The Most Probable Transition Paths of Stochastic Dynamical Systems: Equivalent Description and Characterization

Yuanfei Huang, Qiao Huang, Jinqiao Duan

Abstract

This work is devoted to show a sufficient and necessary description for the most probable transition paths of stochastic dynamical systems with Brownian noise. The equivalence is established by studying the relations between Markovian bridge measures and Onsager-Machlup action functionals. This cannot be achieved by existing methods because Markovian bridge measures are not quasi translation invariant. We overcome this problem by showing that the Onsager-Machlup action functional can be derived from a Markovian bridge process. We then demonstrate that, for some special cases of linear stochastic systems and nonlinear stochastic systems with small noise, the most probable transition path can be determined by a first order deterministic differential equation with an initial value. Finally, we illustrate our results with several examples.

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1 Introduction

Stochastic differential equations (SDEs) have been widely used to describe complex phenomena in physical, biological, and engineering systems. Due to the random fluctuations, transition phenomena between dynamically significant states occur in nonlinear systems. Hence a practical issue is to capture the transition behavior between two metastable states and determine the most probable transition path (which will be introduced in next section) for the stochastic dynamical systems. This problem can be traced back to the derivation of the Onsager-Machlup action functional (OM functional for short), which was firstly introduced by Onsager and Machlup to consider the probability of paths of a diffusion process, as the starting point of a theory of fluctuations [1, 2]. Their work was restricted to processes with linear drifts and constant diffusion coefficients. Later on, Tisza and Manning focused on the same issue for nonlinear equations [3]. The key observation was that the transition probability of a diffusion process can be expressed by a functional integral over paths, i.e., a Feynman path integral.

Some authors followed the idea of [3] to interpret the OM functional as a Lagrangian for determining the most probable transition path of a diffusion process, via a variational principle. This seems to be meaningless, since a solution curve of the variational principle is supposed to be twice differentiable while almost all paths of a diffusion process are nowhere differentiable, and the probability of a single path is zero anyhow. Instead, we can seek for the probability that a path lies within a “neighborhood” of a differentiable curve [4, 5]. Such a neighborhood is a tube along the curve. Then we can compare the probabilities of different tubes of same “thinness”. So the OM functional may be defined as the Lagrangian giving the most probable infinitesimal tube. We shall still use the terminology “most probable transition path” as in those earlier references, to indicate a solution of the variational principle, even though it is not a genuine path. This theory is the basis for many topics in physics and biochemistry, such as path integrals [6, 7, 8, 9, 10], path sampling [11, 12], transition rates [13, 14], transitions for non-Gaussian systems [15, 16], and biomolecular folding [17, 18], etc.

1 School of Mathematics and Statistics & Center for Mathematical Sciences & Hubei Key Laboratory of Engineering Modeling and Scientific Computing, Huazhong University of Science and Technology, Wuhan 430074, P.R. China. Email: yfhuang@hust.edu.cn
2 Group of Mathematical Physics (GFMUL), Department of Mathematics, Faculty of Sciences, University of Lisbon, Campo Grande, Edificio C6, PT-1749-016 Lisboa, Portugal. Email: qhuang@fc.ul.pt
3 Department of Applied Mathematics, Illinois Institute of Technology, Chicago, IL 60616, USA. Email: duan@iit.edu
In this paper, we consider the following SDE in the state space $\mathbb{R}^k$:
\[
\begin{aligned}
dX_t &= -\nabla U(X_t)dt + \sigma dW_t, \quad t > 0, \\
X_0 &= x_0,
\end{aligned}
\]  
where $U : \mathbb{R}^k \to \mathbb{R}$ is a given potential function, $W = \{W_t\}_{t \geq 0}$ is a standard $k$-dimensional Brownian motion, and $\sigma$ is a positive constant (see the next section for all assumptions on coefficients). We assume that $x_0 \in \mathbb{R}^k$ is a metastable state of (1.1), that is, $x_0$ is a stable state of the corresponding deterministic system $dX_t = -\nabla U(X_t)dt$ [16]. For instance, when $k = 1$ and $U = \frac{1}{2}x^4 - \frac{1}{2}x^2$ is the Ginzburg-Landau double-well potential, the corresponding metastable states are $\pm 1$. See Section 5 for more discussions about this example.

For the system (1.1) with a given transition time $l$, the common setup for studying transitions between two metastable states is the following [5, Chapter 6, Section 9]: Among all possible differentiable curves connecting $x_0$ and another metastable state $x_l$, which one is “most probable” for the solution process of (1.1)? This question aims to characterize the transition phenomena of system (1.1), i.e., the solution process $X$ starts from $x_0$ and transfers to a neighborhood of $x_l$ at time $l$. One way to answer this question is to evaluate the measure of tubes around a differentiable curve.

This problem has been studied by several authors in probabilistic perspective [5, 19, 20, 21]. The significant result therein is that (under some regularity assumptions) the probability of the solution process of (1.1) staying in a $\delta$-neighborhood (or a $\delta$-tube) of a curve $\psi$ is given asymptotically by the following:
\[
P(\|X - \psi\|_t < \delta) \sim \exp(-S_{X}^{OM}(\psi))P(\|W\|_t < \delta), \quad \delta \downarrow 0,
\]
where $S_{X}^{OM}$ is called the Onsager-Machlup action functional (OM functional) and defined by
\[
S_{X}^{OM}(\psi) = \frac{1}{2} \int_0^l \left[ \frac{\left| \dot{\psi}(s) + \nabla U(\psi(s)) \right|^2}{\sigma^2} - \Delta U(\psi(s)) \right] ds,
\]
and $\| \cdot \|_t$ denotes the uniform norm on the space $C([0,l],\mathbb{R}^k)$ of all continuous functions from $[0,l]$ to $\mathbb{R}^k$. The most probable transition path of (1.1) is determined by the minimizer of OM functional in a suitable space. The study of the OM functional $S_{X}^{OM}$ indicates some properties of most probable transition paths [22, 23]. Via the standard calculus of variation, the OM functional can deduce an Euler-Lagrange (E-L) equation, based on which a number of numerical algorithms have been proposed to seek for the most probable transition path [24, 25]. This approach has also been used to analyze the geometrical structure of most probable transition paths [26]. Notice that the Euler-Lagrange equation is a sufficient but not necessary description for the most probable transition path, and it is a second order equation with two boundary values which is in general hard to solve either analytically or numerically. Hence there are some natural and crucial questions left, such as whether there are sufficient and necessary descriptions for most probable transition paths. Furthermore, can we have simpler and more efficient descriptions for most probable transition paths? These two questions are what motivate us in the present paper.

The similar objects to transition paths are Markovian bridges. A Markovian bridge is obtained by conditioning a Markov process (in the sequel we always refer to the solution process $X$ of (1.1)) to start from the initial state $x_0$ at time 0 and arrive at another state $x_l$ at time $l$. Once the definition is made precisely, we call the resulting process the $(x_0,l,x_l)$-bridge derived from $X$. It follows from the definition that the $(x_0,l,x_l)$-bridge has sample paths almost surely in the space $C_{x_0,x_l}[0,l]$ of all continuous $\mathbb{R}^k$-valued curves on time interval $[0,l]$ connecting $x_0$ and $x_l$.

In Markovian theory, the transition density function of the Markov process $X$ is usually assumed to be continuous in all of its variables. This assumption implies that the path space $C_{x_0,x_l}[0,l]$ of the $(x_0,l,x_l)$-bridge is a null subset of the total space of all continuous functions on $[0,l]$ starting from $x_0$, under the pushforward measure of $X$. Besides, we know that the measures induced by Markovian bridges are no longer quasi translation invariant. For these two reasons, the previous methods of deriving OM functionals and corresponding results in [4, 5, 19, 20, 21] cannot be applied directly to the Markovian bridges. Thus, do the most probable transition paths determined by the solution process $X$ of (1.1) and by its corresponding Markovian bridge process coincide? We cannot have a positive answer based on the existing results.
In the present paper, we will discuss the relations between the solution process of (1.1) and its derived \((x_0, l, x_l)\)-bridge. These relations will help us to gain more insights in finding the most probable transition paths of the system (1.1). We show that the most probable transition paths of (1.1) and those of its corresponding Markovian bridge process coincide. For the cases of linear stochastic systems and of nonlinear stochastic systems with small noise, we show that the most probable transition path can be determined by some deterministic first order differential equations with initial values.

This paper is organized as follows. In Section 2, we recall some preliminaries. Some results for Markovian bridges are introduced in Section 3: We first study the finite dimensional distributions of Markovian bridges in Subsection 3.1; then we use SDE representations with only initial values to model Markovian bridge processes in Subsection 3.2; we also discuss in Subsection 3.3 the usage of SDE representations in path sampling, and make a few comments and comparisons with existing sampling approaches; in Subsection 3.4, we show that the OM functional can also be derived from bridge measures using different methods with those in [4, 5]; based on these, we obtain our main result in Subsection 3.5 that the most probable transition path(s) of a stochastic dynamical system coincide(s) with that (those) of its corresponding Markovian bridge system. The discussions of a class of linear systems and small noise case are shown in Section 4. In Section 5, we present some examples to illustrate our results. Finally, we summarize our work in Section 6.

2 Preliminaries on Measures Induced by Diffusion Processes

We consider the following SDE on \(\mathbb{R}^k\):

\[
    dX_t = -\nabla U(X_t)dt + \sigma dW_t,
\]

where \(W = (W_1, \ldots, W^k)\) is a standard \(k\)-dimensional Brownian motion.

We denote by \(C[0, l]\) the space \(C([0, l], \mathbb{R}^k)\) of all continuous functions from interval \([0, l]\) to \(\mathbb{R}^k\), and equip it with the uniform topology induced by the following uniform norm so that it is a Banach space,

\[
    \|\psi\|_t = \sup_{t \in [0,l]} |\psi(t)|, \quad \psi \in C[0,l].
\]

We also endow \(C[0, l]\) with corresponding Borel \(\sigma\)-field \(\mathcal{B}\) and canonical filtration \(\{\mathcal{B}_t\}_{t \in [0,l]}\) given by

\[
    \mathcal{B}_t = \sigma\{\omega(s) \mid \omega \in C[0,l], 0 \leq s \leq t\}.
\]

Let \(A\) be the informal generator of \(X\), i.e.,

\[
    A = - \nabla U \cdot \nabla + \frac{1}{2} \sigma^2 \Delta.
\]

We suppose the following:

**Assumption H1.** (1) The potential satisfies \(U \in C^3(\mathbb{R}^k, \mathbb{R})\).

(2) The local martingale problem associated with \(A\) is well-posed in \(C[0, l]\) (e.g., [27, Chapter 5, Definition 4.5]). That is, for every \((s, x) \in [0, l] \times \mathbb{R}^k\), there exists a probability measure \(P_{s,x}\) on \((C[0,l], \mathcal{B})\), such that \(P_{s,x}(\omega(r) = x, r \leq s) = 1\), and for every \(f \in C^2(\mathbb{R}^k)\), \(M_f = \{M_f^t\}_{t \in [s,l]}\) is a local martingale with respect to the right continuous augmentation of \(\{\mathcal{B}_t\}_{t \in [s,l]}\) under \(P_{s,x}\), where

\[
    M_f^t(\omega) := f(\omega(t)) - f(\omega(s)) - \int_s^t Af(\omega(r))dr, \quad \omega \in C[0,l].
\]

The regularity assumption for potential \(U\) in H1-(1) can guarantee the pathwise uniqueness of (2.1) (e.g., [5, Chapter IV, Theorem 3.1]). On the other hand, the existence of solutions for the local martingale problem associated with \(A\) is equivalent to the existence of weak solutions for its corresponding SDE (2.1) [27, Chapter 5, Corollary 4.8, Corollary 4.9], so that there exist a filtered probability space \((\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t \geq 0}, \mathbb{P})\) satisfying usual conditions (e.g., [27, Chapter 1, Definition 2.25]), a \(k\)-dimensional Brownian motion \(W\) on it and a continuous, adapted \(\mathbb{R}^k\)-valued process \(X\) such that the equation (2.1) holds (in the sense of stochastic integral). Applying the result of Yamada–Watanabe [27, Chapter 5, Corollary 3.23], we obtain the strong well-posedness of (2.1). Moreover, Assumption H1-(2) implies that \(X\) is strong Markov under \(\mathbb{P}\) [28, Theorem 4.4.2]. We denote the conditional probability measure \(\mathbb{P}(\cdot \mid X_0 = x_0)\) shortly by \(\mathbb{P}^{x_0}(\cdot)\). Therefore, we have
Lemma 2.1. Under Assumption H1, the SDE \( (2.1) \) has a pathwisely unique strong solution \( X = \{X_t\}_{t \in [0,l]} \) on the probability space \((\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t \geq 0}, \mathbb{P}^x)\), which is strong Markov and satisfies \( \mathbb{P}^x(X_0 = x_0) = 1 \).

