Mathematical foundation of nonequilibrium fluctuation-dissipation theorems for inhomogeneous diffusion processes with unbounded coefficients

Xian Chen\textsuperscript{1}, Chen Jia\textsuperscript{2,∗}

\textsuperscript{1} School of Mathematical Sciences, Xiamen University, Xiamen, 361005, China.
\textsuperscript{2} Department of Mathematical Sciences, The University of Texas at Dallas, Richardson, Texas 75080, U.S.A.
Correspondence: jiac@utdallas.edu

Abstract

Nonequilibrium fluctuation-dissipation theorems (FDTs) are one of the most important advances in stochastic thermodynamics over the past two decades. Here we provide a rigorous mathematical theory of two types of nonequilibrium FDTs for inhomogeneous diffusion processes with unbounded drift and diffusion coefficients by using the Schauder estimates for partial differential equations of parabolic type and the theory of weak generators. The FDTs proved in this paper apply to any forms of nonlinear external perturbations. Furthermore, we prove the uniqueness of the conjugate observables and clarify the precise mathematical conditions and ranges of applicability for the two types of FDTs. Examples are also given to illustrate the main results of this paper.

Keywords: stochastic thermodynamics, linear response, fluctuation relation, nonsymmetric Markov process, stochastic differential equation; parabolic equation

Mathematics Subject Classifications: 60J60, 82C05, 60H10, 82C31, 35K10

1 Introduction

Over the past two decades, significant progress has been made in the field of nonequilibrium stochastic thermodynamics \cite{1-3}, which has grown to become one of the most important branches of statistical physics. The mathematical framework of this theory turns out to be nonstationary and nonsymmetric Markov processes, where the breaking of stationarity characterizes irreversibility described by Boltzmann and the breaking of symmetry characterizes irreversibility described by Prigogine \cite{4-6}. In this theory, an equilibrium state is defined as a stationary and symmetric Markov process and the deviation from equilibrium is usually characterized by the concept of entropy production \cite{7}. When an open system has a sustained external driving, it will approach a nonequilibrium steady state (NESS), which is defined as a stationary but nonsymmetric Markov process.

The fluctuation-dissipation theorem (FDT) for equilibrium states is one of the classical results in equilibrium statistical physics \cite{8-10}. In equilibrium, the FDT expresses the response of an observable to a small external perturbation by the correlation function of this observable and another one that is conjugate to the perturbation with respect to the energy. Mathematically, a small impulsive perturbation at time $s$ will give rise to a response of an observable $f$ at time
that only depends on the time difference \( t - s \) with the form of

\[
R_f(t - s) = -\frac{1}{k_B T} \frac{\partial}{\partial s} \mathbb{E}[f(X_t)]g(X_s),
\]

(1)

where \( k_B \) is the Boltzmann constant, \( T \) is the temperature, and \( g \) is another observable conjugate to the perturbation with respect to the energy.

In recent years, many efforts have been devoted to generalizing the classical equilibrium FDT to systems far from equilibrium [11–25]. The study of the nonequilibrium FDT dated back to the work of Agarwal [11]. Recently, Seifert and Speck [19] have developed a new type of FDT by using the concept of stochastic thermodynamics. They found that in an NESS, the response of an observable to a small external perturbation can be represented by the correlation function of this observable and another one that is conjugate to the perturbation with respect to the stochastic entropy. When a system is in equilibrium, the stochastic entropy reduces to the energy and the nonequilibrium FDT reduces to the classical equilibrium one. The nonequilibrium FDTs have also been successfully applied to solve practical biological problems [26].

