{\exp(-11LR^2/4)}{200}\right) f(((1 + 2/(c\kappa))\|z_t\|_2 + \|z_t + w_t\|_2 + \xi_t + T_{sync}) \\
    \leq \exp\left(-\frac{\exp(-11LR^2/4)}{200}\right) f(((1 + 2/(c\kappa))\|z_t\|_2 + \|z_t + w_t\|_2) + \xi_t + T_{sync} \\
    = e^{-c\kappa T_{sync}R_f} f(((1 + 2/(c\kappa))\|z_t\|_2 + \|z_t + w_t\|_2) + \xi_t + T_{sync},
\end{align*}
$$

where the last equality follows from fact (C2).

## D Discretization Analysis of Underdamped Langevin Diffusion

Some of the notation used in this section is defined in Section 3.

The following proposition is the main discretization result for underdamped dynamics. At a high level the proof follows in a similar vein to the analysis in Appendix B.

**Proposition D.1.** Let $p_0$ be the point mass at $(x_0, 0)$, where $\|x_0\|_2 \leq R$. Let $\delta \leq \frac{1}{2000m}$, we have

$$
\mathbb{E} \left[ \|\nabla U(x_t) - \nabla U(x_{t/\delta}\delta)\|_2^2 \right] \leq 10^9 L^2 \delta^2 (R^2 + d/m), \quad \text{for all } t > 0.
$$

**Proof** We begin by analyzing the following,

$$
\begin{align*}
    \|\nabla U(x_t) - \nabla U(x_{t/\delta}\delta)\|_2^2 &\leq L^2 \|x_t - x_{t/\delta}\|_2^2 \\
    &= L^2 \left\| \int_{t/\delta}^t u_s ds \right\|_2^2 \\
    &\leq L^2 \delta \int_{t/\delta}^t \|u_s\|_2^2 ds,
\end{align*}
$$

where the last inequality is Jensen’s inequality. We bound the second moment of the velocity $\mathbb{E} \left[ \|u_t\|_2^2 \right]$ for all $t > 0$. For some arbitrary $p_0$, let $(x_0, u_0, y_0, v_0) \sim \Gamma^*(p_0, p^*)$. Consider a synchronous coupling between $(x_t, u_t) \sim p_0$ and the invariant distribution $(y_t, v_t) \sim p^*$:

$$
\begin{align*}
    dx_t &= u_t dt; \quad du_t = \left(-2w_t - \frac{1}{c\kappa L} \nabla U(x_{t/\delta}\delta)\right) dt + \sqrt{\frac{4}{c\kappa L}} dB_t, \\
    dy_t &= v_t dt; \quad dv_t = \left(-2v_t - \frac{1}{c\kappa L} \nabla U(y_t)\right) dt + \sqrt{\frac{4}{c\kappa L}} dB_t \\
    dz_t &= d(x_t - y_t) = w_t dt = (u_t - w_t) dt; \quad dw_t = \left(-2w_t - \frac{1}{c\kappa L} \nabla v_t\right) dt.
\end{align*}
$$
Because $p^*$ is the stationary distribution, we have that for all $t > 0$, $(y_t, v_t) \sim p^*$. Repeating the argument in the proof of Corollary C.5 (but note the square here), we get

$$
\frac{d}{dt} E \left[ \left( \sqrt{\|z_t\|^2 + \|z_t + w_t\|^2} - \sqrt{2.2R} \right)^2 \right] \\
\leq - \frac{1}{3(c\kappa)^2} E \left[ \left( \sqrt{\|z_t\|^2 + \|z_t + w_t\|^2} - \sqrt{2.2R} \right)^2 \right] \\
+ \frac{2}{c\kappa L} E \left[ \left( \sqrt{\|z_t\|^2 + \|z_t + w_t\|^2} - \sqrt{2.2R} \right)^2 \right] \|\nabla U(x_t) - \nabla U(x_{t/\delta})\|_2 \\
\leq \frac{1}{3(c\kappa)^2} E \left[ \left( \sqrt{\|z_t\|^2 + \|z_t + w_t\|^2} - \sqrt{2.2R} \right)^2 \right] \\
+ \frac{2}{c\kappa L} \sqrt{E \left[ \left( \sqrt{\|z_t\|^2 + \|z_t + w_t\|^2} - \sqrt{2.2R} \right)^2 \right]} \sqrt{E \left[ \|\nabla U(x_t) - \nabla U(x_{t/\delta})\|_2^2 \right]} \\
\leq \frac{1}{3(c\kappa)^2} E \left[ \left( \sqrt{\|z_t\|^2 + \|z_t + w_t\|^2} - \sqrt{2.2R} \right)^2 \right] \\
+ \frac{2}{c\kappa L} \sqrt{E \left[ \left( \sqrt{\|z_t\|^2 + \|z_t + w_t\|^2} - \sqrt{2.2R} \right)^2 \right]} \sqrt{\delta \int_{t/\delta}^t E [\|u_s\|_2^2] \, ds}, \tag{36}
$$