We suppose that \( x_0 \) is a fixed state of system \( (2.1) \). And let \( x_t \) denote another given state of system \( (2.1) \). The space of paths of \( X \) is the space \( C_{x_0}[0,l] \) of continuous functions
\[
C_{x_0}[0,l] = \{ \psi : [0,l] \to \mathbb{R}^k \text{ is continuous}, \; \psi(0) = x_0 \}.
\]
Note that \( C_{x_0}[0,l] \) is not a linear space unless \( x_0 = 0 \). We equip \( C_{x_0}[0,l] \) with the subspace topology of \( C^0[0,l] \), and denote the corresponding Borel \( \sigma \)-field by \( \mathcal{B}_{x_0}[0,l] \). There is another way to realize elements in \( \mathcal{B}_{x_0}[0,l] \) in terms of cylinder sets, instead of open sets. A cylinder set of \( \mathcal{B}_{x_0}[0,l] \) is of the form
\[
I = \{ \psi \in C_{x_0}[0,l] \mid \psi(t_1) \in E_1, \ldots, \psi(t_n) \in E_n \},
\]
where \( 0 \leq t_1 < \cdots < t_n \leq l \) and \( E_i \)'s are Borel sets of \( \mathbb{R}^k \). It is well known \([27]\) that \( \mathcal{B}_{x_0}[0,l] \) is the \( \sigma \)-field generated by all cylinder sets, that is, the smallest \( \sigma \)-field containing all cylinder sets. An open tube set \( K_\delta(\psi, \delta) \) is defined as
\[
K_\delta(\psi, \delta) = \{ z \in C_{x_0}[0,l] \mid \| \psi - z \|_l < \delta \},
\]
where \( \delta > 0 \) is called the tube size. The corresponding closed tube set is
\[
\bar{K}_\delta(\psi, \delta) = \{ z \in C_{x_0}[0,l] \mid \| \psi - z \|_l \leq \delta \},
\]
which is the closure of \( K_\delta(\psi, \delta) \) under the uniform topology. Let \( B_\rho(x) \) denote the open ball centered at \( x \in \mathbb{R}^k \) with radius \( \rho > 0 \), we denote by \( \bar{B}_\rho(x) \) the corresponding closed ball.

The measure \( \mu^X_{x_0} \) induced by \( X \) on the space \( (C_{x_0}[0,l], \mathcal{B}_{x_0}[0,l]) \) is defined by
\[
\mu^X_{x_0}(B) = \mathbb{P}^x(\{ \omega \in \Omega \mid X(\omega) \in B \}),
\]
for all \( B \in \mathcal{B}_{x_0}[0,l] \). Recall that the measure \( \mu^W_{\sigma W} \) induced by the Brownian motion \( \sigma W \) is called the Wiener measure. Once a positive \( \delta \) is given, we can compare the probabilities of closed tubes for all \( \psi \in C_{x_0}[0,l] \) using \( \mu^X_{x_0}(\bar{K}_\delta(\psi, \delta)) \). And this enables us to discuss the problem of finding the most probable transition path of \( X \).

In general, we have the following definition for the most probable transition path.

Definition 2.2. The most probable transition path of the system \( (2.1) \) connecting two given states \( x_0 \) and \( x_1 \), is a path \( \psi^* \) that makes the OM functional achieve its minimum value in the following path space,
\[
C^2_{x_0,x_1}[0,l] := \{ \psi : [0,l] \to \mathbb{R}^k \mid \psi, \bar{\psi} \text{ exist and are continuous}, \; \psi(0) = x_0, \; \psi(l) = x_1 \}.
\]
In mathematical language, the most probable transition path \( \psi^* \) is a path in \( C^2_{x_0,x_1}[0,l] \) such that
\[
S^{OM}(\psi^*) = \inf_{\psi \in C^2_{x_0,x_1}[0,l]} S^{OM}(\psi).
\]
This is equivalent to that for all \( \psi \in C^2_{x_0,x_1}[0,l] \),
\[
\lim_{\delta \downarrow 0} \frac{\mu^X_{x_0}(K_\delta(\psi^*, \delta))}{\mu^X_{x_0}(\bar{K}_\delta(\psi^*, \delta))} \geq 1,
\]
as a straightforward consequence of \((1.2)\). One can replace the open tubes in the description \((2.2)\) by closed tube sets, adopting a slight modification of the proof of \([5, \text{Theorem 9.1}]\) (or \([4, \text{Section 4}]\) or \([21, \text{Theorem 1}]\)).

Now we show that under given probability measure on path space, the probability of a closed tube set can be approximated by the probabilities of a family of cylinder sets. This property helps us to study the tube probability easily.
Lemma 2.3 (Approximation for probabilities of closed tube sets). Let $\mu$ be a probability measure on $(C_{x_0}[0,l],B_{x_0}^{C_{x_0}[0,l]})$. For each closed tube set $K_t(\psi, \delta)$ with $\psi \in C_{x_0}[0,l]$ and $\delta > 0$, there exists a family of cylinder sets $\{\bar{I}_n(\psi, \delta)\}_{n=1}^\infty$ such that

$$\mu(\bar{K}_t(\psi, \delta)) = \lim_{n \to \infty} \mu(\bar{I}_n(\psi, \delta)).$$

Proof. The proof is separated to two steps.

Step 1. Let $Q$ denote the countable set of rational numbers in $\mathbb{R}$. Since $(0, l) \cap Q$ is a countable set, we denote it as a sequence $\{q_1, q_2, \ldots, q_n, \ldots\}$. Define a family of incremental sequences $\{Q_n\}_{n=1}^\infty$ by

$$Q_n := \{q_1, \cdots, q_n\}.$$

Then we have $(0, l) \cap Q = \bigcup_{n=1}^\infty Q_n$. By the continuity, we can derive the following equalities:

$$\left\{ w \in C_{x_0}[0,l] \bigg| \sup_{t \in [0,l]} |w(t) - \psi(t)| \leq \delta \right\} = \bigcap_{n=1}^\infty \left\{ w \in C_{x_0}[0,l] \big| |w(t) - \psi(t)| \leq \delta \right\}, \quad \text{(2.3)}$$

$$= \bigcap_{n=1}^\infty \bigcap_{t \in Q_n} \left\{ w \in C_{x_0}[0,l] \big| |w(t) - \psi(t)| \leq \delta, \forall t \in Q_n \right\}.$$

Step 2. Noting that the family $\{\{w \in C_{x_0}[0,l] \big| |w(t) - \psi(t)| \leq \delta, \forall t \in Q_n\} : n = 1, \cdots, \infty\}$ is decreasing since $\{Q_n\}_{n=1}^\infty$ is increasing, we have

$$\mu(\bar{K}_t(\psi, \delta)) = \mu \left( \left\{ w \in C_{x_0}[0,l] \bigg| \sup_{t \in [0,l]} |w(t) - \psi(t)| \leq \delta \right\} \right) = \mu \left( \bigcap_{n=1}^\infty \left\{ w \in C_{x_0}[0,l] \big| |w(t) - \psi(t)| \leq \delta, \forall t \in Q_n \right\} \right) = \lim_{n \to \infty} \mu\{w \in C_{x_0}[0,l] \big| |w(t) - \psi(t)| \leq \delta, \forall t \in Q_n\} = \lim_{n \to \infty} \mu(\bar{I}_n(\psi, \delta)),$$

where $\bar{I}_n(\psi, \delta) = \{\phi \in C_{x_0}[0,l] \big| \phi(t) \in B_\delta(\psi(t)), \forall t \in Q_n\}$ is a cylinder set. The proof is complete. \qed

Remark 2.4. In general, this lemma does not work for open tubes. Indeed, if we replace the closed tubes $\bar{K}_t$ and closed cylinder sets $\bar{I}_n$ by their open versions, then the first two equalities of (2.3) should read

$$\left\{ w \in C_{x_0}[0,l] \bigg| \sup_{t \in [0,l]} |w(t) - \psi(t)| < \delta \right\} = \bigcap_{n=1}^\infty \left\{ w \in C_{x_0}[0,l] \bigg| \sup_{t \in (0,l)\cap Q} |w(t) - \psi(t)| < \delta \right\} \subset \bigcap_{n=1}^\infty \left\{ w \in C_{x_0}[0,l] \big| |w(t) - \psi(t)| < \delta \right\}.$$
3 Equivalent Description and Characterization of Most Probable Transition Paths: Markovian Bridges and Onsager-Machlup Functionals

In this section we present some results for Markovian bridges that we will use later. The transition semigroup \( (T_{s,t})_{0 \leq s < t} \) of the solution process \( X \) of system (2.1) is defined as

\[
(T_{s,t}f)(x) = \mathbb{E}(f(X_t) \mid X_s = x),
\]

for each \( f \in \mathfrak{B}_b(\mathbb{R}^k) \) and \( x \in \mathbb{R}^k \), here \( \mathfrak{B}_b(\mathbb{R}^k) \) denotes the space of all measurable and bounded functions \( f : \mathbb{R}^k \to \mathbb{R}^k \). The notation \( \mathbb{E}(\cdot \mid X_s = x) \) denotes the expectation with respect to the regular conditional probability measure \( \mathbb{P}(\cdot \mid X_s = x) \). We suppose that \( T_{s,t} \) admits a transition density \( p(\cdot, t|x,s) \) with respect to a \( \sigma \)-finite measure \( \nu \) on \( \mathbb{R}^k \), in the sense that

\[
T_{s,t}f(x) = \int_{\mathbb{R}^k} f(y)p(y,t|x,s)\nu(dy).
\]

For simplicity, we assume that \( \nu \) is the Lebesgue measure. Since the drift term \( -\nabla U \) and diffusion coefficient \( \sigma \) do not depend on time, we know that this transition density is time homogenous [5], i.e.,

\[
p(y, t + s|z, t) = p(y, s|z, 0),
\]

for every \( t, s \in (0, \infty) \) and \( y, z \in \mathbb{R}^k \).

