New results on relative entropy production, time reversal, and optimal control of time-inhomogeneous nonequilibrium diffusion processes

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Abstract

This paper studies time-inhomogeneous nonequilibrium diffusion processes, including both Brownian dynamics and Langevin dynamics. We derive upper bounds of the relative entropy production of the time-inhomogeneous process with respect to the transient invariant probability measures. We also study the time reversal of the reverse process in Crooks’ fluctuation theorem. We show that the time reversal of the reverse process coincides with the optimally controlled forward process that leads to zero variance importance sampling estimator based on Jarzynski’s equality.

Keywords time-inhomogeneous process, fluctuation theorem, optimal control, relative entropy estimate, time reversal

1 Introduction

In recent years, there has been growing research interest in understanding time-inhomogeneous systems in various research fields, such as in nonequilibrium physics [8, 48, 43], molecular dynamics [15, 9], complex networks [19, 23], and biology [51, 25]. In nonequilibrium physics, in particular, one theoretical focus in the study of time-inhomogeneous systems has been the nonequilibrium work relations, which concern dynamical processes that are out of equilibrium under nonequilibrium driving forces. Notably, Jarzynski’s equality relates the free energy differences between two equilibrium states to the nonequilibrium work needed to drive the system from one state to another within finite time [27, 29], while fluctuation relations reveal the connections between the forward process and the corresponding reverse nonequilibrium process [7, 8, 33, 48, 21].

In this paper we study time-inhomogeneous nonequilibrium diffusion processes, including both Brownian dynamics (or overdamped Langevin dynamics) and Langevin dynamics [50], which are widely used in modeling the dynamics of particle systems in different application areas. Our aim is to provide mathematical analysis on several topics of time-inhomogeneous processes, namely the relative entropy, time reversal, as well as a type of optimal control problem that is related to Jarzynski’s equality [21]. Since the results for Brownian dynamics and Langevin dynamics are similar, in the following we summarize our results for Brownian dynamics and then discuss the differences in the case of Langevin dynamics.

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Given smooth functions $J : \mathbb{R}^n \times [0, T] \to \mathbb{R}^n$, $V : \mathbb{R}^n \times [0, T] \to \mathbb{R}$ and $\sigma : \mathbb{R}^n \times [0, T] \to \mathbb{R}^{n \times m}$, where $T > 0$ and $m \geq n$, we consider the Brownian dynamics (forward process) on $\mathbb{R}^n$ which satisfies the stochastic differential equation (SDE)

$$dx(s) = b(x(s), s) \, ds + \sqrt{2\beta^{-1}} \sigma(x(s), s) \, dw(s),$$

$$= \left( -J - \gamma \nabla V + \frac{1}{\beta} \nabla \cdot \gamma \right)(x(s), s) \, ds + \sqrt{2\beta^{-1}} \sigma(x(s), s) \, dw(s), \quad s \in [0, T],$$

where $\beta > 0$, $\gamma = \sigma \sigma^T$, $b = J - \gamma \nabla V + \frac{1}{\beta} \nabla \cdot \gamma$, $\nabla \cdot \gamma : \mathbb{R}^n \times [0, T] \to \mathbb{R}^n$ denotes the vector whose components are $\left( \nabla \cdot \gamma \right)_i = \sum_{j=1}^{n} \frac{\partial \gamma_{ij}}{\partial x_j}$ for $1 \leq i \leq n$, and $w(s)$ is an $m$-dimensional Brownian motion. Note that both the drift $b$ and the diffusion coefficient $\sigma$ are time-dependent. The matrix-valued function $\gamma : \mathbb{R}^n \times [0, T] \to \mathbb{R}^{n \times n}$ is assumed to be uniformly positive definite. For each $s \in [0, T]$, we denote by $\nu_s$ the probability distribution of $x(s) \in \mathbb{R}^n$, and we make the assumption that the process (for fixed $s$)

$$dx(t) = b(x(t), s) \, dt + \sqrt{2\beta^{-1}} \sigma(x(t), s) \, dw(t), \quad t \geq 0$$

is ergodic with respect to a unique invariant measure $\nu_s^\infty$, which will be called the transient invariant measure of (1) at time $s$.

Our first result for Brownian dynamics (2) (Theorem 1) concerns upper bound estimate for the relative entropy of $\nu_s$ with respect to $\nu_s^\infty$ as a function of $s$, defined as

$$\mathcal{R}(s) = D_{KL}(\nu_s | \nu_s^\infty) = \int_{\mathbb{R}^n} \frac{d\nu_s}{d\nu_s^\infty} \ln \frac{d\nu_s}{d\nu_s^\infty} \, d\nu_s,$$

where $D_{KL}(\cdot | \cdot)$ denotes the Kullback-Leibler divergence between two probability measures. The derivation of the upper bound of $\mathcal{R}(s)$ relies on the formula of the relative entropy production rate (Proposition 2):

$$\frac{d\mathcal{R}(s)}{ds} = -\beta \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} \, d\nu_s^\infty + \beta \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} \, d\nu_s - \frac{1}{\beta} \int_{\mathbb{R}^n} \sigma^T \nabla \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right)^2 \, d\nu_s,$$

as well as the logarithmic Sobolev inequality of $\nu_s^\infty$. We point out that (1) generalizes the known results in literature for time-homogeneous processes [17, 44] with respect to a fixed invariant measure to time-inhomogeneous processes (1) with respect to the transient invariant measures $\nu_s^\infty$.

Our second result for Brownian dynamics (3) (Theorem 2) is about the connection between the time reversal $x^{R,-}(s) = x^R(T-s)$ of the so-called reverse process $x^R(s)$ of (1), which satisfies [8, 29]

$$dx^R(s) = \left( -J - \gamma \nabla V + \frac{1}{\beta} \nabla \cdot \gamma \right)(x^R(s), T-s) \, ds + \sqrt{2\beta^{-1}} \sigma(x^R(s), T-s) \, dw(s),$$

for $s \in [0, T]$, and the stochastic optimal control problem [16]

$$\min_{u_s} \mathbb{E} \left( \int_0^T \frac{\partial V}{\partial s}(x^n(s), s) \, ds + \frac{1}{4} \int_0^T |u_s|^2 \, ds \mid x^n(0) = x \right), \quad x \in \mathbb{R}^n.$$
of the controlled forward process

\[ dx^n(s) = b(x^n(s), s) \, ds + \sigma(x^n(s), s) \, u_s \, ds + \sqrt{2\beta^{-1}}\sigma(x^n(s), s) \, dw(s), \]  

where \( u_s \in \mathbb{R}^m \), \( 0 \leq s \leq T \), is the feedback control force. While (6) involves initial conditions, there is a function \( u^* : \mathbb{R}^n \times [0, T] \to \mathbb{R}^m \), such that \( u^*_s = u^*(x, s) \) is the optimal control of the problem (6)–(7), when the state of the process at time \( s \) is \( x \in \mathbb{R}^n \). We show that the time reversal \( x^{R, -}(s) \) coincides with the optimally controlled process \( x^{u^*}(s) \), i.e. they have the same law on the path space \( C([0, T], \mathbb{R}^n) \), provided that both processes \( x^{R, -}(s) \) and \( x^{u^*}(s) \) start from the same initial distribution. This result may be interesting as it relates processes in two different contexts. In fact, the time reversal \( x^{R, -}(s) \) is the process considered in the celebrated Crooks’ fluctuation theorem [7, 8], while the optimally controlled process \( x^{u^*}(s) \), as well as the optimal control problem (6)–(7), arises in the study of optimal Monte Carlo estimators based on Jarzynski’s inequality [21].

Similar results are obtained for time-inhomogeneous Langevin dynamics, namely the relative entropy estimate (Theorem 4) as well as the connection between the time reversal of reverse process and certain optimally controlled forward process (Theorem 4). In the following, we briefly discuss the main difference in estimating relative entropy in the case of Langevin dynamics. Consider the time-inhomogeneous Langevin dynamics

\[
\begin{align*}
dq(s) &= p(s) \, ds \\
dp(s) &= -\nabla_q V(q(s), s) \, ds - \xi p(s) \, ds + \sqrt{2\beta^{-1}}\xi \, dw(s)
\end{align*}
\]  

with the corresponding Hamiltonian \( H(q, p, s) = V(q, s) + |p|^2/2 \) for \( q, p \in \mathbb{R}^n \), where \( \xi > 0 \) is a positive constant and \( \nabla_q \) denotes the gradient with respect to \( q \). Denote by \( \pi_s \) the probability measure of \( (q(s), p(s)) \in \mathbb{R}^n \times \mathbb{R}^n \) at time \( s \) and by \( \nu_{\pi_s}^\infty \) the transient invariant measure at time \( s \) (similarly defined as \( \nu_{\pi_s}^\infty \) in the Brownian dynamics above). Due to the hypoelliptic structure of (8), extra difficulties arise when estimating the upper bound of the relative entropy, which is defined as

\[ R_{\text{Lan}}(s) = D_{KL}(\pi_s \| \pi_{\pi_s}^\infty) = \int_{\mathbb{R}^n \times \mathbb{R}^n} \ln \frac{d\pi_{\pi_s}^\infty}{d\pi_s} \, d\pi_{\pi_s}^\infty. \]  

In fact, we will derive the formula of the relative entropy production rate (Proposition 4):

\[ \frac{dR_{\text{Lan}}(s)}{ds} = -\beta \int_{\mathbb{R}^n \times \mathbb{R}^n} \frac{\partial H}{\partial s} \, d\pi_{\pi_s}^\infty + \beta \int_{\mathbb{R}^n \times \mathbb{R}^n} \frac{\partial H}{\partial s} \, d\pi_s - \frac{\xi}{\beta} \int_{\mathbb{R}^n \times \mathbb{R}^n} \left| \nabla_p \left( \ln \frac{d\pi_s}{d\pi_{\pi_s}^\infty} \right) \right|^2 \, d\pi_s. \]  

However, different from (4) which contains the full gradient, only the partial gradient \( \nabla_p \) with respect to the momentum \( p \) appears in the last integral of (10). This brings obstacles when we estimate the upper bound of \( R_{\text{Lan}}(s) \) by applying logarithmic Sobolev inequality of \( \pi_{\pi_s}^\infty \). To overcome this difficulty, we will need the hypocoercivity theory developed in [53] and estimate \( R_{\text{Lan}}(s) \) by considering a modified functional.

Let us next mention several previous work in which related topics were considered. Note that relative entropy (estimate) has been widely considered in the study of partial differential equations [5, 53], functional inequalities [30, 52], gradient flows [1],
coarse-graining of stochastic processes \cite{31,12} in mathematics community, as well as in the study of nonequilibrium thermodynamics in physics community \cite{7,17,44}. The convergence of Langevin dynamics towards equilibrium has been studied using hypocoercivity theory \cite{53,11,10} (see \cite{38,2} for the approach using Lyapunov techniques, and \cite{14} for coupling approach). In particular, the weak convergence of Langevin dynamics in the long-time small-friction limit was studied in \cite{20}. The asymptotics in the overdamped limit as well as numerical splitting schemes based on Langevin dynamics has been analyzed in \cite{35,32}. The recent work \cite{24} has considered the convergence rate of nonequilibrium Langevin dynamics under external forcing. In other directions, we note that the reverse process has drawn considerable attentions in nonequilibrium thermodynamics \cite{7,6,29}. The optimal control problem \cite{21} related to Jarzynski’s equality has been considered in \cite{21}. Backward SDEs and controlled dynamics are also related to the so-called Schrödinger bridge problem, which has been used in the study of data assimilation \cite{45} and the development of new Monte Carlo schemes \cite{3}. Lastly, the time reversal of a diffusion process has been studied in \cite{22}.

The current paper has the following novelties. First, concerning the results on the upper bound of relative entropy, while this topic has been extensively studied, it seems that time-inhomogeneous processes as well as the associated relative entropy with respect to transient invariant probability measures are less studied in literature. Let us also emphasize that, different from the previous work \cite{20,24} where an in-depth analysis on the convergence rate of the processes in terms of certain parameters were carried out, the aim of the current paper is to derive the equations of the relative entropy production rate in time-inhomogeneous case (see \cite{11} and \cite{10}) and demonstrate their usefulness in analyzing properties of the corresponding processes. Second, concerning the results on the connection between the time reversal of the reverse process and the optimally controlled process, the results are new to the best of the author’s knowledge. At the technical level, in particular, the nonequilibrium thermodynamics community seems less aware of the SDE of the time reversal process obtained in mathematics community \cite{22}, and the time reversal is typically studied by considering time discretization. In this paper, we make use of the SDE of the time reversal process obtained in \cite{22} and hopefully show its usefulness to different communities.

The paper is organized as follows. In Section 2 we study time-inhomogeneous Brownian dynamics and obtain the aforementioned results. The Langevin dynamics and the corresponding results are studied in Section 3. In Appendix A we present concise derivations of the fluctuation relations for both Brownian dynamics and Langevin dynamics. The optimal control problems and their relations to Jarzynski’s equality are discussed in Appendix B. Finally, the proof of relative entropy estimate for Langevin dynamics is given in Appendix C.