where (i) is by Cauchy-Schwarz and (ii) is by Jensen’s inequality. For any $t > 0$ suppose that for all $0 \leq s \leq t$, we have

$$
E \left[ \|u_s\|_2^2 \right] \leq 2E \left[ \|x_s\|_2^2 + \|x_s + u_s\|_2^2 \right] \\
\leq 4E \left[ \|z_s\|^2 + \|z_s + w_s\|^2 \right] + 4E \left[ \|y_s\|^2 + \|y_s + v_s\|^2 \right] \\
\leq 4E \left[ \|z_s\|^2 + \|z_s + w_s\|^2 \right] + 36(R^2 + d/m) \\
\leq 8E \left[ \|z_s\|^2 + \|z_s + w_s\|^2 \right] + 5R^2 + 36(R^2 + d/m) \\
\leq 100(R^2 + d/m) + 8E_t, \tag{37}
$$

where (i), (ii), (iv) are by Young’s inequality, (iii) is by Lemma E.4, (iv) is once again by Young’s inequality and by $a_+ \geq a$. Combined with the earlier result in Eq. (36),

$$
\frac{d}{dt} E \left[ \left( \sqrt{\|z_t\|^2 + \|z_t + w_t\|^2} - \sqrt{2.2R} \right)^2 \right] \\
\leq - \frac{1}{3(c\kappa)^2} E_t + \frac{2\delta}{c\kappa} \sqrt{E_t} \cdot \sqrt{100(R^2 + d/m) + 8E_t} \\
\leq - \frac{1}{3(c\kappa)^2} \sqrt{E_t} \left( \sqrt{E_t} - 1500\delta \kappa \cdot \sqrt{100(R^2 + d/m) + 8E_t} \right) \\
\leq - \frac{1}{3(c\kappa)^2} \sqrt{E_t} \left( (1 - 6c\delta \kappa) \sqrt{E_t} - 1500\delta \kappa \sqrt{(R^2 + d/m)} \right) \\
\leq - \frac{1}{3(c\kappa)^2} \sqrt{E_t} \left( \frac{1}{2} \sqrt{E_t} - 1500\delta \kappa \sqrt{(R^2 + d/m)} \right),
$$

32
where (i) is because $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$ for $a, b \in \mathbb{R}^+$ and (ii) is by the assumption that $\delta \leq \frac{1}{12cn}$.

It follows that

$$\frac{d}{dt} \mathbb{E} \left[ \left( \sqrt{\|z_t\|^2 + \|z_t + w_t\|^2} - \sqrt{2.2R} \right)^2 \right] \leq 0 \quad \text{if } \mathcal{E}_t \geq 30000^2 (R^2 + d/m).$$

So if initially,

$$\mathbb{E} \left[ \left( \sqrt{\|z_0\|^2 + \|z_0 + w_0\|^2} - \sqrt{2.2R} \right)^2 \right] = \mathcal{E}_0 \leq 30000^2 (R^2 + d/m),$$

then for all $t > 0$, $\mathcal{E}_t \leq 30000(R^2 + d/m)$. By picking $p_0$ to be the point mass inside of a ball of radius $R$, and by using Lemma E.4, we get that $\mathcal{E}_t \leq 36(R^2 + d/m)$ for all $t > 0$. Using the earlier upper bound on $\mathbb{E} \left[ \|u_t\|^2 \right]$ in Eq. (37), we get $\mathbb{E} \left[ \|u_t\|^2 \right] \leq 10^3(R^2 + d/m)$.

Using Eq. (35), we obtain the desired upper bound

$$\mathbb{E} \left[ \|\nabla U(x_t) - \nabla U(x_{\lfloor t/\delta \rfloor})\|^2 \right] \leq 10^9 L^2 h^2(R^2 + d/m) \text{ for all } t > 0.$$ 

\[ \square \]

### E Other Technical Results

**Theorem E.1** (Itô’s Formula for semi-martingales, Theorem 33 in Chapter 2 of Protter (2005)). Let $X$ be a $d$-dimensional semi-martingale and let $h : \mathbb{R}^d \to \mathbb{R}$ be a $C^2$ real function. Then $h(X)$ is again a semi-martingale, and the following formula holds:

$$h(X_t) - h(X_0) = \sum_{i=1}^d \int_{0+}^t \frac{\partial h}{\partial x_i}(X_{s-})dX^i_s + \frac{1}{2} \sum_{1 \leq i, j \leq d} \int_{0+}^t \frac{\partial^2 h}{\partial x_i \partial x_j}(X_{s-})d[X^i, X^j]_s \left. \right|_{s=t} + \sum_{0 < s \leq t} \left\{ h(X_s) - h(X_{s-}) - \sum_{i=1}^d \frac{\partial h}{\partial x_i}(X_{s-})\Delta X^i_s \right\}. $$