Under Assumption H1, the transition densities satisfy the following properties (see Chapter 6 of [29]):

(i) \((s, y, x) \mapsto p(y, s|x, 0)\) is joint continuous,

(ii) The transition density function satisfies the Kolmogorov forward equation (or Fokker-Planck equation)

\[
\frac{\partial p(x,t|x_0,0)}{\partial t} = \nabla(\nabla U(x)p(x,t|x_0,0)) + \frac{1}{2} \sigma^2 \Delta p(x,t|x_0,0),
\]

and the Kolmogorov backward equation

\[
\frac{\partial p(x,t|x_0,0)}{\partial t} = \nabla U(x) \cdot \nabla p(x,t|x_0,0) - \frac{1}{2} \sigma^2 \Delta p(x,t|x_0,0),
\]

both in the sense of generalized functions.

Due to the strong Markov property of the process \( X \), the Chapman-Kolmogorov equations

\[
p(y, l|x_0, 0) = \int_{\mathbb{R}^k} p(z, l - s|x_0, 0)p(y, s|z, 0)dz,
\]

hold for all \( y \in \{x \mid p(x, l | x_0, 0) > 0\} \) and all \( 0 < s < l \).

3.1 Finite dimensional distributions of Markovian bridges

The Lemma 2.3 enables us to use cylinder sets to approximate the tube probabilities. So it is essential for us to consider the finite dimensional distributions of Markovian bridges.

Recall that we have fixed an \( x_0 \in \mathbb{R}^k \). Under our setting, we know that the conditional probability distribution \( \mathbb{P}^{x_0}(X \in \cdot \mid X_l) \) has a regular version, that is, it determines a regular conditional distribution of \( X \) given \( X_l \) under \( \mathbb{P}^{x_0} \) [30, 31]. We denote by \( \mu_{X_l}^{x_0} \) the corresponding probability kernel from \( \mathbb{R}^k \) to \( C_{x_0}[0,l] \), and call it the bridge measure. This means that \( \mathbb{P}^{x_0} \)-a.s. for all \( B \in B_{[0,l]} \),

\[
\mu_{X_l}^{x_0}(B) = \mathbb{P}^{x_0}(X \in B \mid X_l),
\]

or equivalently,

\[
\mu_{X_l}^{x_0}(B) = \mathbb{P}^{x_0}(X \in B \mid X_l = x_l), \quad \text{for } (\mathbb{P}^{x_0} \circ X_l^{-1}) \text{-a.e. } x_l \in \mathbb{R}^k.
\]
Under $\mathbb{P}^{x_0}(\cdot \mid X_t = x_l)$, the process $\{X_t\}_{0 \leq t \leq l}$ is the $(x_0, l, x_l)$-bridge derived from $X$. And this bridge is still strong Markovian \cite{30, 31}, with transition densities

$$p^{x_0,x_l}(y, t | x, s) = \frac{p(y, t - s | x, 0)p(x, l - t | y, 0)}{p(x, l - s | x, 0)}, \quad 0 \leq s < t < l. \quad (3.3)$$

Moreover $\mu^{x_0,x_l}(\{\psi \in C_{x_0}[0, l] \mid \psi(l) = x_l\}) = 1$.

For a cylinder set $I = \{\psi \in C_{x_0}[0, l] \mid \psi(t_1) \in E_1, \ldots, \psi(t_n) \in E_n\}$ with $0 < t_1 < t_2 < \cdots < t_n < l$ and $E_i$’s being Borel sets of $\mathbb{R}^k$, we have that

$$\mu^{x_0,x_l}(I) = \int_{\{x \in E_i, i = 1, \ldots, n\}} p^{x_0,x_l}(x_1, t_1 | x_0, 0) \cdots p^{x_0,x_l}(x_n, t_n | x_{n-1}, t_{n-1}) dx_1 \cdots dx_n$$

$$= \int_{\{x \in E_i, i = 1, \ldots, n\}} \frac{p(x_1, t_1 | x_0, 0)p(x_2, t_2 | x_1, t_1)}{p(x_1, t_1 | x_0, 0)} \cdots \frac{p(x_n, t_n | x_{n-1}, t_{n-1})}{p(x_1, t_1 | x_0, 0)} dx_1 \cdots dx_n$$

$$= \frac{1}{p(x_1, t_1 | x_0, 0)} \int_{\{x \in E_i, i = 1, \ldots, n\}} p(x_1, t_1 | x_0, 0)p(x_2, t_2 | x_1, t_1) \cdots p(x_n, t_n | x_{n-1}, t_{n-1}) dx_1 \cdots dx_n. \quad (3.4)$$

### 3.2 SDE representation for Markovian bridges

In this subsection we represent Markovian bridges via SDEs only with initial values.

Combining equations (3.1), (3.2) and (3.3), the transition probability density function $p^{x_0,x_l}(x, t | x_0, 0)$ satisfies the following partial differential equation \cite{32}:

$$\frac{\partial p^{x_0,x_l}(x, t | x_0, 0)}{\partial t} = \nabla \left[ (\nabla U(x) - \sigma^2 \nabla \ln p(x, l | x, t)) p^{x_0,x_l}(x, t | x_0, 0) \right] + \frac{1}{2} \sigma^2 \Delta p^{x_0,x_l}(x, t | x_0, 0).$$

Formally, this equation has the form of a Fokker-Planck equation. Thus we can associate to the transition density $p^{x_0,x_l}(x, t | x_0, 0)$ a new $k$-dimensional SDE on a certain probability space $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t \geq 0}, \mathbb{P})$ that is rich enough to support a standard $k$-dimensional Brownian motion $W = (W^1, \ldots, W^k)$:

$$dY_t = [-\nabla U(Y_t) + \sigma^2 \nabla \ln p(x, l | Y_t, t)] dt + \sigma dW_t, \quad t \in [0, l]. \quad (3.5)$$

We refer to (3.5) as the bridge SDE associated to (2.1). This equation was originally obtained by Doob \cite{33} from the probabilistic point of view and is known as the Doob h-transform of SDE (2.1).

The existence and uniqueness of weak and strong solutions of (3.5) were established in \cite{32} under some mild assumptions. Specifically, under Assumption H1 (and the following Assumption H2 if $k \geq 2$), the existence and uniqueness of the strong solution of (3.5) are promised \cite{32, Theorem 4.1}. Denote, similar as before, by $\mathbb{P}^{x_0}$ the conditional probability $\mathbb{P}(\cdot | Y_0 = x_0)$. Then, it concluded that for each Borel set $E$ of $\mathbb{R}^k$,

$$\mathbb{P}^{x_0}(Y_t \in E) = \int_E \frac{p(y, t | x_0, 0)p(x, l | y, t)}{p(x, l | x_0, 0)} dy, \quad 0 < t < l, \quad (3.6)$$

and automatically $\mathbb{P}^{x_0}(Y_t = x_l) = 1$.

**Assumption H2.** When $k \geq 2$, we assume in addition that $p(x, l | x_0, 0) > 0$ and $-\Delta U \geq \xi$, where $\xi \in \mathbb{R}$ is a constant.

**Lemma 3.1.** Under Assumptions H1 and H2, the SDE (3.5) has a pathwisely unique strong solution $Y = \{Y_t\}_{t \in [0, l]}$ on the probability space $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t \geq 0}, \mathbb{P}^{x_0})$, which satisfies $\mathbb{P}^{x_0}(Y_0 = x_0, Y_l = x_l) = 1$. 
Remark 3.2. (i). The configurations \((\tilde{\Omega}, \tilde{\mathcal{F}}, \{\tilde{\mathcal{F}}_t\}_{t \geq 0}, \tilde{\mathbb{P}})\), \(\tilde{W}\) of bridge SDE (3.5) do not need to coincide with the configuration \((\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t \geq 0}, \mathbb{P})\), \(W\) of original SDE (2.1), since the ways of obtaining their strong well-posedness in Lemmas 2.1 and 3.1 are both via the Yamada–Watanabe argument, which means that as soon as the probability space is rich enough to support a Brownian motion, the SDE can have a unique strong solution on it, cf. [27, Section 5.3].

(ii). Comparing bridge SDE (3.5) and original SDE (2.1), it can be seen that it is the extra potential \(\sigma^2 \ln p(x_l, l|x_0, 0)\) that “force” the process to reach \(x_l\) at time \(t = l\). The physical realization for (3.5) is to add a virtual potential to the original non-equilibrium thermodynamical system, to force (almost) all paths of the process to pass from an initial metastable state to a particular final metastable state.

3.3 Relations to path sampling

As we have seen in the last remark, the probabilistic configurations of strong solutions of two SDEs (2.1) and (3.5) are not necessarily the same. On the one hand, if we specify different probability spaces for them, or we just consider weak solutions of them rather than strong ones, then the only relation between the solutions that we can talk about is their distributional information. In fact, we will show in Lemma 3.9 that the solution of the bridge SDE (3.5) shares the same law with the \((x_0, l, x_l)\)-bridge derived from the original SDE (2.1). However, in general, no path information for their solutions can be clarified or everything for their paths can be possible in this case.

On the other hand, if we choose the same configuration for them, that is, \((\tilde{\Omega}, \tilde{\mathcal{F}}, \{\tilde{\mathcal{F}}_t\}_{t \geq 0}, \tilde{\mathbb{P}}) = (\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t \geq 0}, \mathbb{P})\) and \(\tilde{W} = W\), then we can construct the strong solution of (3.5) directly from the strong solution of (2.1). More precisely, by replacing the noise terms in (2.1) and (3.5), we obtain the following

Theorem 3.3. Let \(X\) and \(Y\) be the unique strong solutions of SDEs (2.1) and (3.5), respectively, on the same probability space \((\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t \geq 0}, \mathbb{P}^{x_0})\) endowed with the same \(k\)-dimensional Brownian motion \(W\). Then the following SDE holds,

\[
dY_t = [\nabla U(X_t) - \nabla U(Y_t) + \sigma^2 \nabla \ln p(x_l, l|Y_t, t)] dt + dX_t, \quad t \in [0, l]. \tag{3.7}
\]

Note that equation (3.7) provides the relation between path information of two strong solutions \(X\) and \(Y\). Even for a path \(X(\omega)\) that reaches \(x_l\) at time \(t = l\), the resulting path \(Y(\omega)\) realized from (3.7) is not the same as \(X(\omega)\), since the extra drift \(\sigma^2 \nabla \ln p(x_l, l|Y_t(\omega), t)\) is not identically zero (see Example 5.1 for an example for Brownian case).

The relation (3.7) suggests a general approach for sampling paths of Markovian bridges: given a sample path \(X(\omega)\) of strong solution of the original SDE (2.1), one can use (3.7) to sample a path \(Y(\omega)\) of the strong solution of bridge SDE (3.5) by many discrete-time schemes, e.g., Euler–Maruyama method.