The mathematical theory for the NESS has been developed for more than three decades [27–31]. However, this theory cannot be directly applied to study the FDTs because the FDTs focus on the nonstationary perturbation and the time-dependent dynamical behavior of a Markov process. Up till now, there is a lack of rigorous mathematical foundation for the nonequilibrium FDTs. In the physics literature, the derivation of the FDTs is formal and not rigorous. As a result, the precise ranges of applicability and key mathematical tools for the FDTs are unclear. For discrete Markov jump processes with finite state space, an attempt has been made to integrate the FDTs into a rigorous mathematical framework [25]. However, if a Markov process has a continuous state space, the proof of the FDTs turns out to be highly nontrivial due to the lack of effective mathematical tools.

In stochastic thermodynamics, the most important mathematical model of a molecular system is the diffusion process, which generalizes the classical Langevin equation describing the stochastic movement of multiple massive particles in a fluid due to collisions with the fluid molecules. As a beneficial attempt, the Jarzynski-Crooks fluctuation theorem (work relation) has been proved rigorously for diffusion processes [28]. However, this work required that both the drift and diffusion coefficients of a diffusion process are bounded and all their partial derivatives are bounded. These bounded assumptions are so strong that they even exclude the classical Ornstein-Uhlenbeck (OU) process, which describes the velocity of a massive Brownian particle under the influence of friction.

In fact, the Kolmogorov forward and backward equations for a diffusion process are partial differential equations of parabolic type. The reason why such strong bounded assumptions are made is because they serve as the basic requirements of the classical parabolic equation theory [32, 33]. In the present paper, we remove the bounded assumptions and provide a rigorous mathematical foundation for two types of FDTs — the Agarwal-type and Seifert-Speck-type FDTs — for inhomogeneous diffusion processes with weak and unbounded coefficients. It turns out that the theory of this paper applies to any form of nonlinear external perturbations,
rather than merely linear perturbations as in most previous papers. Furthermore, we also prove the uniqueness of the conjugate observables and clarify the mathematical conditions and ranges of applicability for the two types of FDTs.

We stress that the present paper is devoted to providing the mathematical foundation of the nonequilibrium fluctuation-dissipation theorems, instead of developing new mathematical tools for diffusion processes. We strive to reach a balance between being too technical to theoretical physicists and being too straightforward to mathematicians working on stochastic analysis and partial differential equations.

The structure of the present work is organized as follows. In Section 2, we introduce the fundamental framework of the FDTs for inhomogeneous diffusion processes and make the basic assumptions. In particular, we give the rigorous mathematical definition of the perturbed process and response function. In Section 3, we provide a mathematical theory of the Agarwal-type FDT for inhomogeneous diffusion processes by using the Schauder estimates for parabolic equations with unbounded coefficients. In Section 4, we provide a mathematical theory of the Seifert-Speck-type FDT for homogeneous diffusion processes by using the theory of weakly continuous semigroups and weak generators. Section 5 is devoted to clarifying the relationship between the two types of FDTs. In Section 6, we use the example of inhomogeneous OU processes to illustrate the main results of the present paper.

2 Model

2.1 Model and basic assumptions

Let $W = \{W_t : t \geq 0\}$ be an $n$-dimensional standard Brownian motion defined on a filtered probability space $(\Omega, F, P)$. In this paper, we consider a molecular system modeled by a $d$-dimensional inhomogeneous diffusion processes $X = \{X_t : t \geq 0\}$, which is the solution to the following SDE:

$$dX_t = b(t, X_t)dt + \sigma(t, X_t)dW_t,$$

where $b : \mathbb{R}^+ \times \mathbb{R}^d \to \mathbb{R}^d$ and $\sigma : \mathbb{R}^+ \times \mathbb{R}^d \to M_{d \times n}(\mathbb{R})$ with $M_{d \times n}(\mathbb{R})$ being the vector space of all $d \times n$ real matrices. Then $X$ is called a diffusion processes with the drift $b = (b^i)$ and diffusion coefficient $a = \sigma \sigma^T = (a^{ij})$. Recall that $X$ is called homogenous if the drift $b = b(t, x)$ and diffusion coefficient $a = a(t, x)$ only depend on the spatial variable $x$ and do not depend on the time variable $t$. Otherwise, $X$ is called inhomogeneous. If $\sigma$ is a constant diagonal matrix, then (2) is also called the Langevin equation. Most of the previous literature focused on the response of a homogeneous Langevin equation to a small external perturbation. Here we consider the response of a general inhomogeneous diffusion process.