Here $[X, X]_s = X^2 - 2 \int_0^s X^-dX$ is the continuous part of the quadratic variation of the sample path (see p. 70 of Protter, 2005, for the formal definition.). If the continuous part of the dynamics is

$$dX_t = u_t \, dt + M_t \, dB_t + Y_t,$$

where $Y_t$ is a pure jump process, then the above reduces to

$$h(X_t) - h(X_0) = \int_{0+}^t \langle \nabla h(X_{s-}), u_t \rangle \, dt + \frac{1}{2} \int_{0+}^t \text{Tr} \left( M_t \nabla^2 h(X_{s-}) M_t \right) \, dt + \sum_{0 < s \leq t} h(X_s) - h(X_{s-})$$

**Lemma E.2.** $\theta_t$, as defined in Eq. (12)-Eq. (17), is a semimartingale, with dynamics

$$d\theta_t(\omega) = u(\omega, t)dt + u'(\omega, t)dB_t + u''(\omega, t),$$

where $\omega$ indexes a sample path and $u$, $u'$ and $u''$ are appropriate measurable functions.
Proof Let $\omega$ index sample paths. Then the dynamics of $\theta_t$, as outlined in Eq. (12)-Eq. (17), can be decomposed as follows:

\[ u(\omega, t)dt \] represents the (deterministic) dynamics

\[
    d\begin{bmatrix} x_t \\ u_t \end{bmatrix} = \left[-2u_t - \frac{u_t}{\kappa L} \nabla U(x_{t/\delta})\right] dt,
    \quad d\begin{bmatrix} y_t \\ v_t \end{bmatrix} = \left[-2v_t - \frac{v_t}{\kappa L} \nabla U(y_t)\right] dt,
\]

$u'(\omega, t)dB_t$ represents the Brownian motion

\[
    d\begin{bmatrix} x_t \\ u_t \end{bmatrix} = \left[\frac{0}{\kappa L} dB_t\right],
    \quad d\begin{bmatrix} y_t \\ v_t \end{bmatrix} = \left[\frac{0}{\kappa L} dB_t\right] \cdot (1 - \mu_t) + \left[\frac{0}{\kappa L} (I - 2\gamma_t \gamma_t^T) dB_t\right] \cdot \mu_t
\]

and $u''(\omega, t)$ represents the jumps (implicit in the following definitions):

\[
    d\tau_t = \mathbb{1} \left[t \geq \tau_t + T_{\text{sync}} \text{ AND } \sqrt{\|z_t\|_2 + \|z_t + w_t\|_2} \geq 12\sqrt{20}R\right] \cdot (t - \tau_t^-);

    \rho_t = (1 + 2/\kappa)\|z_{\tau_t^-}\|_2 + \|z_{\tau_t^-} + w_{\tau_t^-}\|_2; \quad \mu_t = \mathbb{1} [t \geq \tau_t + T_{\text{sync}}]
\]

\[
    \xi_t = 8/(\kappa L) \int_{\tau_t}^{t} e^{(s-t)/(8\kappa^2)} \left\| \nabla s - \nabla s_t \right\|_2 ds.
\]

To show that $\theta_t$ is a semimartingale, we will show that $u''(\omega, t)$ has locally finite variation. For a fixed $t$, by Lemma E.8, we see that the number of jumps is finite. We thus only need to show that the magnitude of each jump is finite.

The jumps in $\tau_t$ and $\mu_t$ are clearly finite, since they are bounded by $t$ and $1$ respectively. For $\rho_t$, observe that when $\|\rho_t - \rho_{t^-}\|_2 > 0$,

\[
    \rho_t - \rho_{t^-} = (1 + 2/\kappa)\|z_{\tau_t^-}\|_2 + \|z_{\tau_t^-} + w_{\tau_t^-}\|_2 - ((1 + 2/\kappa)\|z_{\tau_t^-}\|_2 + \|z_{\tau_t^-} + w_{\tau_t^-}\|_2)
\]

\[
    = (1 + 2/\kappa)\|z_{\tau_t^-}\|_2 + \|z_{\tau_t^-} + w_{\tau_t^-}\|_2 - ((1 + 2/\kappa)\|z_{\tau_t^-}\|_2 + \|z_{\tau_t^-} + w_{\tau_t^-}\|_2).
\]

Observe that $x_t, u_t, y_t, v_t$ evolve according to an Ito diffusion where the drift is the gradient of an $L$-smooth function. Thus for any $s < t, \|x_t - x_s\|_2 + \|u_s - u_t\|_2 + \|y_s - y_t\|_2 + \|v_s - v_t\|_2 < \infty$ almost surely. By the triangle inequality, $\rho_t - \rho_{t^-} < \infty$ for all $t$ almost surely.