In particular, for the Brownian and Ornstein-Uhlenbeck cases, many explicit representations for the solutions of bridge SDE (3.5) can be found in the literature [35]. Consider the Ornstein-Uhlenbeck (OU) process satisfying the following scalar SDE:

\[
dX_t = -\theta X_t dt + \sigma dW_t, \quad X_0 = 0 \in \mathbb{R}, \tag{3.8}
\]
which recovers Brownian motions when $\theta = 0$ and $\sigma = 1$. Three representations, anticipative version, integral representation and space-time transform, are proposed in [35], respectively to construct Brownian and OU bridges. These representations are equal in law, as they are all solutions to the bridge SDE (3.5) for Brownian and OU cases respectively. Specifically, the integral representation is the unique strong solution to the associated bridge SDE, while other two representations are only weak solutions. It was also demonstrated and partially proved that when a path $X_t(\omega)$ of strong solution of (3.8) reaches 0 at time $t = l$, the sample path realized from the integral representation as strong solution does not coincide with $X_t(\omega)$, while the sample paths realized from other two representations as weak solutions may and may not coincide. These match with our above observations. We will discuss the MPTPs for Brownian and OU bridges later in Section 5.

Different from the bridge SDE construction and the three representations in [35], an intuitive and ingenious construction of Brownian and OU bridges was introduced in [36, Appendix B], by taking a linear combination of two unconstrained independent paths and setting the endpoint of the linear combination to zero. That is, we suppose $Z^1_t$ and $Z^2_t$ to be two mutually independent copies of solution of (3.8), on probability spaces $(\Omega^1, \mathcal{F}^1, (\mathcal{F}^1_t), \mathbb{P}^1)$ and $(\Omega^2, \mathcal{F}^2, (\mathcal{F}^2_t), \mathbb{P}^2)$ respectively. Define a new process $Z$ on the product probability space $(\Omega^1 \times \Omega^2, \mathcal{F}^1 \otimes \mathcal{F}^2, (\mathcal{F}^1_t \otimes \mathcal{F}^2_t), \mathbb{P}^1 \otimes \mathbb{P}^2)$ by

$$Z(\omega_1, \omega_2) = Z^1(\omega_1) \cos(\kappa(\omega_1, \omega_2)) + Z^2(\omega_2) \sin(\kappa(\omega_1, \omega_2)),$$

where $\kappa$ is a random variable on the product space $\Omega^1 \times \Omega^2$ determined by the following terminal condition,

$$Z^1_t \cos \kappa + Z^2_t \sin \kappa = 0,$$

that is, $\kappa = \arctan(-Z^1_t/Z^2_t)$, using the conventions that $\arctan(0/0) = 0$, $\arctan(+\infty) = \frac{\pi}{2}$ and $\arctan(-\infty) = -\frac{\pi}{2}$. This construction implies that the new process $Z$ satisfies $Z_0 = Z_t = 0$ and

$$dZ_t = -\theta Z_t dt + \sigma d(\cos \kappa W^1_t + \sin \kappa W^2_t),$$

(3.9)

Therefore, $Z$ is indeed a $(0,l,0)$-bridge process. But it remains unclear if $Z$ has the same law with the bridge of the original OU process (3.8), as the noise $\cos \kappa W^1_t + \sin \kappa W^2_t$ in SDE (3.9) is not an $\{\mathcal{F}^1_t \otimes \mathcal{F}^2_t\}$-adapted process due to the fact that the random variable $\kappa$ depends on the information at time $t = l$.

### 3.4 Onsager-Machlup functionals and bridge measures

In this subsection, we prove one of the main results of this paper which is described as the following theorem:

**Theorem 3.4** (OM functionals and bridge measures). There exists a constant $C > 0$, such that for each $\psi \in C^2_{x_0,x_l}[0,l]$,

$$\mu^\psi_{x_0,x_l}(\bar{K}_t(\psi, \delta)) \sim C \exp \left(-S^\psi_{x_0,x_l}(\psi)\right) \mu^{0,0}_{\sigma W}(\bar{K}_t(\psi, \delta))$$

as $\delta \downarrow 0$.

**Remark 3.5.** This theorem will be proved by adopting Lemma 2.3, thus the result holds only for closed tubes but not for open tubes.

Conditioning on the event that the solution process $X$ of (2.1) hits the point $x_l$ at time $l$, the regular conditional probability measure (i.e., the bridge measure) $\mu^\psi_{x_0,x_l}$ obeys the following informal stochastic boundary value problem, called *conditioned SDE* [37],

$$\begin{cases}
    dX_t = -\nabla U(X_t) dt + \sigma dW_t, \\
    X_0 = x_0, X_l = x_l,
\end{cases}$$

(3.10)

which should still be understood as the original SDE (2.1) under the conditional probability $P^\psi_{x_0}(\cdot|X_l = x_l)$. A significant difference between the bridge SDE (3.5) and the conditioned SDE (3.10) is that the former is only conditioned on initial value while the later is conditioned on initial and final boundary values.

Now, the measure $\mu^\psi_{x_0,x_l}$ can be characterized via its density with respect to the Brownian bridge measure $\mu^\psi_{\sigma W}$ corresponding to the case $\nabla U \equiv 0$. To see this, for the unconditioned process $X$ in (2.1), the Girsanov
Now we condition on the boundary value $X_l = x_l$. This expression contains a stochastic integral term. Using Itô’s formula we obtain that

$$\frac{d\mu_{x_0}^x}{d\mu_{\sigma W}}(x) = \exp \left\{ -\int_0^l \frac{\nabla U(x(t))}{\sigma} dx(t) - \frac{1}{2} \int_0^l \frac{\nabla U(x(t))^2}{\sigma^2} dt \right\}. \quad (3.11)$$

This expression contains a stochastic integral term. Using Itô’s formula we obtain that

$$\frac{d\mu_{x_0}^x}{d\mu_{\sigma W}}(x) = \exp \left\{ -\frac{1}{\sigma} \left( U(x(l)) - U(x_0) \right) - \frac{1}{2} \int_0^l \frac{\nabla U(x(t))^2}{\sigma^2} dt \right\} = \exp \left\{ -\frac{U(x(l)) - U(x_0)}{\sigma^2} + \frac{1}{2} \int_0^l \left( \Delta U(x(t)) - \frac{\nabla U(x(t))^2}{\sigma^2} \right) dt \right\}.$$

Now we condition on the boundary value $X_l = x_l$, we find by [38, Lemma 5.3] that

$$\frac{d\mu_{x_0,x_l}}{d\mu_{\sigma W}}(x) = C_0 \exp \left\{ \frac{1}{2} \int_0^l \left( \Delta U(x(t)) - \frac{\nabla U(x(t))^2}{\sigma^2} \right) dt \right\},$$

where $C_0$ is a normalized constant, depending only on $x_0, x_l, \sigma$ and $U$. This result has been used in [12, 37].

For each $\psi \in C_{x_0,x_l}[0,l]$ and $x \in \bar{K}_i(\psi, \delta)$, there exists $h \in \{ z \in C_0[0,l] \mid \| z \| \leq \delta \}$ such that

$$x = \psi + h,$$

and

$$\left| \int_0^l \left( \Delta U - \frac{\nabla U^2}{\sigma^2} \right)(x(t))dt \right| - \left| \int_0^l \left( \Delta U - \frac{\nabla U^2}{\sigma^2} \right)(\psi(t))dt \right| = \left| \int_0^l \left( \Delta U - \frac{\nabla U^2}{\sigma^2} \right)(\psi(t) + h(t))dt \right| - \left| \int_0^l \left( \Delta U - \frac{\nabla U^2}{\sigma^2} \right)(\psi(t))dt \right| \leq C_1 \delta,$$

where

$$C_1 = \sup_{x \in \bar{K}_i(\psi, \delta)} \sup_{t \in [0,l]} \left| \nabla \left( \Delta U - \frac{\nabla U^2}{\sigma^2} \right)(x(t)) \right|.$$

So we know that

$$\mu_{x_0,x_l}^x(\bar{K}_i(\psi, \delta)) = \int_{x \in \bar{K}_i(\psi, \delta)} C_0 \exp \left\{ \frac{1}{2} \int_0^l \left( \Delta U(x(t)) - \frac{\nabla U(x(t))^2}{\sigma^2} \right) dt \right\} d\mu_{\sigma W}^{x_0,x_l}(x) \leq C_0 \exp \left\{ C_1 \delta + \frac{1}{2} \int_0^l \left( \Delta U(\psi(t)) - \frac{\nabla U(\psi(t))^2}{\sigma^2} \right) dt \right\} \mu_{\sigma W}^{x_0,x_l}(\bar{K}_i(\psi, \delta)). \quad (3.12)$$

Let $pW(\cdot, t, s) \ (0 \leq s < t \leq l)$ denote the transition density of Brownian motion $\sigma W$. For each
\[
\psi \in C^2_{x_0, x_l}[0, l] \text{ and tube size } \delta > 0, \text{ according to Lemma 2.3 and equation (3.4) we have that }
\]
\[
P_W(x_l, l|x_0, 0) \mu_{\sigma^2 W}^{x_0, x_l}(\bar{K}_t(\psi, \delta)) = p_W(x_l, l|x_0, 0) \lim_{n \to \infty} \mu_{\sigma^2 W}^{x_0, x_l}((\bar{I}_n(\psi, \delta))
\]
\[
= \lim_{n \to \infty} \int_{\{z_i \in B(\psi(t_i), \delta), i=1, \ldots, n\}} \left( \frac{1}{2\pi \sigma^2 \Delta t} \right)^{n+1} \exp \left\{ -\sum_{i=1}^{n+1} \frac{|z_i - z_{i-1}|^2}{2\sigma^2 \Delta t} \right\} dz_1 \cdots dz_n \quad (z_0 = x_0, z_{n+1} = x_l)
\]
\[
= \lim_{n \to \infty} \int_{\{y_i \in B(0, \delta), i=1, \ldots, n\}} \left( \frac{1}{2\pi \sigma^2 \Delta t} \right)^{n+1} \exp \left\{ -\sum_{i=1}^{n+1} \frac{|y_i + \psi(t_i) - y_{i-1} - \psi(t_{i-1})|^2}{2\sigma^2 \Delta t} \right\} dy_1 \cdots dy_n
\]
(Variable substitution: \( y_i = z_i - \psi(t_i), \ i = 0, \cdots, n + 1, \) in particular, \( y_0 = y_{n+1} = 0 \).)
\[
= \lim_{n \to \infty} \exp \left\{ -\sum_{i=1}^{n+1} \frac{|\psi(t_i) - \psi(t_{i-1})|^2}{2\sigma^2 \Delta t} \right\} \int_{\{y_i \in B(0, \delta), i=1, \ldots, n\}} \left( \frac{1}{2\pi \sigma^2 \Delta t} \right)^{n+1} \exp \left\{ -\sum_{i=1}^{n+1} \frac{|y_i - y_{i-1}|^2}{2\sigma^2 \Delta t} \right\} dy_1 \cdots dy_n
\]
\[
\leq \exp \left\{ \frac{l\delta \|\dot{\psi}\|_l}{\sigma^2} \right\} \lim_{n \to \infty} \exp \left\{ -\sum_{i=1}^{n+1} \frac{|\psi(t_i) - \psi(t_{i-1})|^2}{2\sigma^2 \Delta t} \right\}
\]
\[
= p_W(y_n, l|y_0, 0) \exp \left\{ \frac{l\delta \|\dot{\psi}\|_l}{\sigma^2} \right\} \lim_{n \to \infty} \exp \left\{ -\frac{1}{2\sigma^2} \sum_{i=1}^{n+1} \frac{|\psi(t_i) - \psi(t_{i-1})|^2}{\Delta t} \right\} \mu_{\sigma^2 W}^{y_0, y_n}((\bar{I}_n(0, \delta))
\]
\[
= p_W(0, l|0, 0) \exp \left\{ \frac{l\delta \|\dot{\psi}\|_l}{\sigma^2} \right\} \exp \left\{ -\frac{1}{2} \int_0^l \frac{|\ddot{\psi}|^2}{\sigma^2} dt \right\} \mu_{\sigma^2 W}^{0, 0}(\bar{K}_t(0, \delta)),
\]
(3.13)

