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Abstract

Classically, the continuous-time Langevin diffusion converges exponentially fast to its stationary distribution π under the sole assumption that π satisfies a Poincaré inequality. Using this fact to provide guarantees for the discrete-time Langevin Monte Carlo (LMC) algorithm, however, is considerably more challenging due to the need for working with chi-squared or Rényi divergences, and prior works have largely focused on strongly log-concave targets. In this work, we provide the first convergence guarantees for LMC assuming that π satisfies either a Latała–Oleszkiewicz or modified log-Sobolev inequality, which interpolates between the Poincaré and log-Sobolev settings. Unlike prior works, our results allow for weak smoothness and do not require convexity or dissipativity conditions.

1 Introduction

The task of sampling from a target distribution $\pi \propto \exp(-V)$ on \mathbb{R}^d , known only up to a normalizing constant, is fundamental in many areas of scientific computing [Mac03; RC04; Bro+11; Gel+13]. As such, there has been a considerable amount of research dedicated to this task, yielding precise and non-asymptotic algorithmic guarantees when the potential V is strongly convex (see e.g. [Dal17; DMM19; Dwi+19; SL19; HBE20; LST20; Che+21a; Che+21b; CLW21; WSC21]). Many distributions encountered in practice, however, are non-log-concave, and it is therefore of central importance to provide sampling guarantees for such distributions. In this work, we address this problem by working under the assumption that π satisfies a suitable functional inequality, which we now motivate.

The canonical sampling algorithm, Langevin Monte Carlo (LMC), is based on a discretization of the continuous-time Langevin diffusion, which is the solution to the stochastic differential equation

$$dz_t = -\nabla V(z_t) dt + \sqrt{2} dB_t.$$
(1.1)

Here, $(B_t)_{t\geq 0}$ is a standard Brownian motion in \mathbb{R}^d . Classically, if π satisfies a functional inequality such as a Poincaré inequality or a log-Sobolev inequality, then the law of the Langevin diffusion (1.1) converges exponentially fast to the target distribution π [BGL14]. Namely, a Poincaré inequality implies exponential convergence in chi-squared divergence, whereas a log-Sobolev inequality (which is stronger than a Poincaré inequality) implies exponential convergence in KL divergence.

The class of measures satisfying a Poincaré inequality is quite large, including all strongly log-concave measures (due the Bakry–Émery criterion) and, more generally, all log-concave measures [KLS95; Bob99; Che21]. It also includes many examples of non-log-concave distributions such as Gaussian convolutions of measures with bounded support [Bar+18; CCN21], and it is closed under bounded perturbations of the log-density. Owing to its broad applicability and its favorable continuous-time convergence properties, this class of measures is thus a natural goal for providing quantitative guarantees for non-log-concave sampling.

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Sampling guarantees under functional inequalities. Our work is inspired by [VW19], which advocated the use of a functional inequality paired with a smoothness condition as a minimal set of assumptions for obtaining sampling guarantees; in their work, Vempala and Wibisono prove convergence of LMC under a log-Sobolev inequality. This result was then improved using the proximal Langevin algorithm under higher-order smoothness in [Wib19] and extended to Riemannian manifolds in [LE20].

Despite the appeal of this program, however, the majority of works on non-log-concave sampling instead make an additional assumption on the growth of the potential known as a dissipativity condition (e.g. [RRT17; EMS18; Mou+19; EH21; EHZ21; NDC21]). A representative example of such a condition is $\langle \nabla V(x), x \rangle \geq a ||x|| - b$ for some constants a, b > 0. Although useful for discretization proofs, dissipativity conditions are arguably less natural from the standpoint of the quantitative theory of Markov processes [BGL14], and ultimately redundant in the presence of an appropriate functional inequality. Other drawbacks include the fact that b is typically dimension-dependent, and that dissipativity conditions are not as stable under perturbations (see Section 4 for an example). Hence, we avoid such conditions in our work.

In our first main result (Theorem 7), we assume that the target π satisfies a Latała–Oleszkiewicz (LO) inequality with parameter $\alpha \in [1, 2]$. LO inequalities are well-studied functional inequalities that elegantly interpolate between Poincaré and log-Sobolev inequalities [LO00]. Notably, the $\alpha = 1$ case reduces to the Poincaré inequality, while the $\alpha = 2$ case reduces to the log-Sobolev inequality; intermediate values of α enable capturing potentials with growth $V(x) \approx ||x||^{\alpha}$ (see Section 2.2). We also complement our result by proving a sampling guarantee (Theorem 8) under the modified log-Sobolev inequalities considered in [EH21], which is useful for treating examples in which the LO constant is dimension-dependent.

Towards weaker notions of smoothness. Since the assumption of a Poincaré inequality allows for a variety of non-convex potentials with at least linear growth, it is restrictive to pair this assumption with the gradient Lipschitz assumption which is usually invoked in the sampling literature. Hence, following [DGN14; Nes15; Cha+20; EH21], we instead assume that ∇V is Hölder-continuous with exponent $s \in (0, 1]$.

An analysis in Rényi divergence. We now describe the main technical challenge of this work. Recall that a log-Sobolev inequality (LSI) implies exponential ergodicity of the diffusion (1.1) in KL divergence, and consequently the analysis of LMC under a LSI naturally proceeds with the KL divergence as the performance metric [VW19; Wib19; LE20]. Similarly, a Poincaré inequality implies exponential ergodicity of (1.1) in chi-squared divergence, and accordingly we analyze LMC in chi-squared divergence, or equivalently, in Rényi divergence. In turn, the techniques we develop for the analysis may be useful for other situations in which only a Poincaré-type inequality is available, such as the state-of-the-art convergence rate for the underdamped Langevin diffusion [CLW20] or for the mirror-Langevin diffusion [Ch+20b].

Via standard comparison inequalities, a convergence guarantee in Rényi divergence implies convergence for other common divergences (e.g. total variation distance, 2-Wasserstein distance, or KL divergence), and is therefore more desirable. Of particular interest in this regard is the role of Rényi divergence guarantees for providing "warm starts" for high-accuracy samplers such as the Metropolis-adjusted Langevin algorithm [Che+21a; WSC21] and the zigzag sampler [LW20].

Unfortunately, working with Rényi divergences introduces substantial new technical hurdles as it prevents the use of standard coupling-based discretization arguments; as such, there are not many prior works to draw upon. The convergence of the diffusion (1.1) in Rényi divergence was first proven in [CLL19; VW19]. The paper [VW19] also takes a first step towards discretization by introducing a technique based on differential inequalities for the Rényi divergence for a continuous-time interpolation of LMC. Although this strategy succeeds for obtaining KL convergence under an LSI, it falls short for Rényi divergence; indeed, the analysis of [VW19] only holds under the (currently unverifiable) assumption that the *biased stationary distribution* of the LMC algorithm satisfies a Poincaré inequality. Moreover, their result only establishes quantitative convergence of LMC to its biased limit; to recover a convergence guarantee to π , this also requires an estimate of the "Rényi bias" (the Rényi divergence between the biased stationary distribution and π), which was unresolved. Instead, [GT20] provided the first Rényi guarantee for LMC by using the adaptive composition theorem from differential privacy to control the discretization error, albeit suboptimally. Subsequently, their result was sharpened in [EHZ21] via a two-stage analysis combining the two papers [VW19; GT20].

In this paper, we first show how to modify the interpolation method of [VW19] to yield a genuine Rényi convergence guarantee for LMC under an LSI, thereby yielding a stronger result than [GT20; EHZ21] with a shorter and more elegant proof. We further extend this to the case when π is log-concave, but this technique

is unable to cover the setting of a weaker functional inequality and smoothness condition. For this, we instead draw inspiration from the stochastic calculus-based analysis of [DT12; Che+21a]. At the heart of our proofs is the introduction of new change-of-measure inequalities which intriguingly rely on the very fact that the analysis is carried out in Rényi divergence (and not any weaker metric). Thus, although the use of Rényi divergences introduces new technical obstructions, it also provides the key tool for overcoming them.

1.1 Contributions

Convergence of the diffusion under functional inequalities. Our first contribution is to establish quantitative Rényi convergence bounds for the Langevin diffusion (1.1) under the following functional inequalities: (1) the Latała–Oleszkiewicz (LO) inequalities [LO00], which interpolate between the Poincaré and log-Sobolev inequalities (Theorem 2), and the modified log-Sobolev inequality (MLSI) used in [EH21] (Theorem 3). LO and MLSI have relative merits, and they capture the tail behavior of the potential, providing an accurate characterization of the speed of convergence for both the diffusion as well as the LMC algorithm.

Improved guarantees for LMC under an LSI or log-concavity. As our second principal contribution (Theorem 4), we provide an elegant proof that under an LSI, the LMC algorithm (with appropriate step size) achieves ε error in Rényi divergence in $\widetilde{O}(d/\varepsilon)$ iterations. This improves upon past works in several respects. First, in the LSI case, a Rényi convergence guarantee for LMC was previously unknown; thus, our work strengthens [VW19] by proving convergence in a stronger metric (Rényi divergence rather than KL divergence). Second, even when the target π is strongly log-concave, our proof is both sharper and significantly shorter than the prior works [GT20; EHZ21] on Rényi convergence; moreover, our guarantee for fixed step size LMC does not degrade if the number of iterations is taken too large. As a corollary, we resolve an open question of [VW19] on the size of the "Rényi bias" in this setting (see Corollary 5).

With additional effort, we are able to extend the techniques to the case when π is (weakly) log-concave, and we obtain a guarantee with explicit dependence on the Poincaré constant of π (however, our guarantee is no longer stable); see Theorem 6. Our result is the state-of-the-art guarantee for LMC for sampling from isotropic log-concave targets.

Convergence of LMC under a functional inequality and weak smoothness. Our main contribution is to provide general sampling guarantees assuming that the potential has a Hölder-continuous gradient of exponent $s \in (0, 1]$ and that π either satisfies LO (Theorem 7) or MLSI (Theorem 8). As noted previously, these assumptions are considerably more general than what are usually considered in the sampling literature and do not require dissipativity. In particular, Theorem 7 completes the program of [VW19] by establishing the first sampling guarantees for LMC under a Poincaré inequality and a weak smoothness condition.

Generically, our final rate is $\widetilde{O}(d^{(2/\alpha)}(1+1/s)-1/s}/\varepsilon^{1/s})$, where s is the Hölder continuity exponent of ∇V and α captures the growth of the potential at infinity. We give a number of illustrative examples in Section 4 and show that our results improve upon the ones in [EH21].

1.2 Notation and organization

Throughout the paper, $\pi \propto \exp(-V)$ denotes the target distribution on \mathbb{R}^d ; the function $V : \mathbb{R}^d \to \mathbb{R}$ is referred to as the "potential". We abuse notation by identifying a measure with its density (w.r.t. Lebesgue measure on \mathbb{R}^d). We write $a \lesssim b$ and a = O(b) to indicate that $a \leq Cb$ for a universal constant C > 0; also, we use $\tilde{O}(\cdot)$ as a shorthand for $O(\cdot)\log^{O(1)}(\cdot)$. Similar remarks apply to the notations \gtrsim , Ω , $\tilde{\Omega}$, and \asymp , Θ , $\tilde{\Theta}$.

The paper is organized as follows. In Section 2, we begin by reviewing functional inequalities and their implications for the continuous-time convergence of the diffusion (1.1) in Rényi divergence. We then state our main theorems on the LMC algorithm in Section 3, and illustrate them with examples in Section 4. We give a technical exposition of our proof techniques in Section 5 and fill in the details in Section 6, with additional lemmas deferred to the Appendix. We conclude in Section 7 with a discussion of future directions of research.

2 Functional inequalities and continuous-time convergence

Our focus in this section is the convergence of the continuous-time Langevin diffusion (1.1) under various functional inequalities. Throughout the paper, we use the Rényi divergence as a measure of distance between two probability laws. The Rényi divergence of order $q \in (1, \infty)$ of μ from π is defined to be

$$\mathcal{R}_q(\mu \parallel \pi) := \frac{1}{q-1} \ln \left\| \frac{\mathrm{d}\mu}{\mathrm{d}\pi} \right\|_{L^q(\pi)}^q$$

where $\mathcal{R}_q(\mu \parallel \pi)$ is understood to be $+\infty$ if $\mu \ll \pi$. Although the Rényi divergence is not a genuine metric (it is not symmetric and it does not satisfy the triangle inequality), it has the property that $\mathcal{R}_q(\mu \parallel \pi) \ge 0$, with equality if and only if $\mu = \pi$.

Rényi divergence is monotonic in the order: if $1 < q \leq q'$, then $\mathcal{R}_q \leq \mathcal{R}_{q'}$. Notable special cases include:

- as $q \searrow 1$, the Rényi divergence $\mathcal{R}_q(\mu \parallel \pi)$ approaches the KL divergence $\mathsf{KL}(\mu \parallel \pi)$ between μ and π ;
- for q = 2, the Rényi divergence is related to the chi-squared divergence via $\mathcal{R}_2(\mu \| \pi) = \ln(1 + \chi^2(\mu \| \pi));$
- and as $q \to \infty$, we have $\Re_q(\mu \parallel \pi) \to \Re_\infty(\mu \parallel \pi) := \ln \parallel \frac{d\mu}{d\pi} \parallel_{L^\infty(\pi)}$.

These divergences are particularly of interest because they conveniently upper bound a variety of distance measures to be discussed shortly.

2.1 Poincaré and log-Sobolev inequalities

In the context of sampling, the most well-studied functional inequalities are the *Poincaré inequality* (PI) and the *log-Sobolev inequality* (LSI). We say that π satisfies a PI with constant C_{PI} if, for all smooth functions $f : \mathbb{R}^d \to \mathbb{R}$, it holds that

$$\operatorname{var}_{\pi}(f) \le C_{\mathsf{PI}} \mathbb{E}_{\pi}[\|\nabla f\|^2].$$
(PI)

Similarly, we say that π satisfies an LSI with constant C_{LSI} if for all smooth $f : \mathbb{R}^d \to \mathbb{R}$,

$$\operatorname{ent}_{\pi}(f^2) \le 2C_{\mathsf{LSI}} \mathbb{E}_{\pi}[\|\nabla f\|^2], \qquad (\mathsf{LSI})$$

where $\operatorname{ent}_{\pi}(f^2) := \mathbb{E}_{\pi}[f^2 \ln(f^2/\mathbb{E}_{\pi}(f^2))]$. An LSI implies a PI with the same constant.

These functional inequalities are classically related to the ergodicity properties of the Langevin diffusion (1.1). Indeed, if π_t denotes the law of the diffusion at time t, then a PI is equivalent to

$$\chi^{2}(\pi_{t} \parallel \pi) \leq \exp\left(-\frac{2t}{C_{\mathsf{PI}}}\right) \chi^{2}(\pi_{0} \parallel \pi), \quad \text{for all } t \geq 0,$$

whereas an LSI is equivalent to

$$\mathsf{KL}(\pi_t \parallel \pi) \le \exp\left(-\frac{2t}{C_{\mathsf{LSI}}}\right) \mathsf{KL}(\pi_0 \parallel \pi), \quad \text{for all } t \ge 0.$$

Functional inequalities are particularly useful for high-dimensional non-log-concave sampling because they tensorize (if two measures satisfy the same functional inequality, then their product also satisfies the functional inequality with the same constant) and they are stable under common operations such as bounded perturbation (replacing the potential V with \tilde{V} , with $\sup |V - \tilde{V}| < \infty$) and Lipschitz mapping (replacing π with $T_{\#}\pi$ where $T : \mathbb{R}^d \to \mathbb{R}^d$ is Lipschitz and the pushforward $T_{\#}\pi$ is the distribution of T(x) when $x \sim \pi$). We refer to [BGL14] for a comprehensive treatment.

Before stating the convergence results, we remark that under (PI), the result of [Liu20] together with standard comparison inequalities imply

$$\max\left\{2\,\|\mu-\pi\|_{\mathsf{TV}}^2,\,\ln\left(1+\frac{1}{2C_{\mathsf{PI}}}\,W_2^2(\mu,\pi)\right),\,\mathsf{KL}(\mu\,\|\,\pi)\right\} \le \mathfrak{R}_2(\mu\,\|\,\pi)\,.$$

Note that in the Poincaré case, a T_2 transportation inequality does not necessarily hold, so a KL guarantee does not imply a matching W_2 guarantee; by working with Rényi divergences, we are able to provide a unified guarantee for all of these metrics simultaneously.

Improving upon the prior result of [CLL19], Vempala and Wibisono [VW19] showed that these inequalities also imply Rényi convergence for the diffusion.

Theorem 1 ([VW19, Theorems 3 and 5]). Let $q \ge 2$, and let π_t denote the law of the continuous-time Langevin diffusion (1.1) at time t.

1. If π satisfies (LSI), then

$$\partial_t \mathcal{R}_q(\pi_t \parallel \pi) \le -\frac{2}{qC_{\mathsf{LSI}}} \,\mathcal{R}_q(\pi_t \parallel \pi) \,.$$

2. If π satisfies (PI), then

$$\partial_t \mathcal{R}_q(\pi_t \parallel \pi) \leq -\frac{2}{qC_{\mathsf{PI}}} \times \begin{cases} 1 \,, & \text{if } \mathcal{R}_q(\pi_t \parallel \pi) \geq 1 \,, \\ \mathcal{R}_q(\pi_t \parallel \pi) \,, & \text{if } \mathcal{R}_q(\pi_t \parallel \pi) \leq 1 \,. \end{cases}$$

The above result states that under LSI, the Rényi divergence decays exponentially fast whereas under PI, dissipation can be explained in two phases; an initial phase of *slow* decay followed by exponential convergence. Thus, to obtain $\Re_q(\pi_T \parallel \pi) \leq \varepsilon$, it suffices to have

1.
$$T \ge \Omega\left(qC_{\mathsf{LSI}}\ln\frac{\mathfrak{R}_q(\pi_0 \| \pi)}{\varepsilon}\right)$$
 and 2. $T \ge \Omega\left(qC_{\mathsf{PI}}\left(\mathfrak{R}_q(\pi_0 \| \pi) + \ln\frac{1}{\varepsilon}\right)\right)$

under LSI and PI respectively.

2.2 Latała–Oleszkiewicz inequalities

In this paper, in order to interpolate between the Poincaré and log-Sobolev cases, we consider a family of functional inequalities known as Latała–Oleszkiewicz (LO) inequalities [LO00]. We say that π satisfies an LO inequality of order $\alpha \in [1, 2]$ and constant $C_{\mathsf{LO}(\alpha)}$ if for all smooth $f : \mathbb{R}^d \to \mathbb{R}$,

$$\sup_{p \in (1,2)} \frac{\mathbb{E}_{\pi}(f^2) - \mathbb{E}_{\pi}(f^p)^{2/p}}{(2-p)^{2(1-1/\alpha)}} \le C_{\mathsf{LO}(\alpha)} \mathbb{E}_{\pi}[\|\nabla f\|^2].$$
(LO)

It is known that an LO inequality of order 1 is equivalent to a PI, and an LO inequality of order 2 is equivalent to an LSI. More generally, an LO inequality of order α captures measures whose potentials "have tail growth α "; indeed, two notable examples of distributions satisfying the LO inequality of order α are $\pi(x) \propto \exp(-\sum_{i=1}^{d} |x_i|^{\alpha})$ and $\pi(x) \propto \exp(-||x||^{\alpha})$ [LO00; Bar01]. LO inequalities are well-studied because they capture intermediate forms of concentration and are related to a number of other important inequalities, such as Sobolev inequalities; we refer readers to [LO00; Bar01; BR03; Cha04; Bou+05; Wan05; BCR06; BCR07; CGG07; Goz10].