Before concluding this section, we introduce notations and recall several useful inequalities related to probability measures. We denote by $I_n \in \mathbb{R}^{n \times n}$ the identity matrix of order $n$. For a vector $v \in \mathbb{R}^n$, $|v|$ is the Euclidean norm of $v$. Let $A \in \mathbb{R}^{n \times n}$ be an $n$ by $n$ matrix. $\|A\|_2$ denotes the 2-matrix norm of $A$, such that $|Av| \leq \|A\|_2 |v|$ for all $v \in \mathbb{R}^n$. The operator $A : \nabla^2$ denotes the contraction between $A$ and the Hessian operator $\nabla^2$, i.e., $A : \nabla^2 f = \sum_{1 \leq i,j \leq n} A_{ij} \frac{\partial^2 f}{\partial x_i \partial x_j}$, for a $C^2$-smooth test function $f : \mathbb{R}^n \to \mathbb{R}$. We denote by $x(s)$, or, respectively, $(q(s), p(s))$, either the process on $[0, T]$ or the state of the process at a fixed time $s$, depending on the concrete context. $E$ is
the mathematical expectation (or path ensemble average) on the path space. Given a function \( f : \mathbb{R}^n \times [0, T] \to \mathbb{R} \) and time \( t \in [0, T] \), \( f(\cdot, t) \) is a function mapping from \( \mathbb{R}^n \) to \( \mathbb{R} \). We assume that a matrix-valued function \( \sigma : \mathbb{R}^n \times [0, T] \to \mathbb{R}^{n \times m} \) is given such that \( \gamma(x, s) = (\sigma \sigma^T)(x, s) \) is uniformly positive definite matrix, for all \( (x, s) \in \mathbb{R}^n \times [0, T] \). Precisely, we assume that there exists a positive constant \( \gamma^- > 0 \), such that (uniform ellipticity condition)

\[
v^T \gamma(x, s)v \geq \gamma^- |v|^2, \quad \forall \, v, x \in \mathbb{R}^n \text{ and } \forall \, s \in [0, T].
\]

Note that this requires in particular that \( m \geq n \) and \( \sigma \) has full rank \( n \). For the matrix-valued function \( \sigma : \mathbb{R}^n \times [0, T] \to \mathbb{R}^{n \times n} \) whose entries are \( \sigma_{ij} \), where \( 1 \leq i, j \leq n \), we denote by \( \nabla \cdot \sigma \) the function mapping from \( \mathbb{R}^n \times [0, T] \) to \( \mathbb{R}^n \), whose \( i \)th components are \( (\nabla \cdot \sigma)_i = \sum_{j=1}^{n} \frac{\partial \sigma_{ij}}{\partial x_j} \), where \( 1 \leq i \leq n \). Finally, let us recall several definitions and inequalities related to probability measures [52]. Given two probability measures \( \mu \) and \( \nu \) on \( \mathbb{R}^d, \, d \geq 1 \), their total variation is

\[
\|\mu - \nu\|_{TV} = 2 \inf P[X \neq Y]
\]

where the infimum is over all couplings \((X, Y)\) of \((\mu, \nu)\). For all bounded measurable functions \( f \in L^\infty(\mathbb{R}^d) \) with uniform bound \( |f|_\infty \), it holds

\[
\left| \int_{\mathbb{R}^d} f \, d\mu - \int_{\mathbb{R}^d} f \, d\nu \right| \leq |f|_\infty \|\mu - \nu\|_{TV}.
\]

We write \( \nu \ll \mu \) whenever \( \nu \) is absolutely continuous with respect to \( \mu \). The relative entropy of \( \nu \) with respect to \( \mu \) (also called the Kullback-Leibler divergence from \( \mu \) to \( \nu \)), where \( \nu \ll \mu \), is

\[
D_{KL}(\nu \mid \mu) = \int_{\mathbb{R}^d} \ln \frac{d\nu}{d\mu} \, d\nu.
\]

Csiszár-Kullback-Pinsker inequality [52, Remark 22.12] states

\[
\|\nu - \mu\|_{TV} \leq \sqrt{2D_{KL}(\nu \mid \mu)}.
\]

We also introduce the Fisher information

\[
\mathcal{I}(\nu \mid \mu) = \int_{\mathbb{R}^d} \left( \frac{d\nu}{d\mu} \right)^2 \, d\nu.
\]

The probability measure \( \mu \) satisfies the logarithmic Sobolev inequality (LSI) with constant \( \kappa > 0 \) (see [52, Definition 21.1] and [30, Chapter 5]), if

\[
D_{KL}(\nu \mid \mu) \leq \frac{1}{2\kappa} \mathcal{I}(\nu \mid \mu),
\]

for all probability measures \( \nu \) such that \( \nu \ll \mu \) and \( \mathcal{I}(\nu \mid \mu) \) is finite. Denote by \( W_1, W_2 \) the \( L^1 \) and \( L^2 \) Wasserstein distances (see [52, Definition 6.1] and [1, Chapter 7]), respectively. The Wasserstein distances satisfy that

\[
W_1(\nu, \mu) \leq W_2(\nu, \mu),
\]

for all probability measures \( \nu \) such that \( \nu \ll \mu \) and \( \mathcal{I}(\nu \mid \mu) \) is finite.
for all probability measures \( \nu, \mu \), whenever \( W_2(\nu, \mu) < \infty \). Furthermore, for all Lipschitz functions \( f \) on \( \mathbb{R}^d \) with Lipschitz constant \( \|f\|_{\text{Lip}} \), we have

\[
\left| \int_{\mathbb{R}^d} f \, d\mu - \int_{\mathbb{R}^d} f \, d\nu \right| \leq \|f\|_{\text{Lip}} \, W_1(\nu, \mu) .
\]  

(19)

When \( \mu \) satisfies LSI with constant \( \kappa > 0 \), it is known that \( \mu \) also satisfies the Talagrand inequality with the same constant \( \kappa \) \[41\], i.e., for any probability measure \( \nu \ll \mu \),

\[
W_2(\nu, \mu) \leq \sqrt{\frac{2}{\kappa} D_{KL}(\nu \| \mu)} .
\]  

(20)

2 Time-inhomogeneous Brownian dynamics

In this section, we consider time-inhomogeneous Brownian dynamics in state space \( \mathbb{R}^n \). After introducing the forward and reverse processes as well as related quantities in Section 2.1, we derive the production rate formula and the upper bounds of relative entropy in Section 2.2. Finally, in Section 2.3, we establish the connection between the time reversal of reverse process and certain optimally controlled forward process.

2.1 Forward and reverse processes

Let \( V : \mathbb{R}^n \times [0, T] \to \mathbb{R} \) be a time-dependent smooth potential function in the time interval \( [0, T] \), where \( T > 0 \). The vector field \( J : \mathbb{R}^n \times [0, T] \to \mathbb{R}^n \) satisfies

\[
\text{div}(J(x, s)e^{-\beta V(x, s)}) = 0 , \quad \text{a.e. } x \in \mathbb{R}^n ,
\]  

(21)

for all \( s \in [0, T] \). Let \( \beta > 0 \) and \( w(s) \) be an \( m \)-dimensional Brownian motion, where \( s \in [0, T] \). We are interested in the time-inhomogeneous forward process on \( \mathbb{R}^n \), which satisfies SDE

\[
dx(s) = b(x(s), s) \, ds + \sqrt{2\beta^{-1}} \sigma(x(s), s) \, dw(s)
\]

\[
= \left( J - \gamma \nabla V + \frac{1}{\beta} \nabla \cdot \gamma \right)(x(s), s) \, ds + \sqrt{2\beta^{-1}} \sigma(x(s), s) \, dw(s) , \quad s \in [0, T] .
\]  

(22)

In (22), the drift vector \( b : \mathbb{R}^n \times [0, T] \to \mathbb{R}^n \) is

\[
b = J - \gamma \nabla V + \frac{1}{\beta} \nabla \cdot \gamma ,
\]  

(23)

and \( \gamma \) is related to \( \sigma \) by \( \gamma = \sigma \sigma^T \) and satisfies the uniform ellipticity condition \([11]\). Following the terminology in \([13]\), we call the operator \( \mathcal{L}_s \), defined by

\[
\mathcal{L}_s f = \left( (J - \gamma \nabla V + \frac{1}{\beta} \nabla \cdot \gamma)(\cdot, s) \right) \cdot \nabla f + \frac{1}{\beta} \gamma(\cdot, s) : \nabla^2 f
\]

\[
= J \cdot \nabla f + \frac{e^{\beta V}}{\beta} \text{div}(e^{-\beta V} \gamma \nabla f) ,
\]  

(24)
for a test function $f : \mathbb{R}^n \to \mathbb{R}$, the generator of (22) at time $s$. Denote by $\mathcal{L}_s^T$ the adjoint operator of $\mathcal{L}_s$ with respect to Lebesgue measure (i.e. in the standard $L^2$ space). Using the expression on the second line of (24), we find

$$\mathcal{L}_s^T f = - \text{div}(f J) + \frac{1}{\beta} \text{div} \left[ e^{-\beta V} \gamma \nabla (e^{\beta V} f) \right]. \quad (25)$$

For each $s \in [0, T]$, we denote by $\nu_s$ the probability distribution of $x(s)$, and we assume that $\nu_s$ has a smooth positive probability density $\rho$ with respect to the Lebesgue measure (see [42, Theorem 4.2] and [4] for conditions required to guarantee smoothness and positiveness, respectively), i.e. $\rho > 0$ and

$$d\nu_s(x) = \rho(x, s) \, dx, \quad s \geq 0.$$  

(26)

It is well known that $\rho$ satisfies the Fokker-Planck equation [46]

$$\frac{\partial \rho}{\partial s} = \mathcal{L}_s^T \rho. \quad (27)$$

Assume that $s \in [0, T]$ is fixed. Under proper conditions (see [38, 47], for instance), the operator $\mathcal{L}_s$ generates a Markovian semigroup which has a unique invariant distribution $\nu_s^{\infty}$, given by

$$d\nu_s^{\infty}(x) = \frac{1}{Z(s)} e^{-\beta V(x, s)} \, dx, \quad \text{where} \quad Z(s) = \int_{\mathbb{R}^n} e^{-\beta V(x, s)} \, dx. \quad (28)$$

Using (21) and (25), it is straightforward to observe that

$$\mathcal{L}_s^T (e^{-\beta V(\cdot, s)}) \equiv 0, \quad \forall \, s \in [0, T]. \quad (29)$$

The free energy of the process (22) at time $s$ is defined as

$$F(s) = -\beta^{-1} \ln Z(s), \quad s \in [0, T]. \quad (30)$$

Corresponding to the forward process (22), let us also introduce the reverse process (31) and for each $s \in [0, T]$, we define the operator

$$\mathcal{L}_s^R f = \left[ -J - \gamma \nabla V + \frac{1}{\beta} \nabla \cdot \gamma \right] (x^R(s), T - s) \cdot \nabla f + \frac{1}{\beta} \gamma (\cdot, T - s) : \nabla^2 f, \quad (32)$$

for a test function $f : \mathbb{R}^n \to \mathbb{R}$. Note that $\mathcal{L}_s^R$ can be obtained from $\mathcal{L}_s$ by changing the sign in front of the vector $J$ in (24), i.e.,

$$\mathcal{L}_s^R f = \left[ -J - \gamma \nabla V + \frac{1}{\beta} \nabla \cdot \gamma \right] (\cdot, s) \cdot \nabla f + \frac{1}{\beta} \gamma (\cdot, s) : \nabla^2 f,$$

$$= -J \cdot \nabla f + \frac{e^{\beta V}}{\beta} \text{div}(e^{-\beta V} \gamma \nabla f). \quad (33)$$

In particular, when $J \equiv 0$, we have $\mathcal{L}_s^R = \mathcal{L}_s$. More generally, we have the following relations.
Lemma 1. Let \( f, g : \mathbb{R}^n \to \mathbb{R} \) be two bounded \( C^2 \)-smooth functions. For all \( s \in [0, T] \), we have

\[
\int_{\mathbb{R}^n} f (L_s + L^R_{T-s}) g \, dv^\infty_s = -\frac{2}{\beta} \int_{\mathbb{R}^n} (\gamma \nabla f) \cdot \nabla g \, dv^\infty_s,
\]

\[
L^T_s f = e^{-\beta V} L^R_{T-s} (e^{\beta V} f).
\]

Furthermore, when \( g \) is positive, we have

\[
\frac{L_s g}{g} = L_s (\ln g) + \frac{1}{\beta} \sigma^T \nabla \ln g^2,
\]

\[
\frac{L^R_{T-s} g}{g} = L^R_{T-s} (\ln g) + \frac{1}{\beta} \sigma^T \nabla \ln g^2.
\]

Proof. The first identity in (34) can be obtained by summing up (24) and (33), and integrating by parts. For the second identity in (34), using (33), (21) and (25), we can compute

\[
e^{-\beta V} L^R_{T-s} (e^{\beta V} f)
\]

\[= - e^{-\beta V} J \cdot \nabla (e^{\beta V} f) + \frac{1}{\beta} \text{div}[e^{-\beta V} \gamma \nabla (e^{\beta V} f)]
\]

\[= e^{\beta V} f \text{div}(e^{-\beta V} J) - \text{div}(f J) + \frac{1}{\beta} \text{div}[e^{-\beta V} \gamma \nabla (e^{\beta V} f)]
\]

\[= L^T_s f.
\]

The identities in (35) can be verified directly using (24) and (33).

Proposition 1. Assume \( \eta : \mathbb{R}^n \times [0, T] \to \mathbb{R} \) is a bounded smooth function. \( x(s) \) and \( x^R(s) \) are the forward process and the reverse process in (22) and (31), respectively. Then, for all \( x, x' \in \mathbb{R}^n \), we have

\[
e^{-\beta V(x,0)} E \left[ \exp \left( - \beta W + \int_0^T \eta(x(s), s) \, ds \right) \delta(x(T) - x') \bigg| x(0) = x \right]
\]

\[= e^{-\beta V(x',T)} E \left[ \exp \left( \int_0^T \eta(x^R(s), T-s) \, ds \right) \delta(x^R(T) - x) \bigg| x^R(0) = x' \right],
\]

where

\[
W = \int_0^T \frac{\partial V}{\partial s}(x(s), s) \, ds
\]

is the path (work) functional, \( E[\cdot | x(0) = x] \) and \( E[\cdot | x^R(0) = x'] \) denote the path ensemble averages of \( x(s) \) and \( x^R(s) \) starting from \( x \) and \( x' \) at time \( s = 0 \), respectively.
Note that the fluctuation relation (36) above involves Dirac delta function. Rigorously, (36) should be understood as an identity in the sense of distributions. We refer to [21, Remark 2] for related discussions. We also point out that Proposition 1 holds for the process (22) involving a general matrix \( \gamma \) and a vector field \( J \) which satisfies (21). In particular, the reversibility assumption \( J \equiv 0 \) is not required (see [21, Remark 3] for further discussions).