where \( \Delta t = t_i - t_{i-1} \), and we have used the discrete version of integration by parts to estimate the cross terms:

\[
\sum_{i=1}^{n+1} \frac{(y_i - y_{i-1}) \cdot (\psi(t_i) - \psi(t_{i-1}))}{\Delta t}
\]
\[
= \left| y_{n+1} \frac{\psi(t_{n+1}) - \psi(t_n)}{\Delta t} - y_0 \frac{\psi(t_1) - \psi(t_0)}{\Delta t} + \sum_{i=1}^{n} y_i \frac{\psi(t_i) - \psi(t_{i-1}) - \psi(t_{i+1}) - \psi(t_i)}{\Delta t} \right|
\]
\[
\leq \sum_{i=1}^{n} |y_i| \left| \frac{\psi(t_i) - \psi(t_{i-1}) - \psi(t_{i+1}) - \psi(t_i)}{\Delta t} \right| \Delta t
\]
\[
\leq \delta \|\dot{\psi}\| \sum_{i=1}^{n} |\Delta t| \leq l\delta \|\dot{\psi}\|_l.
\]
Now we combine (3.12) and (3.13) to derive that
\[
\mu_X^{\infty-i}(K_i(\psi, \delta)) \leq C_0 \exp \left\{ C_1 \delta l + \frac{l \delta \| \psi \|_l}{\sigma^2} \int_0^l \left( \Delta U(\psi(t)) - \frac{\left| \nabla U(\psi(t)) \right|^2}{\sigma^2} \right) dt \right\} \exp \left\{ \frac{-l \delta \| \psi \|_l}{\sigma^2} \right\} \exp \left\{ -\frac{1}{2} \int_0^l \frac{\left| \psi(t) \right|^2}{\sigma^2} dt \right\} \mu_{\sigma W}^{0,0}(K_i(0, \delta))
\]
\[
= C_0 \exp \left\{ C_1 \delta l + \frac{l \delta \| \psi \|_l}{\sigma^2} \right\} \frac{p_W(0, l|0, 0)}{p_W(x_l, l|x_0, 0)} \exp \left\{ \frac{-1}{2} \int_0^l \frac{\left| \psi(t) \right|^2}{\sigma^2} dt \right\} \mu_{\sigma W}^{0,0}(K_i(0, \delta))
\]
\[
= C_0 \exp \left\{ C_1 \delta l + \frac{l \delta \| \psi \|_l}{\sigma^2} + \frac{l \int_0^l \left( \psi(t) \cdot \nabla U(\psi(t)) \right) dt}{\sigma^2} \right\} \frac{p_W(0, l|0, 0)}{p_W(x_l, l|x_0, 0)} \exp \left\{ -S_X^{OM}(\psi) \right\} \mu_{\sigma W}^{0,0}(K_i(0, \delta)).
\]
Similarly, we have that
\[
\mu_X^{\infty-i}(K_i(\psi, \delta)) \geq C_0 \exp \left\{ -C_1 \delta l - \frac{l \delta \| \psi \|_l}{\sigma^2} - \frac{U(x_l) - U(x_0)}{\sigma^2} \right\} \frac{p_W(0, l|0, 0)}{p_W(x_l, l|x_0, 0)} \exp \left\{ -S_X^{OM}(\psi) \right\} \mu_{\sigma W}^{0,0}(K_i(0, \delta)).
\]
These give the desire results of the Theorem 3.4 with
\[
C = C_0 \exp \left\{ \frac{U(x_l) - U(x_0)}{\sigma^2} \right\} \frac{p_W(0, l|0, 0)}{p_W(x_l, l|x_0, 0)}.
\]

Remark 3.6. (i). In [4, 5] the OM functionals were derived from the measure \(\mu_X^\infty\) using Girsanov formula twice. This works since \(\mu_X^\infty\) is absolutely continuous with respect to \(\mu_{\sigma W}^\infty\), and both measures are quasi translation invariant (see [4] for details). However, the bridge measures \(\mu_X^{\infty-xi}\) and \(\mu_{\sigma W}^{\infty-xi}\) are not quasi translation invariant in \(C_{x_l}[0, l]\). This is the difference between our method and the methods in [4, 5] to derive the OM functionals.

(ii). Note that when we applied Girsanov transform in (3.11), the path \(x(\cdot)\) at the right hand side (RHS) is understood as a path of Brownian motion under \(\mu_{\sigma W}^\infty\), instead of a path of the solution process \(X\).

(iii). In the paper [39], the authors used a one-dimensional potential \(U\) that has two wells with one narrow and one broad, to investigate path sampling schemes. They observed that the Laplacian term \(U''\) has a huge influence on the OM functional. In an ensemble that was generated from a hybrid Monte Carlo sampling scheme, the resulting paths spent the largest amount of time in the narrow well, where the curvature of \(U\) is the largest. They pointed out that such a result is unphysical, by a reason that such paths are inconsistent with the equilibrium thermodynamical distribution where the particle would be expected to be found in the broad well in most of time. Other potentials appeared to be unphysical may also be found in [40]. Possible interpretations for the origin of unphysical phenomena of MPPs are the following: firstly, minimizing a OM functional is in general a non-convex optimization problem as its Lagrangian is non-convex (at least for double-well potentials), and the Euler-Lagrange equation for a OM functional, which may have many solutions, is merely a sufficient but not necessary condition for its minimizers, so numerical scheme based on this approach can only find (an approximation of) some (local) minimizers which we are in general not able to know if it is global, except for some special cases like the linear one, cf. Section 4; secondly, the first author of the present paper showed with his collaborators in [41] that it can occur that the (local) minimizer for the OM functional with a double-well potential has multiple back and forth transitions, when the given transition time \(t\) is large; thirdly, the equilibrium thermodynamical distribution only appears when the time is large.
enough so that the system is in equilibrium state, but it was proved in [42] and [43] that when transition
time \( t \) goes to infinity, the MPP converges under the Fréchet distance which allows a nonhomogeneous time
scaling.

### 3.5 Equivalence of most probable transition paths of Markovian bridge process

in different forms

First of all, we need to define the most probable transition paths for the system (3.5). Note that the
modified drift \( b \) in (4.1) is singular at time \( t = l \). In fact, it is this singular attractive potential which forces
all the paths of \( Y \) to \( x_l \) at time \( l \) [32]. In other words, the process \( Y \) must “transit” to \( x_l \) at time \( l \). So
formally we do not need to emphasis the transition behaviour for the process \( Y \). That is, the problem reduces to:
among all possible smooth paths starting at \( x_0 \), which one is most probable for the solution process \( Y \)
of (3.5)?

The solution process \( Y \) of (3.5) induces a measure \( \mu_{x_0}^{x_l} \) on \( \mathcal{B}_{[0,l]}^{x_0} \) as its law by

\[
\mu_{Y}^{x_0}(B) = \bar{\mathbb{P}}^{x_0}(\{\omega \in \tilde{\Omega} \mid Y(\omega) \in B\}), \quad B \in \mathcal{B}_{[0,l]}^{x_0}.
\]

Inspired by (2.2) and Theorem 3.4, we have the following definition.

**Definition 3.7.** The most probable path of the system (3.5) is a path \( \psi^* \) such that for each path \( \psi \) in
\( C_{2x_0}^2[0,l] \), we have

\[
\lim_{\delta \downarrow 0} \frac{\mu_{Y}^{x_0}(K_{l}(\psi^*, \delta))}{\mu_{\tilde{\psi}}^{x_0}(K_{l}(\psi, \delta))} \geq 1.
\]

**Remark 3.8.** Since we have known that \( \bar{\mathbb{P}}^{x_0}(Y_l = x_l) = 1 \), the most probable paths of system (3.5) must
reach point \( x_l \) at time \( l \).

To figure out the relation between the most probable transition paths of \( X \) and the most probable paths of
\( Y \), we need the help of the bridge measure \( \mu_{x_0}^{x_l} \). Note that although the two system (3.5) and (3.10)
may be defined on different probability spaces, their associate induced measures \( \mu_{Y}^{x_0} \) and \( \mu_{X}^{x_0, x_l} \) are defined
on the same path space \( (C_{x_0}[0,l], \mathcal{B}_{[0,l]}^{x_0}) \). The following lemma gives the relation between measures \( \mu_{Y}^{x_0} \) and
\( \mu_{X}^{x_0, x_l} \).

**Lemma 3.9 (Bridge measures = laws of bridge SDEs).** The two measures \( \mu_{X}^{x_0, x_l} \) and \( \mu_{Y}^{x_0} \) coincide.

**Proof.** The equations (3.3) and (3.6) show us that the transition density functions of process \( X \) under
\( \mathbb{P}^{x_0}(\cdot \mid X_t = x_l) \) and process \( Y \) under \( \bar{\mathbb{P}}^{x_0} \) are identical. Let \( I = \{\psi \in C_{x_0}[0,l] \mid \psi(t_l) \in E_1, \cdots, \psi(t_n) \in E_n\} \)
be a cylinder set with \( 0 \leq t_1 < t_2 < \cdots < t_n \leq l \) and Borel sets \( E_i \subset \mathbb{R}^l \). In the case that \( t_n < l \), we have
the following equalities:

\[
\begin{aligned}
\mu_{Y}^{x_0}(I) &= \bar{\mathbb{P}}^{x_0}(Y_{t_i} \in E_i, i = 1, \cdots, n) \\
&= \int_{E_1} \cdots \int_{E_n} \bar{p}^{x_0}(y_1, t_1|x_0, 0) \cdots \bar{p}^{x_0}(y_n, t_n|y_{n-1}, t_{n-1})dy_1 \cdots dy_n \\
&= \bar{\mathbb{P}}^{x_0}(X_{t_i} \in E_i, i = 1, \cdots, n \mid X_l = x_l) \\
&= \mu_{X}^{x_0, x_l}(I).
\end{aligned}
\]

In the case that \( t_n = l \), due to the fact \( \bar{\mathbb{P}}^{x_0}(Y_l = x_l) = 1 \) and \( \mathbb{P}^{x_0}(X_l = x_l | X_l = x_l) = 1 \), we know that

\[
\begin{aligned}
\mu_{Y}^{x_0}(I) &= \mu_{Y}^{x_0}(\{\psi \in C_{x_0}[0,l] \mid \psi(t_l) \in E_i, i = 1, \cdots, n - 1\}) \\
&= \mu_{X}^{x_0, x_l}(\{\psi \in C_{x_0}[0,l] \mid \psi(t_l) \in E_i, i = 1, \cdots, n - 1\}) = \mu_{X}^{x_0, x_l}(I), \quad \text{if } x_l \in E_n, \\
\mu_{Y}^{x_0}(I) &= 0 = \mu_{X}^{x_0, x_l}(I), \quad \text{if } x_l \notin E_n.
\end{aligned}
\]

Thus the measures \( \mu_{Y}^{x_0} \) and \( \mu_{X}^{x_0, x_l} \) coincide on all cylinder sets of \( C_{x_0}[0,l] \). Recall that, the field \( \mathcal{B}_{[0,l]}^{x_0} \) is the
\( \sigma \)-field generated by all cylinder sets. By the Carathéodory measure extension theorem, we know that the
two probability measures \( \mu_{Y}^{x_0} \) and \( \mu_{X}^{x_0, x_l} \) coincide on \( \mathcal{B}_{[0,l]}^{x_0} \). And this completes the proof. \( \square \)
Remark 3.10. The bridge measure $\mu^{x_0,x_l}_X$ contains the thermodynamic (or statistical) information of all paths of the underlying process $X$ that happen to end at the particular metastable state $x_l$, while the law $\mu^{x_0}_Y$ of bridge SDE (3.5) contains the information of the process $Y$ that are forced to end at the state $x_l$ by an additional virtual potential, cf. Remark 3.2. Lemma 3.9 tells that the thermodynamic information of the above two different thermodynamic systems is equivalent.