As our first result in this section, we extend Theorem 1 to cover LO inequalities. Our proof, which uses as an intermediary the super Poincaré inequality introduced in [Wan00], is deferred to Section 6.1.

Theorem 2. Let $q \ge 2$, and let π_t denote the law of the continuous-time Langevin diffusion (1.1) at time t. Suppose that π satisfies (LO) with order α . Then,

$$\partial_t \mathcal{R}_q(\pi_t \parallel \pi) \le -\frac{1}{68qC_{\mathsf{LO}(\alpha)}} \times \begin{cases} \mathcal{R}_q(\pi_t \parallel \pi)^{2-2/\alpha}, & \text{if } \mathcal{R}_q(\pi_t \parallel \pi) \ge 1, \\ \mathcal{R}_q(\pi_t \parallel \pi), & \text{if } \mathcal{R}_q(\pi_t \parallel \pi) \le 1. \end{cases}$$

The above theorem can be used to obtain $\mathcal{R}_q(\pi_T \parallel \pi) \leq \varepsilon$ whenever

$$T \ge \Omega\left(qC_{\mathsf{LO}(\alpha)}\left(\frac{\mathcal{R}_q(\mu_0 \parallel \pi)^{2/\alpha - 1} - 1}{2/\alpha - 1} + \ln\frac{1}{\varepsilon}\right)\right);$$

we refer to Lemma 28 for details. We also remark that Theorem 2 reduces to Theorem 1 in the edge cases $\alpha = 2$ (LSI) and $\alpha = 1$ (PI) up to an absolute constant. For $\alpha \in (1, 2)$, the initial phase of convergence interpolates between the *slow* decay induced by PI and the exponential decay under LSI.

2.3 Modified log-Sobolev inequalities

In addition, we also consider the modified log-Sobolev inequality (MLSI) used in [EH21]. The MLSI of order $\alpha_0 \in [-1, 2]$ states that for all $f : \mathbb{R}^d \to \mathbb{R}$ with $\mathbb{E}_{\pi}(f^2) = 1$,

$$\operatorname{ent}_{\pi}(f^{2}) \leq 2C_{\mathsf{MLSI}} \inf_{p \geq 2} \left\{ \mathbb{E}_{\pi}[\|\nabla f\|^{2}]^{1-\delta(p)} \widetilde{\mathfrak{m}}_{p} \left((1+f^{2})\pi \right)^{\delta(p)} \right\}, \qquad \delta(p) := \frac{2-\alpha_{0}}{p+2-2\alpha_{0}}, \quad (\mathsf{MLSI})$$

where for a measure μ (not necessarily a probability measure) we write $\tilde{\mathfrak{m}}_p(\mu) := \int (1 + ||\cdot||^2)^{p/2} d\mu$. The inequality (MLSI) is a careful refinement of [TV00], and provides convergence guarantees for both the Langevin diffusion and LMC under various tail growth conditions [EH21]. Further, the functional inequalities in [BZ99; Zeg01] are also similar to MLSI (termed log-Nash inequalities), yet their main focus is infinite-dimensional semigroups. We focus on (MLSI) as used in [EH21] as other MLSI-type results are stated by absorbing various dimension-dependent constants into C_{MLSI} , and thus they cannot provide sharp rates for LMC.

For technical reasons, we also pair this assumption with a concentration property of the target: for some $\mathfrak{m} \geq 0$ and $\alpha \in [0, 1]$,

$$\pi\{\|\cdot\| \ge \mathfrak{m} + \lambda\} \le 2\exp\{-\left(\frac{\lambda}{C_{\mathsf{tail}}}\right)^{\alpha_1}\}, \quad \text{for all } \lambda \ge 0.$$
 (\$\alpha_1\$-tail)

The parameters α_0 and α_1 are analogous to the parameter α in the LO inequality; we refer to [EH21] and the examples in Section 4 for further discussion of (MLSI).

Similarly to Theorem 2, we can prove a quantitative continuous-time convergence rate for the Langevin diffusion (1.1) under an MLSI. The proof is deferred to Section 6.5.

Theorem 3. Suppose that π satisfies (MLSI) and $(\alpha_1$ -tail), and assume that $\varepsilon^{-1}, \mathfrak{m}, C_{\mathsf{MLSI}} \geq 1$ and that $\mathfrak{m}, C_{\mathsf{tail}}, \mathfrak{R}_{2q}(\pi_0 \parallel \pi) \leq d^{O(1)}$. Let $(\pi_t)_{t\geq 0}$ denote the law of the continuous-time Langevin diffusion (1.1). Then, it holds that $\mathfrak{R}_q(\pi_T \parallel \pi) \leq \varepsilon$ for

$$T \ge \Omega \left(q C_{\mathsf{MLSI}}^2 \left(\mathfrak{m} + q C_{\mathsf{tail}} \, \mathcal{R}_{2q} (\pi_0 \parallel \pi)^{1/\alpha_1} \right)^{2-\alpha_0} \operatorname{polylog} \frac{d \, \mathcal{R}_q(\pi_0 \parallel \pi)}{\varepsilon} \right).$$

We remark that when $\alpha_0 = \alpha_1 = \alpha$, the dependence on the Rényi divergence at initialization in Theorems 2 and 3 match up to a logarithmic factor, and hence LO and MSLI provide similar results in continuous time. However, as we discuss in Section 4, MLSI is useful for treating certain examples in which the LO constant $C_{LO(\alpha)}$ may be dimension-dependent whereas C_{MLSI} is not.

3 Main results on Langevin Monte Carlo

In this section, we present our main results on the Rényi convergence of LMC. Denoting the step size with h > 0, the LMC algorithm is defined by the iteration

$$x_{(k+1)h} = x_{kh} - h\nabla V(x_{kh}) + \sqrt{2h}\,\xi_k\,, \qquad k \in \mathbb{N}\,, \tag{LMC}$$

where $(\xi_k)_{k \in \mathbb{N}}$ is a sequence of i.i.d. standard Gaussian random variables. Here, the indexing of the LMC iterates is chosen so that the iterate x_{kh} is comparable to the continuous-time diffusion (1.1) at time kh. We let μ_{kh} denote the law of x_{kh} .

Our first result deals with the LSI and gradient Lipschitz case.

Theorem 4. Assume that π satisfies (LSI) and that ∇V is L-Lipschitz; assume for simplicity that $C_{\text{LSI}}, L \ge 1$ and $q \ge 3$. Let μ_{Nh} denote the N-th iterate of LMC with step size h satisfying $0 < h < 1/(192q^2C_{\text{LSI}}L^2)$. Then, for all $N \ge N_0$, it holds that

$$\mathcal{R}_q(\mu_{Nh} \parallel \pi) \le \exp\left(-\frac{(N-N_0)h}{4C_{\mathsf{LSI}}}\right) \mathcal{R}_2(\mu_0 \parallel \pi) + \widetilde{O}(dhqC_{\mathsf{LSI}}L^2) \,,$$

where $N_0 = \lceil \frac{2C_{\mathsf{LSI}}}{h} \ln \frac{q-1}{2} \rceil$. In particular, if we choose $h = \widetilde{\Theta}(\frac{\varepsilon}{dqC_{\mathsf{LSI}}L^2} \min(1, \frac{d}{q\varepsilon}))$, then

$$\Re_q(\mu_{Nh} \parallel \pi) \le \varepsilon$$
, for all $N \ge \widetilde{\Omega}\left(\frac{dqC_{\mathsf{LSI}}^2 L^2 \log \Re_2(\mu_0 \parallel \pi)}{\varepsilon} \max\{1, \frac{q\varepsilon}{d}\}\right)$.

The comparison of Theorem 4 with [VW19; GT20; EHZ21] is summarized as Table 1. Since our guarantee is stable with respect to the number of iterations N, we can let $N \to \infty$ and obtain an estimate on the asymptotic bias of (LMC) in Rényi divergence; this answers an open question of [VW19].

Corollary 5. Assume that π satisfies (LSI) and that ∇V is L-Lipschitz; assume for simplicity that $C_{\text{LSI}}, L \geq 1$. 1. Let $\mu_{\infty}^{(h)}$ denote the stationary distribution of LMC with step size h satisfying $0 < h < 1/(192q^2C_{\text{LSI}}L^2)$. Then,

$$\mathfrak{R}_{q}(\mu_{\infty}^{(h)} \parallel \pi) \leq \widetilde{O}(dhqC_{\mathsf{LSI}}L^{2}).$$

Source	Assumption	Metric	Complexity	Stable Bound
[VW19]	(LSI)	KL divergence $(q = 1)$	$dC_{\rm LSI}^2L^2/\varepsilon$	1
[GT20]	C_{SC}^{-1} -strongly log-concave	Rényi divergence	$dq^2 C_{\rm SC}^4 L^4/\varepsilon^2$	×
[EHZ21]	C_{SC}^{-1} -strongly log-concave	Rényi divergence	$dq^4 C_{\rm SC}^4 L^4/\varepsilon$	×
Theorem 4	(LSI)	Rényi divergence	$dqC_{\rm LSL}^2L^2/\varepsilon$	1

Table 1: We compare the guarantee of Theorem 4 with prior results, omitting polylogarithmic factors. The last column refers to whether the bound is stable as the number of iterations of LMC tends to infinity. The complexity bound in the last row is stated for moderate values of q; when $q \gg d/\varepsilon$, then the dependence on q becomes $\tilde{O}(q^2)$.

Extending the techniques of Theorem 4, we next give a result for the log-concave (which implies (PI)) and gradient Lipschitz case.

Theorem 6. Assume that π is log-concave (and hence satisfies (PI)) and that ∇V is L-Lipschitz. For simplicity, assume that V is minimized at 0. Let μ_{Nh} denote the N-th iterate of LMC with step size h satisfying $h = \widetilde{\Theta}(\frac{\varepsilon}{dq^2 C_{\text{Pl}}L^2} \min\{1, \frac{1}{q\varepsilon}, \frac{dC_{\text{Pl}}}{\varepsilon L}\})$ and initialized at $\mu_0 = \operatorname{normal}(0, L^{-1}I_d)$. Then,

$$\mathcal{R}_q(\mu_{Nh} \parallel \pi) \leq \varepsilon \qquad after \ N = \widetilde{\Theta}\Big(\frac{d^2q^3C_{\mathsf{Pl}}^2L^2}{\varepsilon} \max\{1, q\varepsilon, \frac{\varepsilon L}{dC_{\mathsf{Pl}}}\}\Big) \ iterations$$

In Table 2, we compare Theorem 6 with the prior works [DMM19; Dwi+19; Che+20a; DKR20]. Theorem 6 is the state-of-the-art result for algorithms based on discretizations of Langevin or underdamped Langevin, only beaten by the result for modified MALA (for which our result reads $\tilde{O}(d^2/\varepsilon^2)$ whereas the result for modified MALA is $\tilde{O}(d^2/\varepsilon^{3/2})$). Moreover, our result is given in the strongest metric (Rényi divergence).

Source	Algorithm	Metric	Complexity
[DMM19]	averaged LMC	$\sqrt{\mathrm{KL}}$	d^2/ε^4
[Dwi+19; Che+20a]	modified MALA	TV	$d^2/\varepsilon^{3/2}$
[DKR20]	modified LMC	W_1	d^2/ε^4
[DKR20]	modified LMC	W_2	d^2/ε^6
[DKR20]	modified ULMC	W_1	d^2/ε^3
[DKR20]	modified ULMC	W_2	d^2/ε^5
Theorem 6	LMC	√Rénvi	d^2/ε^2

Table 2: We compare convergence guarantees for sampling from an isotropic log-concave distribution with $C_{\mathsf{Pl}}, L = O(1)$. MALA refers to the Metropolis-adjusted Langevin algorithm, whereas ULMC refers to underdamped Langevin Monte Carlo algorithm.

Subsequently, we consider the general case of an LO inequality. We also assume weak smoothness for some $s \in (0, 1]$ and L > 0:

$$\|\nabla V(x) - \nabla V(y)\| \le L \, \|x - y\|^s \quad \text{for all } x, y \in \mathbb{R}^d \,. \tag{s-Hölder}$$

We note that the LO order α and the Hölder exponent s need to satisfy $s + 1 \ge \alpha$.

Theorem 7. Assume that the potential satisfies $\nabla V(0) = 0$, (LO) of order α , and (s-Hölder). For simplicity, assume that $\varepsilon^{-1}, \mathfrak{m}, C_{\mathsf{LO}(\alpha)}, L, \mathcal{R}_2(\mu_0 \parallel \hat{\pi}) \geq 1$ and $q \geq 2$; here, $\mathfrak{m} := \int \|\cdot\| d\pi$ and $\hat{\pi}$ is a slightly modified version of π which is introduced in the analysis (Section 6.4). Then, LMC with an appropriate step size (given in (6.11)) satisfies $\mathcal{R}_q(\mu_{Nh} \parallel \pi) \leq \varepsilon$ after

$$N = \widetilde{\Theta}_{s} \Big(\frac{dq^{1+2/s} C_{\mathsf{LO}(\alpha)}^{1+1/s} L^{2/s} \, \mathcal{R}_{2q-1}(\mu_{0} \parallel \pi)^{(2/\alpha-1)\,(1+1/s)}}{\varepsilon^{1/s}} \max \Big\{ 1, q^{1/s} \varepsilon^{1/s}, \frac{\mathfrak{m}^{s}}{d}, \frac{\mathcal{R}_{2}(\mu_{0} \parallel \hat{\pi})^{s/2}}{d} \Big\} \Big)$$

iterations. Here, $\widetilde{\Theta}_s(\cdot)$ hides polylogarithmic factors and constants depending only on s.

We now make a few remarks to simplify the rate. First, although initialization is more subtle in the nonlog-concave case, it is reasonable to take $\mathcal{R}_2(\mu_0 \parallel \hat{\pi}), \mathcal{R}_{2q-1}(\mu_0 \parallel \pi) = \widetilde{O}(d)$; we defer a detailed discussion of initialization to Appendix A. Next, it is also reasonable to assume¹ $\mathfrak{m} = O(d)$, in which case the third term in the maximum will never dominate. Focusing on the dependence on the dimension and target accuracy, we therefore obtain the simplified rate $\widetilde{O}(d^{(2/\alpha)}(1+1/s)-1/s}/\varepsilon^{1/s})$; in particular, in the smooth (s = 1) case, the rate is $\widetilde{O}(d^{4/\alpha-1}/\varepsilon)$. Regarding prior works which handle a wide variety of growth rates and smoothness conditions for the potential, the closest to the present work is [EH21], which obtains a rate of $\widetilde{O}(d^{(2/\alpha+1\{\alpha=1\})}(1+1/s)-1/\varepsilon^{1/s})$ for potentials of tail growth α satisfying (*s*-Hölder); note that our rate is strictly better as soon as s < 1 and avoids the jump in the rate at $\alpha = 1$. We emphasize, however, that despite the superficial similarity with [EH21], our result is the first one under a purely functional analytic condition on the target (together with weak smoothness).

Remark. The case $\alpha = 1$ yields the convergence rate $\tilde{O}(d^{2+1/s}q^{1+2/s}C_{\mathsf{Pl}}^{1+1/s}L^{2/s}/\varepsilon^{1/s})$ for LMC under the Poincaré inequality and weak smoothness. In the case $\alpha = 2$ and s = 1 (LSI and smooth case), the rate reduces to $\tilde{O}(dq^3C_{\mathsf{LSI}}^2L^2/\varepsilon)$, which recovers the guarantee of Theorem 4 up to the dependence on q.

When the LO constant $C_{LO(\alpha)}$ is dimension-dependent, Theorem 7 may not give the sharpest rates. We therefore complement Theorem 7 with a result assuming (MLSI).

Theorem 8. Assume that the potential satisfies $\nabla V(0) = 0$, (MLSI) of order α_0 , (α_1 -tail), and (s-Hölder). For simplicity, assume that ε^{-1} , \mathfrak{m} , C_{MLSI} , C_{tail} , L, $\mathcal{R}_2(\mu_0 \| \hat{\pi}) \ge 1$, $q \ge 2$, and \mathfrak{m} , C_{tail} , $\mathcal{R}_2(\pi_0 \| \pi) \le d^{O(1)}$; here, $\hat{\pi}$ is a slightly modified version of π which is introduced in the analysis (Section 6.4). Then, LMC with an appropriate step size (given in (6.12)) satisfies $\mathcal{R}_q(\mu_{Nh} \| \pi) \le \varepsilon$ after

$$N = \widetilde{\Theta} \Big(\frac{d \mathcal{R}_{2q}(\mu_0 \| \pi)^{(2-\alpha_0)(1+1/s)/\alpha_1}}{\varepsilon^{1/s}} \max \Big\{ 1, \varepsilon^{1/s}, \frac{\mathfrak{m}^s}{d}, \frac{\mathcal{R}_2(\mu_0 \| \hat{\pi})^{s/2}}{d}, \Big(\frac{\mathfrak{m}}{\mathcal{R}_{2q}(\mu_0 \| \pi)^{1/\alpha_1}} \Big)^{(2-\alpha_0)/s} \Big\} \Big)$$

iterations. Here, the $\tilde{\Theta}(\cdot)$ notation hides polylogarithmic factors as well as constants depending on α_0 , α_1 , q, s, C_{MLSI} , C_{tail} , and L; a more precise statement is given in Section 6.5.

For potentials of tail growth $\alpha \in (1, 2]$, we can suppose that (MLSI) and (α_1 -tail) are satisfied with $\alpha_0 = \alpha_1 = \alpha$, where we take $\mathfrak{m} = O(d^{1/\alpha})$. Also, assuming $\mathcal{R}_2(\mu_0 \parallel \hat{\pi}), \mathcal{R}_{2q}(\mu_0 \parallel \pi) = O(d)$, the rate is then simplified to $\widetilde{O}(d^{(2/\alpha)}(1+1/s)-1/s/\varepsilon^{1/s})$ as before. As discussed in the next section, the case $\alpha = 1$ is special and (MLSI) may not hold with $\alpha_0 = \alpha$.

Remark. A number of recent works [DMM19; Cha+20; LC21; Leh21; NDC21] consider non-smooth and mixed-smooth potentials. By incorporating Gaussian smoothing, it seems possible to extend our techniques to cover these settings, but we do not pursue this direction here.

4 Examples

In this section, we illustrate our results on simple examples and compare our guarantees with prior work.

¹This holds for e.g. the potentials $V(x) = ||x||^{\alpha}$ for all $\alpha \in [1, 2]$.

Example 9 (tail growth $\alpha \in (1,2]$). Consider the target $\pi_{\alpha}(x) \propto \exp(-\|x\|^{\alpha})$ for $\alpha \in (1,2]$, which satisfies (LO) of order α and (s-Hölder) with $s = \alpha - 1$. Since π_{α} satisfies (PI) with $C_{\text{PI}} = \Theta(d^{2/\alpha-1})$ [Bob03], then Theorem 7 does not yield a good result. Previously, [EH21] showed that π_{α} satisfies (MLSI) of order α , obtaining the complexity $\tilde{O}(d^{(3-\alpha)/(\alpha-1)}/\varepsilon^{1/(\alpha-1)})$ to achieve ε -accuracy in KL divergence for this target. From Theorem 8, we have improved this rate to $\tilde{O}((d/\varepsilon)^{1/(\alpha-1)})$ in Rényi divergence. Since (MLSI) is stable under bounded perturbations, the same rate holds for the perturbed potential $V(x) = \|x\|^{\alpha} + \cos \|x\|$.