### 2.2 Relative entropy estimate

For \( s \in [0, T] \), recall that \( \nu_s \) is the probability distribution of \( x(s) \) whose density is \( \rho(\cdot, s) \) in (26) and that \( \nu_s^\infty \) is defined in (28). In this section, we study the relative entropy of \( \nu_s \) with respect to \( \nu_s^\infty \) (as a function of \( s \)), defined as

\[
\mathcal{R}(s) = D_{KL}(\nu_s | \nu_s^\infty) = \int_{\mathbb{R}^n} \ln \frac{d\nu_s}{d\nu_s^\infty}(x) d\nu_s(x) = \int_{\mathbb{R}^n} \rho(x, s) \ln \frac{d\nu_s}{d\nu_s^\infty}(x) dx.
\]

The main result of this section is Theorem 1, which provides upper bounds of \( \mathcal{R}(s) \).

Before stating Theorem 1, let us first present the following useful results.

**Lemma 2.** For \( s \in [0, T] \), we have

\[
\frac{\partial}{\partial s} \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) = \beta \left( \frac{\partial V}{\partial s} \frac{d\nu_s}{ds} + dF \right) + \mathcal{L}_{R}^{T-s} \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) + \frac{1}{\beta} \left| \sigma^T \nabla \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) \right|^2.
\]

**Proof.** From (26) and (28), we know that the density

\[
\frac{d\nu_s}{d\nu_s^\infty}(x) = e^{\beta V(x, s)} \rho(x, s) Z(s), \quad x \in \mathbb{R}^n.
\]

Using the Fokker-Planck equation (27), the second identity in (34) of Lemma 1, and the free energy in (30), we can derive

\[
\frac{\partial}{\partial s} \left( \frac{d\nu_s}{d\nu_s^\infty} \right) = (e^{\beta V} \mathcal{L}_s^T \rho) Z(s) + \beta \frac{\partial V}{\partial s} \frac{d\nu_s}{d\nu_s^\infty} + e^{\beta V} \rho \frac{dZ}{ds} = \mathcal{L}_{R}^{T-s} (e^{\beta V} \rho) Z(s) + \beta \frac{\partial V}{\partial s} \frac{d\nu_s}{d\nu_s^\infty} - \beta e^{\beta V} \rho Z(s) \frac{dF}{ds} = \beta \left( \frac{\partial V}{\partial s} - \frac{dF}{ds} \right) \frac{d\nu_s}{d\nu_s^\infty} + \mathcal{L}_{R}^{T-s} \left( \frac{d\nu_s}{d\nu_s^\infty} \right).
\]

Therefore, (39) is obtained after applying (35) of Lemma 1.

**Remark 1.** We work with the operator \( \mathcal{L}_s^T \) which is the adjoint of \( \mathcal{L}_s \) with respect to Lebesgue measure (see Section 2.1). Alternatively, for each \( s \in [0, T] \), one can also consider the operator \( \mathcal{L}_s^* \), which is the adjoint of \( \mathcal{L}_s \) with respect to \( \nu_s^\infty \). In fact, it is straightforward to verify that \( \mathcal{L}_s^*f = e^{\beta V} \mathcal{L}_s^T (e^{-\beta V} f) \) for a test function \( f \). Therefore, Lemma 1 implies

\[
\mathcal{L}_s^* = \mathcal{L}_{R}^{T-s}, \quad \int_{\mathbb{R}^n} f (\mathcal{L}_s + \mathcal{L}_s^*) g d\nu_s^\infty = -\frac{2}{\beta} \int_{\mathbb{R}^n} (\gamma \nabla f) \cdot \nabla g d\nu_s^\infty,
\]

and

\[
\frac{\mathcal{L}_s^* g}{g} = \mathcal{L}_s^*(\ln g) + \frac{1}{\beta} \left| \sigma^T \nabla \ln g \right|^2, \quad \text{when} \ g > 0.
\]
while (39) of Lemma 2 becomes

$$\frac{\partial}{\partial s} \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) = \beta \left( \frac{\partial V}{\partial s} - \frac{dF}{ds} \right) + L_s^* \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) + \frac{1}{\beta} \left| \sigma^T \nabla \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) \right|^2.$$

Using Lemma 2 we can derive an expression of the time derivative of $\mathcal{R}(s)$, i.e., the expression of the relative entropy production rate.

**Proposition 2.** For all $s \in [0, T]$, we have

$$\frac{d\mathcal{R}(s)}{ds} = -\beta \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d\nu_s^\infty + \beta \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d\nu_s - \frac{1}{\beta} \int_{\mathbb{R}^n} \sigma^T \nabla \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right)^2 d\nu_s. \quad (41)$$

**Proof.** Using the Fokker-Planck equation (27), integration by parts formula, the identities in (34), as well as Lemma 2, we can compute from (38) that

$$\frac{d\mathcal{R}(s)}{ds} = \int_{\mathbb{R}^n} \ln \frac{d\nu_s}{d\nu_s^\infty} \frac{\partial \rho}{\partial s} dx + \int_{\mathbb{R}^n} \frac{\partial}{\partial s} \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) dx$$

$$= \int_{\mathbb{R}^n} \ln \frac{d\nu_s}{d\nu_s^\infty} L_s^\ast \rho dx + \int_{\mathbb{R}^n} \left[ \beta \left( \frac{\partial V}{\partial s} - \frac{dF}{ds} \right) + L_s^* \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) + \frac{1}{\beta} \left| \sigma^T \nabla \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) \right|^2 \right] \rho dx$$

$$= -\beta \frac{dF(s)}{ds} \left[ (L_s + L_{T-s}^R) \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) + \beta \frac{\partial V}{\partial s} + \frac{1}{\beta} \left| \sigma^T \nabla \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) \right|^2 \right] \rho dx$$

$$= -\beta \frac{dF(s)}{ds} + \beta \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d\nu_s + \int_{\mathbb{R}^n} \left[ (L_s + L_{T-s}^R) \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) \right] d\nu_s^\ast$$

$$+ \frac{1}{\beta} \int_{\mathbb{R}^n} \left| \sigma^T \nabla \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) \right|^2 d\nu_s$$

$$= -\beta \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d\nu_s + \beta \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d\nu_s - \frac{2}{\beta} \int_{\mathbb{R}^n} \nabla \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) \cdot \nabla \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) d\nu_s$$

$$+ \frac{1}{\beta} \int_{\mathbb{R}^n} \left| \sigma^T \nabla \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right) \right|^2 d\nu_s$$

$$= -\beta \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d\nu_s + \beta \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d\nu_s - \frac{1}{\beta} \int_{\mathbb{R}^n} \sigma^T \nabla \left( \ln \frac{d\nu_s}{d\nu_s^\infty} \right)^2 d\nu_s. \quad (43)$$

In the above, we have used that $\frac{dF(s)}{ds} = \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d\nu_s^\infty$, which can be verified from (28) and (30).
In particular, when the potential \( V \) is time-independent, (41) becomes
\[
\frac{d R(s)}{ds} = - \frac{1}{\beta} \int_\mathbb{R}^n \left| \sigma^T \nabla \ln \frac{d \nu_s}{d \nu_s^\infty} \right|^2 d \nu_s \leq 0,
\]
which shows that the relative entropy \( R(s) \) is non-increasing. It is interesting to note that (44) is true for time-inhomogeneous processes \( x(s) \) (i.e., the vector \( J \), coefficients \( \gamma \) and \( \sigma \) in (22) can be time-dependent), as long as \( V \), or equivalently \( \nu_s^\infty \), is time-independent.

We are ready to state Theorem 1.

**Theorem 1.** Assume that \( \gamma \) satisfies the uniform ellipticity assumption (11) and that the probability measure \( \nu_s^\infty \) satisfies LSI with a uniform constant \( \kappa > 0 \) at any time \( s \in [0, T] \). Let \( L, L_1 \geq 0 \) be constants which are independent of \( s \).

1. Suppose that \( \left| \frac{\partial V}{\partial s}(x, s) \right| \leq L_1 \), for all \( (x, s) \in \mathbb{R}^n \times [0, T] \). We have
\[
\sqrt{R(s)} \leq e^{-\kappa \gamma^{-s/\beta}} \sqrt{R(0)} + \frac{\beta^2 L_1}{\sqrt{2 \kappa \gamma^-}}, \quad \forall s \in [0, T].
\]
(45)

2. For all \( s \in [0, T] \), suppose that \( \frac{\partial V}{\partial s}(\cdot, s) \) is a Lipschitz function on \( \mathbb{R}^n \) with a uniform Lipschitz constant \( L \). We have
\[
\sqrt{R(s)} \leq e^{-\kappa \gamma^{-s/\beta}} \sqrt{R(0)} + \frac{\beta^2 L}{\sqrt{2 \kappa \gamma^-}}, \quad \forall s \in [0, T].
\]
(46)

**Proof.** 1. Consider the terms in (41) of Proposition 2. Since \( \left| \frac{\partial V}{\partial s}(x, s) \right| \leq L_1 \), applying (13) and Csiszár-Kullback-Pinsker inequality (15), we have
\[
\left| \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d \nu_s^\infty - \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d \nu_s \right| \leq L_1 \| \nu_s^\infty - \nu_s \|_{TV}
\leq L_1 \sqrt{2 D_{KL}(\nu_s \| \nu_s^\infty)}
= L_1 \sqrt{2 R(s)}.
\]
(47)

Substituting (47) into (41), using the uniform ellipticity condition (11), the definition of Fisher information (16), and LSI in (17), we can compute
\[
\frac{d R(s)}{ds} = -\beta \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d \nu_s^\infty + \beta \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d \nu_s - \frac{1}{\beta} \int_{\mathbb{R}^n} \left| \sigma^T \nabla \left( \ln \frac{d \nu_s}{d \nu_s^\infty} \right) \right|^2 d \nu_s
\leq \beta L_1 \sqrt{2 R(s)} - \frac{\gamma^\cdot \mathcal{I}(\nu_s \| \nu_s^\infty)}{\beta}
\leq \beta L_1 \sqrt{2 R(s)} - \frac{2 \kappa \gamma^-}{\beta} R(s),
\]
(48)
which implies
\[
\frac{d}{ds} \sqrt{R(s)} \leq -\frac{\kappa \gamma^-}{\beta} \sqrt{R(s)} + \frac{\beta L_1}{\sqrt{2}}.
\]
The upper bound (45) is implied by Gronwall’s inequality.
2. Since $\frac{\partial V}{\partial s}$ is Lipschitz, applying the inequalities (18) and (19), we find
\[
\left| \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d\nu_s^\infty - \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d\nu_s \right| \leq L \mathcal{W}_1(\nu_s, \nu_s^\infty) \leq L \mathcal{W}_2(\nu_s, \nu_s^\infty). \tag{49}
\]
Since $\nu_s^\infty$ satisfies LSI with the constant $\kappa$, the Talagrand inequality (20) holds, i.e.
\[
\mathcal{W}_2(\nu_s, \nu_s^\infty) \leq \sqrt{\frac{2}{\kappa} D_{KL}(\nu_s^\infty \| \nu_s)} = \sqrt{\frac{2\mathcal{R}(s)}{\kappa}}. \tag{50}
\]
Applying (49)–(50), a similar argument as (48) shows that
\[
\frac{d\mathcal{R}(s)}{ds} \leq \beta L \sqrt{\frac{2\mathcal{R}(s)}{\kappa}} - \frac{2\kappa \gamma - \beta}{\beta} \mathcal{R}(s).
\]
The upper bound (46) again follows from Gronwall’s inequality.

We conclude this section with two remarks on Theorem 1.

Remark 2. Obviously, when the process is defined on $[0, +\infty)$, i.e. $T = +\infty$, the conclusions of Theorem 1 are true on $[0, +\infty)$ as well.

In the proof above, the key step to derive upper bounds of $\mathcal{R}(s)$ is to estimate the difference $\left| \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d\nu_s^\infty - \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d\nu_s \right|$. Instead of assuming boundedness or Lipschitz condition for $\frac{\partial V}{\partial s}$, one can also assume that $\frac{\partial V}{\partial s}(x, s) - \frac{\partial V}{\partial s}(y, s) \leq L|x - y|^\alpha$ for all $x, y \in \mathbb{R}^n$ and $s \in [0, T]$, where $L \geq 0$. In this case, one can in fact show that
\[
\left| \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d\nu_s^\infty - \int_{\mathbb{R}^n} \frac{\partial V}{\partial s} d\nu_s \right| \leq L \mathcal{W}_2(\nu_s, \nu_s^\infty)^\alpha \leq L \left( \frac{2\mathcal{R}(s)}{\kappa} \right)^{\frac{\alpha}{2}},
\]
from which we obtain
\[
\frac{d\mathcal{R}(s)}{ds} \leq \beta L \left( \frac{2\mathcal{R}(s)}{\kappa} \right)^{\frac{\alpha}{2}} - \frac{2\kappa \gamma - \beta}{\beta} \mathcal{R}(s).
\]
This again allows us to derive upper bound of $\mathcal{R}(s)$ using a Gronwall type inequality. We omit the details for simplicity.