The proof that $\xi_t \leq \infty$ almost surely is very similar and is omitted.

Lemma E.3. The second moment of the invariant distribution $p^*(x) \propto \exp(-U(x))$ is bounded by

\[
    \mathbb{E}_{x \sim p^*} \left[\|x\|_2^2\right] \leq \frac{2d}{m} + 18R^2.
\]

Proof First, let $\varepsilon > 0$ be any positive real number. We will define the function $h : \mathbb{R} \to \mathbb{R}$ as follows:

\[
    h(r) = \begin{cases} 
    0 & \text{if } r \leq R, \\
    \frac{1}{6\varepsilon}(r - R)^3 & \text{if } r \in [R, R + \varepsilon], \\
    \frac{\varepsilon^2}{2} + \frac{(r - (R + \varepsilon)^2)^2}{2} & \text{if } r \geq R + \varepsilon.
    \end{cases}
\]

It can be easily verified that this function is twice differentiable with the derivatives given by,

\[
    h'(r) = \begin{cases} 
    0 & \text{if } r \leq R, \\
    \frac{(r - R)^2}{2\varepsilon} & \text{if } r \in [R, R + \varepsilon], \\
    r - (R + \varepsilon/2) & \text{if } r \geq R + \varepsilon.
    \end{cases}
\]
and
\[
    h''(r) = \begin{cases} 
        0 & \text{if } r \leq R, \\
        \frac{r-R}{\varepsilon} & \text{if } r \in [R, R+\varepsilon], \\
        1 & \text{if } r \geq R+\varepsilon.
    \end{cases}
\]

Intuitively, \(h(r)\) is intended to be a smooth approximation to \(\frac{(r-R)^2}{\varepsilon}\). In particular,
\[
    \forall r, h(r) \in \left[ \frac{(r-(R+\varepsilon))^2}{2}, \frac{(r-R)^2}{2} \right].
\]

The lower bound is obvious from the definition of \(h(r)\), so we will only prove the upper bound. To see this, consider two cases (the case when \(r \leq R\) is obvious):

**Case 1** \(r \in (R, R+\varepsilon)\):
\[
    \frac{\varepsilon^2}{24} + \frac{(r-(R+\varepsilon/2))^2}{2} \leq \frac{\varepsilon^2}{4} + \frac{(r-(R+\varepsilon/2))^2}{2} + \varepsilon(r-(R+\varepsilon/2)) = \frac{(r-(R+\varepsilon/2)+\varepsilon/2)^2}{2} = \frac{(r-R)^2}{2},
\]

the desired upper bound thus follows. Let \(x_0 \sim p^*\), and consider the SDE
\[
    dx_t = -\nabla U(x_t)dt + \sqrt{2}dB_t.
\]

Clearly, \(x_t \sim p^*\) for all \(t\) as \(p^*\) is invariant under Langevin diffusion. We will study the evolution of \(\mathbb{E}[h(\|x_t\|)]\). Let \(\ell(x) := \|x\|\), so that \(h(\|x_t\|) = h(\ell(x))\) then
\[
    \nabla h(\ell(x)) = h'(\ell(x))\nabla \ell(x)
\]
\[
    \nabla^2 h(\ell(x)) = h''(\ell(x))\nabla \ell(x)\nabla \ell(x)^T + h'(\ell(x))\nabla^2 \ell(x).
\]

Consider \(x_t\) for \(t > 0\). We will now consider three cases and study the evolution of \(h(\ell(x_t))\).

**Case 1** \(\|x_t\| \leq R\):
\[
    \nabla h(\ell(x)) = 0 \\
    \nabla^2 h(\ell(x)) = 0,
\]

and hence by Itô’s Lemma,
\[
    dh(\ell(x_t)) = -\langle \nabla U(x_t), 0 \rangle dt + \text{Tr}(0)dt - \sqrt{2}\langle \nabla h(x_t), dB_t \rangle = 0.
\]

**Case 2** \(\|x_t\| \in [R, R+\varepsilon]\):
\[
    \nabla h(\ell(x)) = \frac{\|x\|_2 - R}{2\varepsilon\|x\|_2} \cdot x \\
    \nabla^2 h(\ell(x)) = \frac{\|x\|_2^2 - R}{\varepsilon\|x\|_2^2} \cdot xx^\top + \frac{(\|x\|_2 - R)^2}{2\varepsilon\|x\|_2^2} \left( I_{d \times d} - \frac{xx^\top}{\|x\|_2^2} \right),
\]