Due to the use of the CKP inequality [BV05], their KL bound yields $\tilde{O}(d^{(5-\alpha)/(\alpha-1)}/\varepsilon^{\alpha/(\alpha-1)})$ complexity to reach ε accuracy in the W_{α}^2 metric. On the other hand, Theorem 8 together with the Poincaré inequality yields the complexity $\tilde{O}(d^{2/(\alpha(\alpha-1))}/\varepsilon^{1/(\alpha-1)})$ to obtain ε accuracy in the W_2^2 metric. Hence, we have both improved the rate in W_{α} and proven a new guarantee in W_2 which previously could not be reached at all.

Example 10 (tail growth $\alpha \in (1, 2]$ for smoothed potential). Consider $\pi_{\alpha}(x) \propto \exp(-(1 + ||x||^2)^{\alpha/2})$, which satisfies (LO) of order α and (*s*-Hölder) with s = 1 (i.e. ∇V is Lipschitz). Previously, [EH21] obtained the complexity $\widetilde{O}(d^{(4-\alpha)/\alpha}/\varepsilon)$ in KL divergence and $\widetilde{O}(d^{(4+\alpha)/\alpha}/\varepsilon^{\alpha})$ in W_{α}^2 . From Theorem 8, we have obtained the rate $\widetilde{O}(d^{(4-\alpha)/\alpha}/\varepsilon)$ in Rényi divergence and $\widetilde{O}(d^{(6-2\alpha)/\alpha}/\varepsilon)$ in W_2^2 . As before, this rate is stable under suitable perturbations of the potential.

Example 11 (tail growth $\alpha = 1$ for smoothed potential). The case of $\alpha = 1$ is worth considering separately for comparison purposes. Consider the target $\pi_1(x) \propto \exp(-\sqrt{1+||x||^2})$, which satisfies (*s*-Hölder) with s = 1 (i.e. ∇V is Lipschitz). Previously, [EH21] showed that π_1 satisfies (MLSI) with $\alpha_0 = -O(\frac{1}{\log d})$ and $C_{\text{MLSI}} = O(\log d)$; also, π_1 satisfies (α_1 -tail) with $\alpha_1 = 1$. Using this, they obtained the complexity $\widetilde{O}(d^5/\varepsilon)$ in KL divergence, whereas Theorem 8 implies the same rate in Rényi divergence. We also remark that their rate only holds for sufficiently small perturbations (e.g. their analysis does not cover $V(x) = ||x|| + \cos ||x||)$ due to the need to preserve a dissipativity assumption, whereas our result has no such requirement. This highlights a benefit of working without dissipativity conditions.

Here, Theorem 6 applies to π_1 with $C_{\mathsf{PI}} = O(d)$ [Bob03] and yields a rate of $\widetilde{O}(d^4/\varepsilon)$ in Rényi divergence; in contrast, [DMM19] yields a rate of $\widetilde{O}(d^3/\varepsilon^2)$ in KL divergence (started from a distribution with $W_2^2(\mu_0, \pi_1) = O(d^2)$) for averaged LMC, and [Dwi+19; Che+20a] yields a rate of $\widetilde{O}(d^{3.5}/\varepsilon^{0.75})$ in $\|\cdot\|_{\mathsf{TV}}^2$ for modified MALA, although none of these rates is stable under perturbation.

Example 12 (tail growth $\alpha \in [1,2]$ for smoothed product potential). For $x \in \mathbb{R}^d$, let $\langle x \rangle_i := \sqrt{1+x_i^2}$. Consider the target $\pi_\alpha(x) \propto \exp(-\|\langle x \rangle\|_\alpha^\alpha)$, which satisfies (LO) of order α (see [LO00]) and (*s*-Hölder) with s = 1 (i.e. ∇V is Lipschitz). The result of [EH21] implies a complexity of $\widetilde{O}(d^{(4-\alpha)/\alpha}/\varepsilon)$ in KL divergence and $\widetilde{O}(d^{(4+\alpha)/\alpha}/\varepsilon^\alpha)$ in W_α^2 for $\alpha \in (1,2]$, and $\widetilde{O}(d^5/\varepsilon)$ in KL divergence when $\alpha = 1$. From Theorem 7, we have obtained the rate $\widetilde{O}(d^{(4-\alpha)/\alpha}/\varepsilon)$ in Rényi divergence and hence also W_2^2 for all $\alpha \in [1,2]$; in particular, there is no jump in the rate at $\alpha = 1$.

Example 13 (LSI case with weakly smooth potential). We also compare the results when $\alpha = 2$ and $s \in (0,1]$. In this case, [Cha+20] obtained the rate $\widetilde{O}(d^{(2+s)/s}/\varepsilon^{1/s})$ in $\|\cdot\|_{\mathsf{TV}}^2$ for strongly log-concave distributions, whereas [EH21] obtained the rate $\widetilde{O}((d/\varepsilon)^{1/s})$ in KL divergence for perturbations of strongly log-concave distributions. In contrast, Theorem 7 yields the rate $\widetilde{O}(d/\varepsilon^{1/s})$ in Rényi divergence under (LSI). An example of such a potential is given by $V(x) = \frac{1}{2} \|x\|^2 + \cos(\|x\|^{1+s})$.

5 Technical overview

5.1 Adapting the interpolation method to Rényi divergences

In the proof of Theorem 4, we follow the interpolation method of [VW19]. Namely, we introduce the following interpolation of (LMC): for $t \in [kh, (k+1)h]$, let

$$x_{t} = x_{kh} - (t - kh) \nabla V(x_{kh}) + \sqrt{2} (B_{t} - B_{kh}), \qquad (5.1)$$

where $(B_t)_{t\geq 0}$ is a standard Brownian motion, and let μ_t denote the law of x_t . Then, [VW19] derives the following differential inequality for the KL divergence:

$$\partial_t \mathsf{KL}(\mu_t \parallel \pi) \le -\frac{3}{4} \times \underbrace{4 \mathbb{E}_{\pi}[\|\nabla \sqrt{\rho_t}\|^2]}_{\text{Fisher information}} + \underbrace{\mathbb{E}[\|\nabla V(x_t) - \nabla V(x_{kh})\|^2]}_{\text{discretization error}}, \qquad t \in [kh, (k+1)h], \tag{5.2}$$

where we write $\rho_t := \frac{d\mu_t}{d\pi}$. This inequality is an analogue of the celebrated de Bruijn identity from information theory for the interpolated process. Assuming that π satisfies (LSI) and that ∇V is *L*-Lipschitz, the Fisher information upper bounds the KL divergence and the discretization error is shown to be of order $O(dh^2L^2)$; this then yields a convergence guarantee in KL divergence.

The analogous differential inequality for the Rényi divergence is, for $t \in [kh, (k+1)h]$,

$$\partial_t \mathcal{R}_q(\mu_t \parallel \pi) \le -\underbrace{\frac{3}{q} \frac{\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)}}_{\text{Rényi Fisher information}} + \underbrace{q \frac{\mathbb{E}[\rho_t^{q-1}(x_t) \|\nabla V(x_t) - \nabla V(x_{kh})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)}}_{\text{discretization error}}.$$
(5.3)

(See the proof of [EHZ21, Lemma 6]; to make the paper more self-contained, we also provide a derivation in Proposition 15.) Note that the q = 1 case of the above inequality formally corresponds to (5.2). Next, as shown in [VW19, Lemma 5], the Rényi Fisher information indeed upper bounds the Rényi divergence under an LSI. However, the discretization term is now far trickier to control.

Write $\psi_t := \rho_t^{q-1} / \mathbb{E}_{\pi}(\rho_t^q)$. Observing that $\mathbb{E} \psi_t(x_t) = 1$, the discretization term can be written as an expectation under a *change of measure*:

discretization error =
$$q \widetilde{\mathbb{E}}[\|\nabla V(x_t) - \nabla V(x_{kh})\|^2]$$
,

where $\widetilde{\mathbb{E}}$ is the expectation under the measure $\widetilde{\mathbb{P}}$ defined via $\frac{d\widetilde{\mathbb{P}}}{d\mathbb{P}} = \psi_t(x_t)$. Also, using the Lipschitzness of ∇V , we obtain $\|\nabla V(x_t) - \nabla V(x_{kh})\|^2 \leq 2h^2 L^2 \|\nabla V(x_{kh})\|^2 + 4L^2 \|B_t - B_{kh}\|^2$. Hence, our task is to bound the expectation of these two terms under a complicated change of measure.

Towards that end, consider first the Brownian motion term. Using the Donsker–Varadhan variational principle, for any random variable X,

$$\widetilde{\mathbb{E}}X \leq \mathsf{KL}(\widetilde{\mathbb{P}} \parallel \mathbb{P}) + \ln \mathbb{E} \exp X$$

Applying this to $X = c \left(\|B_t - B_{kh}\| - \mathbb{E} \|B_t - B_{kh}\| \right)^2$ for a constant c > 0 to be chosen later, we can bound

$$\widetilde{\mathbb{E}}[\|B_t - B_{kh}\|^2] \le 2 \mathbb{E}[\|B_t - B_{kh}\|^2] + \frac{2}{c} \widetilde{\mathbb{E}}X \le 2 \mathbb{E}[\|B_t - B_{kh}\|^2] + \frac{2}{c} \left\{ \mathsf{KL}(\widetilde{\mathbb{P}} \| \mathbb{P}) + \ln \mathbb{E} \exp\left(c \left(\|B_t - B_{kh}\| - \mathbb{E}\|B_t - B_{kh}\|\right)^2\right) \right\}.$$
(5.4)

Note that the first and third terms in the right-hand side of the above expression are expectations under the original measure \mathbb{P} , and can therefore be controlled; to ensure that the third term is bounded, we can take $c \approx 1/h$. For the second term, a surprising calculation involving a judicious application of the LSI for π (see (6.3), (6.4), and (6.5)) shows that it is bounded by h times the Rényi Fisher information, and can therefore be absorbed into the first term of the differential inequality (5.3) for h sufficiently small.

The expectation of the drift term $\|\nabla V(x_{kh})\|^2$ under the change of measure can also be handled via similar methods, but this can be bypassed via a duality principle for the Fisher information; see Lemma 16. We also remark that naïvely, this proof incurs a cubic dependence on q, but this can be sharpened via an argument based on hypercontractivity (Proposition 17).

In the above proof outline, the LSI for π plays a crucial role in the arguments. In Theorem 6, we show that the method can be somewhat extended to the case when π does not satisfy an LSI, but is instead assumed to be (weakly) log-concave. In this case, we show that with an appropriate Gaussian initialization, the law μ_{kh} of the *iterate* x_{kh} of (LMC) satisfies an LSI, albeit with a constant which grows with the number of iterations (Lemma 18). In turn, this fact together with a suitable modification of the preceding proof strategy also allows us to obtain a convergence guarantee in this case (see Section 6.3 for details).

5.2 Controlling discretization error via Girsanov's theorem

In the general case of a weaker functional inequality and smoothness condition, the preceding arguments do not apply. Instead, we start with the weak triangle inequality for the Rényi divergence:

$$\mathfrak{R}_{q}(\mu_{T} \parallel \pi) \leq \mathfrak{R}_{2q}(\mu_{T} \parallel \pi_{T}) + \mathfrak{R}_{2q-1}(\pi_{T} \parallel \pi) + \mathfrak{R}_{2q-1}(\pi) +$$

Here, $(\mu_t)_{t\geq 0}$ is the law of the interpolated process (5.1), whereas $(\pi_t)_{t\geq 0}$ is the law of the continuous-time Langevin diffusion (1.1) initialized at a draw from μ_0 . The second term is handled via the continuous-time convergence results, either under the LO inequality (Theorem 2) or under the MLSI (Theorem 3), and the crux of the proof is to control the first term (the discretization error).

The discretization error $\mathcal{R}_{2q}(\mu_T \parallel \pi_T)$ was controlled in the prior works [GT20; EHZ21] via the adaptive composition theorem, albeit under stronger assumptions (strong convexity/dissipativity). Briefly, this theorem controls the Rényi divergence between the paths of the interpolated and original (continuous-time) processes by summing up the contribution to the Rényi divergence in each infinitesimal time step. In turn, due to the Brownian motion driving the SDEs, this reduces to a computation of the Rényi divergence between Gaussians. Making this approach rigorous, however, requires first applying it to the discrete-time algorithm and then performing a cumbersome limiting argument. In this paper, we streamline this technique by instead invoking Girsanov's theorem from stochastic calculus.

First, the data processing inequality implies that $\mathcal{R}_{2q}(\mu_T \parallel \pi_T) \leq \mathcal{R}_{2q}(P_T \parallel Q_T)$, where P_T and Q_T are measures on path space representing the laws of the trajectories (on the interval [0, T]) of the interpolated and diffusion processes respectively. Next, Girsanov's theorem provides a closed-form formula for the Radon-Nikodym derivative $\frac{dP_T}{dQ_T}$, which leads to the inequality

$$\mathcal{R}_{2q}(P_T \parallel Q_T) \le \frac{1}{2(2q-1)} \ln \mathbb{E} \exp\left(4q^2 \int_0^T \|\nabla V(z_t) - \nabla V(z_{\lfloor t/h \rfloor h})\|^2 \,\mathrm{d}t\right),$$

where $(z_t)_{t\geq 0}$ is the continuous-time Langevin diffusion (1.1). The use of Girsanov's theorem for deriving quantitative estimates on the discretization error in this manner was likely first introduced in [DT12] for the KL divergence, although the current application to Rényi divergences is closer to the calculation for MALA in [Che+21a]. However, to the best our knowledge, this paper is the first to adapt the Girsanov technique to provide a complete Rényi convergence result for LMC.

Controlling the discretization error over an interval [0, h] corresponding to a single iteration of LMC is straightforward using the tools of stochastic calculus, and was in fact carried out in [Che+21a]. Extending this to the full time interval [0, T] is more challenging; indeed, if we bound the discretization error on [h, 2h]conditional on $(z_t)_{t\in[0,h]}$, then the resulting bound depends on $||z_h||^2$, which prevents us from straightforwardly iterating the one-step discretization bound. To address this, we instead control intermediate error terms conditioned on the event $\mathcal{E}_{\delta,T} := \max_{k \in \mathbb{N}, kh \leq T} ||z_{kh}|| \leq R_{\delta,T}$, and $R_{\delta,T}$ is chosen so that $\mathbb{P}(\mathcal{E}_{\delta,T}) \geq 1-\delta$. Subsequently, we can use Lemma 22 to remove the conditioning, and hence providing a bound on $\mathcal{R}_{2q}(P_T ||Q_T)$ if $R_{\delta,T}$ does not grow too fast in $1/\delta$; in particular, it is required that $R_{\delta,T} \leq \sqrt{\log(1/\delta)}$.

The requirement on $R_{\delta,T}$ is equivalent to requiring that for each $t \in [0,T]$, the random variable z_t has sub-Gaussian tails. Observe however that the stationary distribution π may not have sub-Gaussian tails under our assumption of an LO inequality (indeed, in the Poincaré case, π may only have subexponential tails). Nevertheless, if the initialization μ_0 has sub-Gaussian tails, then for each $t \in [0,T]$ it may still be the case that π_t has sub-Gaussian tails. This turns out to be true, but it is quite non-trivial to prove without any dissipativity conditions on the potential V, and therefore constitutes our primary technical challenge.

To overcome this challenge, we introduce a novel technique based on comparison of the diffusion (1.1) with an auxiliary Langevin diffusion $(\hat{\pi}_t)_{t\geq 0}$ corresponding to a modified stationary distribution $\hat{\pi}$. The distribution $\hat{\pi}$ is constructed to have sub-Gaussian tails. To transfer the sub-Gaussianity of $\hat{\pi}$ to π_t , we apply the following change of measure inequality: for probability measures μ and ν , and any event $E \subseteq \mathbb{R}^d$,

$$\mu(E) = \nu(E) + \int \mathbb{1}_E \left(\frac{\mathrm{d}\mu}{\mathrm{d}\nu} - 1\right) \mathrm{d}\nu \le \nu(E) + \sqrt{\chi^2(\mu \parallel \nu) \nu(E)},$$

where the last inequality is the Cauchy–Schwarz inequality. This simple inequality states that in order to control the probability of an event E under a measure μ in terms of its probability under ν , it suffices to

control the chi-squared divergence between μ and ν . Applying this to our context, we can establish sub-Gaussian tail bounds for π_t if we can control the Rényi divergences $\mathcal{R}_2(\pi_t \parallel \hat{\pi}_t)$ and $\mathcal{R}_2(\hat{\pi}_t \parallel \hat{\pi})$; the former is again controlled via Girsanov's theorem. We stress that the auxiliary process $(\hat{\pi}_t)_{t\geq 0}$ is introduced only for analysis purposes and does not affect the implementation of the algorithm.

The details of this strategy are carried out in Section 6.4.

6 Proofs

6.1 Proof of Theorem 2

In this section, we prove Theorem 2 on the Rényi convergence of the continuous-time Langevin diffusion (1.1) under an LO inequality. Using capacity inequalities as an intermediary, [BCR06; Goz10] established the equivalence of LO inequalities with other functional inequalities such as modified Sobolev inequalities. For our purposes, it is convenient to work with *super Poincaré inequalities*, which were introduced in [Wan00].

We say that π satisfies a super Poincaré inequality with function $\beta : \mathbb{R}_+ \to \mathbb{R}_+$ if for all smooth $f : \mathbb{R}^d \to \mathbb{R}$,

$$\mathbb{E}_{\pi}(f^2) \le \beta(s) \mathbb{E}_{\pi}[\|\nabla f\|^2] + s \left(\mathbb{E}_{\pi}|f|\right)^2 \quad \text{for all } s \ge 1.$$
(6.1)

For $\alpha \in [1, 2]$, define the function $\beta_{\alpha} : \mathbb{R}_+ \to \mathbb{R}_+$ via

$$\beta_{\alpha}(s) := \frac{96C_{\mathsf{LO}(\alpha)}}{\ln(e+s)^{2-2/\alpha}} \,.$$

Then, it is known that (LO) with order α implies a super Poincaré inequality with function β_{α} (see [Goz10, Remark 5.16]). The following proof is inspired by the proof of [VW19, Theorem 5].

Proof. [Proof of Theorem 2] From [VW19, Lemma 6], we have

$$\partial_t \mathcal{R}_q(\pi_t \parallel \pi) = -\frac{4}{q} \frac{\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)},$$

where $\rho_t := \frac{\mathrm{d}\pi_t}{\mathrm{d}\pi}$. Applying the super Poincaré inequality (6.1) with $f = \rho_t^{q/2}$ and $\beta = \beta_{\alpha}$ yields

$$\mathbb{E}_{\pi}[\|\nabla(\rho_{t}^{q/2})\|^{2}] \geq \frac{1}{\beta_{\alpha}(s)} \mathbb{E}_{\pi}(\rho_{t}^{q}) - \frac{s}{\beta_{\alpha}(s)} \{\mathbb{E}_{\pi}(\rho_{t}^{q/2})\}^{2} = \frac{1}{\beta_{\alpha}(s)} \exp\{(q-1) \mathcal{R}_{q}(\pi_{t} \| \pi)\} - \frac{s}{\beta_{\alpha}(s)} \exp\{(q-2) \mathcal{R}_{q/2}(\pi_{t} \| \pi)\}.$$

Using the fact that $\mathcal{R}_{q/2} \leq \mathcal{R}_q$, we can further lower bound this by

$$\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2] \ge \frac{\exp\{(q-1)\mathcal{R}_q(\pi_t \| \pi)\}}{\beta_{\alpha}(s)} \left(1 - s \exp\{-\mathcal{R}_q(\pi_t \| \pi)\}\right) = \frac{\mathbb{E}_{\pi}(\rho_t^q)}{\beta_{\alpha}(s)} \left(1 - s \exp\{-\mathcal{R}_q(\pi_t \| \pi)\}\right).$$

We now distinguish two cases. If $\Re_q(\pi_t \parallel \pi) \ge 1$, then we choose $s = \frac{1}{2} \exp\{\Re_q(\pi_t \parallel \pi)\}$, yielding

$$\partial_t \mathcal{R}_q(\pi_t \parallel \pi) \le -\frac{2}{q\beta_\alpha(s)} = -\frac{\ln(\mathbf{e} + \frac{1}{2}\exp\mathcal{R}_q(\pi_t \parallel \pi))^{2-2/\alpha}}{48qC_{\mathsf{LO}(\alpha)}} \le -\frac{1}{68qC_{\mathsf{LO}(\alpha)}}\mathcal{R}_q(\pi_t \parallel \pi)^{2-2/\alpha} = -\frac{1}{68qC_{\mathsf{LO}(\alpha)$$

Otherwise, if $\mathcal{R}_q(\pi_t \parallel \pi) \leq 1$, then we choose s = 1, yielding

$$\partial_t \mathcal{R}_q(\pi_t \parallel \pi) \le -\frac{4}{q\beta_\alpha(1)} \left(1 - \exp\{-\mathcal{R}_q(\pi_t \parallel \pi)\} \right) \le -\frac{2}{q\beta_\alpha(1)} \mathcal{R}_q(\pi_t \parallel \pi) \le -\frac{1}{68qC_{\mathsf{LO}(\alpha)}} \mathcal{R}_q(\pi_t \parallel \pi) \,,$$

where we used the elementary inequality $1 - \exp(-x) \ge x/2$ for $x \in [0, 1]$.