Remark 3. Since the probability measure $\nu_s^\infty$ (28) depends on $\beta$, the constant $\kappa$ in Theorem 1 in general depends on $\beta$ as well. In particular, assuming that $\nabla^2 V(x, s) \geq \kappa_0 I_n$ for some $\kappa_0 > 0$ which is independent of $\beta$, for all $(x, s) \in \mathbb{R}^n \times [0, T]$, then it is known that $\nu_s^\infty$ satisfies LSI with the constant $\kappa = \beta \kappa_0$ [52, Remark 21.4]. In this case, (45) and (46) become
\[
\sqrt{\mathcal{R}(s)} \leq e^{-\kappa_0 \gamma - s} \sqrt{\mathcal{R}(0)} + \frac{\beta L_1}{\sqrt{2 \kappa_0 \gamma}}, \quad \forall s \in [0, T],
\]
and
\[
\sqrt{\mathcal{R}(s)} \leq e^{-\kappa_0 \gamma - s} \sqrt{\mathcal{R}(0)} + \sqrt{\frac{\beta}{2\kappa_0}} \frac{L}{\kappa_0}, \quad \forall s \in [0, T],
\]
respectively.
2.3 Connection between time reversal of reverse process and optimally controlled forward process

First of all, let us introduce a stochastic optimal control problem \([16]\) that is related to Jarzynski’s equality (we refer to Appendix \([B.1]\) for further motivations). We consider the stochastic optimal control problem

\[
U(x, t) = \min_{u_s} \mathbb{E} \left( W^u_{(t,T)} + \frac{1}{4} \int_t^T |u_s|^2 \, ds \mid x^u(t) = x \right), \quad (x, t) \in \mathbb{R}^n \times [0, T],
\]

of the controlled process

\[
dx^u(s) = \left(J - \gamma \nabla V + \frac{1}{\beta} \nabla \cdot \gamma \right)(x^u(s), s) \, ds + \sqrt{2 \beta - 1} \sigma(x^u(s), s) \, dw(s) + \sigma(x^u(s), s) u_s \, ds,
\]

where the minimum is over all adapted processes \(u_s \in \mathbb{R}^m\) such that (52) is well-defined, and the work functional is (cf. \([37]\))

\[
W^u_{(t,T)} = \int_t^T \frac{\partial V}{\partial s}(x^u(s), s) \, ds, \quad 0 \leq t \leq T.
\]

The function \(U : \mathbb{R}^n \times [0, T] \rightarrow \mathbb{R}\) is called the value function of the optimal control problem \((51)-(52)\). It is known that the optimal control \(u^*_s\) exists and is given in the feedback form as \([16]\)

\[
u
\]

\[
W^u_{(t,T)} = \int_t^T \frac{\partial V}{\partial s}(x^u(s), s) \, ds,
\]

\[
u
\]

when the state of the system is at \(x \in \mathbb{R}^n\) at time \(s \in [0, T]\). We also introduce the probability measure \(\nu^*_0\) on \(\mathbb{R}^n\), defined by

\[
\frac{d\nu^*_0}{dx}(x) = \frac{e^{-\beta V(x,0)}}{Z(T)} \mathbb{E} \left( e^{-\beta W} \mid x(0) = x \right), \quad x \in \mathbb{R}^n,
\]

where \(W\) is in \([37]\) and \(\mathbb{E}(: \mid x(0) = x)\) denotes the path ensemble average of the (uncontrolled) dynamics \([22]\) starting from \(x(0) = x\) at \(s = 0\). Note that Jarzynski’s equality \([112]\) in Appendix \([B.1]\) implies that the integration of \(\nu^*_0\) over \(\mathbb{R}^n\) equals to one. Moreover, the optimal control \(u^*\) and the probability measure \(\nu^*_0\) give the optimal Monte Carlo estimators based on Jarzynski’s equality (see Appendix \([B.1]\) and \([21]\)).

The following result connects the time reversal of the reverse process \((31)\) and the controlled process \((52)\) under the optimal control in \((54)\).

**Theorem 2.** Let \(\nu^\infty_T\) and \(\nu^*_0\) be the probability measures in \((28)\) and \((55)\), respectively. Consider the reverse process \(x^R(s)\) in \((31)\) starting from the distribution \(\nu^\infty_T\) at \(s = 0\). Assume the probability distribution of \(x^R(s)\) has a positive smooth density with respect to Lebesgue measure for all \(s \in [0, T]\). Define the time reversal \(x^{R,-}(s) = x^R(T-s)\), where \(s \in [0, T]\). \(x^{u^*}(s)\) denotes the controlled process \((52)\) under the optimal control \(u^*\) in \((54)\) starting from the initial distribution \(\nu^*_0\). Then, \(x^{R,-}(s)\) and \(x^{u^*}(s)\) have the same law on the path space \(C([0,T], \mathbb{R}^n)\).

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Proof. Let us denote by $\nu_s^R$ the probability distribution of $x^R(s)$ at time $s$. Let $\rho^R(\cdot, s)$ be the probability density of $\nu_s^R$ with respect to Lebesgue measure. Similar to (27), $\rho^R$ satisfies the Fokker-Planck equation

$$\frac{\partial \rho^R}{\partial s} = (\mathcal{L}_s^R)^T \rho^R, \quad s \in [0,T],$$

where $\mathcal{L}_s^R$ is the operator in (32).

In the following, we show that both processes $x^{R,-}(s)$ and $x^{u^*}(s)$ satisfy the same SDE with the same initial probability distribution.

1. First, we consider the SDEs of $x^{R,-}(s)$ and $x^{u^*}(s)$. For the optimally controlled process $x^{u^*}(s)$, combining (52) and (54), using $\gamma = \sigma \sigma^T$, we find

$$dx^{u^*}(s) = \left( J - \gamma \nabla V + \frac{1}{\beta} \nabla \cdot \gamma \right)(x^{u^*}(s)) ds + \sqrt{2\beta^{-1}} \sigma(x^{u^*}(s),s) dw(s)$$

$$- 2(\gamma \nabla U)(x^{u^*}(s),s) ds, \quad s \in [0,T],$$

where $U$ is the value function in (51).

For the time reversal $x^{R,-}(s)$, let us recall the reverse process (31), which we rewrite as

$$dx^R(s) = \hat{b}(x^R(s),s) ds + \sqrt{2\beta^{-1}} \hat{\sigma}(x^R(s),s) dw(s),$$

where, for all $(x, s) \in \mathbb{R}^n \times [0,T],$

$$\hat{b}(x, s) = \left( - J - \gamma \nabla V + \frac{1}{\beta} \nabla \cdot \gamma \right)(x, T - s),$$

$$\hat{\sigma}(x, s) = \sigma(x, T - s), \quad \hat{\gamma}(x, s) = (\hat{\sigma} \hat{\sigma}^T)(x, s) = \gamma(x, T - s).$$

Since $\rho^R$ is both smooth and positive, it is shown in [22] that $x^{R,-}(s) = x^R(T - s)$ is again a diffusion process which satisfies the SDE

$$dx^{R,-}(s) = \hat{b}^-(x^{R,-}(s), T - s) ds + \sqrt{2\beta^{-1}} \hat{\sigma}(x^{R,-}(s), T - s) dw(s), \quad s \in [0,T],$$

with the initial distribution $\nu_s^R$ (i.e. the distribution of $x^R(T)$), where the drift term $\hat{b}^-$ is

$$\hat{b}^-(x, s) = \left(- \hat{b} + \frac{2}{\beta \rho^R} \nabla \cdot (\rho^R \hat{\gamma})\right)(x, s), \quad (x, s) \in \mathbb{R}^n \times [0,T].$$

Substituting (59) in (61), we can derive

$$\hat{b}^-(x, T - s) = \left(- \hat{b} + \frac{2}{\beta \rho^R} \nabla \cdot (\rho^R \hat{\gamma})\right)(x, T - s)$$

$$= \left( J + \gamma \nabla V - \frac{1}{\beta} \nabla \cdot \gamma + \frac{2}{\beta \rho^R} \nabla \cdot (\rho^R \hat{\gamma}) \right)(x, s)$$

$$= \left( J + \gamma \nabla V - \frac{1}{\beta} \nabla \cdot \gamma + \frac{2}{\beta \rho^R} \gamma \nabla \rho^R \hat{\gamma} \right)(x, s)$$

$$= \left( J + \gamma \nabla V + \frac{1}{\beta} \nabla \cdot \gamma + \frac{2}{\beta} \gamma \nabla \ln(\rho^R) \right)(x, s)$$

$$= \left( J - \gamma \nabla V + \frac{1}{\beta} \nabla \cdot \gamma + \frac{2}{\beta} \gamma \nabla \ln(e^{\beta V} \rho^R) \right)(x, s),$$
where we have used the notation $\rho^{R,-}(\cdot, s) = \rho^{R}(\cdot, T - s)$, for all $s \in [0, T]$. Using (62) and (59), we can write SDE (60) more explicitly as

$$
dx_{R}^{-}(s) = \hat{b}^{-}(x_{R}^{-}(s), T - s) \, ds + \sqrt{2\beta^{-1}\sigma}(x_{R}^{-}(s), T - s) \, dw(s)
$$

$$
= \left( J - \gamma \nabla V + \frac{1}{\beta} \nabla \cdot \gamma \right)(x_{R}^{-}(s), s) \, ds + \sqrt{2\beta^{-1}\sigma}(x_{R}^{-}(s), s) \, dw(s)
$$

$$
+ \frac{2}{\beta} \left( \gamma \nabla \ln(e^{\beta V} \rho^{R,-}) \right)(x_{R}^{-}(s), s) \, ds.
$$

(63)

To show that the two SDEs (67) and (63) are the same, we define

$$
g(x, s) = e^{\beta V(x, s)} \rho^{R}(x, T - s) Z(T), \quad (x, s) \in \mathbb{R}^n \times [0, T].
$$

(64)

Since the initial distribution of $x^{R}(s)$ is $\nu^{R}_0 = \nu^{\infty}_T$, we have $\rho^{R}(x, 0) = \frac{1}{Z(T)} e^{-\beta V(x, T)}$, which implies $g(x, T) = 1$. Using (66) and the identity (34) in Lemma 1 i.e., $L_s f = e^{\beta V} (L_{T-s}^R)^T (e^{-\beta V} f)$ for a test function $f$, we can derive

$$
\frac{\partial g}{\partial s} = -Z(T) e^{\beta V} \frac{\partial \rho^{R}}{\partial s}(x, T - s) + \beta \frac{\partial V}{\partial s} g
$$

$$
= -Z(T) e^{\beta V} [ (L_{T-s}^R)^T \rho^{R}(\cdot, T - s)] + \beta \frac{\partial V}{\partial s} g
$$

$$
= -e^{\beta V} (L_{T-s}^R)^T (e^{-\beta V} g) + \beta \frac{\partial V}{\partial s} g
$$

$$
= -L_s g + \beta \frac{\partial V}{\partial s} g.
$$

(65)

In fact, the derivations above show that $g$ and the value function $U$ are related by the logarithmic transformation (we refer to (123)–(124) in Appendix B.1 for details), i.e.

$$
U = -\beta^{-1} \ln g.
$$

(66)

Combining (64) and (66), we see that both SDEs (67) and (63) are the same.

2. Next, we show that the initial distribution of $x_{R}^{-}(s)$ is $\nu^{R}_0$ in (55). Since $x_{R}^{-}(s) = x^{R}(T - s)$, it is enough to verify $\nu^{R}_T = \nu^{\infty}_0$, or, equivalently, the density $\rho^{R}(x, T)$ coincides with the one in (55). In fact, applying Feynmann-Kac formula, from (65) we obtain

$$
g(x, t) = \mathbb{E} \left[ \exp \left( -\beta \int_{t}^{T} \frac{\partial V}{\partial s}(x(s), s) \, ds \right) \mid x(t) = x \right], \quad (x, t) \in \mathbb{R}^n \times [0, T],
$$

(67)

where $\mathbb{E}(\cdot \mid x(t) = x)$ denotes the path ensemble average of the (uncontrolled) dynamics (22) starting from $x(t) = x$ at time $t$. Comparing (67) with (55), using (67) and (61), we obtain

$$
d\nu^{R}_T = \rho^{R}(x, T) \, dx = \frac{1}{Z(T)} e^{-\beta V(x, 0)} g(x, 0) \, dx = d\nu^{\infty}_0.
$$

(68)

This shows that the initial distribution of $x_{R}^{-}(s)$ is indeed $\nu^{\infty}_0$. 

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To summarize, both \( x^{R_1}(s) \) and \( x^{u^*_1}(s) \) satisfy the same SDE with the same initial distribution \( \nu_0^* \). Therefore, we conclude that they have the same law on the path space.

\[ \Box \]

### 3 Time-inhomogeneous Langevin dynamics

In this section, we study time-inhomogeneous (underdamped) Langevin dynamics in phase space. The analysis is similar to that in the previous section. We introduce Langevin dynamics and useful notations in Section 3.1. Then, in Section 3.2 we study the relative entropy estimate for time-inhomogeneous Langevin dynamics. Finally, in Section 3.3 we establish the connection between the time reversal of reverse Langevin process and certain optimally controlled forward Langevin process.

#### 3.1 Forward and reverse processes

Denote by \((q, p)\) the state of the system in phase space \( \mathbb{R}^n \times \mathbb{R}^n \). \( \nabla_q, \nabla_p \) are the gradient operators with respect to the \( q \) and \( p \) components, respectively. Given a time-dependent smooth Hamiltonian \( H : \mathbb{R}^n \times \mathbb{R}^n \times [0, T] \rightarrow \mathbb{R} \) within time \([0, T]\), we consider the forward Langevin dynamics [33, Section 2.2.3]

\[
\begin{align*}
    dq(s) &= \nabla_p H(q(s), p(s), s) \, ds \\
    dp(s) &= -\nabla_q H(q(s), p(s), s) \, ds - \gamma(q(s), s) \nabla_p H(q(s), p(s), s) \, ds + \sqrt{2\beta^{-1}} \sigma(q(s), s) \, dw(s)
\end{align*}
\]

for \( s \in [0, T] \), where \( \sigma : \mathbb{R}^n \times [0, T] \rightarrow \mathbb{R}^{n \times m} \) is smooth, \( w(s) \) is an \( m \)-dimensional Brownian motion, and \( \beta > 0 \) is related to the (inverse) temperature of the system. We assume that \( \gamma = \sigma \sigma^T : \mathbb{R}^n \times [0, T] \rightarrow \mathbb{R}^{n \times n} \) such that the uniform ellipticity condition (11) holds.