35
so again by Itô’s Lemma,
\[
\begin{align*}
\frac{dh(\ell(x_t))}{dt} & = \mathsf{Tr}\left(\left(\frac{\|x_t\|_2 - R}{\|x_t\|_2} x_t x_t^\top \right) + \frac{\|x_t\|_2 - R}{\varepsilon\|x_t\|_2^2} \left(I_{d \times d} - \frac{x_t x_t^\top}{\|x_t\|_2^2}\right)\right) dt \\
& \quad - \langle \nabla U(x_t), x_t \rangle \frac{(\|x_t\|_2 - R)^2}{2\varepsilon\|x_t\|_2} dt + \sqrt{2} \frac{(\|x_t\|_2 - R)^2}{2\varepsilon} \left\langle \frac{x_t}{\|x_t\|_2}, dB_t \right\rangle \\
& \leq -m\|x_t\|_2 \left(\frac{(\|x_t\|_2 - R)^2}{2\varepsilon} + \frac{\|x_t\|_2 - R}{\varepsilon} \left(1 + \frac{\varepsilon(d-1)}{2R}\right)\right) dt \\
& \quad + \sqrt{2} \frac{(\|x_t\|_2 - R)^2}{2\varepsilon} \left\langle \frac{x_t}{\|x_t\|_2}, dB_t \right\rangle \\
& \leq \left[1 + \frac{(\|x_t\|_2 - R - \varepsilon/2)^2}{2(\|x_t\|_2 - R - \varepsilon/2)}\right] dt + \sqrt{2} \frac{(\|x_t\|_2 - R - \varepsilon/2)}{\|x_t\|_2} \left\langle \frac{x_t}{\|x_t\|_2}, dB_t \right\rangle.
\end{align*}
\]

**Case 3** \(\|x_t\|_2 \geq R + \varepsilon\):
\[
\begin{align*}
\nabla h(\ell(x)) &= \frac{(\|x\|_2 - R - \varepsilon/2) \cdot x}{\|x\|_2} \\
\nabla^2 h(\ell(x)) &= \frac{xx^\top}{\|x\|^2} + \frac{(\|x\|_2 - R - \varepsilon/2)}{\|x\|_2} \cdot \left(I_{d \times d} - \frac{xx^\top}{\|x\|^2}\right).
\end{align*}
\]

By Itô’s Lemma,
\[
\begin{align*}
\frac{dh(\ell(x_t))}{dt} & = -\frac{(\|x_t\|_2 - R - \varepsilon/2)}{\|x_t\|_2} \langle \nabla U(x_t), x_t \rangle dt \\
& \quad + \mathsf{Tr}\left(\frac{1}{\|x_t\|_2^2} x_t x_t^\top + \frac{(\|x_t\|_2 - R - \varepsilon/2)}{\|x_t\|_2} \left(I - \frac{x_t x_t^\top}{\|x_t\|_2^2}\right)\right) dt \\
& \quad + \sqrt{2} \left(\|x_t\|_2 - R - \varepsilon/2\right) \left\langle \frac{x_t}{\|x_t\|_2}, dB_t \right\rangle \\
& \leq -m\|x_t\|_2 \langle \frac{(\|x_t\|_2 - R - \varepsilon/2)^2}{2}, dB_t \rangle \\
& \quad + \left[1 + \frac{(R - \varepsilon/2)^2}{2(\|x_t\|_2 - R - \varepsilon/2)}\right] dt + \sqrt{2} \left(\|x_t\|_2 - R - \varepsilon/2\right) \left\langle \frac{x_t}{\|x_t\|_2}, dB_t \right\rangle.
\end{align*}
\]

We now choose \(\varepsilon = 2R\) to get
\[
\|x_t\|_2 \cdot (\|x_t\|_2 - R - \varepsilon/2) = (\|x_t\|_2 - R - \varepsilon/2)^2 + (R + \varepsilon/2) \cdot (\|x_t\|_2 - R - \varepsilon/2) \\
\geq \frac{(\|x_t\|_2 - R - \varepsilon/2)^2}{2} + \frac{3\varepsilon (4R + \varepsilon)}{8} \\
\geq \frac{(\|x_t\|_2 - R - \varepsilon/2)^2}{2} + \frac{\varepsilon^2}{24}.
\]