Proof of Theorem 4 6.2

Throughout this section, recall the notation $\rho_t := \frac{d\mu_t}{d\pi}$ and $\psi_t := \rho_t^{q-1} / \mathbb{E}_{\pi}(\rho_t^q)$. We begin by proving the differential inequality (5.3). Although this has appeared in the previous works [VW19; EHZ21], we include the proofs for the sake of completeness.

Proposition 14. Let $(\mu_t)_{t>0}$ denote the law of the interpolation (5.1) of LMC. Then, for $t \in [kh, (k+1)h]$,

$$\partial_t \mu_t = \operatorname{div} \left(\left\{ \nabla \ln \frac{\mathrm{d}\mu_t}{\mathrm{d}\pi} + \mathbb{E} [\nabla V(x_{kh}) - \nabla V(x_t) \mid x_t = \cdot] \right\} \mu_t \right).$$

Proof. For $s, t \in \mathbb{R}_+$, let $\mu_{t|s}(\cdot \mid x_s)$ denote the conditional law of x_t given x_s , and let $\mu_{s,t}$ denote the joint law of (x_s, x_t) . Conditioned on x_{kh} , the Fokker-Planck equation for the interpolation (5.1) takes the form

$$\partial_t \mu_{t|kh}(\cdot \mid x_{kh}) = \Delta \mu_{t|kh}(\cdot \mid x_{kh}) + \operatorname{div}(\nabla V(x_{kh}) \mu_{t|kh}(\cdot \mid x_{kh})).$$

Taking the expectation over x_{kh} yields

$$\partial_t \mu_t = \Delta \mu_t + \operatorname{div}(\nabla V \,\mu_t) + \int \operatorname{div}\left(\left\{\nabla V(x_{kh}) - \nabla V(\cdot)\right\} \mu_{t|kh}(\cdot \mid x_{kh})\right) \mathrm{d}\mu_{kh}(x_{kh})$$
$$= \operatorname{div}\left(\nabla \ln \frac{\mathrm{d}\mu_t}{\mathrm{d}\pi} \,\mu_t\right) + \operatorname{div}\left(\left(\int \left\{\nabla V(x_{kh}) - \nabla V(\cdot)\right\} \mathrm{d}\mu_{kh|t}(x_{kh} \mid \cdot)\right) \mu_t(\cdot)\right)$$
$$= \operatorname{div}\left(\nabla \ln \frac{\mathrm{d}\mu_t}{\mathrm{d}\pi} \,\mu_t\right) + \operatorname{div}\left(\left\{\mathbb{E}[\nabla V(x_{kh}) \mid x_t = \cdot] - \nabla V\right\} \mu_t\right).$$

Combining the two terms yields the result.

Proposition 15. Let $(\mu_t)_{t\geq 0}$ denote the law of the interpolation (5.1) of LMC. Also, let $\rho_t := \frac{d\mu_t}{d\pi}$ and $\psi_t := \rho_t^{q-1} / \mathbb{E}_{\pi}(\rho_t^q). \text{ Then, } \bar{for} \ t \in [kh, (k+1)h],$

$$\partial_t \mathcal{R}_q(\mu_t \| \pi) \le -\frac{3}{q} \frac{\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)} + q \,\mathbb{E}[\psi_t(x_t) \|\nabla V(x_t) - \nabla V(x_{kh})\|^2]$$

Proof. For brevity, in this proof we write $\Delta_t := \mathbb{E}[\nabla V(x_{kh}) \mid x_t = \cdot] - \nabla V$. Elementary calculus together with Proposition 14 yields

$$\begin{aligned} \partial_t \mathcal{R}_q(\mu_t \parallel \pi) &= \frac{q}{(q-1) \mathbb{E}_{\pi}(\rho_t^q)} \int \left(\frac{\mathrm{d}\mu_t}{\mathrm{d}\pi}\right)^{q-1} \partial_t \mu_t = \frac{q}{(q-1) \mathbb{E}_{\pi}(\rho_t^q)} \int \rho_t^{q-1} \operatorname{div}(\{\nabla \ln \rho_t + \Delta_t\} \mu_t) \\ &= -\frac{q}{(q-1) \mathbb{E}_{\pi}(\rho_t^q)} \int \langle \nabla(\rho_t^{q-1}), \nabla \ln \rho_t + \Delta_t \rangle \,\mathrm{d}\mu_t \\ &= -\frac{1}{\mathbb{E}_{\pi}(\rho_t^q)} \left\{ \frac{4}{q} \mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2] + 2 \mathbb{E}_{\mu_t}[\rho_t^{q/2-1} \langle \nabla(\rho_t^{q/2}), \Delta_t \rangle] \right\}. \end{aligned}$$

For the second term, Young's inequality implies

$$\begin{aligned} -\mathbb{E}_{\mu_{t}}[\rho_{t}^{q/2-1}\langle\nabla(\rho_{t}^{q/2}),\Delta_{t}\rangle] &= -\iint\rho_{t}^{q/2-1}(x_{t})\langle\nabla(\rho_{t}^{q/2})(x_{t}),\nabla V(x_{kh})-\nabla V(x_{t})\rangle\,\mu_{kh|t}(\mathrm{d}x_{kh}\mid x_{t})\,\mu_{t}(\mathrm{d}x_{t})\\ &= -\iint\rho_{t}^{q/2-1}(x_{t})\langle\nabla(\rho_{t}^{q/2})(x_{t}),\nabla V(x_{kh})-\nabla V(x_{t})\rangle\,\mu_{kh,t}(\mathrm{d}x_{kh},\mathrm{d}x_{t})\\ &= -\mathbb{E}[\rho_{t}^{q/2-1}(x_{t})\langle\nabla(\rho_{t}^{q/2})(x_{t}),\nabla V(x_{kh})-\nabla V(x_{t})\rangle]\\ &\leq \frac{1}{2q}\,\mathbb{E}_{\pi}[\|\nabla(\rho_{t}^{q/2})\|^{2}] + \frac{q}{2}\,\mathbb{E}[\rho_{t}^{q-1}(x_{t})\,\|\nabla V(x_{kh})-\nabla V(x_{t})\|^{2}]\,.\end{aligned}$$

Substituting this into the previous expression completes the proof.

Next, we formulate a lemma to control the expectation of $\|\nabla V\|^2$ under a change of measure. Although this is not strictly necessary for the proof, it streamlines the argument.

Lemma 16. Assume that ∇V is L-Lipschitz. For any probability measure μ , it holds that

$$\mathbb{E}_{\mu}[\|\nabla V\|^{2}] \leq 4 \mathbb{E}_{\pi}[\|\nabla \sqrt{\frac{\mathrm{d}\mu}{\mathrm{d}\pi}}\|^{2}] + 2dL = \mathbb{E}_{\mu}[\|\nabla \ln \frac{\mathrm{d}\mu}{\mathrm{d}\pi}\|^{2}] + 2dL$$

Proof. Let \mathcal{L} denote the infinitesimal generator of the Langevin diffusion (1.1), i.e. $\mathcal{L}f = \langle \nabla V, \nabla f \rangle - \Delta f$. Observe that $\mathcal{L}V = \|\nabla V\|^2 - \Delta V$. Applying integration by parts and recalling that $\mathbb{E}_{\pi} \mathcal{L}f = 0$ for any f,

$$\mathbb{E}_{\mu}[\|\nabla V\|^{2}] = \mathbb{E}_{\mu} \mathcal{L}V + \mathbb{E}_{\mu} \Delta V \leq \int \mathcal{L}V\left(\frac{\mathrm{d}\mu}{\mathrm{d}\pi} - 1\right) \mathrm{d}\pi + dL = \int \left\langle \nabla V, \nabla \frac{\mathrm{d}\mu}{\mathrm{d}\pi} \right\rangle \mathrm{d}\pi + dL \\ = 2 \int \left\langle \sqrt{\frac{\mathrm{d}\mu}{\mathrm{d}\pi}} \nabla V, \nabla \sqrt{\frac{\mathrm{d}\mu}{\mathrm{d}\pi}} \right\rangle \mathrm{d}\pi + dL \leq \frac{1}{2} \mathbb{E}_{\mu}[\|\nabla V\|^{2}] + 2 \mathbb{E}_{\pi}\left[\left\| \nabla \sqrt{\frac{\mathrm{d}\mu}{\mathrm{d}\pi}} \right\|^{2} \right] + dL.$$

Rearrange this inequality to obtain the desired result.

We are now ready to give the proof of Theorem 4. In order to emphasize the main ideas, we first present a proof which incurs a suboptimal dependence on q and explain how to sharpen the argument afterwards.

Proof. [Proof of Theorem 4] As encapsulated in the differential inequality of Proposition 15, the crux of the proof is to control the discretization error term $\mathbb{E}[\psi_t(x_t) \| \nabla V(x_t) - \nabla V(x_{kh}) \|^2]$ for $t \in [kh, (k+1)h]$. Since ∇V is *L*-Lipschitz, we have $\| \nabla V(x_t) - \nabla V(x_{kh}) \|^2 \leq 2L^2 (t-kh)^2 \| \nabla V(x_{kh}) \|^2 + 4L^2 \| B_t - B_{kh} \|^2$. However, it is more convenient to have a bound in terms of $\| \nabla V(x_t) \|$ rather than $\| \nabla V(x_{kh}) \|$, so we use

$$\|\nabla V(x_{kh})\| \le \|\nabla V(x_t)\| + L \|x_t - x_{kh}\| \le \|\nabla V(x_t)\| + hL \|\nabla V(x_{kh})\| + \sqrt{2}L \|B_t - B_{kh}\|.$$

If $h \leq 1/(3L)$, we can rearrange this inequality to obtain $\|\nabla V(x_{kh})\| \leq \frac{3}{2} \|\nabla V(x_t)\| + \frac{3L}{\sqrt{2}} \|B_t - B_{kh}\|$, so

$$\begin{aligned} \|\nabla V(x_t) - \nabla V(x_{kh})\|^2 &\leq 9L^2 \left(t - kh\right)^2 \|\nabla V(x_t)\|^2 + \left(18h^2 L^4 + 4L^2\right) \|B_t - B_{kh}\|^2 \\ &\leq 9L^2 \left(t - kh\right)^2 \|\nabla V(x_t)\|^2 + 6L^2 \|B_t - B_{kh}\|^2 \,. \end{aligned}$$

We will control the two error terms in turn.

For the first error term, applying Lemma 16 to the measure $\psi_t \mu_t$ yields

$$\mathbb{E}_{\psi_t \mu_t}[\|\nabla V\|^2] \le \mathbb{E}_{\mu_t} \left[\psi_t \left\| \nabla \ln \left(\psi_t \frac{\mathrm{d}\mu_t}{\mathrm{d}\pi} \right) \right\|^2 \right] + 2dL = \frac{\mathbb{E}_{\pi} \left[\rho_t^q \|\nabla \ln (\rho_t^q)\|^2 \right]}{\mathbb{E}_{\pi} (\rho_t^q)} + 2dL = \frac{4 \mathbb{E}_{\pi} [\|\nabla (\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi} (\rho_t^q)} + 2dL.$$

Note the calculation

$$\mathbb{E}_{\mu_t} \left[\psi_t \left\| \nabla \ln \left(\psi_t \frac{\mathrm{d}\mu_t}{\mathrm{d}\pi} \right) \right\|^2 \right] = \frac{4 \,\mathbb{E}_{\pi} \left[\left\| \nabla \left(\rho_t^{q/2} \right) \right\|^2 \right]}{\mathbb{E}_{\pi}(\rho_t^q)} \,, \tag{6.2}$$

which will be used below as well.

For the second error term, we apply the Donsker–Varadhan variational principle as in (5.4).

$$\mathbb{E}[\psi_t(x_t) \| B_t - B_{kh} \|^2] \le 2 \mathbb{E}[\| B_t - B_{kh} \|^2] + \frac{2}{c} \left\{ \mathsf{KL}(\widetilde{\mathbb{P}} \| \mathbb{P}) + \ln \mathbb{E} \exp\left(c \left(\| B_t - B_{kh} \| - \mathbb{E} \| B_t - B_{kh} \|\right)^2\right) \right\}$$
$$\le 2d \left(t - kh\right) + \frac{2}{c} \left\{ \mathsf{KL}(\widetilde{\mathbb{P}} \| \mathbb{P}) + \ln \mathbb{E} \exp\left(c \left(\| B_t - B_{kh} \| - \mathbb{E} \| B_t - B_{kh} \|\right)^2\right) \right\},$$

where $\frac{d\tilde{\mathbb{P}}}{d\mathbb{P}} = \psi_t(x_t)$. Due to Gaussian concentration, if we set $c = \frac{1}{8(t-kh)}$, then

$$\mathbb{E}\exp\frac{\left(\|B_t - B_{kh}\| - \mathbb{E}\|B_t - B_{kh}\|\right)^2}{8\left(t - kh\right)} \le 2,$$

c.f. [BLM13, Section 2.3, Theorem 5.5]. Next, using the LSI for π , we compute

$$\mathsf{KL}(\widetilde{\mathbb{P}} \parallel \mathbb{P}) = \mathbb{E}_{\psi_t \mu_t} \ln \psi_t = \mathbb{E}_{\psi_t \mu_t} \ln \frac{\rho_t^{q-1}}{\mathbb{E}_{\mu_t}(\rho_t^{q-1})} = \frac{q-1}{q} \mathbb{E}_{\psi_t \mu_t} \ln \frac{\rho_t^q}{\mathbb{E}_{\mu_t}(\rho_t^{q-1})^{q/(q-1)}}$$
(6.3)

$$= \frac{q-1}{q} \left\{ \mathbb{E}_{\psi_t \mu_t} \ln \frac{\rho_t^q}{\mathbb{E}_{\mu_t}(\rho_t^{q-1})} - \underbrace{\frac{1}{q-1} \ln \mathbb{E}_{\mu_t}(\rho_t^{q-1})}_{\geq 0} \right\} \leq \frac{q-1}{q} \operatorname{\mathsf{KL}}(\psi_t \mu_t \parallel \pi)$$
(6.4)

$$\leq \frac{(q-1)C_{\mathsf{LSI}}}{2q} \mathbb{E}_{\psi_t \mu_t} \left[\left\| \nabla \ln(\psi_t \frac{\mathrm{d}\mu_t}{\mathrm{d}\pi}) \right\|^2 \right] = \frac{2(q-1)C_{\mathsf{LSI}}}{q} \frac{\mathbb{E}_{\pi} \left[\left\| \nabla(\rho_t^{q/2}) \right\|^2 \right]}{\mathbb{E}_{\pi}(\rho_t^q)}, \tag{6.5}$$

where the last equality is (6.2). We have proved

$$\begin{split} \mathbb{E}[\psi_t(x_t) \, \|B_t - B_{kh}\|^2] &\leq 2d \, (t - kh) + \frac{32h \, (q - 1) \, C_{\mathsf{LSI}}}{q} \, \frac{\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)} + (16 \ln 2) \, (t - kh) \\ &\leq 14d \, (t - kh) + 32h C_{\mathsf{LSI}} \, \frac{\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)} \, . \end{split}$$

Finally, collecting together the error terms and applying Proposition 15, we see that

$$\begin{split} \partial_t \mathcal{R}_q(\mu_t \parallel \pi) &\leq -\frac{3}{q} \, \frac{\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)} + 9qL^2 \left(t - kh\right)^2 \left\{ \frac{4 \, \mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)} + 2dL \right\} \\ &+ 6qL^2 \left\{ 14d \left(t - kh\right) + 32hC_{\mathsf{LSI}} \, \frac{\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)} \right\}. \end{split}$$

Assuming for simplicity that $C_{LSI}, L \ge 1$, then $h \le 1/(192q^2C_{LSI}L^2)$ implies

$$\begin{split} \partial_t \mathcal{R}_q(\mu_t \parallel \pi) &\leq -\frac{1}{q} \, \frac{\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)} + 18 dq L^3 \left(t - kh\right)^2 + 84 dq L^2 \left(t - kh\right) \\ &\leq -\frac{1}{2q C_{\mathsf{LSI}}} \, \mathcal{R}_q(\mu_t \parallel \pi) + 18 dq L^3 \left(t - kh\right)^2 + 84 dq L^2 \left(t - kh\right), \end{split}$$

where the last line uses the fact that π satisfies LSI (see [VW19, Lemma 5]). This then implies the differential inequality

$$\begin{aligned} \partial_t \left\{ \exp\left(\frac{t-kh}{2qC_{\mathsf{LSI}}}\right) \mathcal{R}_q(\mu_t \parallel \pi) \right\} &\leq \exp\left(\frac{t-kh}{2qC_{\mathsf{LSI}}}\right) \left\{ 18dqL^3 \left(t-kh\right)^2 + 84dqL^2 \left(t-kh\right) \right\} \\ &\leq 19dqL^3 \left(t-kh\right)^2 + 85dqL^2 \left(t-kh\right). \end{aligned}$$

Integrating this inequality over $t \in [kh, (k+1)h]$ yields the recursion

$$\begin{split} \mathcal{R}_q(\mu_{(k+1)h} \parallel \pi) &\leq \exp\left(-\frac{h}{2qC_{\mathsf{LSI}}}\right) \mathcal{R}_q(\mu_k \parallel \pi) + \frac{19}{3} dh^3 q L^3 + \frac{85}{2} dh^2 q L^2 \\ &\leq \exp\left(-\frac{h}{2qC_{\mathsf{LSI}}}\right) \mathcal{R}_q(\mu_k \parallel \pi) + 43 dh^2 q L^2 \,. \end{split}$$

Iterating this yields

$$\mathcal{R}_q(\mu_{Nh} \parallel \pi) \le \exp\left(-\frac{Nh}{2qC_{\mathsf{LSI}}}\right) \mathcal{R}_q(\mu_0 \parallel \pi) + 86dhq^2 C_{\mathsf{LSI}}L^2,$$

which completes the proof.

We now outline the hypercontractivity argument to improve the dependence on q.