Under mild assumptions on \( H \), it is known that, for fixed \( s \in [0, T] \), the operator \( Q_s \), defined by (note that \( \gamma \) is independent of \( p \))

\[
Q_s f = \nabla_p H \cdot \nabla_q f - \nabla_q H \cdot \nabla_p f - \gamma \nabla_p H \cdot \nabla_p f + \frac{1}{\beta} \gamma : \nabla_p^2 f
\]

\[
= \nabla_p H \cdot \nabla_q f - \nabla_q H \cdot \nabla_p f + \frac{e^{\beta H}}{\beta} \text{div} \left( e^{-\beta H} \gamma \nabla_p f \right),
\]

for a test function \( f : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R} \), is hypoelliptic [37, 38, 42], and the corresponding Markovian semigroup is ergodic with respect to the unique invariant measure \( \pi^\infty_s \) on \( \mathbb{R}^n \times \mathbb{R}^n \), which is defined by

\[
d\pi^\infty_s = \frac{1}{Z(s)} e^{-\beta H(q, p, s)} \, dq dp, \quad \text{where } Z(s) = \int_{\mathbb{R}^n \times \mathbb{R}^n} e^{-\beta H(q, p, s)} \, dq dp.
\]

The free energy of the system is

\[
\mathcal{F}(s) = -\beta^{-1} \ln Z(s), \quad s \in [0, T].
\]
Let us denote by $\pi_s$ the probability measure of $(q(s), p(s))$ in the space $\mathbb{R}^n \times \mathbb{R}^n$ at time $s \in [0, T]$. We assume that $\pi_s$ has a positive smooth probability density $\varrho$ with respect to Lebesgue measure, such that

$$d\pi_s = \varrho(q, p, s) \, dq \, dp,$$

where $\int_{\mathbb{R}^n \times \mathbb{R}^n} \varrho(q, p, s) \, dq \, dp = 1$. (73)

$\varrho$ satisfies the Fokker-Planck equation

$$\frac{\partial \varrho}{\partial s} = Q^T_s \varrho, \quad s \in [0, T].$$

(74)

We note that the existence of the smooth density $\varrho$ can be obtained from Hörmander’s Theorem, which also implies that the Fokker-Planck equation (74) is actually valid in a classical sense [42, Section 6.2.1].

The following two concrete (time-homogeneous) cases are often studied in the literature.

(1) Both $\sigma$ and $\gamma$ are independent of $s$. The Hamiltonian is

$$H = H(q, p) = V(q) + \frac{p^T M^{-1} p}{2}, \quad (q, p) \in \mathbb{R}^n \times \mathbb{R}^n,$$

where $V : \mathbb{R}^n \to \mathbb{R}$ is a smooth potential function that grows sufficiently fast at infinity, and $M \in \mathbb{R}^{n \times n}$ is a constant symmetric positive definite matrix. In this case, (69) becomes

$$dq(s) = M^{-1} p(s) \, ds$$

$$dp(s) = - \nabla_q V(q(s)) \, ds - \gamma(q(s)) M^{-1} p(s) \, ds + \sqrt{2 \beta^{-1}} \sigma(q(s)) \, dw(s).$$

(76)

We refer to [33, 34] for previous studies of (76).

(2) Both $\sigma$ and $\gamma$ are independent of $s$, and more generally, $H(q, p, s) = V(q) + V_1(p)$, where $V, V_1 : \mathbb{R}^n \to \mathbb{R}$ are two smooth potential functions, both of which grow sufficiently fast at infinity. In this case, (69) becomes

$$dq(s) = \nabla_p V_1(p(s)) \, ds$$

$$dp(s) = - \nabla_q V(q(s)) \, ds - \gamma(q(s)) \nabla_p V_1(p(s)) \, ds + \sqrt{2 \beta^{-1}} \sigma(q(s)) \, dw(s).$$

(77)

Apparently, (77) reduces to (76) when $V_1(p) = \frac{p^T M^{-1} p}{2}$, for $p \in \mathbb{R}^n$. We refer to [36, 49] for known results related to (77).

Similar to the case of Brownian dynamics in Section 2.1, let us also introduce the reverse Langevin dynamics

$$dq^R(s) = - \nabla_p H(q^R(s), p^R(s), T - s) \, ds$$

$$dp^R(s) = \nabla_q H(q^R(s), p^R(s), T - s) \, ds - \gamma(q^R(s), T - s) \nabla_p H(q^R(s), p^R(s), T - s) \, ds$$

$$+ \sqrt{2 \beta^{-1}} \sigma(q^R(s), T - s) \, dw(s).$$

(78)
Lemma 3. Omit its proof and we refer to the proof of Lemma 1 for details.

\[ R_s f = - \nabla_p H(q, p, T - s) \cdot \nabla_q f + \nabla_q H(q, p, T - s) \cdot \nabla_p f - \gamma(q, T - s) \nabla_p H(q, p, T - s) \cdot \nabla_p f + \frac{1}{\beta} \gamma(q, T - s) : \nabla_p^2 f, \]  

(79)

for a test function \( f : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R} \). The following results can be directly verified. We omit its proof and we refer to the proof of Lemma 1 for details.

**Lemma 3.** Let \( f, g : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R} \) be two bounded \( C^2 \)-smooth functions. Then, the following identities hold: for all \( s \in [0, T] \),

\[
\int_{\mathbb{R}^n \times \mathbb{R}^n} f(Q_s + Q_{T-s}^R) g d\pi_s^\infty = -\frac{2}{\beta} \int_{\mathbb{R}^n \times \mathbb{R}^n} \gamma \nabla_p f \cdot \nabla_q g d\pi_s^\infty, \\
Q_s f = e^{-\beta H} Q_{T-s}^R (e^{\beta H} f).
\]

Further, when \( g \) is positive, we have

\[
\frac{Q_s g}{g} = Q_s (\ln g) + \frac{1}{\beta} |\sigma^T \nabla_p \ln g|^2,
\]

\[
\frac{Q_{T-s}^R g}{g} = Q_{T-s}^R (\ln g) + \frac{1}{\beta} |\sigma^T \nabla_p \ln g|^2.
\]

(81)

We mention that (81) has been used in [24] to study Langevin dynamics under external forcing.

We conclude this section with the following fluctuation relation [6] concerning the forward Langevin dynamics (69) and the reverse Langevin dynamics (78), respectively. A concise proof using Lemma 3 is given in Appendix A.2.

**Proposition 3.** Let \( \eta : \mathbb{R}^n \times \mathbb{R}^n \times [0, T] \to \mathbb{R} \) be a bounded smooth function. \((q(s), p(s))\) and \((q^R(s), p^R(s))\) are the dynamics in (69) and (78), respectively. For all \( q, q', p, p' \in \mathbb{R}^n \), we have

\[
e^{-\beta H(q,p,0)} \mathbb{E} \left[ \exp \left( -\beta W + \int_0^T \eta(q(s), p(s), s) ds \right) \times \delta(q(T) - q') \delta(p(T) - p') \right| q(0) = q, p(0) = p \]  

\[
e^{-\beta H(q',p',T)} \mathbb{E} \left[ \exp \left( \int_0^T \eta(q^R(s), p^R(s), T - s) ds \right) \times \delta(q^R(T) - q) \delta(p^R(T) - p) \right| q^R(0) = q', p^R(0) = p' \]  

(82)

where \( W \) is the path functional (work)

\[
W = \int_0^T \frac{\partial H}{\partial s}(q(s), p(s), s) ds,
\]

(83)

\( \mathbb{E} \cdot |q(0) = q, p(0) = p| \) and \( \mathbb{E} \cdot |q^R(0) = q', p^R(0) = p'| \) denote the path ensemble averages of (69) and (78), starting from \((q, p)\) and \((q', p')\) at \( s = 0 \), respectively.
3.2 Relative entropy estimate

Given \( s \in [0, T] \), recall that \( \pi^\infty_s \) and \( \pi_s \) are the probability measures defined in (71) and (73), respectively. The goal of this section is to estimate the relative entropy

\[
\mathcal{R}^{\text{Lan}}(s) = D_{KL}(\pi_s \| \pi^\infty_s) = \int_{\mathbb{R}^n \times \mathbb{R}^n} \rho(q, p, s) \ln \frac{d\pi_s}{d\pi^\infty_s}(q, p) \, dq dp .
\]  

(84)

Let us first state the following two results (for Langevin dynamics in the general form (69)), which can be verified using Lemma 3. We omit their proofs since they are similar to the proofs of Lemma 2 and Proposition 2 in Section 2.2, respectively.

**Lemma 4.** For \( s \in [0, T] \), we have

\[
\frac{\partial}{\partial s} \left( \ln \frac{d\pi_s}{d\pi^\infty_s} \right) = \beta \left( \frac{\partial H}{\partial s} - \frac{dF(s)}{ds} \right) + Q^R_{T-s} \left( \ln \frac{d\pi_s}{d\pi^\infty_s} \right) + \frac{1}{\beta} \left| \sigma^T \nabla_p \left( \ln \frac{d\pi_s}{d\pi^\infty_s} \right) \right|^2,
\]

(85)

where \( F \) is the free energy in (72), and \( Q^R_{T-s} \) is the operator in (79) at time \( T - s \).

**Proposition 4.** For \( s \in [0, T] \), we have

\[
\frac{d\mathcal{R}^{\text{Lan}}(s)}{ds} = -\beta \int_{\mathbb{R}^n \times \mathbb{R}^n} \frac{\partial H}{\partial s} d\pi^\infty_s + \beta \int_{\mathbb{R}^n \times \mathbb{R}^n} \frac{\partial H}{\partial p} d\pi_s - \frac{1}{\beta} \int_{\mathbb{R}^n \times \mathbb{R}^n} \left| \sigma^T \nabla_p \left( \ln \frac{d\pi_s}{d\pi^\infty_s} \right) \right|^2 d\pi_s .
\]

(86)

We are ready to state the main result on the upper bound of the relative entropy (84). For simplicity, we only consider the case where

\[
\sigma = \sqrt{\xi I_n}, \quad H(q, p, s) = V(q, s) + \frac{|p|^2}{2}, \quad (q, p, s) \in \mathbb{R}^n \times \mathbb{R}^n \times [0, T],
\]

(87)

for some time-dependent potential function \( V \) and some constant \( \xi > 0 \). In this case, (71) reads \( d\pi^\infty_s = Z(s)^{-1} e^{-\beta(V(q, s) + |p|^2/2)} \, dq dp \), whose marginal probability measure in position \( q \) is (cf. (28))

\[
d\nu^\infty_s(q) = \frac{1}{Z(s)} e^{-\beta V(q, s)} \, dq, \quad \text{where} \quad Z(s) = \int_{\mathbb{R}^n} e^{-\beta V(q, s)} \, dq.
\]

(88)

**Theorem 3.** Let \( \mathcal{R}^{\text{Lan}}(s) \) be the relative entropy in (84). Consider the case (87), for some time-dependent potential function \( V \) and some constant \( \xi > 0 \). Assume the following two conditions are met.

1. \( V \) is \( C^2 \)-smooth. There exist constants \( L_1, L_2, L \geq 0 \), such that

\[
\left| \frac{\partial V}{\partial s} \right| \leq L_1, \quad \left| \frac{\partial^2 V}{\partial s^2} \right| \leq L_2, \quad \| \nabla^2 V \|_2 \leq L,
\]

(89)

for all \( (q, s) \in \mathbb{R}^n \times [0, T] \).

2. The marginal probability measure (88) satisfies LSI with constant \( \kappa > 0 \), for all \( s \in [0, T] \).
Then, we can find constants $a, b, c, \omega, C_1, C_2 > 0$, which depend on $L, \xi, \beta, \kappa$ but are independent of $L_1$ and $L_2$, such that
\[
\mathcal{R}^{\text{Lan}}(s) \leq \mathcal{E}(s) \leq \mathcal{E}(0)e^{-\omega s} + (C_1 L_1^2 + C_2 L_2^2), \quad \forall \ s \in [0, T],
\]
where
\[
\mathcal{E}(s) = \mathcal{R}^{\text{Lan}}(s) + \int_{\mathbb{R}^n \times \mathbb{R}^n} \left( a \left| \nabla_p \left( \ln \frac{d\pi_s}{d\pi_{s}^\infty} \right) \right|^2 + 2b \nabla_p \left( \ln \frac{d\pi_s}{d\pi_{s}^\infty} \right) \cdot \nabla_q \left( \ln \frac{d\pi_s}{d\pi_{s}^\infty} \right) 
+ c \left| \nabla_q \left( \ln \frac{d\pi_s}{d\pi_{s}^\infty} \right) \right|^2 \right) d\pi_s.
\]

The proof of Theorem 3 is adapted from [53] where a general hypocoercivity theory was developed. We present its proof in Appendix C due to its technicality. Let us conclude this section with several remarks on Theorem 3.

**Remark 4.** Note that, in the case of (87), the marginal measure of $\pi_s^\infty$ in momentum $p$ is $Z_p^{-1}e^{-\beta|p|^2/2}dp$, where $Z_p = \int_{\mathbb{R}^n} e^{-\beta|p|^2/2}dp$, which satisfies LSI with constant $\beta$. See Remark 3 and [52, Example 21.3]. The second assumption in Theorem 3 on the spatial marginal measure (88) implies that $\pi_s^\infty$ itself as a product measure satisfies LSI with constant $\min\{\kappa, \beta\}$ [30, Section 5.2], i.e.,
\[
D_{KL}(\pi \mid \pi_s^\infty) \leq \frac{1}{2 \min\{\kappa, \beta\}} \mathcal{I}(\pi \mid \mu_s^\infty) = \frac{1}{2 \min\{\kappa, \beta\}} \int_{\mathbb{R}^n \times \mathbb{R}^n} \left( \left| \nabla_p \left( \ln \frac{d\pi}{d\pi_{s}^\infty} \right) \right|^2 + \left| \nabla_q \left( \ln \frac{d\pi}{d\pi_{s}^\infty} \right) \right|^2 \right) d\pi,
\]
for all $\pi$, such that $\pi \ll \pi_s^\infty$ and $\mathcal{I}(\pi \mid \pi_s^\infty)$ is finite.

**Remark 5.** We make two comments on the estimate of Theorem 3.

1. Since $L_1, L_2$ are the upper bounds of $\frac{\partial V}{\partial s}$ and $\frac{\partial^2 V}{\partial s^2}$ respectively, the estimate (90) implies that the relative entropy (84) is small when the potential $V$ (and its gradient) varies slowly in time. In particular, when $L_1 = L_2 = 0$, it states the exponential entropy decay of Langevin dynamics under a fixed potential $V = V(q)$ [53].