Under Theorem 3.4 and Lemma 3.9, for $\psi_1, \psi_2 \in C^2_{x_0,x_l}[0,l]$ we have that

$$\lim_{\delta \downarrow 0} \frac{\mu^{x_0}_Y(\tilde{K}_1(\psi_1, \delta))}{\mu^{x_0}_X(\tilde{K}_1(\psi_2, \delta))} = \lim_{\delta \downarrow 0} \frac{\mu^{x_0}_X(\tilde{K}_1(\psi_1, \delta))}{\mu^{x_0}_X(\tilde{K}_1(\psi_2, \delta))} = \exp(S^{QM}_X(\psi_2) - S^{QM}_X(\psi_1)) = \lim_{\delta \downarrow 0} \frac{\mu^{x_0}_X(\tilde{K}_1(\psi_1, \delta))}{\mu^{x_0}_X(\tilde{K}_1(\psi_2, \delta))}.$$ 

Thus the main result of this paper can be verified easily and we summarize it as the following theorem.

Theorem 3.11 (Equivalence of most probable transition paths in different forms). Under the Assumptions $H1$ and $H2$, if the most probable transition path(s) of the system (2.1) exist(s), then it (they) coincide(s) with the most probable path(s) of the associated bridge SDE (3.5).

Remark 3.12. As we have mentioned in the introduction, neither the most probable transition paths of system (2.1) nor the most probable paths of the bridge SDE (3.5) are genuine paths since they are differentiable curves. This means the MPPs/MPTPs are statistical predictions rather than actual observations or measurements. Theorem 3.11 infers that such statistical predictions for the two thermodynamic systems in Remark 3.10 are equivalent. In many cases the path matters, however, changes in the thermodynamic properties depend only on the initial and final states and not upon the path [44].

4 Two Special Cases: Linear Stochastic Systems and Stochastic Systems with Small Noise

For the sake of notational simplicity, we introduce the modified drift $b$ by

$$b(t, x) := -\nabla U(x) + \sigma^2 \nabla \ln p(x_l | x),$$

Due to Theorem 3.11, we know that if we want to find the most probable transition paths of system (2.1), an alternative way is to find the most probable paths of system (3.5). In other words, the optimization problem

$$\inf_{\psi \in C^2_{x_0,x_l}[0,l]} S^{QM}_X(\psi)$$

turns to another optimization problem

$$\inf_{\psi \in C^2_{x_0,x_l}[0,l]} S^{QM}_Y(\psi),$$

where $S^{QM}_Y$ is the OM functional for the system (3.5) over time interval $[0,l]$, i.e.,

$$S^{QM}_Y(\psi) = \frac{1}{2} \int_0^l \left[ \frac{|\dot{\psi}(s) - b(s, \psi(s))|^2}{\sigma^2} + \nabla \cdot b(s, \psi(s)) \right] ds.$$

Remark 4.1. The two optimization problems (4.2) and (4.3) can be both translated to optimal control problems. That is, (4.2) can be translated into

$$\text{minimizing} \quad J_X[\psi, u] := \frac{1}{2} \int_0^l \left[ \frac{|u(s)|^2}{\sigma^2} - \Delta U(\psi(s)) \right] ds + \Theta(\psi(l)),$$

subject to

$$\begin{cases}
\dot{\psi}(s) = -\nabla U(\psi(s)) + u(s), & s \in [0, l], \\
\psi(0) = x_0,
\end{cases}$$

subject to
where the functional $J_X$ is called the payoff functional, the function $\Theta$ is given by
\[
\Theta(x) = \begin{cases} 
0, & x = x_l, \\
+\infty, & \text{otherwise}. 
\end{cases}
\]
and called the terminal cost, equation (4.4) is called the state equation. Similarly, (4.3) can be translated into
\[
\text{minimizing } J_Y[\psi, u] := \frac{1}{2} \int_0^l \left( |u(s) - \sigma^2 \nabla \ln p(x_l, |\psi(s), s)|^2 + \nabla \cdot b(s, \psi(s)) \right) ds,
\]
subject to the same state equation (4.4). The singularities of $\Theta$ and $p$ at $x_l$ imply that the minimizers of $J_X$ and $J_Y$ both satisfy $\psi(l) = x_l$. The equivalence between (4.2) and (4.3) provides an indirect way to obtain that $J_X$ and $J_Y$ share the same minimizer, which is not so obvious from their forms. We refer to [45, 46] for more discussions on optimal control problems arising from path or entropic information of processes.

A special case is that the divergence term $\nabla \cdot b(t, x)$ is independent of $x$. In this case,
\[
\inf_{\psi \in C^2_{[0, l]}} S^O_M(\psi) = \frac{1}{2} \int_0^l (\nabla \cdot b)(s) ds + \inf_{\psi \in C^2_{[0, l]}} \frac{1}{2} \int_0^l |\dot{\psi}(s) - b(s, \psi(s))|^2 \sigma^2 ds,
\]
this will achieve its minimum if the quadratic term can vanish. Therefore, the most probable path is described by the following first-order ordinary differential equation (ODE) if it is solvable,
\[
\begin{aligned}
\dot{\psi}^*(t) &= b(t, \psi^*(t)), \quad t \in [0, l) \\
\psi^*(0) &= x_0.
\end{aligned}
\] (4.5)

The existence and uniqueness of the solution of system (4.5) can be promised by the regularity of the function $b$ on $[0, l) \times \mathbb{R}^k$.

In the following subsections, we will show the utilization of this special case by studying two typical classes of stochastic systems: linear systems, and nonlinear systems with small noise.

### 4.1 Linear systems

Consider the following linear equation [27, Section 5.6]:
\[
\begin{cases}
\dot{X}_t = [G X_t + a] dt + \sigma dW_t, \quad 0 \leq t < \infty \\
X_0 = x_0,
\end{cases}
\]
(4.6)
where $W$ is a $k$-dimensional Brownian motion independent of the initial vector $x_0 \in \mathbb{R}^k$, $G$ is a $(k \times k)$ constant nondegenerate symmetric matrix, $a$ is a $(k \times 1)$ matrix and the noise intensity $\sigma$ is a positive constant. Under these settings, it is easy to check that the drift term is the gradient of the potential function
\[
U(x) = -\frac{1}{2} x^T G x - a^T x + \text{constant},
\]
which satisfies $\Delta U = -\text{Tr} \ G$. The solution of the system (4.6) has the following representation,
\[
X_t = \Phi(t) \left[ x_0 + \int_0^t \Phi^{-1}(s) a ds + \sigma \int_0^t \Phi^{-1}(s) dW_s \right], \quad 0 \leq t < \infty,
\]
(4.8)
where $\Phi^{-1}$ is the matrix inverse of the solution $\Phi(t) = e^{G t}$ of the differential equation
\[
\begin{aligned}
\dot{\Phi}(t) &= G \Phi(t) \\
\Phi(0) &= I,
\end{aligned}
\] (4.9)
and \( I \) is the \( k \times k \) identity matrix. Clearly, the solution \( X \) in (4.8) is a Gaussian process, whose mean vector and covariance matrix are given by

\[
\begin{align*}
\mu(t) & \triangleq \mathbb{E}X_t = \Phi(t) \left[ x_0 + \int_0^t \Phi^{-1}(s)ads \right], \\
\Sigma(t) & \triangleq \mathbb{E}[(X_t - \mathbb{E}X_t)(X_t - \mathbb{E}X_t)^T] = \sigma^2 \Phi(t) \left[ \int_0^t \Phi^{-1}(s)(\Phi^{-1}(s))^Tds \right] \Phi^T(t).
\end{align*}
\]

Hence the probability density function of \( X \) is

\[
p(x,t|x_0,0) = \frac{1}{(2\pi)^{k/2}\sqrt{\det \Sigma(t)}} \exp \left\{ -\frac{1}{2} [x - \mu(t)]^T \Sigma^{-1}(t) [x - \mu(t)] \right\}.
\]

Now the divergence of the modified drift (in (4.1)) of the corresponding Markovian bridge system (3.5) is

\[
\nabla \cdot [Gx + a + \sigma^2 \nabla \ln p(x,l|x,t)]
\]

\[
= \text{Tr} G - \frac{\sigma^2}{2} \Delta \left\{ \left[ x_l - \Phi(l-t) \left( x + \int_0^{l-t} \Phi^{-1}(s)ads \right) \right]^T \Sigma^{-1}(l-t) \left[ x_l - \Phi(l-t) \left( x + \int_0^{l-t} \Phi^{-1}(s)ads \right) \right] \right\}.
\]

Observe that the term in the braces at the RHS of the above equality is a quadratic form in \( x \). Hence, the Laplacian of the whole term in the braces is independent of \( x \), so is the divergence of the modified drift. To sum up, we have the following corollary.

**Corollary 4.2.** The most probable transition path of the linear system (4.6) is described by the following ordinary differential equation

\[
\begin{align*}
\dot{\psi}(t) & = G\psi(t) + a + \left[ \int_0^{l-t} \Phi^{-1}(s)(\Phi^{-1}(s))^Tds \right]^{-1} \left( \Phi^{-1}(l-t)x_l - \psi(t) - \int_0^{l-t} \Phi^{-1}(s)ads \right), \\
\psi(0) & = x_0,
\end{align*}
\]

where \( \Phi(t) = e^{Gt} \) is the solution of the differential equation (4.9).

### 4.2 Systems with small noise

Now we turn to nonlinear systems. We consider the small-noise version of system (2.1) as follows:

\[
\begin{align*}
\left\{ \begin{array}{l}
\frac{dX^\varepsilon_t}{dt} = -\nabla U(X^\varepsilon_t) dt + \varepsilon dW_t, \quad t \in (0,l], \\
X^\varepsilon_0 = x_0,
\end{array} \right.
\end{align*}
\]

(4.10)

where \( \varepsilon \) is a positive constant and \( x \mapsto U(x) \) is a real function on \( \mathbb{R}^k \). This system has been studied with a rich history, see for example [47] and references therein.