Following standard notations, for any multi-index $\beta = (\beta_1, \cdots, \beta_d)$, set $|\beta| = \beta_1 + \cdots + \beta_d$ and $D^\beta = \partial_1^{\beta_1} \cdots \partial_d^{\beta_d}$, where $\partial_i = \partial / \partial_i$ denotes the ith weak or strong partial derivative. In this paper, we need the following function spaces.
Definition 2.1. In the following definitions, $[0, T]$ and $\mathbb{R}^d$ may be also replaced by subsets of $[0, T]$ and $\mathbb{R}^d$, respectively.

Let $B(\mathbb{R}^d)$ denote the space of all bounded measurable functions on $\mathbb{R}^d$.

Let $C^k_c(\mathbb{R}^d)$ with $k \in \mathbb{Z}^+ \cup \{\infty\}$ denote the space of all $f \in C^k(\mathbb{R}^d)$ with compact support.

Let $C_b(\mathbb{R}^d)$ denote the Banach space of all bounded continuous functions on $\mathbb{R}^d$ endowed with the supremum norm $\| \cdot \|$.

Let $C^k_b(\mathbb{R}^d)$ with $k \in \mathbb{Z}^+$ denote the Banach space of all $f \in C^k(\mathbb{R}^d)$ such that

$$\|f\|_{C^k_b(\mathbb{R}^d)} := \sum_{|\beta| \leq k} \|D^\beta f\| < \infty.$$ 

Let $C^\alpha_b(\mathbb{R}^d)$ with $0 < \alpha < 1$ denote the Banach space of all bounded $\alpha$-Hölder continuous functions on $\mathbb{R}^d$ with norm defined as

$$\|f\|_{C^\alpha_b(\mathbb{R}^d)} = \|f\| + \sup_{x,y \in \mathbb{R}^d, x \neq y} \frac{|f(x) - f(y)|}{|x - y|^\alpha}.$$

Let $C^\alpha_{loc}(\mathbb{R}^d)$ with $0 < \alpha < 1$ denote the space of all measurable functions $f$ on $\mathbb{R}^d$ such that $f \in C^\alpha_b(U)$ for any bounded open subsets $U \subset \mathbb{R}^d$.

Let $C^{k+\alpha}_b(\mathbb{R}^d)$ with $k \in \mathbb{Z}^+$ and $0 < \alpha < 1$ denote the Banach space of all $f \in C^k_b(\mathbb{R}^d)$ whose all $k$th-order partial derivatives are $\alpha$-Hölder continuous with norm defined as

$$\|f\|_{C^{k+\alpha}_b(\mathbb{R}^d)} = \|f\|_{C^k_b(\mathbb{R}^d)} + \sum_{|\beta| = k} \|D^\beta f\|_{C^\alpha_b(\mathbb{R}^d)}.$$ 

Let $C^{l,k}([0, T] \times \mathbb{R}^d)$ with $l, k \in \mathbb{Z}^+$ denote the space of all continuous functions $f$ on $[0, T] \times \mathbb{R}^d$ that are $l$th-order continuously differentiable with respect to the time variable and $k$th-order continuously differentiable with respect to the spatial variable.