Plugging this into Eq. (38) gives
\[
\begin{align*}
\frac{dh(\ell(x_t))}{dt} & \leq -m \cdot h(\ell(x_t)) dt + d \cdot dt + \sqrt{2} (\|x_t\|_2 - R - \varepsilon/2) \left\langle \frac{x_t}{\|x_t\|_2}, dB_t \right\rangle,
\end{align*}
\]
Combining all three cases and taking expectations, under our choice of $\varepsilon = 2R$ we get
\[
d\mathbb{E} [h(\ell(x_t))] \leq -m\mathbb{E} [h(\ell(x_t))] dt + d \cdot dt.
\]
Because $p^*$ is stationary, we have $\mathbb{E} [h(\ell(x_t))] = 0$, so
\[
0 = d\mathbb{E} [h(\ell(x_t))] \leq (-m\mathbb{E} [h(\ell(x_t))] + d) dt,
\]
which implies that
\[
\mathbb{E}_{x \sim p^*} [h(\ell(x))] \leq \frac{d}{m}.
\]
Finally, using the lower bound on $h(\ell(x))$, we get
\[
\mathbb{E} [\|x\|_2^2] \leq 2\mathbb{E} [(\|x\|_2 - (R + \varepsilon))^2] + 2(R + \varepsilon)^2 \leq 2\mathbb{E} [(\|x\|_2 - (R + \varepsilon))^2] + 2\varepsilon^2 \\
\leq 2\mathbb{E} [h(\ell(x))] + 2(R + \varepsilon)^2.
\]
We thus conclude that
\[
\mathbb{E}_{x \sim p^*} [\|x\|_2^2] \leq \frac{2d}{m} + 18R^2.
\]

**Lemma E.4.** Let $p^*(x, u) \propto \exp(-U(x) - \frac{c\kappa L}{2} \|u\|_2^2)$ be the target distribution, then
\[
\mathbb{E}_{(x, u) \sim p^*} [\|x\|_2^2 + \|x + u\|_2^2] \leq 36(R^2 + d/m).
\]

**Proof** The result follows from the facts that (i) $x$ and $u$ are independent, (ii) $\mathbb{E}_{u \sim p^*(u)} [\|u\|_2^2] \leq d/(\kappa L) \leq d/m$ and (iii) by Lemma E.3.

**Lemma E.5.** Given $(x_{k\delta}, u_{k\delta})$, the solution $(x_t, u_t)$ (for $t \in (k\delta, (k + 1)\delta]$) of the discrete underdamped Langevin diffusion (2) is
\[
u_t = u_{k\delta}e^{-\lambda_1 t} - \lambda_2 \left( \int_{k\delta}^t e^{-\lambda_1 (t-s)} \nabla f(x_{k\delta}) \, ds \right) + \sqrt{2\lambda_1\lambda_2} \int_{k\delta}^t e^{-\lambda_1 (t-s)} \, dB_s
\]
\[
x_t = x_{k\delta} + \int_{k\delta}^t u_s \, ds.
\]

**Proof** It can be easily verified that the above expressions have the correct initial values $(x_{k\delta}, u_{k\delta})$.

By taking derivatives, one also verifies that they satisfy the differential equations in Eq. (10).

**Lemma E.6.** Conditioned on $(x_{k\delta}, u_{k\delta})$, the solution $(x_{(k+1)\delta}, u_{(k+1)\delta})$ of (10) is a Gaussian with mean,
\[
\mathbb{E} [u_t] = u_{k\delta}e^{-2t} - \frac{1}{2c\kappa L} \left( 1 - e^{-2t} \right) \nabla f(x_{k\delta})
\]
\[
\mathbb{E} [x_t] = x_{k\delta} + \frac{1}{2} \left( 1 - e^{-2t} \right) u_{k\delta} - \frac{1}{2c\kappa L} \left( t - \frac{1}{2} \left( 1 - e^{-2t} \right) \right) \nabla U(x_{k\delta}),
\]
and covariance,
\[
\mathbb{E} [(x_t - \mathbb{E} [x_t]) (x_t - \mathbb{E} [x_t])^\top] = \frac{1}{c\kappa L} \left[ t - \frac{1}{4} e^{-4t} - \frac{3}{4} + e^{-2t} \right] \cdot I_d \times d
\]
\[
\mathbb{E} [(u_t - \mathbb{E} [u_t]) (u_t - \mathbb{E} [u_t])^\top] = \frac{1}{c\kappa L} \left( 1 - e^{-4t} \right) \cdot I_d \times d
\]
\[
\mathbb{E} [(x_t - \mathbb{E} [x_t]) (u_t - \mathbb{E} [u_t])^\top] = \frac{1}{2c\kappa L} \left[ 1 + e^{-4t} - 2e^{-2t} \right] \cdot I_d \times d.
\]
Proof It follows from the definition of Brownian motion that the distribution of \((x_t, u_t)\) is a 2d-dimensional Gaussian distribution. We will compute its moments below, using the expression in Lemma E.5. Computation of the conditional means is straightforward, as we can simply ignore the zero-mean Brownian motion terms:

\[
\mathbb{E}[u_t] = u_{k\delta} e^{-2t} - \frac{1}{2ckL} (1 - e^{-2t}) \nabla f(x_{k\delta}) \\
\mathbb{E}[x_t] = x_{k\delta} + \frac{1}{2} (1 - e^{-2t}) u_{k\delta} - \frac{1}{2ckL} \left( t - \frac{1}{2} (1 - e^{-2t}) \right) \nabla f(x_{k\delta}).
\]