Proposition 17 (Hypercontractivity). Let $(\mu_t)_{t\geq 0}$ denote the law of the interpolation (5.1) of LMC. Also, let $q(t) := 1 + (q_0 - 1) \exp \frac{t}{2C_{\text{LSI}}}$ for $t \geq 0$, and write $\rho_t := \frac{d\mu_t}{d\pi}$, $\psi_t := \rho_t^{q(t)-1} / \mathbb{E}_{\pi}(\rho_t^{q(t)})$. Then, for $t \in [kh, (k+1)h]$,

$$\partial_t \left(\frac{1}{q(t)} \ln \int \rho_t^{q(t)} \, \mathrm{d}\pi \right) \le -\frac{2 \left(q(t) - 1 \right)}{q(t)^2} \frac{\mathbb{E}_{\pi} [\|\nabla(\rho_t^{q(t)/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^{q(t)})} + \left(q(t) - 1 \right) \mathbb{E}[\psi_t(x_t) \|\nabla V(x_t) - \nabla V(x_{kh})\|^2].$$

Proof. Using calculus together with Proposition 14, we compute the derivative in time as in Proposition 15, only now taking into account the additional time-dependent function q. Since the calculation is very similar to Proposition 15, we only record the final result:

$$\begin{aligned} \partial_t \Big(\frac{1}{q(t)} \ln \int \rho_t^{q(t)} \, \mathrm{d}\pi \Big) &= -\frac{1}{\mathbb{E}_\pi(\rho_t^{q(t)})} \int \langle \nabla(\rho_t^{q(t)-1}), \nabla \ln \rho_t + \Delta_t \rangle \, \mathrm{d}\mu_t + \frac{\dot{q}(t) \operatorname{ent}_\pi(\rho_t^{q(t)})}{q(t)^2 \, \mathbb{E}_\pi(\rho_t^{q(t)})} \\ &\leq -\frac{3 \left(q(t)-1\right)}{q(t)^2} \, \frac{\mathbb{E}_\pi[\|\nabla(\rho_t^{q(t)/2})\|^2]}{\mathbb{E}_\pi(\rho_t^{q(t)})} + \left(q(t)-1\right) \mathbb{E}[\psi_t(x_t) \, \|\nabla V(x_t) - \nabla V(x_{kh})\|^2] + \frac{\dot{q}(t) \operatorname{ent}_\pi(\rho_t^{q(t)})}{q(t)^2 \, \mathbb{E}_\pi(\rho_t^{q(t)})} \end{aligned}$$

where \dot{q} is the derivative of q, we write $\Delta_t := \mathbb{E}[\nabla V(x_{kh}) \mid x_t = \cdot] - \nabla V$, and the entropy functional is defined in Section 2. Applying (LSI),

$$\frac{\dot{q}(t)\operatorname{ent}_{\pi}(\rho_t^{q(t)})}{q(t)^2 \,\mathbb{E}_{\pi}(\rho_t^{q(t)})} \le \frac{2\dot{q}(t)C_{\mathsf{LSI}} \,\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q(t)/2})\|^2]}{q(t)^2 \,\mathbb{E}_{\pi}(\rho_t^{q(t)})} = \frac{q(t)-1}{q(t)^2} \,\frac{\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q(t)/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^{q(t)})}$$

where the last equality follows from our choice of q.

Proof. [Proof of Theorem 4] **Initial waiting phase**. Let $\bar{q} \geq 3$. We apply Proposition 17 with $q_0 = 2$ and for $t \leq N_0 h$, where $N_0 = \lceil \frac{2C_{\text{LSI}}}{h} \ln(\bar{q}-1) \rceil$. As in the earlier proof of Theorem 4, we take $h \leq 1/(192q^2C_{\text{LSI}}L^2)$; note that, $\bar{q} \leq q(N_0 h) \leq 2\bar{q}$. Then, the bound on the error term from the previous proof implies

$$\partial_t \left(\frac{1}{q(t)} \ln \int \rho_t^{q(t)} \,\mathrm{d}\pi \right) \le 18 dq(t) L^3 \left(t - kh \right)^2 + 84 dq(t) L^2 \left(t - kh \right).$$

Integrating this over $t \in [kh, (k+1)h]$ yields

$$\frac{1}{q((k+1)h)}\ln\int\rho_{(k+1)h}^{q((k+1)h)}\mathrm{d}\pi - \frac{1}{q(kh)}\ln\int\rho_{kh}^{q(kh)}\mathrm{d}\pi \le 12dh^3\bar{q}L^3 + 84dh^2\bar{q}L^2 \le 85dh^2\bar{q}L^2 \,.$$

Iterating this yields

$$\frac{1}{q(N_0h)}\ln\int\rho_{N_0h}^{q(N_0h)}\,\mathrm{d}\pi - \frac{1}{2}\ln\int\rho_0^2\,\mathrm{d}\pi \le 85dh^2\bar{q}L^2N_0 \le 170dh\bar{q}C_{\mathsf{LSI}}L^2\ln\bar{q}$$

Remainder of the convergence analysis. After shifting the time indices and applying the preceding proof of Theorem 4 with q = 2,

$$\begin{aligned} \Re_{\bar{q}}(\mu_{(N+N_{0})h} \parallel \pi) &\leq \frac{3}{2\bar{q}} \ln \int \rho_{(N+N_{0})h}^{\bar{q}} \,\mathrm{d}\pi \leq \frac{3}{4} \,\Re_{2}(\mu_{Nh} \parallel \pi) + 255 dh \bar{q} C_{\mathsf{LSI}} L^{2} \ln \bar{q} \\ &\leq \frac{3}{4} \exp\left(-\frac{Nh}{4C_{\mathsf{LSI}}}\right) \,\Re_{2}(\mu_{0} \parallel \pi) + 258 dh C_{\mathsf{LSI}} L^{2} + 255 dh \bar{q} C_{\mathsf{LSI}} L^{2} \ln \bar{q} \\ &\leq \exp\left(-\frac{Nh}{4C_{\mathsf{LSI}}}\right) \,\Re_{2}(\mu_{0} \parallel \pi) + 513 dh \bar{q} C_{\mathsf{LSI}} L^{2} \ln \bar{q} \,. \end{aligned}$$

This completes the proof.

6.3 Proof of Theorem 6

To prove Theorem 6, we show that the iterates of LMC satisfy (LSI) with a growing constant.

Lemma 18. Assume that V is convex and ∇V is L-Lipschitz. Let $(\mu_{kh})_{k \in \mathbb{N}}$ denote the law of the iterates of LMC initialized at $\mu_0 = \operatorname{normal}(0, L^{-1}I_d)$ and run with step size $h \leq 1/L$. Then, the LSI constant $C_{\mathsf{LSI}}(\mu_{kh})$ of μ_{kh} satisfies $C_{\mathsf{LSI}}(\mu_{kh}) \leq L + 2kh$.

Proof. With the condition on the step size, $id - h\nabla V$ is a contraction. Using standard facts about the behavior of the log-Sobolev constant under contractions ([BGL14, Proposition 5.4.3]) and convolutions (see e.g. [Cha04, Corollary 3.1]), we obtain

$$C_{\mathsf{LSI}}(\mu_{(k+1)h}) \le C_{\mathsf{LSI}}((\mathrm{id} - h\nabla V)_{\#}\mu_{kh}) + 2h \le C_{\mathsf{LSI}}(\mu_{kh}) + 2h.$$

The result follows via iteration.

We are now ready to prove Theorem 6, which builds upon the proof of Theorem 4.

Proof. [Proof of Theorem 6] Using again the differential inequality of Proposition 15, assuming $h \leq 1/(3L)$, we want to control the error term

$$\mathbb{E}[\psi_t(x_t) \|\nabla V(x_t) - \nabla V(x_{kh})\|^2] \le 9L^2 (t - kh)^2 \mathbb{E}[\psi_t(x_t) \|\nabla V(x_t)\|^2] + 6L^2 \mathbb{E}[\psi_t(x_t) \|B_t - B_{kh}\|^2]$$

see the first proof of Theorem 4. For the first term, an application of Lemma 16 again yields

$$\mathbb{E}[\psi_t(x_t) \| \nabla V(x_t) \|^2] \le \frac{4 \mathbb{E}_{\pi}[\| \nabla (\rho_t^{q/2}) \|^2]}{\mathbb{E}_{\pi}(\rho_t^q)} + 2dL$$

For the second term, the Donsker–Varadhan variational principle (5.4) implies

$$\mathbb{E}[\psi_t(x_t) \| B_t - B_{kh} \|^2] \le 2d (t - kh) + 16 (t - kh) \{ \mathsf{KL}(\tilde{\mathbb{P}} \| \mathbb{P}) + \ln 2 \}.$$

Now comes a key difference in the proof: in Theorem 4, we bounded $\mathsf{KL}(\widetilde{\mathbb{P}} \parallel \mathbb{P}) \leq \frac{q-1}{q} \mathsf{KL}(\psi_t \mu_t \parallel \pi)$ and applied the LSI for π . Here, we instead use $\mathsf{KL}(\widetilde{\mathbb{P}} \parallel \mathbb{P}) = \mathsf{KL}(\psi_t \mu_t \parallel \mu_t)$ and apply the LSI from Lemma 18 which worsens over time. We thus obtain

$$\mathsf{KL}(\widetilde{\mathbb{P}} \,\|\, \mathbb{P}) \leq 2C_{\mathsf{LSI}}(\mu_t) \, \frac{\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)} \leq 2\left(L + 2\left(k+1\right)h\right) \frac{\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)} \,.$$

Let N denote the total number of iterations that we run LMC. Collecting together all of the error terms and using Proposition 15, we see that

$$\begin{aligned} \partial_t \mathcal{R}_q(\mu_t \parallel \pi) &\leq -\frac{3}{q} \, \frac{\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)} + 9qL^2 \, (t-kh)^2 \left\{ \frac{4 \, \mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)} + 2dL \right\} \\ &+ 6qL^2 \left\{ 14d \, (t-kh) + 32h \, (L+2Nh) \, \frac{\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)} \right\}. \end{aligned}$$

Assuming $h \leq \frac{1}{384qL\sqrt{N}} \min\{1, \frac{\sqrt{N}}{qL^2}\}$, it yields

$$\begin{split} \partial_t \mathcal{R}_q(\mu_t \parallel \pi) &\leq -\frac{1}{q} \frac{\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)} + 18dqL^3 \left(t - kh\right)^2 + 84dqL^2 \left(t - kh\right) \\ &\leq -\frac{1}{qC_{\mathsf{PI}}} \left\{1 - \exp(-\mathcal{R}_q(\mu_t \parallel \pi))\right\} + 18dqL^3 \left(t - kh\right)^2 + 84dqL^2 \left(t - kh\right), \end{split}$$

where the last inequality follows from [VW19, Lemma 17].

We now split the analysis into two phases. In the first phase, we consider $t \leq N_0 h$, where N_0 is the largest integer such that $\Re_q(\mu_{N_0h} \parallel \pi) \geq 1$. Then,

$$\partial_t \mathcal{R}_q(\mu_t \parallel \pi) \le -\frac{1}{2qC_{\mathsf{Pl}}} + 18dqL^3 (t-kh)^2 + 84dqL^2 (t-kh)$$

Integration yields

$$\Re_q(\mu_{(k+1)h} \parallel \pi) - \Re_q(\mu_{kh} \parallel \pi) \le -\frac{h}{2qC_{\mathsf{PI}}} + 6dh^3qL^3 + 42dh^2qL^2 \le -\frac{h}{2qC_{\mathsf{PI}}} + 43dh^2qL^2 \,.$$

If $h \leq \frac{1}{172dq^2 C_{\mathsf{Pl}L^2}}$, then we deduce that $\mathcal{R}_q(\mu_{kh} \parallel \pi) \leq \mathcal{R}_q(\mu_0 \parallel \pi) - \frac{kh}{4qC_{\mathsf{Pl}}}$, and hence that the first phase ends after at most $N_0 \leq 4qC_{\mathsf{PI}}\mathcal{R}_q(\mu_0 \parallel \pi)/h$ iterations.

In the second phase, we consider t such that $\Re_q(\mu_t \parallel \pi) \leq 1$. Using $1 - \exp(-x) \geq x/2$ for $x \in [0, 1]$, in this phase we have the inequality

$$\partial_t \mathcal{R}_q(\mu_t \| \pi) \le -\frac{1}{2qC_{\mathsf{PI}}} \,\mathcal{R}_q(\mu_t \| \pi) + 18dqL^3 \left(t - kh\right)^2 + 84dqL^2 \left(t - kh\right).$$

As in the proof of Theorem 4, it implies

$$\begin{aligned} \Re_q(\mu_{Nh} \parallel \pi) &\leq \exp\left(-\frac{(N-N_0-1)h}{2qC_{\mathsf{Pl}}}\right) \Re_q(\mu_{(N_0+1)h} \parallel \pi) + 88dhq^2 C_{\mathsf{Pl}}L^2 \\ &\leq \exp\left(-\frac{(N-N_0-1)h}{2qC_{\mathsf{Pl}}}\right) + 88dhq^2 C_{\mathsf{Pl}}L^2 \,. \end{aligned}$$

To make this at most ε , we take $h \leq \frac{\varepsilon}{176dq^2 C_{\mathsf{Pl}}L^2}$ and $N \geq N_0 + 1 + \frac{2qC_{\mathsf{Pl}}}{h}\ln(2/\varepsilon)$. From Lemma 29, we see that $\mathcal{R}_q(\mu_0 \parallel \pi) = \widetilde{O}(d)$, so that $N = \widetilde{\Theta}(\frac{dqC_{\mathsf{Pl}}}{h})$. Substituting this into our earlier constraints on h, we see that if we take

$$h = \widetilde{\Theta} \Big(\frac{\varepsilon}{dq^2 C_{\mathsf{PI}} L^2} \min \big\{ 1, \frac{1}{q\varepsilon}, \frac{dC_{\mathsf{PI}}}{\varepsilon L} \big\} \Big) \,,$$

then the iteration complexity is

$$N = \widetilde{\Theta} \left(\frac{d^2 q^3 C_{\mathsf{Pl}}^2 L^2}{\varepsilon} \max\{1, q\varepsilon, \frac{\varepsilon L}{dC_{\mathsf{Pl}}}\} \right).$$

This completes the proof.

6.4 Proof of Theorem 7

6.4.1Girsanov's theorem and change of measure

As discussed in Section 5.2, our main technical tool is Girsanov's theorem, stated below in a form which is convenient for our purposes.

Theorem 19 (Girsanov's theorem, [Oks13, Theorem 8.6.8]). Let $(x_t)_{t\geq 0}$, $(b_t^P)_{t\geq 0}$, $(b_t^Q)_{t\geq 0}$ be stochastic processes adapted to the same filtration. Let P_T and Q_T be probability measures on the path space $C([0,T]; \mathbb{R}^d)$ such that $(x_t)_{t>0}$ evolves according to

$$\begin{aligned} \mathrm{d}x_t &= b_t^P \,\mathrm{d}t + \sqrt{2} \,\mathrm{d}B_t^P \qquad \text{under } P_T \,, \\ \mathrm{d}x_t &= b_t^Q \,\mathrm{d}t + \sqrt{2} \,\mathrm{d}B_t^Q \qquad \text{under } Q_T \,, \end{aligned}$$

where B^P is a P_T -Brownian motion and B^Q is a Q_T -Brownian motion. Assume that Novikov's condition

$$\mathbb{E}^{Q_T} \exp\left(\frac{1}{4} \int_0^T \|b_t^P - b_t^Q\|^2 \,\mathrm{d}t\right) < \infty$$

holds. Then,

$$\frac{\mathrm{d}P_T}{\mathrm{d}Q_T} = \exp\left(\frac{1}{\sqrt{2}}\int_0^T \langle b_t^P - b_t^Q, \mathrm{d}B_t^Q \rangle - \frac{1}{4}\int_0^T \|b_t^P - b_t^Q\|^2 \,\mathrm{d}t\right)$$

Remark. In our applications of Girsanov's theorem, although we do not check Novikov's condition explicitly, the validity of Novikov's condition follows from the proof.

Actually, we only need the following corollary.

Corollary 20. For any event \mathcal{E} and $q \geq 1$,

$$\mathbb{E}^{Q_T} \left[\left(\frac{\mathrm{d}P_T}{\mathrm{d}Q_T} \right)^q \mathbb{1}_{\mathcal{E}} \right] \le \sqrt{\mathbb{E} \left[\exp \left(q^2 \int_0^T \| b_t^P - b_t^Q \|^2 \, \mathrm{d}t \right) \mathbb{1}_{\mathcal{E}} \right]}$$

Proof. Applying the Cauchy–Schwarz inequality,

$$\begin{split} \mathbb{E}^{Q_T} \left[\left(\frac{\mathrm{d}P_T}{\mathrm{d}Q_T} \right)^q \mathbb{1}_{\mathcal{E}} \right] &= \mathbb{E}^{Q_T} \left[\exp\left(\frac{q}{\sqrt{2}} \int_0^T \langle b_t^P - b_t^Q, \mathrm{d}B_t^Q \rangle - \frac{q}{4} \int_0^T \|b_t^P - b_t^Q\|^2 \, \mathrm{d}t \right) \, \mathbb{1}_{\mathcal{E}} \right] \\ &\leq \sqrt{\mathbb{E}^{Q_T} \left[\exp\left(\left(q^2 - \frac{q}{2} \right) \int_0^T \|b_t^P - b_t^Q\|^2 \, \mathrm{d}t \right) \, \mathbb{1}_{\mathcal{E}} \right]} \\ & \times \underbrace{\sqrt{\mathbb{E}^{Q_T} \exp\left(\sqrt{2}q \int_0^T \langle b_t^P - b_t^Q, \mathrm{d}B_t^Q \rangle - q^2 \int_0^T \|b_t^P - b_t^Q\|^2 \, \mathrm{d}t \right)}}_{=1} \\ &\leq \sqrt{\mathbb{E}^{Q_T} \left[\exp\left(q^2 \int_0^T \|b_t^P - b_t^Q\|^2 \, \mathrm{d}t \right) \, \mathbb{1}_{\mathcal{E}} \right]}, \end{split}$$

where we used Itô's lemma to show that the underlined term equals 1.

Next, we state and prove the change of measure principle described in Section 5.2. This lemma will be invoked repeatedly in the main arguments.

Lemma 21 (change of measure). Let μ , ν be probability measures and let E be any event. Then,

$$\mu(E) \le \nu(E) + \sqrt{\chi^2(\mu \parallel \nu) \nu(E)}.$$

In particular, if μ and ν are probability measures on \mathbb{R}^d and

$$\nu\{\|\cdot\| \ge R_0 + \eta\} \le C \exp(-c\eta^2) \quad \text{for all } \eta \ge 0,$$

where $C \geq 1$, then

$$\mu\Big\{\|\cdot\| \ge R_0 + \sqrt{\frac{1}{c} \mathcal{R}_2(\mu \| \nu)} + \eta\Big\} \le 2C \exp\left(-\frac{c\eta^2}{2}\right) \quad \text{for all } \eta \ge 0.$$

Proof.

$$\mu(E) = \nu(E) + \int \mathbb{1}_E \left(\frac{\mathrm{d}\mu}{\mathrm{d}\nu} - 1\right) \mathrm{d}\nu \le \nu(E) + \sqrt{\chi^2(\mu \parallel \nu) \nu(E)},$$

where the last inequality is the Cauchy–Schwarz inequality.

For the second statement, applying the change of measure principle to $E = \{ \| \cdot \| \ge R_0 + \bar{\eta} \}$ yields

$$\mu\{\|\cdot\| \ge R_0 + \bar{\eta}\} \le C \exp(-c\bar{\eta}^2) + \sqrt{C} \exp\{-(c\bar{\eta}^2 - \mathcal{R}_2(\mu \| \nu))\}$$

Now take $\bar{\eta} = \sqrt{\frac{1}{c} \mathcal{R}_2(\mu \parallel \nu)} + \eta.$

Finally, we use the following lemma used to remove the conditioning on events.