Let $C^{0,k+\alpha}_b([0, T] \times \mathbb{R}^d)$ with $k \in \mathbb{Z}^+$ and $0 < \alpha < 1$ denote the Banach space of all continuous functions $f$ on $[0, T] \times \mathbb{R}^d$ such that

$$\|f\|_{C^{0,k+\alpha}_b([0, T] \times \mathbb{R}^d)} := \sup_{t \in [0, T]} \|f(t, \cdot)\|_{C^{k+\alpha}_b(\mathbb{R}^d)} < \infty.$$ 

Let $C^{0,0,k+\alpha}_b([0, T] \times [-1, 1] \times \mathbb{R}^d)$ with $k \in \mathbb{Z}^+$ and $0 < \alpha < 1$ denote the Banach space of all continuous functions $f$ on $[0, T] \times [-1, 1] \times \mathbb{R}^d$ such that

$$\|f\|_{C^{0,0,k+\alpha}_b([0, T] \times [-1, 1] \times \mathbb{R}^d)} := \sup_{(t, h) \in [0, T] \times [-1, 1]} \|f(t, h, \cdot)\|_{C^{k+\alpha}_b(\mathbb{R}^d)} < \infty.$$ 

Let $L^p_{loc}(\mathbb{R}^d)$ with $p \geq 1$ denote the space of all measurable functions $f$ on $\mathbb{R}^d$ such that $f \in L^p(U)$ for any bounded open subset $U \subset \mathbb{R}^d$.

Let $W^{k,p}(\mathbb{R}^d)$ with $k \in \mathbb{Z}^+$ and $p \geq 1$ denote the Banach space of all $k$th-order weakly differentiable functions $f$ on $\mathbb{R}^d$ such that

$$\|f\|_{W^{k,p}(\mathbb{R}^d)} := \sum_{|\beta| \leq k} \|D^\beta f\|_{L^p(\mathbb{R}^d)} < \infty.$$
The space \( W^{k,2}(\mathbb{R}^d) \) is also denoted by \( H^k(\mathbb{R}^d) \).

- Let \( W^{k,p}_{\text{loc}}(\mathbb{R}^d) \) with \( k \in \mathbb{Z}^+ \) and \( p \geq 1 \) denote the space of all measurable functions \( f \) on \( \mathbb{R}^d \) such that \( f \in W^{k,p}(U) \) for any bounded open subsets \( U \subset \mathbb{R}^d \). The space \( W^{k,2}_{\text{loc}}(\mathbb{R}^d) \) is also denoted by \( H^k_{\text{loc}}(\mathbb{R}^d) \).

- For any open subset \( U \subset \mathbb{R}^d \), let \( W^{k,p}_0(U) \) with \( k \in \mathbb{Z}^+ \) and \( p \geq 1 \) denote the closure of \( C_c^\infty(\mathbb{R}^d) \) in \( W^{k,p}(U) \). The space \( W^{k,2}_0(U) \) is also denoted by \( H^k_0(U) \). We stress here that if we take \( U = \mathbb{R}^d \), then \( W^{k,p}_0(\mathbb{R}^d) = W^{k,p}(\mathbb{R}^d) \) [34, Corollary 3.23]. However, this equality may not hold for general open subset \( U \).

Recall that the generator \( \{A_t : t \geq 0\} \) of \( X \) is defined as the following second-order elliptic operators:

\[
A_t f = \sum_{i=1}^{d} b^i(t, x) \partial_i f + \frac{1}{2} \sum_{i,j=1}^{d} a^{ij}(t, x) \partial_{ij} f, \quad f \in W^{2,1}_{\text{loc}}(\mathbb{R}^d).
\]

The transition semigroup \( \{P_{s,t} : 0 \leq s \leq t\} \) of \( X \) is defined as

\[
P_{s,t} f(x) = \mathbb{E}_{s,x} f(X_t) := \mathbb{E}\{f(X_t) | X_s = x\}, \quad f \in B(\mathbb{R}^d).
\]

In the following, we always fix a time \( T > 0 \) and consider the dynamics of \( X \) up to time \( T \).

**Definition 2.2.** We say that \( X \) satisfies the **regular conditions** if there exists \( 0 < \alpha < 1 \), two constants \( \lambda, C > 0 \), and a function \( \eta : [0, T] \times \mathbb{R}^d \to \mathbb{R} \) such that the following five conditions hold.