(40) (41)

The conditional variance for \(u_t\) only involves the Brownian motion term:

\[
\mathbb{E} \left[ (u_t - \mathbb{E}[u_t]) (u_t - \mathbb{E}[u_t])^\top \right] = \frac{4}{ckL} \mathbb{E} \left[ \left( \int_{k\delta}^t e^{-2(t-s)} dB_s \right) \left( \int_{k\delta}^t e^{-2(s-t)} dB_s \right)^\top \right] \\
= \frac{4}{ckL} \left( \int_{k\delta}^t e^{-4(t-s)} ds \right) \cdot I_{d \times d} \\
= \frac{1}{ckL} (1 - e^{-4t}) \cdot I_{d \times d}.
\]

The Brownian motion term for \(x_t\) is given by

\[
\sqrt{\frac{4}{ckL}} \int_{k\delta}^t \left( \int_{k\delta}^r e^{-2(r-s)} dB_s \right) dr = \sqrt{\frac{4}{ckL}} \int_{k\delta}^t e^{2s} \left( \int_s^t e^{-2r} dr \right) dB_s \\
= \sqrt{\frac{1}{ckL}} \int_{k\delta}^t (1 - e^{-2(t-s)}) dB_s.
\]

Here the second equality follows by Fubini’s theorem. The conditional covariance for \(x_t\) now follows as

\[
\mathbb{E} \left[ (x_t - \mathbb{E}[x_t]) (x_t - \mathbb{E}[x_t])^\top \right] = \frac{1}{ckL} \mathbb{E} \left[ \left( \int_{k\delta}^t (1 - e^{-2(t-s)}) dB_s \right) \left( \int_{k\delta}^t (1 - e^{-2(t-s)}) dB_s \right)^\top \right] \\
= \frac{1}{ckL} \left[ \int_{k\delta}^t (1 - e^{-2(t-s)})^2 ds \right] \cdot I_{d \times d} \\
= \frac{1}{ckL} \left[ t - \frac{1}{4} e^{-4t} - \frac{3}{4} + e^{-2t} \right] \cdot I_{d \times d}.
\]

Finally we compute the cross-covariance between \(x_t\) and \(u_t\),

\[
\mathbb{E} \left[ (x_t - \mathbb{E}[x_t]) (u_t - \mathbb{E}[u_t])^\top \right] = \frac{1}{500\kappa L} \mathbb{E} \left[ \left( \int_{k\delta}^t (1 - e^{-2(t-s)}) dB_s \right) \left( \int_{k\delta}^t e^{-2(t-s)} dB_s \right)^\top \right] \\
= \frac{1}{500\kappa L} \left[ \int_{k\delta}^t (1 - e^{-2(t-s)})(e^{-2(t-s)}) ds \right] \cdot I_{d \times d} \\
= \frac{1}{2ckL} \left[ 1 + e^{-4t} - 2e^{-2t} \right] \cdot I_{d \times d}.
\]

We thus have an explicitly defined Gaussian. Notice that we can sample from this distribution in time linear in \(d\), since all \(d\) coordinates are independent.

Let \(\mathcal{L}(\theta_t)\) be the Lyapunov function defined in Section 3.

Lemma E.7. Let \(p^*\) be the invariant distribution then

\[
\mathbb{E} [\mathcal{L}(\theta_t)] \geq \frac{1}{5} W_1(p_t, p^*)
\]

(42)

\[
\mathbb{E} [\mathcal{L}(\theta_0)] \leq W_1(p_0, p^*).
\]

(43)
Proof We first show
\[ \mathbb{E} \left[ \mathcal{L}(\theta_t) \geq \frac{e^{-\frac{11LR^2}{4}}}{5} W_1(p_t, p^*) \right]. \]

By Lemma 1.2, we know if \( \alpha_f = L/4 \) and \( R_f = \sqrt{11} R \) as defined in (21), then
\[ f((1 + 2/(c\kappa))/\|z_t\|_2 + \|z_t + w_t\|_2) \geq \frac{1}{2} e^{-\frac{11LR^2}{4}} ((1 + 2/(c\kappa))/\|z_t\|_2 + \|z_t + w_t\|_2) \]
\[ \geq \frac{1}{4} e^{-\frac{11LR^2}{4}} (\|z_t\|_2 + \|w_t\|_2). \quad (44) \]