2. Instead of assuming (89) on $[0, T]$ where $L_1, L_2$ are constants, let us suppose
\[
\left| \frac{\partial V}{\partial s} \right| \leq L_1(s), \quad \left| \frac{\partial^2 V}{\partial s^2} \right| \leq L_2(s), \quad \| \nabla^2 V \|_2 \leq L,
\]
for all $(q, s) \in \mathbb{R}^n \times [0, \infty)$, where $L > 0$ is constant, both functions $L_1(s)$ and $L_2(s)$ decrease to zero monotonically, as $s \to +\infty$. Also assume that the second assumption of Theorem 3 on the spatial margin (88) is true for all $s \geq 0$. Then, the same proof of Theorem 3 actually gives
\[
\mathcal{R}^{\text{Lan}}(s) \leq \mathcal{E}(s) \leq \mathcal{E}(0)e^{-\omega s} + (C_1 L_1^2(s) + C_2 L_2^2(s)), \quad \forall \ s \geq 0,
\]
which clearly implies that $\lim_{s \to +\infty} \mathcal{R}^{\text{Lan}}(s) = 0$ in this case.
Remark 6. We discuss the choice of $\omega$ in two different asymptotic regimes of $\xi$. In fact, as shown in the proof in Appendix C, it is necessary that the constants $a, b, c > 0$ are chosen such that both the $2 \times 2$ matrices $S$ and $\tilde{S}$ in (141) are positive definite, and $\omega$ can be defined explicitly as $\omega = \frac{\lambda_1}{2} \left( \frac{1}{\min(q, p)} + \lambda_2 \right)^{-1}$, where $\lambda_i$ and $\tilde{\lambda}_i$, $i = 1, 2$, are the eigenvalues of $S$ and $\tilde{S}$, respectively, such that $0 < \lambda_1 \leq \lambda_2$ and $0 < \tilde{\lambda}_1 \leq \tilde{\lambda}_2$. See (152). By analyzing the conditions that guarantee the positive definiteness of matrices $S$ and $\tilde{S}$, we can draw the following conclusions.

1. When $\xi \to 0$, one can choose $a, b, c > 0$, which are all $O(\xi)$. In this case, both eigenvalues $\tilde{\lambda}_1$ and $\lambda_2$ are $O(\xi)$. Therefore, $\omega = O(\xi)$ as well.

2. When $\xi \to +\infty$, one can choose $a, b, c > 0$, which are all $O(\xi^{-1})$. As a result, both $\tilde{\lambda}_1$ and $\lambda_2$ are $O(\xi^{-1})$. Therefore, $\omega = O(\xi^{-1})$ as well.

To summarize, although the problems are different, the asymptotics of $\omega$ in terms of $\xi$ are indeed consistent with the previous results \cite{20, 10, 24}.

3.3 Connection between time reversal of reverse process and optimally controlled forward process

In this section we study the connection between an optimally controlled Langevin process and the time reversal of the reverse Langevin process \cite{78}. Let us first introduce the optimal control problem

$$
\mathcal{U}(q, p, t) = \min_{u_s} \mathbb{E} \left( \mathcal{W}_n^{u_{(t,T)}} + \frac{1}{4} \int_t^T |u_s|^2 \, ds \left| q^n(t) = q, p^n(t) = p \right) , \quad q, p \in \mathbb{R}^n, \quad t \in [0, T],
$$

(95)
of the controlled process

$$
dq^n(s) = \nabla_p H(q^n(s), p^n(s), s) \, ds,
$$

$$
dp^n(s) = -\nabla_q H(q^n(s), p^n(s), s) \, ds - \gamma(q^n(s), s) \nabla_p H(q^n(s), p^n(s), s) \, ds + \sigma(q^n(s), s) u_s \, ds + \sqrt{2\beta^{-1}} \sigma(q^n(s), s) \, dw(s),
$$

(96)

where $u_s \in \mathbb{R}^m$, $0 \leq s \leq T$, is the control force, the minimum is over all adapted processes $u_s$ such that (96) is well-defined, and (cf. \cite{83})

$$
\mathcal{W}_n^{u_{(t,T)}} = \int_t^T \frac{\partial H}{\partial s} (q^n(s), p^n(s), s) \, ds, \quad 0 \leq t \leq T.
$$

(97)

It is known that the optimal control $u^*$ of (95)–(96) exists under mild conditions, and is given by

$$
u_s^* = u_s^*(q, p) = -2\sigma^T(q, s) \nabla_p \mathcal{U}(q, p, s),
$$

(98)
when the system’s state is at $(q, p) \in \mathbb{R}^n \times \mathbb{R}^n$ at time $s$. We also introduce the probability measure $\pi^*_0$ on $\mathbb{R}^n \times \mathbb{R}^n$, which is defined as

$$
d\pi^*_0(q, p) = \frac{1}{Z(T)} \mathbb{E} \left( e^{-\beta H} \left| q(0) = q, p(0) = p \right) e^{-\beta H(q, p, 0)} \, dq dp,
$$

(99)
where $Z(T)$ and $W$ are defined in (71) and (83), respectively, and $E(\cdot | q(0) = q, p(0) = p)$ denotes the path ensemble average of (69) starting from $(q, p)$ at $s = 0$. (Note that, from Jarzynski’s equality (125) in Appendix B.2, one directly sees that the integration of $\pi^*_0$ over $\mathbb{R}^n \times \mathbb{R}^n$ is indeed one.) It turns out that the optimal control $u^*$ and the probability measure $\pi^*_0$ provide the optimal importance sampling Monte Carlo estimators based on the Jarzynski’s equality for Langevin dynamics. We refer to Appendix B.2 for further motivations of (95)–(96).

Our main result is stated below, which relates the optimally controlled Langevin process (96) with $u = u^*$ in (98) to the time reversal of the reverse Langevin process (78).

**Theorem 4.** Let $(q^R(s), p^R(s))$ be the reverse process (78) starting from the initial distribution $\pi^R_0$ at $s = 0$. Assume that the probability distribution of $(q^R(s), p^R(s))$ has a positive smooth density with respect to Lebesgue measure for all $s \in [0, T]$. Define $(q^{R-}(s), p^{R-}(s)) = (q^R(T - s), p^R(T - s))$ for $s \in [0, T]$. Denote by $(q^{a^*}(s), p^{a^*}(s))$ the controlled process (96) under the optimal control $u^*$ in (98) starting from the distribution $\pi^*_0$ in (99). Then, $(q^{R-}(s), p^{R-}(s))$ and $(q^{a^*}(s), p^{a^*}(s))$ have the same law on the path space $C([0, T], \mathbb{R}^n \times \mathbb{R}^n)$.

**Proof.** We sketch the proof since it is similar to the proof of Theorem 2.

Let $\rho^R$ be the probability distribution of $(q^R(s), p^R(s))$ at $s \in [0, T]$. Denote by $\rho^R(q, p, s)$ the probability density of $\pi^R_s$ with respect to Lebesgue measure. Similar to (104), $\rho^R$ satisfies the Fokker-Planck equation

$$\frac{\partial \rho^R}{\partial s} = (Q^R)T \rho^R, \quad s \in [0, T],$$

(100)

where $Q^R_s$ is the generator in (29).

Recall the reverse process (78), which we rewrite as

$$\frac{dq^R(s)}{ds} = - \nabla_p \tilde{H}(q^R(s), p^R(s), s) ds$$

$$\frac{dp^R(s)}{ds} = \nabla_q \tilde{H}(q^R(s), p^R(s), s) ds - \tilde{\gamma}(q^R(s), s) \nabla_p \tilde{H}(q^R(s), p^R(s), s) ds$$

$$+ \sqrt{2\beta^{-1}}\tilde{\sigma}(q^R(s), s) dw(s),$$

(101)

where we have defined, for all $(q, p, s) \in \mathbb{R}^n \times \mathbb{R}^n \times [0, T]$,

$$\tilde{H}(q, p, s) = H(q, p, T - s),$$

$$\tilde{\sigma}(q, s) = \sigma(q, T - s), \quad \tilde{\gamma}(q, s) = (\tilde{\sigma}^T)(q, s) = \gamma(q, T - s).$$

(102)

Since $\rho^R$ is both smooth and positive, the result in (22) asserts that the time reversal $(q^{R-}(s), p^{R-}(s)) = (q^R(T - s), p^R(T - s))$, $s \in [0, T]$, is again a diffusion process which satisfies the SDE

$$\frac{d q^{R-}(s)}{ds} = \nabla_q \tilde{H}(q^{R-}(s), p^{R-}(s), T - s) ds$$

$$\frac{d p^{R-}(s)}{ds} = b^{-}(q^{R-}(s), p^{R-}(s), T - s) ds + \sqrt{2\beta^{-1}}\tilde{\sigma}(q^{R-}(s), T - s) dw(s)$$

(103)

on $s \in [0, T]$, with the initial distribution $\pi^R_T$, where the drift $b^-$ is, for all $(q, p, s) \in \mathbb{R}^n \times \mathbb{R}^n \times [0, T]$,

$$b^-(q, p, s) = \left(- \nabla_q \tilde{H} + \tilde{\gamma} \nabla_p \tilde{H} + \frac{2}{\beta \rho^R} \nabla_p \cdot (\rho^R \tilde{\gamma}) \right)(q, p, s).$$

(104)
Substituting (102) in (104), we find
\[
\begin{align*}
b^-(q, p, T - s) &= \left( -\nabla_q \hat{H} + \gamma \nabla_p \hat{H} + \frac{2}{\beta g^R} \nabla_p \cdot (\rho^R \gamma) \right)(q, p, T - s) \\
&= \left( -\nabla_q H + \gamma \nabla_p H + \frac{2}{\beta g^R} \nabla_p \cdot (\rho^R \gamma) \right)(q, p, s) \\
&= \left( -\nabla_q H + \gamma \nabla_p H + \frac{2}{\beta g^R} \gamma \nabla_p g^R \right)(q, p, s) \\
&= \left( -\nabla_q H - \gamma \nabla_p H + \frac{2}{\beta} \gamma \nabla_p \ln(e^{\beta H} \rho^R \gamma) \right)(q, p, s),
\end{align*}
\]
(105)
where we have used the notation \(\rho^R, -\gamma(g^R, p, s) = \rho^R(q, p, T - s)\) and the fact that \(\gamma\) is independent of \(p\). Using (102) and (105), (103) can be written more explicitly as
\[
\begin{align*}
dq^R(-) &= \nabla_p H(q^R, p^R, s) ds \\
p^R(-) &= -\nabla_q H(q^R, p^R, s) ds - \gamma(q^R, p^R, s) \nabla_p H(q^R, p^R, s) ds \\
&\quad + \frac{2}{\beta} \left( \gamma \nabla_p \ln(e^{\beta H} \rho^R) \right)(q^R, p^R, s) ds \\
&\quad + \sqrt{2\beta^{-1}} \sigma(q^R, p^R, s) dw(s).
\end{align*}
\]
(106)
Define \(g(q, p, s) = e^{\beta H} (q, p, s) \rho^R(q, p, T - s) Z(T)\), where \(Z(T)\) is defined in (71). Similar to the proof of Theorem 2, one can again show that \(g\) and the value function \(U\) in (95) are related by
\[
U = -\beta^{-1} \ln g.
\]
(107)
We refer to (64)–(66) in Section 2.3 and (130)–(131) in Appendix B.2 for details. Combining (96), (98), (106) and (107), we see that both processes \((q^R(-), p^R(-))\) and \((q^\ast(-), p^\ast(-))\) satisfy the same SDE.

Using Feynman-Kac formula, the PDE of \(g\) (see (129)–(130) in Appendix B.2), as well as \(W\) in (83), we can verify that the distribution \(\pi_0^R\) is the same as the distribution \(\pi_0^\ast\) in (99). To summarize, we have proved that both \((q^R(-), p^R(-))\) and \((q^\ast(-), p^\ast(-))\) satisfy the same SDE with the same initial distribution \(\pi_0^\ast\). Therefore, they have the same law on the path space.

\section*{Acknowledgements}

Some preliminary results of this paper were presented at a Focus Retreat organized by Carsten Hartmann, Tim Sullivan and Sebastian Reich at Potsdam, Germany, in January 2019. The author would like to thank them for helpful discussions. The author also benefited from discussions with Gabriel Stoltz on hypo-coercivity of Langevin dynamics. This work is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany’s Excellence Strategy — The Berlin Mathematics Research Center MATH+ (EXC-2046/1, project ID: 390685689).
A Proofs of fluctuation relations

In this section, we present concise derivations of the fluctuation relations for both Brownian dynamics in Section 2.1 and Langevin dynamics in Section 3.1.

A.1 Fluctuation relation for Brownian dynamics

Proof of Proposition 1. Consider the PDE
\[
\frac{\partial f}{\partial s} = \mathcal{L}_s^T f + \left( \eta - \beta \frac{\partial V}{\partial s} \right) f, \quad s \in [0, T],
\]
\[
f(\cdot, 0) = f_0,
\]
where \( f_0 : \mathbb{R}^n \to \mathbb{R} \) is a bounded continuous function. One can verify that its solution can be expressed as (similar to the derivation of Kolmogorov’s forward equation [46], for instance, by introducing a test function and applying Ito’s formula)
\[
f(x', t) = \int_{\mathbb{R}^n} \mathbb{E} \left[ \exp \left( \int_0^t \eta(x(s), s) \, ds - \beta \int_0^t \frac{\partial V}{\partial s}(x(s), s) \, ds \right) \delta(x(t) - x') \ \bigg| \ x(0) = x \right] f_0(x) \, dx,
\]
(108)
for \((x', t) \in \mathbb{R}^n \times [0, T]\). On the other hand, using the second identity in (34) of Lemma 1, from (108) we find
\[
\frac{\partial (e^{\beta V} f)}{\partial s} = (e^{\beta V} f) \eta + e^{\beta V} \mathcal{L}_s^T f = (e^{\beta V} f) \eta + \mathcal{L}_s^{R} (e^{\beta V} f).
\]
(110)
Define
\[
\phi(x, s) = e^{\beta V(x,T-s)} f(x, T-s), \quad \forall \ (x, s) \in \mathbb{R}^n \times [0, T].
\]
(111)
Then, (110) implies
\[
\frac{\partial \phi}{\partial s} + \eta(x, T-s) \phi + \mathcal{L}_s^{R} \phi = 0, \quad s \in [0, T],
\]
\[
\phi(x, T) = e^{\beta V(x,0)} f_0(x), \quad x \in \mathbb{R}^n.
\]
(112)
Since \(\mathcal{L}_s^{R}\) is the generator of the reverse dynamics (31) at time \(s\), applying Feynman-Kac formula and using the terminal condition in (112), we know
\[
\phi(x', t) = \mathbb{E} \left[ \exp \left( \int_t^T \eta(x^{R}(s), T-s) \, ds \right) \phi(x^{R}(T), T) \ \bigg| \ x^{R}(t) = x' \right] f_0(x) e^{\beta V(x,0)} \, dx,
\]
(113)
for all \((x', t) \in \mathbb{R}^n \times [0, T]\). Combining (109), (111) and (113), we can derive

\[
\int_{\mathbb{R}^n} \mathbb{E} \left[ \exp \left( \int_0^T \eta(x^R(s), T - s) ds \right) \delta \left( x^R(T) - x' \right) \right] f_0(x) e^{\beta V(x, 0)} dx
\]

\[= \phi(x', 0)
\]

\[= e^{\beta V(x', T)} f(x', T)
\]

\[= e^{\beta V(x', T)} \int_{\mathbb{R}^n} \mathbb{E} \left[ \exp \left( \int_0^T \eta(x(s), s) ds - \beta \int_0^T \frac{\partial V}{\partial s}(x(s), s) ds \right) \delta(x(T) - x') \right] f_0(x) dx.
\]

Therefore, we obtain (36), since (114) holds for all bounded continuous functions \(f_0\).