Lemma 22 ([GT20, Lemma 14]). Let Y > 0 be a random variable. Assume that for all $0 < \delta < 1/2$ there exists an event \mathcal{E}_{δ} with probability at least $1 - \delta$ such that $\mathbb{E}[Y^2 \mid \mathcal{E}_{\delta}] \leq \frac{v}{\delta\xi}$ for some $\xi < 1$. Then, $\mathbb{E}Y \leq 4\sqrt{v}$.

6.4.2 Sub-Gaussianity of the Langevin diffusion

In this section, we introduce a modified distribution: for $\gamma, R > 0$,

$$\hat{\pi} \propto \exp(-\hat{V}), \qquad \hat{V}(x) := V(x) + \frac{\gamma}{2} (||x|| - R)_+^2.$$
 (6.6)

Here, $(||x|| - R)^2_+$ is interpreted as $\max\{||x|| - R, 0\}^2$. Although $\hat{\pi}$ and \hat{V} depend on the parameters γ and R, we will suppress this in the notation for simplicity. Note that by construction, $V = \hat{V}$ on the ball B(0, R) of radius R centered at the origin. Also, the probability measure $\hat{\pi}$ has sub-Gaussian tails. We record this and other useful facts below.

Lemma 23 (properties of the modified potential). Let $\hat{\pi}$ and \hat{V} be defined as in (6.6). Assume that $\nabla V(0) = 0$ and that ∇V satisfies (s-Hölder). Then, the following assertions hold.

1. (sub-Gaussian tail bound) Assume that R is chosen so that $\pi(B(0,R)) \ge 1/2$. Then, for all $\eta \ge 0$,

$$\hat{\pi}\{\|\cdot\| \ge R+\eta\} \le 2\exp\left(-\frac{\gamma\eta^2}{2}\right).$$

2. (gradient growth) The gradient $\nabla \hat{V}$ satisfies

$$\left\|\nabla \hat{V}(x)\right\| \le L + (L + \gamma) \left\|x\right\|.$$

Proof.

1. We can write

$$\int \exp\left(\frac{\gamma}{2} \left(\left\|\cdot\right\| - R\right)_{+}^{2}\right) \mathrm{d}\hat{\pi} = \frac{\int \exp(-V)}{\int \exp(-\hat{V})}$$

Next, we bound

$$\frac{\int \exp(-\hat{V})}{\int \exp(-V)} = \int \exp\left(-\frac{\gamma}{2} \left(\|\cdot\| - R\right)_{+}^{2}\right) \mathrm{d}\pi \ge \pi \left(B(0, R)\right) \ge \frac{1}{2}$$

by our assumption on R. The sub-Gaussian tail bound follows from Markov's inequality via

$$\hat{\pi}\{\|\cdot\|-R \ge \eta\} \le \hat{\pi}\left\{\exp\left(\frac{\gamma}{2}\left(\|\cdot\|-R\right)_{+}^{2}\right) \ge \exp\left(\frac{\gamma\eta^{2}}{2}\right) \le 2\exp\left(-\frac{\gamma\eta^{2}}{2}\right).$$

2. First, note that $\|\nabla V(x)\| \leq L \|x\|^s \leq L (1 + \|x\|)$, using $\nabla V(0) = 0$ and (s-Hölder). Then,

$$\|\nabla \hat{V}(x)\| \le \|\nabla V(x)\| + \gamma (\|x\| - R)_+ \le L + (L + \gamma) \|x\|.$$

Throughout this section, we will assume that $R \ge \max\{1, 2\mathfrak{m}\}$, where $\mathfrak{m} := \int \|\cdot\| d\pi$, so that the sub-Gaussian tail bound in Lemma 23 is valid.

We now begin transferring the sub-Gaussianity of $\hat{\pi}$ to π_t . First, we establish sub-Gaussian tail bounds for $\hat{\pi}_t$, where $(\hat{\pi}_t)_{t>0}$ is the law of the continuous-time Langevin diffusion

$$\mathrm{d}\hat{x}_t = -\nabla \hat{V}(\hat{x}_t) \,\mathrm{d}t + \sqrt{2} \,\mathrm{d}B_t \tag{6.7}$$

with potential \hat{V} , initialized at $\hat{x}_0 \sim \mu_0$.

Lemma 24. Let $(\hat{z}_t)_{t\geq 0}$ denote the modified diffusion (6.6) with potential \hat{V} . Assume that $h \leq 1/(2(L+\gamma))$ and $R \geq \max\{1, 2\mathfrak{m}\}$. Then, for all $\delta \in (0, 1)$, with probability at least $1 - \delta$,

$$\sup_{t \in [0,Nh]} \left\| \hat{z}_t \right\| \le R + 4h\left(L + \gamma\right)R + \sqrt{\frac{8}{\gamma} \mathcal{R}_2(\mu_0 \parallel \hat{\pi})} + \sqrt{\left(96dh + \frac{32}{\gamma}\right) \ln \frac{8N}{\delta}}$$

Proof. Apply the change of measure principle (Lemma 21) together with the sub-Gaussian tail bound in Lemma 23 to see that with probability at least $1 - \delta$,

$$\|\hat{z}_{kh}\| \le R + \sqrt{\frac{2}{\gamma}} \,\mathcal{R}_2(\hat{\pi}_t \parallel \hat{\pi}) + \sqrt{\frac{4}{\gamma} \ln \frac{4}{\delta}} \,.$$

Since the Rényi divergence is decreasing along the diffusion (6.7), then $\mathcal{R}_2(\hat{\pi}_t \parallel \hat{\pi}) \leq \mathcal{R}_2(\mu_0 \parallel \hat{\pi})$. Therefore, a union bound implies that with probability at least $1 - \delta$,

$$\max_{k=0,1,\dots,N-1} \|\hat{z}_{kh}\| \le R + \sqrt{\frac{2}{\gamma} \mathcal{R}_2(\mu_0 \| \hat{\pi})} + \sqrt{\frac{4}{\gamma} \ln \frac{4N}{\delta}}.$$
(6.8)

Next, for $t \leq h$,

$$\begin{aligned} \|\hat{z}_{kh+t} - \hat{z}_{kh}\| &\leq \int_{0}^{t} \|\nabla \hat{V}(\hat{z}_{kh+r})\| \,\mathrm{d}r + \sqrt{2} \,\|B_{kh+t} - B_{kh}\| \\ &\leq hL + (L+\gamma) \int_{0}^{t} \|\hat{z}_{kh+r}\| \,\mathrm{d}r + \sqrt{2} \,\|B_{kh+t} - B_{kh}\| \\ &\leq hL + (L+\gamma) \left(h \,\|\hat{z}_{kh}\| + \int_{0}^{t} \|\hat{z}_{kh+r} - \hat{z}_{kh}\| \,\mathrm{d}r\right) + \sqrt{2} \,\|B_{kh+t} - B_{kh}\| \,, \end{aligned}$$

where we used Lemma 23. Grönwall's inequality implies

$$\sup_{t \in [0,h]} \|\hat{z}_{kh+t} - \hat{z}_{kh}\| \le \left(hL + h\left(L + \gamma\right) \|\hat{z}_{kh}\| + \sqrt{2} \sup_{t \in [0,h]} \|B_{kh+t} - B_{kh}\|\right) \exp\left(h\left(L + \gamma\right)\right)$$
$$\le 2hL + 2h\left(L + \gamma\right) \|\hat{z}_{kh}\| + \sqrt{8} \sup_{t \in [0,h]} \|B_{kh+t} - B_{kh}\|$$

provided $h \leq 1/(2(L+\gamma))$. Now, a union bound shows that

$$\mathbb{P}\left\{\sup_{t\in[0,Nh]} \|\hat{z}_{t}\| \geq \eta\right\} \leq \mathbb{P}\left\{\max_{k=0,1,\dots,N-1} \|\hat{z}_{kh}\| \geq R'\right\} + \sum_{k=0}^{N-1} \mathbb{P}\left\{\sup_{t\in[0,h]} \|\hat{z}_{kh+t} - \hat{z}_{kh}\| \geq \eta - R', \max_{k=0,1,\dots,N-1} \|\hat{z}_{kh}\| \leq R'\right\} \\ \leq \mathbb{P}\left\{\max_{k=0,1,\dots,N-1} \|\hat{z}_{kh}\| \geq R'\right\} + \sum_{k=0}^{N-1} \mathbb{P}\left\{\sqrt{8}\sup_{t\in[0,h]} \|B_{kh+t} - B_{kh}\| \geq \eta - R' - 2hL - 2h(L+\gamma)R'\right\}$$

Taking $R' = R + \sqrt{\frac{2}{\gamma} \mathcal{R}_2(\mu_0 \| \hat{\pi})} + \sqrt{\frac{4}{\gamma} \ln \frac{8N}{\delta}}$ and applying a standard bound on the tail probability of Brownian motion (Lemma 32) shows that with probability at least $1 - \delta$, if $R \ge 1$,

$$\sup_{t \in [0,Nh]} \|\hat{z}_t\| \le R' + 2hL + 2h(L+\gamma)R' + \sqrt{48dh\ln\frac{6N}{\delta}}$$
$$\le R + 4h(L+\gamma)R + \sqrt{\frac{8}{\gamma}\mathcal{R}_2(\mu_0\|\hat{\pi})} + \sqrt{\left(96dh + \frac{32}{\gamma}\right)\ln\frac{8N}{\delta}}$$

after simplifying some terms.

Next, we control the Rényi divergence between π_t and $\hat{\pi}_t$, which ultimately allows us to transfer the sub-Gaussianity to π_t .

Proposition 25. Let T := Nh. Let Q_T , \hat{Q}_T be the measures on path space corresponding to the original diffusion (1.1) and the modified diffusion (6.7) respectively, both initialized at μ_0 . Assume that $h \leq \frac{1}{3} \min\{\frac{1}{L+\gamma}, \frac{T}{d}\}$ and $\gamma \leq \frac{1}{3072T}$. Also, suppose that $R \geq \max\{1, 2\mathfrak{m}\}$ and $\mathcal{R}_2(\mu_0 \parallel \hat{\pi}) \geq 1$. Then,

$$\Re_2(Q_T \parallel \hat{Q}_T) \le \frac{h \left(L + \gamma\right)^2 R^2}{d} + 5 \Re_2(\mu_0 \parallel \hat{\pi}) \ln(8N).$$

Proof. For all $0 < \delta < 1/2$, let \mathcal{E}_{δ} denote the event that the conclusion of Lemma 24 holds, i.e.

$$\mathcal{E}_{\delta} := \left\{ \sup_{t \in [0, Nh]} \| \hat{z}_t \| \le R + 4h \left(L + \gamma \right) R + \sqrt{\frac{8}{\gamma} \mathcal{R}_2(\mu_0 \| \hat{\pi})} + \sqrt{\left(96dh + \frac{32}{\gamma}\right) \ln \frac{8N}{\delta}} \right\}.$$

Then, we know that $\mathbb{P}(\mathcal{E}_{\delta}) \geq 1 - \delta$. Applying Girsanov's theorem in the form of Corollary 20,

$$\begin{aligned} \ln \mathbb{E}\left[\left(\frac{\mathrm{d}Q_T}{\mathrm{d}\hat{Q}_T}\right)^4 \mathbb{1}_{\mathcal{E}_{\delta}}\right] &\leq \frac{1}{2} \ln \mathbb{E}\left[\exp\left(16\int_0^T \|\nabla V(\hat{z}_t) - \nabla \hat{V}(\hat{z}_t)\|^2 \,\mathrm{d}t\right) \mathbb{1}_{\mathcal{E}_{\delta}}\right] \\ &= \frac{1}{2} \ln \mathbb{E}\left[\exp\left(16\gamma^2\int_0^T \left(\|\hat{z}_t\| - R\right)_+^2 \,\mathrm{d}t\right) \mathbb{1}_{\mathcal{E}_{\delta}}\right] \\ &\leq \left(384\gamma^2 h^2 \left(L + \gamma\right)^2 R^2 + 192\gamma \,\mathcal{R}_2(\mu_0 \parallel \hat{\pi}) + (2304\gamma^2 dh + 768\gamma) \ln \frac{8N}{\delta}\right) T.\end{aligned}$$

In order to apply Lemma 22 and remove the conditioning, we require $2304\gamma^2 dhT + 768\gamma T < 1$. This can be achieved by taking $\gamma \leq \frac{1}{3072T}$ and $h \leq \frac{T}{3d}$. Then, Lemma 22 implies

$$\begin{aligned} \mathcal{R}_{2}(Q_{T} \parallel \hat{Q}_{T}) &= \ln \mathbb{E}\left[\left(\frac{\mathrm{d}Q_{T}}{\mathrm{d}\hat{Q}_{T}}\right)^{2}\right] \\ &\leq \ln 8 + \left(192\gamma^{2}h^{2}\left(L+\gamma\right)^{2}R^{2}+96\gamma\,\mathcal{R}_{2}(\mu_{0}\parallel\hat{\pi})+\left(1152\gamma^{2}dh+384\gamma\right)\ln(8N)\right)T \\ &\leq \ln 8 + \frac{h^{2}\left(L+\gamma\right)^{2}R^{2}}{T} + \mathcal{R}_{2}(\mu_{0}\parallel\hat{\pi}) + \frac{dh\ln(8N)}{T} + \ln(8N) \\ &\leq \frac{h\left(L+\gamma\right)^{2}R^{2}}{d} + 5\mathcal{R}_{2}(\mu_{0}\parallel\hat{\pi})\ln(8N)\,, \end{aligned}$$

where we have combined terms using $\mathcal{R}_2(\mu_0 \parallel \hat{\pi}) \geq 1$ to simplify the final bound.

Proposition 26. Let $(z_t)_{t\geq 0}$ denote the continuous-time diffusion (1.1) initialized at μ_0 . Assume that $h \leq \frac{1}{3} \min\{\frac{1}{L+T^{-1}}, \frac{T}{d}\}$ and $\mathfrak{m}, \mathcal{R}_2(\mu_0 \parallel \hat{\pi}) \geq 1$. Then, for all $\delta \in (0, 1/2)$, with probability at least $1 - \delta$,

$$\max_{k=0,1,\dots,N-1} \|z_{kh}\| \le 2\mathfrak{m} + 490\sqrt{T\mathcal{R}_2(\mu_0 \| \hat{\pi})\ln(8N)} + \frac{230h^{1/2}\mathfrak{m}\left(L+T^{-1}\right)T^{1/2}}{d^{1/2}} + 160\sqrt{T\ln\frac{1}{\delta}},$$

where we write T := Nh.

Proof. Recall from the proof of Lemma 24 that with probability at least $1 - \delta$,

$$\max_{k=0,1,...,N-1} \|\hat{z}_{kh}\| \le R + \sqrt{\frac{2}{\gamma} \,\mathcal{R}_2(\mu_0 \parallel \hat{\pi})} + \sqrt{\frac{4}{\gamma} \ln \frac{4N}{\delta}}$$

(see (6.8)). Equivalently,

$$\mathbb{P}\Big\{\max_{k=0,1,...,N-1} \|\hat{z}_{kh}\| \ge R + \sqrt{\frac{2}{\gamma} \,\mathcal{R}_2(\mu_0 \| \hat{\pi})} + \eta \Big\} \le 4N \exp\left(-\frac{\gamma \eta^2}{4}\right).$$

Applying the change of measure principle (Lemma 21) again to Q_T and \hat{Q}_T with the choice $\gamma = \frac{1}{3072T}$ and $R = 2\mathfrak{m}$ reveals that for all $\delta \in (0, 1/2)$, with probability at least $1 - \delta$,

$$\begin{aligned} \max_{k=0,1,...,N-1} \|z_{kh}\| &\leq R + \sqrt{\frac{2}{\gamma}} \,\mathcal{R}_2(\mu_0 \parallel \hat{\pi}) + \sqrt{\frac{4}{\gamma}} \,\mathcal{R}_2(Q_T \parallel \hat{Q}_T) + \sqrt{\frac{8}{\gamma}} \ln \frac{8N}{\delta} \\ &\leq 2\mathfrak{m} + 490\sqrt{T\mathcal{R}_2(\mu_0 \parallel \hat{\pi}) \ln(8N)} + \frac{230h^{1/2}\mathfrak{m} \left(L + T^{-1}\right) T^{1/2}}{d^{1/2}} + 160\sqrt{T \ln \frac{1}{\delta}} \,, \end{aligned}$$
simplifying the bound.

after simplifying the bound.

Bounding the discretization error 6.4.3

In this section, we prove our main bound on the discretization error.

Proposition 27. Let $(\mu_t)_{t>0}$ denote the law of the interpolated process (5.1) and let $(\pi_t)_{t>0}$ denote the law of the continuous-time Langevin diffusion (1.1), both initialized at μ_0 . Assume that ∇V satisfies $\nabla V(0) = 0$ and (s-Hölder). For simplicity, assume that ε^{-1} , $\mathfrak{m}, L, T, \mathfrak{R}_2(\mu_0 \parallel \hat{\pi}) \geq 1$ and $q \geq 2$. If the step size h satisfies

$$h \leq \widetilde{O}_s\left(\frac{\varepsilon^{1/s}}{dq^{1/s}L^{2/s}T^{1/s}}\min\left\{1,\frac{1}{q^{1/s}\varepsilon^{1/s}},\frac{d}{\mathfrak{m}^s},\frac{d}{\mathcal{R}_2(\mu_0 \parallel \hat{\pi})^{s/2}}\right\}\right),$$

where the notation \widetilde{O}_s hides constants depending on s as well as polylogarithmic factors, then for T := Nh,

$$\mathfrak{R}_q(\mu_T \parallel \pi_T) \le \varepsilon \,.$$

Proof. Let P, Q denote the measures on path space corresponding to the interpolated process (5.1) and the continuous-time diffusion (1.1) respectively, both initialized at μ_0 . Also, let

$$G_t := \frac{1}{\sqrt{2}} \int_0^r \langle \nabla V(z_r) - \nabla V(z_{\lfloor r/h \rfloor h}), \mathrm{d}B_r \rangle - \frac{1}{4} \int_0^r \|\nabla V(z_r) - \nabla V(z_{\lfloor r/h \rfloor h})\|^2 \,\mathrm{d}r \,,$$

where $(z_t)_{t\geq 0}$ is the continuous-time diffusion (1.1). By applying Girsanov's theorem (Theorem 19) and Itô's formula, we obtain

$$\mathbb{E}^{Q_T} \left[\left(\frac{\mathrm{d}P_T}{\mathrm{d}Q_T} \right)^q \right] - 1 = \mathbb{E} \exp(qG_T) - 1 = \frac{q \left(q - 1 \right)}{4} \mathbb{E} \int_0^T \exp(qG_t) \left\| \nabla V(z_t) - \nabla V(z_{\lfloor t/h \rfloor h}) \right\|^2 \mathrm{d}t \\ \leq \frac{q^2}{4} \int_0^T \sqrt{\mathbb{E}[\exp(2qG_t)] \mathbb{E}[\left\| \nabla V(z_t) - \nabla V(z_{\lfloor t/h \rfloor h}) \right\|^4]} \, \mathrm{d}t \,.$$

$$(6.9)$$

We bound the two expectations in turn. From Corollary 20 and $(s-H\"{o}lder)$,

$$\mathbb{E}\exp(2qG_t) \le \sqrt{\mathbb{E}\exp\left(4q^2\int_0^t \|\nabla V(z_r) - \nabla V(z_{\lfloor r/h \rfloor h})\|^2 \,\mathrm{d}r\right)} \le \sqrt{\mathbb{E}\exp\left(4q^2L^2\int_0^t \|z_r - z_{\lfloor r/h \rfloor h}\|^{2s} \,\mathrm{d}r\right)}$$

and we control this term by conditioning on the event

$$\mathcal{E}_{\delta,kh} := \left\{ \max_{j=0,1,\dots,k-1} \|z_{jh}\| \le \underbrace{2\mathfrak{m} + 490\sqrt{T\mathcal{R}_2(\mu_0 \| \hat{\pi})\ln(8N)} + \frac{230h^{1/2}\mathfrak{m}\left(L+T^{-1}\right)T^{1/2}}{d^{1/2}} + 160\sqrt{T\ln\frac{1}{\delta}} \right\}}_{=:R_{\delta}}$$

By Proposition 26, we know that $\mathbb{P}(\mathcal{E}_{\delta,kh}) \geq 1 - \delta$.