(a) For any \( R > 0 \), we have \( b, a \in C^{0,3+\alpha}_b([0, T] \times B_R) \), where \( B_R = \{x \in \mathbb{R}^d : |x| < R\} \) is the ball in \( \mathbb{R}^d \) with radius \( R \) centered at the origin.

(b) The diffusion coefficient \( a \) satisfies

\[
\xi^T a(t, x) \xi \geq \eta(t, x) |\xi|^2, \quad \forall t \in [0, T], \xi, x \in \mathbb{R}^d,
\]

where

\[
\inf_{(t,x) \in [0,T] \times \mathbb{R}^d} \eta(t, x) \geq \lambda > 0.
\]

(c) The drift \( b \) and diffusion coefficient \( a \) are controlled by

\[
b(t, x)^T x \leq C \eta(t, x) (1 + |x|^2),
\]

\[
|a(t, x)| + \text{tr}(a(t, x)) \leq C \eta(t, x) (1 + |x|^2), \quad \forall t \in [0, T], x \in \mathbb{R}^d.
\]

(d) For any multi-index \( \beta = (\beta_1, \cdots, \beta_d) \) with \( 1 \leq |\beta| \leq 3 \),

\[
|D^\beta b(t, x)| + |D^\beta a(t, x)| \leq C \eta(t, x), \quad \forall t \in [0, T], x \in \mathbb{R}^d.
\]

(e) There exists a function \( \phi \in C^2(\mathbb{R}^d) \) satisfying \( \phi(x) \to \infty \) as \( |x| \to \infty \) such that

\[
A_t \phi(x) \leq C \phi(x), \quad \forall t \in [0, T], x \in \mathbb{R}^d.
\]
Here the function $\phi$ is called the Lyapunov function. If $X$ is homogenous, then the regular condition (c) can be removed [35].

**Remark 2.3.** The classical parabolic equation theory focused on the case when $b$ and $a$, together with all their spatial partial derivatives, are bounded and continuous [32, 33]. In this case, the regular conditions (a), (c), and (d) are automatically satisfied. If we take $\phi(x) = 1 + |x|^2$, then the regular condition (e) is also satisfied. Therefore, the regular conditions are much weaker than the requirements of the classical parabolic equation theory.

**Remark 2.4.** If $X$ is homogenous, then $b$, $a$, and $r$ only depend on the spatial variable $x$ and thus the constants $\alpha$, $\lambda$, and $C$ do not depend on the time $T$. In this case, we do not need to fix the time $T$ and all the results of this paper will not change if we replace $T$ by $\infty$.

In the following, unless otherwise specified, we always assume that the regular conditions are satisfied. For any $R > 0$, let $\tau_R$ be the hitting time of the sphere $\partial B_R$ by $X$. Recall that the explosion time $\tau$ of $X$ is defined as
\[
\tau = \lim_{R \to \infty} \tau_R.
\]
The following proposition shows that regular conditions guarantee the existence, uniqueness, and nonexplosion of $X$.

**Proposition 2.5.** Assume that $\sigma = a^{1/2}$ is taken as the square root $a$. Then the following two statements hold.

(a) If the regular conditions (a) and (b) hold, then the strong solution of (2) exists and is unique up to time $T$.

(b) If the regular condition (e) holds, then $X$ is nonexplosive up to time $T$, that is, $\tau > T$ almost surely.

**Proof.** We first prove (a). The regular condition (a) implies that $b$ and $a$ are locally Lipschitz up to time $T$: for any $R > 0$, there exists a constant $K > 0$ such that
\[
|b(t, x) - b(t, y)| \leq K|x - y|, \quad |a(t, x) - a(t, y)| \leq K|x - y|, \quad \forall \ t \in [0, T], x, y \in B_R.
\]
By [33, Theorem 5.2.2], the regular condition (b) implies that
\[
|a^{1/2}(t, x) - a^{1/2}(t, y)| \leq \frac{K}{2\lambda^{1/2}}|x - y|, \quad \forall \ t \in [0, T], x \in B_R.
\]
This shows that $\sigma$ is also locally Lipschitz up to time $T$. Then Ito’s existence and uniqueness theorem gives the desired result.