A.2 Fluctuation relation for Langevin dynamics

Proof of Proposition 3. The proof is similar to that of Proposition 1 in Appendix A.1. Consider the PDE

\[
\frac{\partial f}{\partial s} = Q_s^T f + (\eta - \beta \frac{\partial H}{\partial s}) f, \quad s \in [0, T],
\]

\[f(\cdot, \cdot, 0) = f_0,
\]

where \(f_0 : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}\) is a bounded continuous function.

Introduce the function \(\phi : \mathbb{R}^n \times \mathbb{R}^n \times [0, T] \rightarrow \mathbb{R}\), where \(\phi(q, p, s) = (e^{\beta H}) q, p, T - s\). Using (115) and the second identity in (80) of Lemma 3, we can verify that

\[
\frac{\partial (e^{\beta H})}{\partial s} = (e^{\beta H}) \eta + Q_s^R (e^{\beta H} f),
\]

from which we obtain

\[
\frac{\partial \phi}{\partial s} + \eta(q, p, T - s) \phi + Q_s^R \phi = 0, \quad s \in [0, T],
\]

\[
\phi(q, p, T) = e^{\beta H(q, p, 0)} f_0(q, p), \quad (q, p) \in \mathbb{R}^n \times \mathbb{R}^n.
\]

(117) is obtained after expressing the solutions of PDEs (115) and (117) in terms of path ensemble averages of the Langevin dynamics (69) and (78), respectively. We refer to (109), (113), and (114) for details.

B Optimal control problems related to Jarzynski’s identity

In this section, we discuss the relevance of both the optimal control problem (51)–(52) in Section 2.3 and the optimal control problem (95)–(96) in Section 3.3 to the study of free energy calculation based on Jarzynski’s identity.

B.1 Brownian dynamics

We consider the forward process (22) and recall the notations in Section 2.1. Jarzynski’s identity states that \(26 \ 27 \)

\[
\Delta F = F(T) - F(0) = -\beta^{-1} \ln \mathbb{E} \left( e^{-\beta W} \bigg| x(0) \sim \nu_0^\infty \right),
\]

(118)
where $F$ is the free energy in (30), $\mathbb{E}(\cdot | x(0) \sim \nu_0^\infty)$ denotes the path ensemble average of (22) with initial distribution $\nu_0^\infty$, and $W$ is the work in (37). (118) provides a way of computing the free energy difference $\Delta F$ by sampling nonequilibrium trajectories, although the sampling variance is an issue of Monte Carlo estimators based on (118). See [15, 28, 39] for previous studies. In the following, we recall some analysis of (118) using change of measures [21], and show how the optimal control problem (51)–(52) arises.

Let $\nu_0$ be a probability measure on $\mathbb{R}^n$ that is absolutely continuous with respect to the Lebesgue measure, and $u_s \in \mathbb{R}^m$, $0 \leq s \leq T$, is a (feedback) control force such that the Novikov’s condition is satisfied [10]. Applying change of measures to (118), we see that the free energy difference can also be estimated using

$$
\Delta F = -\beta^{-1} \ln \mathbb{E} \left( e^{-\beta W} \frac{\partial P}{\partial \nu} \bigg| x^n(0) \sim \nu_0 \right)
$$

(119)

where $\mathbb{E}(\cdot | x^n(0) \sim \nu_0)$ denotes the path ensemble average of the controlled nonequilibrium process

$$
dx^n(s) = \left( J - \gamma \nabla V + \frac{1}{\beta} \nabla \cdot \gamma \right)(x^n(s), s) \, ds + \sqrt{2\beta^{-1}} \sigma(x^n(s), s) \, dw(s)
$$

$$
+ \sigma(x^n(s), s) u_s \, ds ,
$$

starting from $x^n(0) \sim \nu_0$, $P$ and $P_{\nu_0}$, are the path measures of the original process (22) and the controlled process (120), respectively. The explicit expression of the likelihood ratio in (119) is given by Girsanov’s theorem [40]. Moreover, there exists an optimal change of measures $P_{\nu_0}^\ast$, which corresponds to an optimal initial distribution $\nu_0^\ast$ and an optimal control force $u^\ast$, such that the variance of the (importance sampling) Monte Carlo estimator based on (119) equals zero [21]. In fact, a simple argument shows that $\nu_0^\ast$ satisfies

$$
d\nu_0^\ast \frac{dx}{dx} = \frac{e^{-\beta V(x,0)}}{Z(T)} \mathbb{E} \left( e^{-\beta W} \bigg| x(0) = x \right) = \frac{e^{-\beta V(x,0)}}{Z(T)} g(x,0) ,
$$

(121)

where

$$
g(x,t) = \mathbb{E} \left( e^{-\beta \int_t^T \frac{\partial V}{\partial s} (x(s),s) \, ds} \bigg| x(t) = x \right) , \quad \forall \ (x,t) \in \mathbb{R}^n \times [0,T] .
$$

(122)

Feynman-Kac formula implies that $g$ solves the PDE

$$
\frac{\partial g}{\partial s} + \mathcal{L}_s g - \beta \frac{\partial V}{\partial s} g = 0 , \quad \text{and} \quad g(\cdot,T) \equiv 1 .
$$

(123)

The optimal control problem (51)–(52) is recovered by considering the logarithmic transformation $U = -\beta^{-1} \ln g$ [16]. In fact, using the identity (33) in Lemma [1] we can deduce from (123) that $U : \mathbb{R}^n \times [0,T] \to \mathbb{R}$ satisfies the HJB equation

$$
\frac{\partial U}{\partial s} + \min_{v \in \mathbb{R}^m} \left\{ \mathcal{L}_s U + (\sigma v) \cdot \nabla U + \frac{|v|^2}{4} + \frac{\partial V}{\partial s} \right\} = 0 , \quad (x,s) \in \mathbb{R}^n \times [0,T] ,
$$

(124)

Therefore, $U$ is the value function of the stochastic optimal control problem (51)–(52) [16]. It is also known that the optimal control of the optimal control problem (51)–(52) is given by $u^\ast$, which coincides with $u^\ast$ that leads to the optimal change of measures (119).
B.2 Langevin dynamics

Similar to the case of Brownian dynamics in Appendix B.1, Jarzynski’s identity
\[
\Delta F = F(T) - F(0) = -\beta^{-1} \ln E \left( e^{-\beta W} \left| (q(0), p(0)) \sim \pi^\infty_0 \right. \right),
\]
holds for Langevin dynamics [29][6], where \( F \) is the free energy in (72), \( E(\cdot \mid (q(0), p(0)) \sim \pi^\infty_0) \) denotes the path ensemble average of the (forward) process (69) starting from the initial distribution \( \pi^\infty_0 \) in (71), and \( W \) is the work in (83). In the following, we explain how the optimal control problem (95)–(96) is related to (125).

Applying change of measures to (125), we get
\[
\Delta F = -\beta^{-1} \ln E \left( e^{-\beta W} \left| \frac{dP}{dP_{\tilde{\pi}_0}} \right| (q^u(0), p^u(0)) \sim \tilde{\pi}_0 \right) \tag{126}
\]
where \( P_u \) and \( E(\cdot \mid (q^u(0), p^u(0)) \sim \tilde{\pi}_0) \) denote respectively the probability measure (in path space) and the path ensemble average of the controlled Langevin process
\[
\begin{align*}
\frac{dq^u(s)}{ds} &= \nabla_q H(q^u(s), p^u(s), s) ds \\
\frac{dp^u(s)}{ds} &= -\nabla_p H(q^u(s), p^u(s), s) ds - \gamma g (q^u(s), s) \frac{\partial H}{\partial q} (q^u(s), s) ds + \sigma q^u(s), s) u_s ds + \sqrt{2\beta^{-1}} \sigma(q^u(s), s) dw(s)
\end{align*}
\tag{127}
\]
starting from the initial distribution \( \tilde{\pi}_0 \) (which may differ from \( \pi^\infty_0 \), \( P \) denotes the probability measure of (69) starting from \( \pi^\infty_0 \), and \( u_s \in \mathbb{R}^m \), \( 0 \leq s \leq T \), is the control force. Note that in (127) the control force is only applied to the equation of momentum \( p \) [54]. The explicit expression of the likelihood ratio in (126) is again given by Girsanov’s theorem [40]. In particular, there is an optimal change of measure, characterized by the optimal initial distribution \( \pi^*_0 \), and the optimal control force \( u^* \), such that the variance of the importance sampling Monte Carlo estimator based on (126) equals zero. A simple analysis shows that
\[
d\pi^*_0 = \frac{1}{Z(T)} g(q, p, 0) e^{-\beta H(q, p, 0)} dqdp, \tag{128}
\]
where
\[
g(q, p, t) = E \left( e^{-\beta \int_t^T \frac{\partial H}{\partial q}(q(s), p(s), s) ds} \left| q(t) = q, p(t) = p \right. \right), \quad \forall (q, p, t) \in \mathbb{R}^n \times \mathbb{R}^n \times [0, T].
\tag{129}
\]
Feymann-Kac formula implies that \( g \) in (129) satisfies the PDE
\[
\frac{\partial g}{\partial s} + Q_s g - \beta \frac{\partial H}{\partial q} g = 0, \quad g(\cdot, \cdot, T) = 1, \tag{130}
\]
where \( Q_s \) is the generator of (69) at time \( s \).

The optimal control problem (95)–(96) is then recovered by considering \( \mathcal{U} = -\beta^{-1} \ln g \). Concretely, applying (81) in Lemma 3 one can derive from (130) the HJB equation
\[
\frac{\partial \mathcal{U}}{\partial s} + \min_{v \in \mathbb{R}^m} \left\{ Q_s \mathcal{U} + (\sigma v) \cdot \nabla_p \mathcal{U} + \frac{|v|^2}{4} + \frac{\partial H}{\partial q} \right\} = 0, \tag{131}
\]
\[
\mathcal{U}(\cdot, \cdot, T) = 0.
\]
Therefore, \( \mathcal{U} \) is the value function of the optimal control problem (95)–(96) [16]. The optimal control of (94)–(96) is given by (89), which coincides with \( u^* \) that leads to the optimal change of measure in (126).
C Relative entropy estimate for Langevin dynamics: Proof of Theorem 3

In this section, we prove Theorem 3 in Section 3.2. The proof is based on the hypocoercivity theory [53] (in the simplest setting), which is a general framework for the study of the convergence of degenerate kinetic equations towards equilibrium. Before presenting the proof, we need to introduce some notations.

First of all, let us define the operators

\[ A = \nabla_p, \quad A_i = \frac{\partial}{\partial p_i}, \quad B = p \cdot \nabla_q - \nabla_q V \cdot \nabla_p, \]

\[ C = \nabla_q, \quad C_i = [A_i, B] = A_i B - B A_i = \frac{\partial}{\partial q_i}, \quad 1 \leq i \leq n, \]

(132)

where \([A_i, B]\) denotes the commutator of \(A_i\) and \(B\), and we have used the fact that \(V = V(q, s)\) is independent of \(p\) to derive the last equality. Note that, since \(V\) is time-dependent, \(B = B_s\) is time-dependent as well. Following [53], for \(s \in [0, T]\), we denote by \(A^*_i\) and \(B^*\) the adjoint operators of \(A_i\) and \(B\) with respect to the probability measure \(\pi_\infty\) (71), respectively. (The notations here should be compared to (25) and (74), which are adjoint operators with respect to Lebesgue measure. Also see Remark 1 for related discussions.) Note that we are considering the special case (87), i.e.,

\[ \sigma = \sqrt{\xi} I_n, \quad H(q, p, s) = V(q, s) + \frac{|p|^2}{2}, \quad (q, p, s) \in \mathbb{R}^n \times \mathbb{R}^n \times [0, T], \]

(133)

where \(\xi > 0\). One can verify that (see [53, Section 7])

\[ A_i^* = -\frac{\partial}{\partial p_i} + \beta p_i, \quad A_i^* A_i = -\frac{\partial^2}{\partial p_i^2} + \beta p_i \frac{\partial}{\partial p_i}, \]

\[ B^* = -B, \]

\[ [C_i, B] = -\sum_{l=1}^n \frac{\partial^2 V}{\partial q_i \partial q_l} \frac{\partial}{\partial p_l}, \quad [A_i, A_j^*] = \beta \delta_{ij}, \quad [A_i, C_j] = 0, \quad [C_i, A_j^*] = 0, \]

for \(1 \leq i, j \leq n\), as well as

\[ Q_s = -\frac{\xi}{\beta} \sum_{i=1}^n A_i^* A_i + B_s, \quad Q^R_{T-s} = Q^*_s = -\frac{\xi}{\beta} \sum_{i=1}^n A_i^* A_i - B_s, \]

(135)

where \(Q_s, Q^R_s\) are defined in (70) and (79) (in the case of (133)), respectively. The identities in (134) and (135) allow us to interchange the order of two first-order differential operators (in the proof of Lemma 5 below). To simplify notations, we introduce functions

\[ h = \frac{d\pi_s}{d\pi_\infty}, \quad \text{and} \quad u = \ln h, \]

(136)

where the probability measure \(\pi_s\) is defined in (73). Also, we will write \(\int f d\pi_s\) or \(\int f d\pi_\infty\) for integrations over the entire phase space \(\mathbb{R}^n \times \mathbb{R}^n\). With these conventions, (51) in Lemma 3 and (85) in Lemma 4 imply

\[ \frac{\partial h}{\partial s} = \beta \left( \frac{\partial V}{\partial s} - \frac{dF(s)}{ds} \right) h + Q^*_s h, \]

(137)

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\[
\frac{\partial u}{\partial s} = \beta \left( \frac{\partial V}{\partial s} - \frac{dF(s)}{ds} \right) + Q^*_s u + \frac{\xi}{\beta} |Au|^2 ,
\] (138)

where we have used \( \frac{dH}{ds} = \frac{\partial V}{\partial s} \) thanks to (133).