The Freidlin-Wentzell theory of large deviations asserts that, for \( \delta > 0 \) and \( \varepsilon > 0 \) and sufficiently small,

\[
\mathbb{P}^{x_0}(\|X^\varepsilon - \psi\|_t < \delta) \sim \exp(-\varepsilon^{-2}S_{X}^{\text{FW}}(\psi)),
\]

where the Freidlin-Wentzell (FW) action functional is defined as

\[
S_{X}^{\text{FW}}(\psi) = \frac{1}{2} \int_0^t |\dot{\psi}(s) + \nabla U(\psi(s))|^2 ds,
\]

which turns out to be the dominant term of OM functional (1.3). Thus as \( \varepsilon \downarrow 0 \), the most probable transition path \( \psi^* \) of system (4.10) is given by the following equation:

\[
S_{X}^{\text{FW}}(\psi^*) = \inf_{\psi \in C^0_{l_0,l}([0,l])} S_{X}^{\text{FW}}(\psi).
\]
The Lagrangian of the FW action functional is

\[ L(\psi, \dot{\psi}) = |\dot{\psi} + \nabla U(\psi)|^2, \]

and the associated Euler-Lagrange equation is a second order boundary value problem which reads

\[
\begin{align*}
\psi - \frac{1}{2} \nabla |\nabla U(\psi)|^2 &= 0, \\
\psi(0) &= x_0, \quad \psi(l) = x_l.
\end{align*}
\]  

The classical variational method tells that the Euler-Lagrange equation is a necessary but not sufficient condition of the most probable transition paths.

On the other hand, the bridge process of system (4.10) is

\[
\begin{align*}
\frac{dY^\varepsilon_l}{dt} &= \left[-\nabla U(Y^\varepsilon_l) + \varepsilon^2 \nabla \ln p_\varepsilon(x_l, l|Y^\varepsilon_l, t)\right] dt + \varepsilon d\tilde{W}_t, \quad t \in (0, l), \\
Y^\varepsilon_0 &= x_0,
\end{align*}
\]  

where \( p_\varepsilon(x_l, l|x, t) \) is the transition density of the solution process of system (4.10). The problem here is how to characterize the limit of the term \( \varepsilon \nabla \ln p_\varepsilon(x_l, l|Y^\varepsilon_l, t) \) as \( \varepsilon \downarrow 0 \). However, in general this is not analytically possible. An alternative way to deal with this problem is to make approximations. The papers [48, 49] for path sampling have given some schemes to do approximations.

The authors in [48] transformed the Fokker-Planck equation (3.1) for \( p_\varepsilon \) to the following imaginary time Schrödinger equation by the transformation \( \Psi(x, t) = \exp\left(\frac{U(x)}{\varepsilon^2}\right)p_\varepsilon(x, t|x_0, t_0) \),

\[
\frac{\partial \Psi}{\partial t} = \varepsilon^2 \frac{\Delta \Psi(x, t)}{2} - \frac{1}{2\varepsilon^2} V(x) \Psi(x, t),
\]

where \( V(x) = |\nabla U(x)|^2 - \varepsilon^2 \Delta U(x) \); they then used Trotter approximation to approximate the Schrödinger kernel and obtained the following asymptotic formula,

\[
p_\varepsilon(x, t|y, s) = \exp \left\{ - \frac{U(x) - U(y)}{\varepsilon^2} - \frac{|x - y|^2}{2\varepsilon^2} - \frac{t - s}{4\varepsilon^2} (V(x) + V(y)) \right\} + O(|t - s|^3).
\]

This formula not only suggests that the SDE (4.12) can be approximated by the following SDE

\[
\begin{align*}
\frac{dY^\varepsilon_l}{dt} &= \left[\frac{x_l - Y^\varepsilon_l}{l - t} - \frac{l - t}{4} \nabla V(Y^\varepsilon_l)\right] dt + \varepsilon d\tilde{W}_t, \quad t \in (0, l), \\
Y^\varepsilon_0 &= x_0,
\end{align*}
\]

when the transition time \( l \) is short, but also quantifies the approximation errors.

The paper [49] provided a different and more complicated approximation approach for the one-dimensional case of SDE (4.12). The approximating SDE in the limit \( \varepsilon \downarrow 0 \) is given by

\[
\begin{align*}
\frac{dY^\varepsilon_l}{dt} &= \left[\frac{x_l - Y^\varepsilon_l}{l - t} - \frac{l - t}{2} \int_0^1 \left(1 - u\right) \frac{d}{dx} \left[ \left(\frac{d}{dx}\right)^2 (x_l u + Y^\varepsilon_l (1 - u)) \right] du \right] dt + \varepsilon d\tilde{W}_t, \quad t \in (0, l), \\
Y^\varepsilon_0 &= x_0.
\end{align*}
\]

See [49] for more discussions and comparisons.

Now we have two approximation schemes for the most probable paths of the system (4.12) in the limit \( \varepsilon \downarrow 0 \). The first one \( \psi_{\text{appr},1} \) is described by a first order differential equation:

\[
\begin{align*}
\frac{d\psi_{\text{appr},1}}{dt} &= \frac{x_l - \psi_{\text{appr},1}}{l - t} - \frac{l - t}{4} \nabla |\nabla U|^2(\psi_{\text{appr},1}), \quad t \in [0, l), \\
\psi_{\text{appr},1}(0) &= x_0,
\end{align*}
\]  

(4.13)
and the other one \( \psi_{\text{appr},2} \) is described by an integro differential equation:

\[
\begin{cases}
\frac{d\psi_{\text{appr},2}}{dt} = \frac{x_l - \psi_{\text{appr},2}}{l - t} - \frac{l - t}{2} \int_0^1 (1 - u) \frac{d^2}{dx^2} \left[ \frac{d^2}{dx^2} \right] (x_l u + \psi_{\text{appr},2}(1 - u)) du, \ t \in [0, l), \\
\psi_{\text{appr},2}(0) = x_0.
\end{cases}
\] (4.14)

Now we have three descriptive equations for the most probable transition paths of the system (4.10)—equation (4.11), (4.13) and (4.14). The Euler-Lagrange equation (4.11) is a conventional result derived from the classical variation method. Thus it is a necessary but not sufficient description for the most probable transition paths of the system (4.10). Besides this, the equation (4.11) is a second order boundary value problem, it is hard to solve analytically or numerically in general. Equations (4.13) and (4.14) are approximations of the most probable paths of the bridge system (4.12), and hence also approximations of the most probable transition paths of the original system (4.10) due to Theorem 3.11. One advantage of these two approximations is that they are much easier and more efficient to perform numerically, since they are first order ODEs without any restrictions on the ending values. Meanwhile, the analytic expressions of equation (4.13) and (4.14) enable us to analyze the most probable transition paths asymptotically in a convenient fashion. Though the disadvantages are also obvious: firstly, the cases having analytic expressions for the most probable transition path are rare; secondly, the approximations is valid on a limited time interval. These will be shown in the example of stochastic double-well systems in the next section.

5 Examples

Let us consider several examples in order to illustrate our results.

Example 5.1 (The free Brownian motion). The simplest case is the free particles in Euclidean space. In this case, the Green’s function \( p(x_l, l|x, t) \) can be written explicitly as follows

\[
p(x_l, l|x, t) = \frac{1}{2\pi(l - t)} e^{-\frac{(x_l - x)^2}{2(l - t)}}.
\]

The corresponding Markovian bridge process is described by the following SDE:

\[
dY_t = \frac{x_l - Y_t}{l - t} dt + d\tilde{W}_t, \quad Y_0 = x_0.
\] (5.1)

The partial derivative of the drift term with respect to the position variable is independent of position variable. Thus by (4.5), the most probable path of (5.1) is

\[
\frac{d\psi^*}{dt} = \frac{x_l - \psi^*}{l - t}, \quad \psi^*(0) = x_0 \implies \psi^*(t) = x_l + \frac{x_0 - x_l}{l}(l - t), \ t \in [0, l),
\]

which can be verified as the extremal path of the OM functional \( S_{OM}(\psi) = \frac{1}{2} \int_0^l \dot{\psi}^2 dt \) over the path space \( C_{x_0,x_l}^2 [0, l] \).

Example 5.2 (Linear systems). In this example we consider the linear system (4.6) in one-dimensional and two-dimensional cases.

Case 1. Consider the scalar case of the system with \( G = -\theta, \ a = \theta \mu \) where \( \theta \) and \( \mu \) are constants. The system turns to

\[
dX_t = \theta(\mu - X_t) dt + \sigma dW_t, \quad X_0 = x_0 \in \mathbb{R}.
\] (5.2)

The solution of (5.2) is called an Ornstein-Uhlenbeck (OU) process [50] (more general than (3.8)). OU process are usually used in finance to model the spread of stocks or to calculate interest rates and currency exchange rates. They also appear in physics to model the motion of a particle under friction.

On the one hand, the potential function of the system (5.2), as in (4.7) satisfies \( U''(x) = -\theta \). So the OM functional of the system is

\[
S_{OM}(\psi) = \frac{1}{2\sigma^2} \int_0^l \left[ (\dot{\psi} - \theta \mu + \theta \psi)^2 + \theta^2 \right] dt.
\]
Figure 1: The most probable transition path starting from $x_0 = 0$ and ending at $x_l = 2$ with transition time $l = 2, 3, 4$ respectively, for the OU process with parameters $\mu = 1, \theta = 2$. The yellow lines are the solutions of the equation (5.4) computed by forward Euler scheme, while red point lines are the solutions of the Euler-Lagrange equation (5.3) computed by the shooting method.

The corresponding Euler-Lagrange (E-L) equation reads
\[
\begin{cases}
\ddot{\psi} + \theta(\theta \mu - \theta \dot{\psi}) = 0, \\
\psi(0) = x_0, \quad \psi(l) = x_l.
\end{cases}
\]

Hence, we can solve the second-order boundary value problem (5.3), if it is uniquely solvable, to obtain the most probable transition path.

On the other hand, the transition probability density function is [51]
\[
p(x_l, l | x, t) = \frac{\sqrt{\theta}}{\sigma \sqrt{\pi(1 - e^{-2\theta(l-t)})}} \exp \left\{ - \frac{\theta}{\sigma^2} \left[ x_l - (e^{-\theta(l-t)}x + \mu e^{-\theta(l-t)}) \right]^2 \right\},
\]
which leads to a Markovian bridge process as in (3.5). Then by Corollary 4.2, the most probable transition path of (5.2) is described by the following first-order ODE,
\[
\frac{d\psi^*(t)}{dt} = \theta(\mu - \psi^*) + 2\theta e^{-\theta(l-t)} x_l - \frac{(e^{-\theta(l-t)} \psi^* + \mu e^{-\theta(l-t)})}{1 - e^{-2\theta(l-t)}}, \quad \psi^*(0) = x_0.
\]

As (5.4) is a first-order linear ODE, it can be numerically solved quite easily. Moreover, its analytical solution can be explicitly found out as follows,
\[
\psi^*(t) = \exp \left( - \int_0^t P(s) ds \right) \left[ x_0 + \int_0^t Q(s) \exp \left( \int_0^s P(u) du \right) ds \right],
\]
where
\[
P(t) = -\theta - \frac{2\theta e^{-2\theta(l-t)}}{1 - e^{-2\theta(l-t)}},
\]
\[
Q(t) = \theta \mu + 2\theta e^{-\theta(l-t)} x_l - \frac{(\mu - e^{-\theta(l-t)})}{1 - e^{-2\theta(l-t)}}.
\]

Figure 1 shows the numerical results of the MPTPs via (5.3) and (5.4). They fit very well, with difference only about $10^{-4}$. But apparently, (5.4) is much easier to treat than (5.3) both analytically and numerically.