One step error. We first consider the error over an interval [0, h] conditionally on z_0 , corresponding to a single step of the LMC algorithm. This step requires bounding the exponential moment of $\sup_{t \in [0,h]} ||z_t - z_0||^{2s}$, which is a slightly tedious exercise in stochastic calculus; hence, we postpone the calculation to Appendix B. We quote the final result here: assuming that $h \lesssim 1/(d^s q^2 L^2)^{1/(1+s)}$, Lemma 33 implies

$$\ln \mathbb{E} \exp\left(8q^2 L^2 \int_0^h \|z_t - z_0\|^{2s} \, \mathrm{d}t\right) \le \ln \mathbb{E} \exp\left(8hq^2 L^2 \sup_{t \in [0,h]} \|z_t - z_0\|^{2s}\right)$$
$$\lesssim h^{2s+1}q^2 L^{2s+2} \left(1 + \|z_0\|^{2s^2}\right) + d^s h^{s+1}q^2 L^2$$

Iterating the bound. Let $(\mathcal{F}_t)_{t\geq 0}$ denote the filtration and write $H_t := \int_0^t ||x_r - x_{\lfloor r/h \rfloor h}||^{2s} dr$. By conditioning on $\mathcal{F}_{(N-1)h}$, we can apply the one step bound to derive the bound

$$\begin{split} &\ln \mathbb{E}[\exp\{8q^2L^2H_{Nh}\} \, \mathbb{1}_{\mathcal{E}_{\delta,Nh}}] \\ &\leq \ln \mathbb{E}[\exp\{8q^2L^2H_{(N-1)h} + O(h^{2s+1}q^2L^{2s+2}\left(1 + \|z_{(N-1)h}\|^{2s^2}\right) + d^sh^{s+1}q^2L^2)\} \, \mathbb{1}_{\mathcal{E}_{\delta,Nh}}] \\ &\leq \ln \mathbb{E}[\exp\{8q^2L^2H_{(N-1)h}\} \, \mathbb{1}_{\mathcal{E}_{\delta,(N-1)h}}] + O(h^{2s+1}q^2L^{2s+2}\left(1 + R_{\delta}^{2s^2}\right) + d^sh^{s+1}q^2L^2). \end{split}$$

Iterating this recursion yields

$$\ln \mathbb{E}[\exp\{8q^2L^2H_{Nh}\} \ \mathbb{1}_{\mathcal{E}_{\delta,Nh}}] \lesssim h^{2s}q^2L^{2s+2}R_{\delta}^{2s^2}T + d^sh^sq^2L^2T.$$

where we recall T := Nh. In order to apply Lemma 22 to remove the conditioning, we require the step size to satisfy $h \leq_s 1/(q^{1/s}L^{(s+1)/s}T^{(s^2+1)/(2s)})$, where the notation \leq_s hides a constant depending only on s. Applying the lemma then yields

$$\begin{split} \ln \mathbb{E} \exp\{4q^2 L^2 H_{Nh}\} &\lesssim 1 + d^s h^s q^2 L^2 T \\ &+ h^{2s} q^2 L^{2s+2} T \left(\mathfrak{m} + \sqrt{T \mathcal{R}_2(\mu_0 \parallel \hat{\pi}) \ln(8N)} + \frac{h^{1/2} \mathfrak{m} \left(L + T^{-1}\right) T^{1/2}}{d^{1/2}}\right)^{2s^2}. \end{split}$$

We pause here to give a remark which may clarify the proof. The +1 term above arises for two reasons. First, Lemma 22 requires a bound on the conditional expectation $\mathbb{E}[\exp\{8q^2L^2H_{Nh}\} | \mathcal{E}_{\delta,Nh}]$ whereas we have bounded $\mathbb{E}[\exp\{8q^2L^2H_{Nh}\} | \mathbb{I}_{\mathcal{E}_{\delta,Nh}}]$; passing from the latter to the former incurs a factor of 2 (for $\delta \leq 1/2$). Second, the conclusion of Lemma 22 also contributes a factor of 4. This shows that the application of Lemma 22 inherently adds a constant to the bound on the logarithm of the expectation. This also explains why, at the beginning of this proof in (6.9), we first applied Itô's formula to $\exp(qG_T)$ rather than applying Lemma 22 to $\mathbb{E}\exp(qG_T)$ directly. If we had done the latter, then it would not be possible to make the Rényi divergence $\mathcal{R}_q(P_T \parallel Q_T)$ arbitrarily small with an appropriate choice of h.

We now choose h in order to make $\mathbb{E} \exp\{4q^2L^2H_{Nh}\} \lesssim 1$. This is accomplished by taking

$$h \leq \widetilde{O}_{s} \left(\frac{1}{dq^{2/s} L^{2/s} T^{1/s}} \min\left\{ 1, \frac{d}{\mathfrak{m}^{s}}, \frac{d}{\mathcal{R}_{2}(\mu_{0} \parallel \hat{\pi})^{s/2}}, \frac{d^{(2s+2)/(s+2)}}{\mathfrak{m}^{2s/(s+2)}} \right\} \right).$$
(6.10)

The last term in the minimum can also be eliminated; indeed, if $d^{(2s+2)/(s+2)}/\mathfrak{m}^{2s/(s+2)} \geq 1$, then it is not active in the minimum. Otherwise, raising this expression to the power $(s+2)/2 \geq 1$,

$$\frac{d^{(2s+2)/(s+2)}}{\mathfrak{m}^{2s/(s+2)}} \geq \frac{d^{s+1}}{\mathfrak{m}^s} \geq \frac{d}{\mathfrak{m}^s}$$

Controlling the remaining term. Next, we must bound $\mathbb{E}[\|\nabla V(z_t) - \nabla V(z_{kh})\|^4]$ for $t \in [kh, (k+1)h]$. Although this can also be handled directly via stochastic calculus, we will deduce the bound from Lemma 33 to avoid repeating work. This yields

$$\mathbb{E}[\exp(\lambda \|z_t - z_{kh}\|^{2s}) \mid z_{kh}] \lesssim 1,$$

provided that λ is chosen as

$$\lambda \asymp \frac{1}{d^s h^s} \wedge \frac{1}{h^{2s} L^{2s} \left(1 + \|z_{kh}\|^{2s^2}\right)}$$

In turn, it implies the tail bound

$$\mathbb{P}\{\|z_t - z_{kh}\|^{4s} \ge \eta \mid z_{kh}\} \lesssim \exp(-\lambda\sqrt{\eta})$$

which is integrated to yield

$$\sqrt{\mathbb{E}[\|\nabla V(z_t) - \nabla V(z_{kh})\|^4]} \le L^2 \sqrt{\mathbb{E}[\|z_t - z_{kh}\|^{4s}]} \lesssim L^2 \sqrt{\mathbb{E}[\frac{1}{\lambda^2}]} \lesssim d^s h^s L^2 + h^{2s} L^{2s+2} \sqrt{1 + \mathbb{E}[\|z_{kh}\|^{4s^2}]}.$$

Integrate the sub-Gaussian tail bound from Proposition 26 to obtain

$$\sqrt{1 + \mathbb{E}[\|z_{kh}\|^{4s^2}]} \le \widetilde{O}\left(\mathfrak{m}^{2s^2} + T^{s^2} \mathcal{R}_2(\mu_0 \| \hat{\pi})^{s^2} + \frac{h^{s^2} \mathfrak{m}^{2s^2} L^{2s^2} T^{s^2}}{d^{s^2}}\right).$$

Finishing the proof. Combining together the previous steps, we have proven

$$\mathbb{E}^{Q_T}\left[\left(\frac{\mathrm{d}P_T}{\mathrm{d}Q_T}\right)^q\right] - 1 \le \widetilde{O}\left(d^s h^s q^2 L^2 T + h^{2s} q^2 L^{2s+2} T\left(\mathfrak{m}^{2s^2} + T^{s^2} \mathcal{R}_2(\mu_0 \parallel \hat{\pi})^{s^2} + \frac{h^{s^2} \mathfrak{m}^{2s^2} L^{2s^2} T^{s^2}}{d^{s^2}}\right)\right).$$

The step size condition from (6.10) makes the right-hand side of the above expression ≤ 1 . Taking logarithms,

$$\Re_{q}(P_{T} \parallel Q_{T}) \leq \widetilde{O}\left(d^{s}h^{s}qL^{2}T + h^{2s}qL^{2s+2}T\left(\mathfrak{m}^{2s^{2}} + T^{s^{2}}\mathfrak{R}_{2}(\mu_{0} \parallel \hat{\pi})^{s^{2}} + \frac{h^{s^{2}}\mathfrak{m}^{2s^{2}}L^{2s^{2}}T^{s^{2}}}{d^{s^{2}}}\right)\right)$$

We now choose h to make the Rényi divergence at most ε . By similar reasoning as before, it suffices to take

$$h \leq \widetilde{O}_s \left(\frac{\varepsilon^{1/s}}{dq^{1/s} L^{2/s} T^{1/s}} \min\left\{ 1, \frac{d}{\mathfrak{m}^s}, \frac{d}{\mathcal{R}_2(\mu_0 \parallel \hat{\pi})^{s/2}} \right\} \right).$$

This completes the proof.

6.4.4 Finishing the proof

Finally, we use Theorem 2 on the continuous-time convergence of the Langevin diffusion (1.1) in Rényi divergence under an LO inequality. Together with our discretization bound, it will imply Theorem 7.

Lemma 28. Let $(\pi_t)_{t\geq 0}$ denote the law of the continuous-time diffusion (1.1) initialized at μ_0 , and assume that π satisfies (LO) with order α . If

$$T \ge 68qC_{\mathsf{LO}(\alpha)} \left(\frac{\mathcal{R}_q(\mu_0 \parallel \pi)^{2/\alpha - 1} - 1}{2/\alpha - 1} + \ln \frac{1}{\varepsilon} \right),$$

we obtain $\mathfrak{R}_q(\pi_T \parallel \pi) \leq \varepsilon$.

Proof. Recall from Theorem 2 that

$$\partial_t \mathcal{R}_q(\pi_t \parallel \pi) \le -\frac{1}{68qC_{\mathsf{LO}(\alpha)}} \times \begin{cases} \mathcal{R}_q(\pi_t \parallel \pi)^{2-2/\alpha} , & \text{if } \mathcal{R}_q(\pi_t \parallel \pi) \ge 1 , \\ \mathcal{R}_q(\pi_t \parallel \pi) , & \text{if } \mathcal{R}_q(\pi_t \parallel \pi) \le 1 . \end{cases}$$

In general, if $R : \mathbb{R}_+ \to \mathbb{R}_+$ satisfies the ODE $R' = -CR^{\beta}$ for some $\beta \in (0, 1)$, then a calculation shows that

$$R(t) = \{R(0)^{1-\beta} - C(1-\beta)t\}^{1/(1-\beta)}$$

Thus, if $\alpha < 2$, we obtain $\Re_q(\pi_{T_0} \parallel \pi) \leq 1$ at time

$$T_0 = \frac{68qC_{\mathsf{LO}(\alpha)}}{2/\alpha - 1} \left\{ \Re_q(\mu_0 \parallel \pi)^{2/\alpha - 1} - 1 \right\}.$$

Observe that as $\alpha \to 2$, then $T_0 \to 68q C_{\mathsf{LO}(2)} \ln \mathfrak{R}_q(\mu_0 \parallel \pi)$ which recovers the continuous-time convergence under (LSI). Then, at time $T = T_0 + 68qC_{\mathsf{LO}(\alpha)}\ln(1/\varepsilon)$, we obtain $\mathcal{R}_q(\pi_T \parallel \pi) \leq \varepsilon$.

Proof. [Proof of Theorem 7] Let $(\mu_t)_{t\geq 0}$ denote the law of the interpolated process (5.1) and let $(\pi_t)_{t\geq 0}$ denote the law of the continuous-time Langevin diffusion (1.1), both initialized at μ_0 . By the weak triangle inequality, we can bound

$$\mathfrak{R}_{q}(\mu_{Nh} \parallel \pi) \leq \mathfrak{R}_{2q}(\mu_{Nh} \parallel \pi_{Nh}) + \mathfrak{R}_{2q-1}(\pi_{Nh} \parallel \pi).$$

For T := Nh, we can make the second term at most $\varepsilon/2$ if we choose $T = \widetilde{\Theta}(qC_{\mathsf{LO}(\alpha)} \mathcal{R}_{2q-1}(\mu_0 \| \pi)^{2/\alpha-1})$ by Lemma 28. Then, by Proposition 27, we can make the first term at most $\varepsilon/2$ taking

$$h = \widetilde{\Theta}_{s} \left(\frac{\varepsilon^{1/s}}{dq^{2/s} C_{\mathsf{LO}(\alpha)}^{1/s} L^{2/s} \,\mathfrak{R}_{2q-1}(\mu_{0} \parallel \pi)^{(2/\alpha-1)/s}} \min\left\{ 1, \frac{1}{q^{1/s} \varepsilon^{1/s}}, \frac{d}{\mathfrak{m}^{s}}, \frac{d}{\mathcal{R}_{2}(\mu_{0} \parallel \hat{\pi})^{s/2}} \right\} \right).$$
(6.11)

Then, the total number of iterations of LMC is

$$N = \frac{T}{h} = \widetilde{\Theta}_{s} \Big(\frac{dq^{1+2/s} C_{\mathsf{LO}(\alpha)}^{1+1/s} L^{2/s} \,\mathfrak{R}_{2q-1}(\mu_{0} \parallel \pi)^{(2/\alpha-1)(1+1/s)}}{\varepsilon^{1/s}} \max \Big\{ 1, q^{1/s} \varepsilon^{1/s}, \frac{\mathfrak{m}^{s}}{d}, \frac{\mathfrak{R}_{2}(\mu_{0} \parallel \hat{\pi})^{s/2}}{d} \Big\} \Big).$$

is completes the proof.

This completes the proof.

Proof of Theorems 3 and 8 6.5

We first prove the continuous-time convergence for the Langevin diffusion (1.1) under (MLSI) and $(\alpha_1$ -tail). **Proof.** [Proof of Theorem 3] From [VW19, Lemma 6], we have

$$\partial_t \mathcal{R}_q(\pi_t \parallel \pi) = -\frac{4}{q} \frac{\mathbb{E}_{\pi}[\|\nabla(\rho_t^{q/2})\|^2]}{\mathbb{E}_{\pi}(\rho_t^q)},$$

where $\rho_t := \frac{\mathrm{d}\pi_t}{\mathrm{d}\pi}$. Following the calculations of [VW19, Lemma 5] and applying (MLSI) to $f^2 = \rho_t^q / \mathbb{E}_{\pi}(\rho_t^q)$,

$$\frac{4}{q} \frac{\mathbb{E}_{\pi}[\|\nabla(\rho_{t}^{q/2})\|^{2}]}{\mathbb{E}_{\pi}(\rho_{t}^{q})} \geq \frac{4}{q} \left(\frac{\operatorname{ent}_{\pi}(\rho_{t}^{q})}{2C_{\mathsf{MLSI}} \mathbb{E}_{\pi}(\rho_{t}^{q}) \widetilde{\mathfrak{m}}_{p}((1+\rho_{t}^{q}/\mathbb{E}_{\pi}(\rho_{t}^{q}))\pi)^{\delta(p)}}\right)^{1/(1-\delta(p))}}{qC_{\mathsf{MLSI}}^{2} \widetilde{\mathfrak{m}}_{p}((1+\rho_{t}^{q})\pi)^{\delta(p)/(1-\delta(p))}} \left(\frac{\operatorname{ent}_{\pi}(\rho_{t}^{q})}{\mathbb{E}_{\pi}(\rho_{t}^{q})}\right)^{1/(1-\delta(p))}}{qC_{\mathsf{MLSI}}^{2} \widetilde{\mathfrak{m}}_{p}((1+\rho_{t}^{q})\pi)^{\delta(p)/(1-\delta(p))}} \mathcal{R}_{q}(\pi_{t} \parallel \pi)^{1/(1-\delta(p))}}} \geq \frac{\varepsilon^{\delta(p)/(1-\delta(p))}}{qC_{\mathsf{MLSI}}^{2} \widetilde{\mathfrak{m}}_{p}((1+\rho_{t}^{q})\pi)^{\delta(p)/(1-\delta(p))}} \mathcal{R}_{q}(\pi_{t} \parallel \pi)}$$

as long as $\Re_q(\pi_t \parallel \pi) \geq \varepsilon$. Next, we bound the moments. It is a standard exercise (see [Ver18, Exercise 2.7.3]) to show that $(\alpha_1$ -tail) implies $\widetilde{\mathfrak{m}}_p(\pi)^{1/p} \lesssim \mathfrak{m} + C_{\mathsf{tail}} p^{1/\alpha_1}$. Also, by a slight modification of the change of measure principle (Lemma 21), we can show that $\widetilde{\mathfrak{m}}_p(\rho_t^q \pi)^{1/p} \lesssim \mathfrak{m} + C_{\mathsf{tail}} \mathcal{R}_2(\rho_t^q \pi \parallel \pi)^{1/\alpha_1} + C_{\mathsf{tail}} p^{1/\alpha_1}$, and that $\mathfrak{R}_2(\rho_t^q \pi \parallel \pi) \lesssim q \mathfrak{R}_{2q}(\pi_t \parallel \pi) \leq q \mathfrak{R}_{2q}(\pi_0 \parallel \pi)$. Therefore,

$$\begin{split} \widetilde{\mathfrak{m}}_p \big((1+\rho_t^q)\pi \big)^{\delta(p)/(1-\delta(p))} &\leq \widetilde{\mathfrak{m}}_p(\pi)^{\delta(p)/(1-\delta(p))} + \widetilde{\mathfrak{m}}_p(\rho_t^q\pi)^{\delta(p)/(1-\delta(p))} \\ &\lesssim \left\{ \mathfrak{m} + qC_{\mathsf{tail}} \, \mathcal{R}_{2q}(\pi_0 \parallel \pi)^{1/\alpha_1} + C_{\mathsf{tail}} \, p^{1/\alpha_1} \right\}^{(2-\alpha_0)\,(1+\alpha_0/(p-\alpha_0))}. \end{split}$$

Using the assumption that $\mathfrak{m}, C_{\mathsf{tail}}, \mathfrak{R}_{2q}(\pi_0 \parallel \pi) \leq d^{O(1)}$, if we choose $p \gtrsim \log d$, then

$$\widetilde{\mathfrak{m}}_p \big((1+\rho_t^q)\pi \big)^{\delta(p)/(1-\delta(p))} \lesssim \big\{ \mathfrak{m} + qC_{\mathsf{tail}} \, \mathcal{R}_{2q} (\pi_0 \parallel \pi)^{1/\alpha_1} + C_{\mathsf{tail}} \, p^{1/\alpha_1} \big\}^{2-\alpha_0}$$

Together, it implies that $\mathcal{R}_q(\pi_T \parallel \pi) \leq \varepsilon$ whenever

$$T \ge \Omega \left(\frac{qC_{\mathsf{MLSI}}^2}{\varepsilon^{2\delta(p)}} \left\{ \mathfrak{m} + qC_{\mathsf{tail}} \, \mathcal{R}_{2q}(\pi_0 \parallel \pi)^{1/\alpha_1} + C_{\mathsf{tail}} \, p^{1/\alpha_1} \right\}^{2-\alpha_0} \ln \frac{\mathcal{R}_q(\pi_0 \parallel \pi)}{\varepsilon} \right).$$

Next, choosing $p \simeq \ln(d/\varepsilon)$, we obtain $\varepsilon^{2\delta(p)} \gtrsim 1$, so that

$$T \ge \Omega \left(q C_{\mathsf{MLSI}}^2 \left\{ \mathfrak{m} + q C_{\mathsf{tail}} \, \mathcal{R}_{2q}(\pi_0 \parallel \pi)^{1/\alpha_1} + C_{\mathsf{tail}} \ln(d/\varepsilon)^{1/\alpha_1} \right\}^{2-\alpha_0} \ln \frac{\mathcal{R}_q(\pi_0 \parallel \pi)}{\varepsilon} \right),$$

completing the proof.