We next prove (b). Let $\phi$ be the Lyapunov function in the regular condition (e). By Ito’s formula, we have
\[
d\phi(X_s) = A_s \phi(X_s) ds + \nabla \phi(X_s)^T \sigma(s, X_s) dW_s.
\]
For any $0 \leq t \leq T$ and $|x| < R$, we have
\[
\mathbb{E}_x \phi(X_{t \wedge \tau_R}) = \phi(x) + \mathbb{E}_x \int_0^t A_s \phi(X_s) I_{\{s \leq \tau_R\}} ds \leq \phi(x) + C \int_0^t \mathbb{E}_x \phi(X_{s \wedge \tau_R}) ds.
\]
By Gronwall’s inequality, we have

$$\mathbb{E}_x \phi(X_{\tau_R}) I_{\{\tau_R \leq t\}} \leq \mathbb{E}_x \phi(X_{t \wedge \tau_R}) \leq \phi(x) e^{Ct}, \quad \forall \ t \in [0, T].$$

This shows that

$$\min_{|y|=R} \phi(y) \cdot P_x(\tau_R \leq T) \leq \phi(x) e^{CT}.$$  

Since $\phi(y) \to \infty$ as $|y| \to \infty$, we have $P_x(\tau_R \leq T) \to 0$ as $R \to \infty$. This indicates that

$$P_x(\tau \leq T) = \lim_{R \to \infty} P_x(\tau_R \leq T) = 0,$$

which gives the desired result. \hfill \Box

### 2.2 Perturbed processes

The FDTs are concerned with the response of the diffusion process $X$ to a small external perturbation. For any $h \in C[0, T]$ with $\|h\| \leq 1$ which characterizes the input protocol of the perturbation, we consider another inhomogeneous diffusion process $X^h = \{X^h_t : t \geq 0\}$ with perturbed drift $b^h : [0, T] \times \mathbb{R}^d \to \mathbb{R}^d$ and diffusion coefficient $a^h : [0, T] \times \mathbb{R}^d \to M_{d \times d}(\mathbb{R})$. Since $X^h$ is a perturbation of $X$, it is natural to assume that they have the same initial distribution and there exist two trivariate functions

$$\bar{b} : [0, T] \times [-1, 1] \times \mathbb{R}^d \to \mathbb{R}^d, \quad \bar{a} : [0, T] \times [-1, 1] \times \mathbb{R}^d \to M_{d \times d}(\mathbb{R})$$

such that

$$\bar{b}(t, x) = b(0, x), \quad a(t, x) = \bar{a}(t, 0, x),$$

$$b^h(t, x) = \bar{b}(t, h(t), x), \quad a^h(t, x) = \bar{a}(t, h(t), x).$$

Here $t$ is the time variable, $h$ is the perturbation variable, and $x$ is the spatial variable. Similarly, we can define the generator $\{A^h_t\}$ and transition semigroup $\{P^h_s\}$ of $X^h$. In the following, we do not distinguish $b^h(t, x)$ and $\bar{b}(t, h(t), x)$ and do not distinguish $a^h(t, x)$ and $\bar{a}(t, h(t), x)$. The notations should be clear from the context.

**Remark 2.6.** In [8], the authors added a linear perturbation to the drift and kept the diffusion coefficient unchanged. In addition, the authors assumed that the perturbed drift has the form of

$$b^h(t, x) = b(t, x) + hF(t)K(x).$$

Here we remove these two restrictions and consider a general nonlinear external perturbation.