On the other hand, by Eq. (34), for any \((t, s) : \tau_i \leq s \leq \tau_t + T_{sync}\),
\[ \sqrt{\|z_{\tau_i}\|^2 + \|z_{\tau_i} + w_{\tau_i}\|^2 + \xi_i} \geq \sqrt{\|z_t\|^2 + \|z_t + w_t\|^2} - \sqrt{2.2R} \]
\[ \geq \sqrt{\|z_t\|^2 + \|z_t + w_t\|^2} - 1/4 \sqrt{\|z_{\tau_i}\|^2 + \|z_{\tau_i} + w_{\tau_i}\|^2}. \]

This implies that
\[ \frac{5}{4} \sqrt{\|z_{\tau_i}\|^2 + \|z_{\tau_i} + w_{\tau_i}\|^2 + \xi_i} \geq \sqrt{\|z_t\|^2 + \|z_t + w_t\|^2}. \quad (45) \]

Note that by definition of \( \mu_t, \mu_t = 0 \Rightarrow t \leq \tau_t + T_{sync} \). We have:
\[ \|z_t\|_2 + \|w_t\|_2 \leq 2(\|z_t\|_2 + \|z_t + w_t\|_2) \]
\[ \leq 4 \sqrt{\|z_{\tau_i}\|^2 + \|z_{\tau_i} + w_{\tau_i}\|^2} \]
\[ \leq 5 \left( \sqrt{\|z_{\tau_i}\|^2 + \|z_{\tau_i} + w_{\tau_i}\|^2} + \xi_i \right) \]
\[ \leq 5 \left( \sqrt{\|z_{\tau_i}\|^2 + \|z_{\tau_i} + w_{\tau_i}\|^2} + \xi_i \right) \]
\[ \leq 5 e^{\frac{11LR^2}{4}} \left( f((1 + 2/(c\kappa))/\|z_{\tau_i}\|_2 + \|z_{\tau_i} + w_{\tau_i}\|_2) + \xi_i \right) \]
\[ = 5 e^{\frac{11LR^2}{4}} (f(\rho_i) + \xi_i), \]

where the third inequality follows from Eq. (45). We put this together with Eq. (44) to get that
\[ \mathbb{E} \left[ \mathcal{L}(\theta_t) \right] \geq \frac{1}{5} e^{-\frac{11LR^2}{4}} \mathbb{E} \left[ \|z_t\|_2 + \|w_t\|_2 \right] \geq \frac{e^{-\frac{11LR^2}{4}}}{5} W_1(p_t, p^*). \]

Finally, for \( t = 0 \), the inequality
\[ \mathbb{E} \left[ \mathcal{L}(\theta_0) \right] \leq W_1(p_0, p^*) \]
is true by definition of \( \theta_0 \) in Eq. (20) and statement (F3) of Lemma 1.2 (in particular, \( f(r) \leq r \)).

Lemma E.8. Consider \( \tau_i, \rho_i, \mu_i \) and \( \xi_i \) defined in Eq. (14)-Eq. (16). For any finite time \( t \), the values of \( \tau_i, \rho_i, \mu_i \) and \( \xi_i \) can only jump a finite number of times almost surely.

Proof With a slight abuse of notation, let \( \theta_t \) be a sample path. Let
\[ \mathcal{H} := \{ t : \tau_t = t \}. \]

Furthermore let \( \mathcal{H}_s \) be the \( s \)th smallest element of \( \mathcal{H} \). Then the dynamics of \( \tau_i \) implies that \( \mathcal{H}_{i+1} \supseteq \mathcal{H}_i + T_{sync} \). Therefore, for any finite time \( s \) \( |\mathcal{H} \cap [0, s]| \leq \left[ \frac{s}{T_{sync}} \right] + 1 \). Thus it follows that there are at most \( \left[ \frac{s}{T_{sync}} \right] + 1 \) jumps before time \( s \) almost surely. 


Lemma E.9. The following statement holds almost surely for sample paths $\theta_t : \mathbb{R}^+ \rightarrow \mathbb{R}^{4d+4}$ (generated by the dynamics in Eq. (12) - Eq. (17)):

$$\mu_t = 1 \Rightarrow \sqrt{\|z_t\|_2^2 + \|w_t\|_2^2} \leq \sqrt{5}R.$$

Proof. From the definition in Eq. (16), we know that

$$\mu_t = 1 \iff t \geq \tau_t + T_{\text{sync}}$$

$$\Rightarrow t \neq \tau_t$$

$$\Rightarrow t < \tau_t + T_{\text{sync}} \text{ OR } \sqrt{\|z_t\|_2^2 + \|z_t + w_t\|_2} < \sqrt{5}R.$$

Combining the first line and last line, and the fact that $\tau_t \geq \tau_{t-}$,

$$\mu_t = 1 \Rightarrow \sqrt{\|z_t\|_2^2 + \|z_t + w_t\|_2} < \sqrt{5}R.$$