We need the following result, which is essentially a special case of the more general result [53, Lemma 32]. We present its proof since in the current setting \( V \) is time-dependent and the calculation is more transparent.

**Lemma 5.** Let \( h \) and \( u \) be the functions in (136). We have the following identities.

\[
\begin{align*}
\frac{d}{ds} \int |Au|^2 d\pi_s &= -\frac{2\xi}{\beta} \sum_{i,j=1}^n \int (A_i A_j u)^2 d\pi_s - 2\xi \int |Au|^2 d\pi_s - 2 \int \langle Au, Cu \rangle d\pi_s , \\
\frac{d}{ds} \int |Cu|^2 d\pi_s &= 2\beta \int \langle Cu, C \frac{\partial V}{\partial s} \rangle d\pi_s - 2\xi \sum_{i,j=1}^n \int (C_j A_i u)^2 d\pi_s \\
&\quad - 2 \int \langle [C, B] u, Cu \rangle d\pi_s , \\
\frac{d}{ds} \int \langle Au, Cu \rangle d\pi_s &= \beta \int \langle Au, C \frac{\partial V}{\partial s} \rangle d\pi_s - \frac{2\xi}{\beta} \sum_{i,j=1}^n \int (A_j A_i u)(A_i C_j u) d\pi_s \\
&\quad - \xi \int \langle Au, Cu \rangle d\pi_s - \int |Cu|^2 d\pi_s - \int \langle Au, [C, B] u \rangle d\pi_s .
\end{align*}
\]

**Proof.** Since the proof is similar to the one of [53, Lemma 32], we only sketch the derivation of the first identity. The other two identities can be derived similarly, using (132), (134) and integration by parts.

Recall that \( Q^T_s \) and \( Q^*_s \) are the adjoint operators of \( Q_s \) with respect to Lebesgue measure and the probability measure \( \pi^\infty_s \), respectively. Using \( d\pi_s = \varrho dqdp \), \( \text{(136)} \), and the Fokker-Planck equation (174), we compute

\[
\begin{align*}
\frac{d}{ds} \int |Au|^2 d\pi_s &= \frac{d}{ds} \int |Au|^2 \varrho dqdp \\
&= \int \left( \frac{\partial}{\partial s} |Au|^2 \right) \varrho dqdp + \int |Au|^2 Q^T_s \varrho dqdp \\
&= 2 \int \langle Au, A \frac{\partial u}{\partial s} \rangle d\pi_s + \int (Q_s |Au|^2) d\pi_s \\
&= 2 \int \langle Au, A \frac{\partial u}{\partial s} \rangle h d\pi^\infty_s + \int (Q_s |Au|^2) h d\pi^\infty_s .
\end{align*}
\]

Using (138), (135), and integration by parts formula, we get

\[
\frac{d}{ds} \int |Au|^2 d\pi_s
\]
where we have used \((Au) = (A \ln h)h = Ah\), as well as \(A(\frac{\partial W}{\partial s}) - \frac{\partial F}{\partial s} = \nabla_p \frac{\partial F}{\partial s} = 0\).

Concerning \(J_1\), using integration by parts formula, the identities

\[ A_i A_j^* = A_j^* A_i + \beta \delta_{ij} \] (see (133)) and \(A_i A_j = A_j A_i\), we can derive

\[
J_1 = -\frac{2\xi}{\beta} \sum_{j=1}^{n} \left( \langle Au, A A_j^* A_j u \rangle h \, d\pi_s^\infty \right) + \frac{\xi}{\beta} \int \langle Ah, A|Au|^2 \rangle \, d\pi_s^\infty
\]

which, using the identities

\[
\sum_{i,j=1}^{n} \left( \langle A_i A_j^* A_j u \rangle h \, d\pi_s^\infty \right) = \sum_{i,j=1}^{n} \left( \langle A_i h \rangle (A_i A_j^* A_j u) \right) h \, d\pi_s^\infty
\]

and

\[
\sum_{i,j=1}^{n} \left( \langle A_i A_j u \rangle^2 h \, d\pi_s^\infty \right) = \sum_{i,j=1}^{n} \left( \langle A_i A_j u \rangle^2 h \, d\pi_s^\infty \right)
\]

leads to

\[
J_1 = -\frac{2\xi}{\beta} \sum_{i,j=1}^{n} \left( \langle A_i A_j^* A_j u \rangle h \, d\pi_s^\infty \right) + \frac{\xi}{\beta} \int \langle Ah, A|Au|^2 \rangle \, d\pi_s^\infty
\]

Concerning \(J_2\), using \(AB = BA + [A, B] = BA + C\) (see (132)), we compute

\[
J_2 = -2 \int \langle Au, ABu \rangle h \, d\pi_s^\infty + \int (B|Au|^2) h \, d\pi_s^\infty
\]

which, using the identities

\[
\sum_{i,j=1}^{n} \left( \langle A_i A_j u \rangle^2 h \, d\pi_s^\infty \right) = \sum_{i,j=1}^{n} \left( \langle A_i A_j u \rangle^2 h \, d\pi_s^\infty \right)
\]

and

\[
\sum_{i,j=1}^{n} \left( \langle A_i u \rangle h \, d\pi_s^\infty \right) = \sum_{i,j=1}^{n} \left( \langle A_i u \rangle h \, d\pi_s^\infty \right)
\]

leads to

\[
J_2 = -2 \int \langle Au, ABu \rangle h \, d\pi_s^\infty + \int (B|Au|^2) h \, d\pi_s^\infty
\]

The first conclusion follows by summing up (140) and (141).
Now we are ready to prove Theorem 3.

Proof of Theorem 3. Recall the quantity \( E(s) \) in (91). Using (132) and (136), we can write

\[
E(s) = R^{\text{Lan}}(s) + a \int |Au|^2 \, d\pi_s + 2b \int \langle Au, Cu \rangle \, d\pi_s + c \int |Cu|^2 \, d\pi_s. \tag{142}
\]

Since the spatial marginal measure of \( \pi_s^\infty \) satisfies LSI with constant \( \kappa \), the measure \( \pi_s^\infty \) itself satisfies LSI with constant \( \min\{\kappa, \beta\} \) (see Remark 4), which implies

\[
R^{\text{Lan}}(s) \leq \frac{1}{2 \min\{\kappa, \beta\}} \int (|Au|^2 + |Cu|^2) \, d\pi_s. \tag{143}
\]

Let us choose constants \( a, b, c > 0 \), such that both matrices

\[
S = \begin{pmatrix} a & b \\ b & c \end{pmatrix}, \quad \tilde{S} = \begin{pmatrix} \xi(\frac{1}{\beta} + 2a) - 2b(1 + L) & -(a + b\xi + cL) \\ -(a + b\xi + cL) & 2b - c \end{pmatrix} \tag{144}
\]

are positive definite, where \( L > 0 \) is the upper bound of \( \|\nabla^2 V\|_2 \) in (89). For instance, this is satisfied when \( a, b, c \) are small enough, such that \( 2b > c \) and \( b^2 < ac \). Denote by \( \lambda_1, \lambda_2 \) the two (real) positive eigenvalues of \( S \), where \( 0 < \lambda_1 \leq \lambda_2 \), and denote by \( \tilde{\lambda}_1, \tilde{\lambda}_2 \) the two (real) positive eigenvalues of \( \tilde{S} \) such that \( 0 < \tilde{\lambda}_1 \leq \tilde{\lambda}_2 \). Then, we have

\[
\lambda_1(x^2 + y^2) \leq ax^2 + 2bxy + cy^2 \leq \lambda_2(x^2 + y^2),
\]

\[
\tilde{\lambda}_1(x^2 + y^2) \leq \left[ \xi\left(\frac{1}{\beta} + 2a\right) - 2b(1 + L) \right] x^2 - 2(a + b\xi + cL)xy + (2b - c)y^2 \tag{145}
\]

\[
\leq \tilde{\lambda}_2(x^2 + y^2),
\]

for all \( x, y \in \mathbb{R} \). (145) and (143) imply

\[
R^{\text{Lan}}(s) \leq E(s) \leq \left( \frac{1}{2 \min\{\kappa, \beta\}} + \lambda_2 \right) \int (|Au|^2 + |Cu|^2) \, d\pi_s, \quad \forall s \in [0, T]. \tag{146}
\]

Applying the identities in both Proposition 4 and Lemma 5, we can derive

\[
\frac{d}{ds} E(s) = -\beta \int \frac{\partial V}{\partial s} \, d\pi_s^\infty + \beta \int \frac{\partial V}{\partial s} \, d\pi_s + 2c\beta \int \langle Cu, C \frac{\partial V}{\partial s} \rangle \, d\pi_s + 2b\beta \int \langle Au, C \frac{\partial V}{\partial s} \rangle \, d\pi_s
\]

\[
- \xi\left(\frac{1}{\beta} + 2a\right) \int |Au|^2 \, d\pi_s - 2(a + b\xi) \int \langle Au, Cu \rangle \, d\pi_s - 2b \int |Cu|^2 \, d\pi_s - 2b \int \langle Au, C, B \rangle \, d\pi_s - 2c \int \langle C, B \rangle \, d\pi_s
\]

\[
- \frac{2c}{\beta} \sum_{i,j=1}^{n} \int \left[ a(A_i A_j u)^2 + 2b(C_j A_i u)(A_i A_j u) + c(C_j A_i u)^2 \right] \, d\pi_s
\]

\[= J_1 + J_2 + J_3 + J_4 + J_5, \tag{147}
\]
where $J_l$, $1 \leq l \leq 5$, denotes the terms on the $l$th line in the second equality above. Clearly, (145) implies $J_5 \leq 0$. In the following, we estimate $J_l$ for $l = 1, 2, 3, 4$.

Recall the constants $L_1$, $L_2$ and $L$ in the assumption (38). Similar to (17), using (13) and Csiszár-Kullback-Pinsker inequality (15), we find

\begin{equation}
J_1 \leq \beta \left| \frac{\partial V}{\partial s} d\pi_s - \int \frac{\partial V}{\partial s} d\pi_s \right| \\
\leq \beta L_1 \sqrt{2DL_1(\pi_s | \pi_s^\infty)} = \beta L_1 \sqrt{2R_L^\lambda(s)} \leq \frac{\beta^2 L_1^2}{2\omega} + \omega \mathcal{E}(s),
\end{equation}

for all $\omega > 0$, while Cauchy-Schwarz inequality implies

\begin{equation}
J_2 \leq 2c\beta \int \langle Cu, C \frac{\partial V}{\partial s} \rangle d\pi_s + 2b\beta \int \langle Au, C \frac{\partial V}{\partial s} \rangle d\pi_s \\
\leq \left( c + \frac{b}{2} \right) \beta^2 L_2^2 + c \int |Cu|^2 d\pi_s + 2b \int |Au|^2 d\pi_s.
\end{equation}

For $J_3$, we clearly have

\begin{equation}
J_3 \leq -\xi \left( \frac{1}{\beta} + 2a \right) \int |Au|^2 d\pi_s + 2(a + b\xi) \int |Au||Cu| d\pi_s - 2b \int |Cu|^2 d\pi_s.
\end{equation}

For $J_4$, since $[C_1, B] = -\sum_{l=1}^n \frac{\partial^2 V}{\partial q_l \partial q_l} \frac{\partial^2}{\partial q_l}$ (see (134)) and $\|\nabla^2 V\|_2 \leq L$, we have

\begin{equation}
|J_4| = -2b \int \langle Au, [C, B]u \rangle d\pi_s - 2c \int \langle [C, B]u, Cu \rangle d\pi_s \\
\leq 2bL \int |Au|^2 d\pi_s + 2cL \int |Au| |Cu| d\pi_s.
\end{equation}

Let us choose $\omega > 0$, such that

\begin{equation}
2\omega = \bar{\lambda}_1 \left( \frac{1}{2 \min\{\kappa, \beta\}} + \lambda_2 \right)^{-1}.
\end{equation}

Substituting the estimates (148)–(151) into (147), applying (145), (146), and using (152), we find

\[
\begin{align*}
\frac{d}{ds} \mathcal{E}(s) &\leq \left[ \frac{\beta^2 L_1^2}{2\omega} + \left( c + \frac{b}{2} \right) \beta^2 L_2^2 \right] + \omega \mathcal{E}(s) - \left\{ \xi \left( \frac{1}{\beta} + 2a \right) - 2b(1 + L) \right\} \int |Au|^2 d\pi_s \\
&\quad - 2(cL + a + b\xi) \int |Au||Cu| d\pi_s + (2b - c) \int |Cu|^2 d\pi_s \\
&\leq \left[ \frac{\beta^2 L_1^2}{2\omega} + \left( c + \frac{b}{2} \right) \beta^2 L_2^2 \right] + \omega \mathcal{E}(s) - \bar{\lambda}_1 \int (|Au|^2 + |Cu|^2) d\pi_s \\
&\leq \left[ \frac{\beta^2 L_1^2}{2\omega} + \left( c + \frac{b}{2} \right) \beta^2 L_2^2 \right] + \omega \mathcal{E}(s) - \bar{\lambda}_1 \left( \frac{1}{2 \min\{\kappa, \beta\}} + \lambda_2 \right)^{-1} \mathcal{E}(s) \\
&= \left[ \frac{\beta^2 L_1^2}{2\omega} + \left( c + \frac{b}{2} \right) \beta^2 L_2^2 \right] - \omega \mathcal{E}(s).
\end{align*}
\]

The conclusion follows by applying Gronwall’s inequality.
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