Case 2. Consider the system (4.6) in $\mathbb{R}^2$ with $a = (0, 0)^T$, $\sigma = 1$ and
\[
G = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.
\]
Now the system turns to the following coupled system,

\[
\begin{aligned}
    dX^1_t &= X^2_t \, dt + dW^1_t, \\
    dX^2_t &= X^1_t \, dt + dW^2_t, \\
    X_0 &= x_0 \in \mathbb{R}^2.
\end{aligned}
\]  

(5.5)

(a) Most probable transition paths in \((x^1, x^2, t)\)-plane (left) and \((x^1, x^2)\)-plane (right) with \(x_0 = (1, -1), x_l = (-1, 1)\) and \(l = 2, 3, 4\).

(b) Most probable transition paths in \((x^1, x^2, t)\)-plane (left) and \((x^1, x^2)\)-plane (right) with \(x_0 = (1, -1), x_l = (1, 1)\) and \(l = 2, 3, 4\).

Figure 2: The most probable transition paths in \((x^1, x^2, t)\)-plane and \((x^1, x^2)\)-plane under different initial and terminal conditions and transition times. The yellow lines are the numerical solutions of (5.7) and the red point lines are the solutions of equation (5.6).

On the one hand, the potential function is given by \(U(x^1, x^2) = -x^1 x^2 + \text{constant}\), so that \(\Delta U \equiv 0\). Then the OM action functional of (5.5) is

\[
S^{OM}(\psi) = \frac{1}{2} \int_0^l \left| \dot{\psi}(s) - G\psi(s) \right|^2 - (\Delta U)(\psi(s)) \right| ds = \frac{1}{2} \int_0^l \left| \psi(s) - G\psi(s) \right|^2 ds,
\]

and the corresponding Euler-Lagrange equation is

\[
\begin{aligned}
    \ddot{\psi}^1 &= \psi^1, \\
    \ddot{\psi}^2 &= \psi^2, \\
    \psi(0) &= x_0, \ \psi(l) = x_l.
\end{aligned}
\]  

(5.6)
Note that the two-dimensional boundary value problem (5.6) can be separated into two independent one-dimensional boundary value problems. Thus we can use shooting method to solve each one-dimensional equation respectively.

On the other hand, observe that
\[ e^{Gt} = \frac{1}{2} \begin{pmatrix} e^t + e^{-t} & e^t - e^{-t} \\ e^{-t} - e^t & e^{-t} + e^t \end{pmatrix}, \quad (e^{Gt})^{-1} = e^{-Gt} = \frac{1}{2} \begin{pmatrix} e^t + e^{-t} & -e^t + e^{-t} \\ -e^{-t} + e^t & e^{-t} + e^t \end{pmatrix}. \]

So the mean \( \mu(t) \) of \( X_t \) is
\[ \mu(t) = e^{Gt}x_0 = \frac{1}{2} \begin{pmatrix} (e^t + e^{-t})x_0^1 + (e^t - e^{-t})x_0^2 \\ (e^{-t} - e^t)x_0^1 + (e^t + e^{-t})x_0^2 \end{pmatrix}, \]

and the covariance matrix \( \Sigma(t) \) is
\[ \Sigma(t) = e^{Gt} \int_0^t (e^{Gs})^{-1} \left[ (e^{Gs})^{-1} \right]^T ds(e^{Gt})T = \frac{1}{4} \begin{pmatrix} e^{2t} - e^{-2t} & e^{-2t} - 2 + e^{2t} \\ e^{-2t} - 2 + e^{2t} & e^{2t} - e^{-2t} \end{pmatrix}, \]

with matrix inverse (when \( t > 0 \)):
\[ \Sigma^{-1}(t) = \begin{pmatrix} -\frac{e^{2t} - e^{-2t}}{2+e^{2t}} & \frac{-e^{-2t} - 2+e^{2t}}{2+e^{2t}} \\ \frac{-e^{-2t} - 2+e^{2t}}{2+e^{2t}} & -\frac{e^{2t} - e^{-2t}}{2+e^{2t}} \end{pmatrix}. \]

According to Corollary 4.2 we know that, the most probable transition path of system (5.5) solves the following system of first-order ODEs:
\[
\begin{cases}
\dot{\psi}^1(t) = \psi^2(t) + (e^{G(t-t)} \Sigma^{-1}(l-t) (x_l - e^{G(0-t)} \psi(t)), \quad t \in [0, l), \\
\psi(0) = x_0.
\end{cases}
\]

Figure 2 shows the numerical solutions of the Euler-Lagrange equation (5.6) and the first-order ODE system (5.7), with different initial or boundary values and different transition times, by using shooting method and forward Euler scheme respectively. In this case, since the Euler-Lagrange equation is already decoupled while the first-order ODE system is still coupled, it is hard to say which one is more efficient. But anyway, they still fit each other quite well. This shows the validity of our method.

**Example 5.3** (Ginzburg-Landau double-well system with small noise). Consider the following scalar double-well system with small noise:
\[ dX_t = (X_t - X_t^3)dt + \varepsilon dW_t, \quad X_0 = x_0 \in \mathbb{R}. \]

It is easy to see that 1 and −1 are stable equilibrium states of the deterministic system and hence metastable states of the stochastic system, while 0 is an unstable equilibrium state of the deterministic system. We consider the transition phenomena between metastable states \( x_0 = -1 \) and \( x_l = 1 \).

The first approximation \( \psi_{\text{appr}, 1} \) of the most probable transition path is
\[
\frac{d\psi_{\text{appr}, 1}}{dt} = \frac{x_l - \psi_{\text{appr}, 1}}{l-t} - \frac{1}{2} (l-t)(\psi_{\text{appr}, 1} - \psi_{\text{appr}, 1}^3)(1 - 3\psi_{\text{appr}, 1}^2), \quad t \in [0, l). \tag{5.8}
\]

And the other one \( \psi_{\text{appr}, 2} \) is
\[
\frac{d\psi_{\text{appr}, 2}}{dt} = \frac{x_l - \psi_{\text{appr}, 2}}{l-t} - (l-t) \int_0^1 (1-u)(Z - Z^3)(1 - 3Z^2)du, \quad t \in [0, l), \tag{5.9}
\]

where \( Z = x_l u + \psi_{\text{appr}, 2}(1-u) \).

The FW action functional of this system is
\[ S_{FW}(\psi) = \frac{1}{2} \int_0^l (\psi - (\psi^3))^2 dt. \]
The most probable transition paths approximated by $\psi_{\text{appr},1}$, $\psi_{\text{appr},2}$ and $\psi_{\text{shoot}}$ under different transition times.

The Euler-Lagrange equation reads
\[
\begin{aligned}
\ddot{\psi} &= (\psi - \psi^3)(1 - 3\psi^2), \\
\psi(0) &= x_0, \psi(l) = x_l.
\end{aligned}
\]

A general numerical way to solve this second order differential equation is the shooting method. And we denote the path computed by the shooting method as $\psi_{\text{shoot}}$.

We choose the transition time $l$ to be $1, 2, 4, 7, 10, 12, 15$ respectively, and compute the corresponding paths $\psi_{\text{appr},1}$, $\psi_{\text{appr},2}$ and $\psi_{\text{shoot}}$. Here we set the time step to be $\Delta t = 10^{-4}$. The paths $\psi_{\text{appr},1}$ and $\psi_{\text{appr},2}$ can be numerically computed by forward Euler scheme according to equations (5.8) and (5.9). And we use the shooting method with Newton iteration to compute the path $\psi_{\text{shoot}}$ and we set the iteration error to be $10^{-4}$, i.e., when $|\psi_{\text{shoot}}(l) - x_l| < 10^{-4}$ we stop the algorithm.

Figure 3 shows the paths computed by the ways mentioned above. And we compute the corresponding discrete Freidlin-Wentzell action functional values of all these paths by
\[
S_{FW}(\psi) = \sum_i \left( \frac{\psi_i - \psi_{i-1}}{\Delta t} - (\psi_{i-1} - \psi_{i-1}^3) \right)^2 \Delta t.
\]

The values are listed in Table 1. From Figure 3 we know that when the transition time $l$ is small such as $l = 1, 2$, the three paths $\psi_{\text{appr},1}$, $\psi_{\text{appr},2}$ and $\psi_{\text{shoot}}$ are almost identical. The path $\psi_{\text{appr},2}$ and $\psi_{\text{shoot}}$ are still quite close for $l = 4, 7, 10$. When $l = 12, 15$, these three paths are away from each others. Since it shows in Table 1 that the FW action value of $\psi_{\text{shoot}}$ keeps smallest among the three FW action values when $l > 2$ (except $l = 12$), we know that the path $\psi_{\text{shoot}}$ may be more suitable to approximate the most probable transition path for large time. However the numerical shooting method failed to find the most probable transition path when $l = 12$. The shooting method did not work because the initial parameter we chose is not suitable and it makes the algorithm divergence. Because the shooting method turns the boundary value problem to an initial value problem. Thus the selection of the initial parameter is very important for this numerical method. The initial problems (i.e. $\psi_{\text{appr},1}$ and $\psi_{\text{appr},2}$) do not have this shortcoming.

6 Conclusion and Discussion

In general, the problem of finding the most probable transition paths of stochastic dynamical systems is solved by Euler-Lagrange equations which are second order equations with two boundary values. In this
Table 1: The Freidlin-Wentzell action functional values of the most probable transition paths in Figure 3.

| Transition Time | $S_{FW}^{\psi_{appr.1}}$ | $S_{FW}^{\psi_{appr.2}}$ | $S_{FW}^{\psi_{shoot}}$ |
|-----------------|-------------------------|-------------------------|-------------------------|
| 1               | 4.0784                  | 4.0760                  | 4.0765                  |
| 2               | 2.1716                  | 2.1510                  | 2.1511                  |
| 4               | 1.4963                  | 1.2940                  | 1.2939                  |
| 7               | 1.4936                  | 1.0510                  | 1.0475                  |
| 10              | 1.4943                  | 1.0264                  | 1.0072                  |
| 12              | 1.4945                  | 1.0356                  | NaN                     |
| 15              | 1.4946                  | 1.1225                  | 1.0003                  |

work, we show that the most probable transition paths of a stochastic dynamical system can be determined by its corresponding Markovian bridge system. This provides a new insight to related topics. The result mainly depends on the derivation of the Onsager-Machlup action functionals from bridge measures. It is worth to notice that the bridge measures are no longer quasi translation invariant. This fact leads to a different method from the existing works to derive the Onsager-Machlup action functionals. The Markovian bridge system has an extra drift term which forces all sample paths to end at a given point. However it is not possible to get an analytical expression for this extra drift for general nonlinear stochastic systems. But there do exist some analytic approximations for this term in small noise cases. Thus an important application of our result is that the most probable transition paths can be determined (for some special cases) or approximated (for general nonlinear cases with small noise) by first order differential equations. These first order differential equations are easier to solve numerically than the Euler-Lagrange equations. And we should notice that, our first order differential equation is a sufficient and necessary description of the most probable transition path, but the Euler-Lagrange equation is a sufficient but not necessary description.

To summarize, in this paper we firstly develop a new method to derive Onsager-Machlup action functional for Markovian bridge measures that the previous theories do not work for such measures. Secondly we show that for a class of linear system and stochastic systems with small noise, the corresponding most probable transition paths can be determined by a first order differential equations. Though such differential equations cannot be presented analytically for general nonlinear systems, our method provides potential point of view to solve more general cases. So our future works will focus on approximating the drift term of the Markovian bridge system on a longer time interval keeping the accuracy.

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Data Availability

The datasets generated during and/or analysed during the current study are available from the corresponding author on reasonable request.

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