With the continuous-time result in hand, it is now straightforward to combine it with the discretization result (Proposition 27) from the previous section.

Proof. [Proof of Theorem 8] Let $(\mu_t)_{t\geq 0}$ denote the law of the interpolated process (5.1) and let $(\pi_t)_{t\geq 0}$ denote the law of the continuous-time Langevin diffusion (1.1), both initialized at μ_0 . By the weak triangle inequality, we can bound

$$\mathfrak{R}_{q}(\mu_{Nh} \parallel \pi) \leq \mathfrak{R}_{2q}(\mu_{Nh} \parallel \pi_{Nh}) + \mathfrak{R}_{2q-1}(\pi_{Nh} \parallel \pi).$$

For T := Nh, we can make the second term at most $\varepsilon/2$ if we choose

$$T = \widetilde{\Theta}(qC_{\mathsf{MLSI}}^2 \left\{ \mathfrak{m} + qC_{\mathsf{tail}} \, \mathfrak{R}_{2q}(\mu_0 \parallel \pi)^{1/\alpha_1} \right\}^{2-\alpha_0})$$

by Theorem 3. Then, by Proposition 27, we can make the first term at most $\varepsilon/2$ taking

$$h = \widetilde{\Theta}_{s} \left(\frac{\varepsilon^{1/s}}{dq^{(4-\alpha_{0})/s} C_{\mathsf{MLSI}}^{2/s} C_{\mathsf{tail}}^{(2-\alpha_{0})/s} L^{2/s} \mathcal{R}_{2q}(\mu_{0} \parallel \pi)^{(2-\alpha_{0})/(\alpha_{1}s)}} \times \min \left\{ 1, \frac{1}{q^{1/s} \varepsilon^{1/s}}, \frac{d}{\mathfrak{m}^{s}}, \frac{d}{\mathcal{R}_{2}(\mu_{0} \parallel \hat{\pi})^{s/2}}, \left(\frac{\mathcal{R}_{2q}(\mu_{0} \parallel \pi)^{1/\alpha_{1}}}{\mathfrak{m}} \right)^{(2-\alpha_{0})/s} \right\} \right).$$
(6.12)

Then, the total number of iterations of LMC is

$$N = \frac{T}{h} = \widetilde{\Theta}_{s} \Big(\frac{dq^{(1+(3-\alpha_{0})(1+s))/s} C_{\mathsf{MLSI}}^{2(1+1/s)} C_{\mathsf{tail}}^{(2-\alpha_{0})(1+1/s)} L^{2/s} \mathcal{R}_{2q}(\mu_{0} \parallel \pi)^{(2-\alpha_{0})(1+1/s)/\alpha_{1}}}{\varepsilon^{1/s}} \times \max \Big\{ 1, q^{1/s} \varepsilon^{1/s}, \frac{\mathfrak{m}^{s}}{d}, \frac{\mathcal{R}_{2}(\mu_{0} \parallel \hat{\pi})^{s/2}}{d}, (\frac{\mathfrak{m}}{\mathcal{R}_{2q}(\mu_{0} \parallel \pi)^{1/\alpha_{1}}})^{(2-\alpha_{0})/s} \Big\} \Big).$$

This completes the proof.

7 Conclusion

In this work, we have given a suite of sampling guarantees for the LMC algorithm which assume only that a functional inequality and a smoothness condition hold. In particular, no such guarantees were previously known beyond the LSI case considered in [VW19]. Consequently, we have resolved the open questions of estimating the Rényi bias of LMC (Corollary 5) and establishing quantitative convergence guarantees for LMC under a Poincaré inequality. Our results and techniques are also of interest because they work with a stronger metric (namely, Rényi divergence) than what is usually considered in the sampling literature.

To conclude, we list a few directions for future research.

• Towards the goal of understanding non-log-concave sampling, it is important to establish sampling guarantees for other algorithms, such as underdamped Langevin Monte Carlo, under suitable functional inequalities. Similarly, it is not clear how sharp our bounds are, and it is worth investigating whether our techniques can be improved.

• As discussed in the introduction, obtaining guarantees in Rényi divergence is useful for applications to differential privacy, as well as for obtaining warm starts for high-accuracy algorithms. Hence, we ask whether Rényi convergence guarantees can be proved for more sophisticated algorithms, such as randomized midpoint discretizations [SL19; HBE20].

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A Initialization

In this section, we give bounds on the Rényi divergence at initialization. We begin with the convex case.

Lemma 29. Suppose that V is convex with V(0) = 0 and $\nabla V(0) = 0$, and assume that ∇V is L-Lipschitz. Let $\mathfrak{m} := \int \|\cdot\| \, d\pi$. Then, for $\mu_0 = \operatorname{normal}(0, L^{-1}I_d)$,

$$\Re_{\infty}(\mu_0 \parallel \pi) \le 2 + \frac{d}{2} \ln(2\mathfrak{m}^2 L)$$

Proof. We can write

$$\sup \frac{\mu_0}{\pi} = \sup_{x \in \mathbb{R}^d} \exp\{V(x) - \frac{L}{2} \|x\|^2\} \frac{\int \exp(-V)}{\int \exp(-V - \delta \|\cdot\|^2)} \frac{\int \exp(-V - \delta \|\cdot\|^2)}{(2\pi/L)^{d/2}}$$
(A.1)

for some $\delta > 0$ to be chosen later. We bound the three ratios in turn. First,

$$\exp\{V(x) - \frac{L}{2} \|x\|^2\} \le 1$$

using $V(x) \leq L ||x||^2/2$. Next,

$$\frac{\int \exp(-V - \delta \, \|\cdot\|^2)}{\int \exp(-V)} = \int \exp(-\delta \, \|\cdot\|^2) \, \mathrm{d}\pi \ge \exp(-4\delta\mathfrak{m}^2) \, \pi\{\|\cdot\|\le 2\mathfrak{m}\} \ge \frac{1}{2} \exp(-4\delta\mathfrak{m}^2)$$

by Markov's inequality. Finally, since $V \ge 0$,

$$\frac{\int \exp(-V - \delta \, \|\cdot\|^2)}{(2\pi/L)^{d/2}} \le \frac{\int \exp(-\delta \, \|\cdot\|^2)}{(2\pi/L)^{d/2}} = \left(\frac{L}{2\delta}\right)^{d/2}.$$

Taking $\delta = 1/(4\mathfrak{m}^2)$, we obtain

$$\mathcal{R}_{\infty}(\mu_0 \parallel \pi) = \ln \sup \frac{\mu_0}{\pi} \le 2 + \frac{d}{2} \ln(2\mathfrak{m}^2 L) \,,$$

which is O(d), up to a logarithmic factor.

We next extend this result to the general case.

Lemma 30. Suppose that $\nabla V(0) = 0$ and that ∇V satisfies (s-Hölder) with constant L > 0. Let $\mathfrak{m} := \int \|\cdot\| d\pi$. Then, for $\mu_0 = \operatorname{normal}(0, (2L)^{-1}I_d)$,

$$\Re_{\infty}(\mu_0 \parallel \pi) \le 2 + L + V(0) - \min V + \frac{d}{2}\ln(4\mathfrak{m}^2 L)$$

Proof. We consider the same decomposition as in (A.1). First, for some $\lambda \in [0, 1]$, we have

$$V(x) - V(0)| = |\langle \nabla V(\lambda x), x \rangle| \le \|\nabla V(\lambda x) - \nabla V(0)\| \, \|x\| \le L \, \|x\|^{1+s}.$$

Therefore,

$$\exp\{V(x) - L \|x\|^2\} \le \exp\{V(x) - V(0) + V(0) - L \|x\|^2\} \le \exp\{V(0) + L \|x\|^{1+s} - L \|x\|^2\} \le \exp\{V(0) + L\}$$

using $t^{1+s} \leq 1 + t^2$ for all $t \geq 0$. Next,

$$\frac{\int \exp(-V - \delta \, \|\cdot\|^2)}{\int \exp(-V)} \ge \frac{1}{2} \exp(-4\delta \mathfrak{m}^2)$$

-	

as before. Lastly,

$$\frac{\int \exp(-V - \delta \|\cdot\|^2)}{(\pi/L)^{d/2}} \le \frac{\exp(-\min V) \int \exp(-\delta \|\cdot\|^2)}{(\pi/L)^{d/2}} = \exp(-\min V) \left(\frac{L}{\delta}\right)^{d/2}$$

This yields

$$\mathcal{R}_{\infty}(\mu_0 \parallel \pi) = \ln \sup \frac{\mu_0}{\pi} \le 2 + L + V(0) - \min V + \frac{d}{2} \ln(4\mathfrak{m}^2 L)$$

with the choice $\delta = 1/(4\mathfrak{m}^2)$.

In order to obtain an initialization with $\mathcal{R}_{\infty}(\mu_0 \parallel \pi) = \tilde{O}(d)$, the lemma requires finding a stationary point $x \in \mathbb{R}^d$ such that the optimality gap $V(x) - \min V$ is not too large, i.e. of order O(d). Since ∇V satisfies (*s*-Hölder), it suffices to find a stationary point which lies in a ball of radius $O(d^{1/(1+s)})$ centered at the minimizer of V. Based on this result, it seems reasonable to assume that the initialization typically satisfies $\mathcal{R}_{\infty}(\mu_0 \parallel \pi) = \tilde{O}(d)$.

Actually, in the setting of Theorem 7, we also need a bound on the Rényi divergence $\mathcal{R}_2(\mu_0 \parallel \hat{\pi})$, where $\hat{\pi}$ is a slight modification of π (see Section 6.4). The following lemma is proven just as in Lemma 30, so the proof is omitted.

Lemma 31. Suppose that $\nabla V(0) = 0$ and that ∇V satisfies (s-Hölder) with constant L > 0. For some $\gamma > 0$, let $\hat{V}(x) := V(x) + \frac{\gamma}{2} (||x|| - R)^2_+$, and let $\hat{\pi} \propto \exp(-\hat{V})$. Also, let $\hat{\mathfrak{m}} := \int ||\cdot|| \, d\hat{\pi}$. Then, for $\mu_0 = \operatorname{normal}(0, (2L + \gamma)^{-1}I_d)$,

$$\Re_{\infty}(\mu_0 \| \hat{\pi}) \le 2 + L + \frac{\gamma}{2} + V(0) - \min V + \frac{d}{2} \ln(4\hat{\mathfrak{m}}^2 L).$$

From the tail bound in Lemma 23, we can deduce an upper bound for $\hat{\mathfrak{m}}$ as follows

$$\begin{split} \hat{\mathfrak{m}} &= \int_{0}^{\infty} \hat{\pi}(\|\cdot\| \ge t) \, \mathrm{d}t \\ &= \int_{0}^{R} \hat{\pi}(\|\cdot\| \ge t) \, \mathrm{d}t + \int_{0}^{\infty} \hat{\pi}(\|\cdot\| \ge R + \eta) \, \mathrm{d}\eta \\ &\leq R + \int_{0}^{\infty} 2 \exp\left(-\frac{\gamma \eta^{2}}{2}\right) \mathrm{d}\eta \\ &\lesssim R + \sqrt{\frac{1}{\gamma}} \,. \end{split}$$

In Proposition 26, we eventually take γ roughly of order $1/d \leq \gamma \leq 1$, and $R \leq \mathfrak{m}$. Hence, if $L + V(0) - \min V = \widetilde{O}(d)$ and $\mathfrak{m} \leq d^{O(1)}$, then $\mathfrak{R}_{\infty}(\mu_0 \parallel \hat{\pi}) = \widetilde{O}(d)$.

B Additional technical lemmas

In this section, we collect together technical lemmas which appear in the proofs of Section 6.4. The proofs rely on standard arguments from stochastic calculus. The first lemma extends [Che+21a, Lemma 23].

Lemma 32. Let $(B_t)_{t>0}$ be a standard Brownian motion in \mathbb{R}^d . Then, if $\lambda \ge 0$ and $h \le 1/(4\lambda)$,

$$\mathbb{E}\exp\left(\lambda \sup_{t\in[0,h]} \|B_t\|^2\right) \le \exp(6dh\lambda)$$

In particular, for all $\eta \geq 0$,

$$\mathbb{P}\left\{\sup_{t\in[0,h]} \|B_t\| \ge \eta\right\} \le 3\exp\left(-\frac{\eta^2}{6dh}\right).$$

Next, for $s \in (0, 1)$ *and* $0 \le \lambda < 1/(12dh)^{s}$ *,*

$$\mathbb{E}\exp\left(\lambda \sup_{t\in[0,h]} \|B_t\|^{2s}\right) \le \exp(144d^s h^s \lambda).$$

Proof. The first statement follows from [Che+21a, Lemma 23], and the second follows from the first by taking $\lambda = 1/(6dh)$ and applying Markov's inequality.

We now turn towards the proof of the third statement. Using the tail bound

$$\mathbb{P}\left\{\sup_{t\in[0,h]} \|B_t\|^{2s} \ge \eta\right\} \le 3\exp\left(-\frac{\eta^{1/s}}{6dh}\right)$$

we now bound $\mathbb{E} \exp(\lambda \sup_{t \in [0,h]} ||B_t||^{2s})$.

$$\mathbb{E}\exp\left(\lambda \sup_{t\in[0,h]} \|B_t\|^{2s}\right) = 1 + \lambda \int_0^\infty \exp(\lambda\eta) \mathbb{P}\left\{\sup_{t\in[0,h]} \|B_t\|^{2s} \ge \eta\right\} \mathrm{d}\eta \le 1 + 3\lambda \int_0^\infty \exp\left(\lambda\eta - \frac{\eta^{1/s}}{6dh}\right) \mathrm{d}\eta.$$

Split the integral into whether or not $\eta \geq (12dh\lambda)^{s/(1-s)}$. For the first part,

$$\lambda \int_{0}^{(12dh\lambda)^{s/(1-s)}} \exp(\lambda\eta) \,\mathrm{d}\eta \le (12dh)^{s/(1-s)} \lambda^{1/(1-s)} \exp\{(12dh)^{s/(1-s)} \lambda^{1/(1-s)}\} \le 3 (12dh)^{s/(1-s)} \lambda^{1/(1-s)}$$

provided that $\lambda \leq 1/(12dh)^s$. For the second part, using the change of variables $\tau = \eta^{1/s}/(12dh)$,

$$\begin{split} \lambda \int_{(12dh\lambda)^{s/(1-s)}}^{\infty} \exp\left(\lambda\eta - \frac{\eta^{1/s}}{6dh}\right) \mathrm{d}\eta &\leq \lambda \int_{(12dh\lambda)^{s/(1-s)}}^{\infty} \exp\left(-\frac{\eta^{1/s}}{12dh}\right) \mathrm{d}\eta \leq (12dh)^s s \lambda \int_0^{\infty} \frac{\exp(-\tau)}{\tau^{1-s}} \,\mathrm{d}\tau \\ &= (12dh)^s s \lambda \Gamma(s) = (12dh)^s \lambda \Gamma(1+s) \leq (12dh)^s \lambda \,, \end{split}$$

where we used Gautschi's inequality to obtain $\Gamma(1+s) \leq 1$. We have therefore proven

$$\mathbb{E} \exp\left(\lambda \sup_{t \in [0,h]} \|B_t\|^{2s}\right) \le 1 + 9 \left(12dh\right)^{s/(1-s)} \lambda^{1/(1-s)} + 3 \left(12dh\right)^s \lambda \le 1 + 144d^s h^s \lambda,$$

which implies the result.

The following lemma extends [Che+21a, Lemma 24].

Lemma 33. Let $(z_t)_{t\geq 0}$ denote the continuous-time Langevin diffusion (1.1) started at z_0 , and assume that the gradient ∇V of the potential satisfies $\nabla V(0) = 0$ and (s-Hölder). Also, assume that $h \leq 1/(6L)$ and $\lambda \leq 1/(96d^sh^s)$. Then,

$$\mathbb{E} \exp\left(\lambda \sup_{t \in [0,h]} \|z_t - z_0\|^{2s}\right) \le \exp\{8h^{2s}L^{2s}\left(1 + \|z_0\|^{2s^2}\right)\lambda + 1152d^sh^s\lambda\}.$$

Proof. Let $f(t) := \sup_{r \in [0,t]} ||z_r - z_0||^2$. Then, for $0 \le t \le h$, since $||\nabla V(x)|| \le L ||x||^s$,

$$\begin{aligned} \|z_t - z_0\|^2 &= \left\| -\int_0^t \nabla V(z_r) \,\mathrm{d}r + \sqrt{2} \,B_t \right\|^2 \le 2t \int_0^t \|\nabla V(z_r)\|^2 \,\mathrm{d}r + 4 \,\|B_t\|^2 \\ &\le 4t \int_0^t \|\nabla V(z_r) - \nabla V(z_0)\|^2 \,\mathrm{d}r + 4t^2 \,\|\nabla V(z_0)\|^2 + 4 \,\|B_t\|^2 \\ &\le 4t L^2 \int_0^t \|z_r - z_0\|^{2s} \,\mathrm{d}r + 4t^2 L^2 \,\|z_0\|^{2s} + 4 \,\|B_t\|^2 \\ &\le 4t L^2 \int_0^t \|z_r - z_0\|^2 \,\mathrm{d}r + 4t^2 L^2 \,(1 + \|z_0\|^{2s}) + 4 \,\|B_t\|^2 \,, \end{aligned}$$

which yields

$$f(t) \le 4t^2 L^2 \left(1 + \|z_0\|^{2s}\right) + 4 \sup_{r \in [0,t]} \|B_r\|^2 + 4t L^2 \int_0^t f(r) \, \mathrm{d}r \, .$$

Grönwall's inequality yields

$$f(h) \le \left(4h^2 L^2 \left(1 + \|z_0\|^{2s}\right) + 4 \sup_{r \in [0,h]} \|B_r\|^2\right) \exp(2h^2 L^2) \le 8h^2 L^2 \left(1 + \|z_0\|^{2s}\right) + 8 \sup_{r \in [0,h]} \|B_r\|^2$$

using $h \leq 1/(6L)$. It also yields

$$\sup_{t \in [0,h]} \|z_t - z_0\|^{2s} \le 8h^{2s}L^{2s} (1 + \|z_0\|^{2s^2}) + 8 \sup_{r \in [0,h]} \|B_r\|^{2s}.$$

The result now follows from Lemma 32.

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