To proceed, we write the perturbed drift $b^h$ and diffusion coefficient $a^h$ as

$$b^h(t, x) = b(t, x) + hq^h(t, x), \quad a^h(t, x) = a(t, x) + hr^h(t, x),$$

where $q^h = (q^h_i)$ and $r^h = (r^h_i)$. We assume that $b^h$ and $a^h$ are differentiable with respect to $h$. For convenience, we write

$$q(t, x) = \partial_h|_{h=0} b^h(t, x), \quad r(t, x) = \partial_h|_{h=0} a^h(t, x),$$

and
where $q = (q^i)$ and $r = (r^{ij})$. For any $0 \leq t \leq T$, we define the following second-order differential operators:

$$
\mathcal{L}^h_t f = \sum_{i=1}^{d} q^i_h(t, x) \partial_i f + \frac{1}{2} \sum_{i,j=1}^{d} r^{ij}_h(t, x) \partial_{ij} f, \quad f \in W^{2,1}_{\text{loc}}(\mathbb{R}^d),
$$

$$
\mathcal{L}_t f = \sum_{i=1}^{d} q^i(t, x) \partial_i f + \frac{1}{2} \sum_{i,j=1}^{d} r^{ij}(t, x) \partial_{ij} f, \quad f \in W^{2,1}_{\text{loc}}(\mathbb{R}^d).
$$

**Assumption 2.7.** In the following, we assume that there exists $0 < \theta < 1$ and a constant $L > 0$ such as the following four conditions hold.

(a) For any $R > 0$, we have $\bar{b}, \bar{a} \in C_b^{0,0.3+\alpha}([0, T] \times [-1, 1] \times B_R)$.

(b) The functions $q_h$ and $r_h$ are controlled by

$$
\|q_h\|_{C_b^{\alpha,\theta}([0, T] \times \mathbb{R}^d)} + \|r_h\|_{C_b^{\alpha,\theta}([0, T] \times \mathbb{R}^d)} \leq L, \quad \forall \ h \in [-1, 1].
$$

(c) For any multi-index $\beta = (\beta_1, \ldots, \beta_d)$ with $1 \leq |\beta| \leq 3$,

$$
|D^\beta q_h(t, x)| + |D^\beta r_h(t, x)| \leq L\eta(t, x), \quad \forall \ t \in [0, T], h \in [-1, 1], x \in \mathbb{R}^d,
$$

where $\eta(t, x)$ is the function introduced in the regular conditions.

(d) The Lyapunov function $\phi$ satisfies

$$
\mathcal{L}^h_t \phi(x) \leq L\phi(x), \quad \forall \ t \in [0, T], h \in [-1, 1], x \in \mathbb{R}^d.
$$

The following lemma follows directly from the above assumptions.

**Lemma 2.8.** When $\|h\|$ is sufficiently small, the perturbed process $X^h$ also satisfies the regular conditions and the constants $\lambda$ and $C$ in the regular conditions can be chosen to be independent of $h$.

**Proof.** By Assumption 2.7(a), it is easy to see that for any $R > 0$,

$$
\sup_{t \in [0,T]} \|b_h(t, \cdot)\|_{C_b^{3+\alpha}(B_R)} \leq \sup_{(t,h) \in [0,T] \times [-1,1]} \|\tilde{b}(t, h, \cdot)\|_{C_b^{3+\alpha}(B_R)} < \infty,
$$

which shows that $b_h \in C_b^{0,3+\alpha}([0, T] \times B_R)$. Similarly, we also have $a_h \in C_b^{0,3+\alpha}([0, T] \times B_R)$. Thus $X^h$ satisfies the regular condition (a). By Assumption 2.7(b), when $\|h\|$ is sufficiently small, for any $0 \leq t \leq T$ and $\xi, x \in \mathbb{R}^d$,

$$
\xi^T a_h(t, x) \xi \geq \xi^T a(t, x) \xi - |a_h(t, x) - a(t, x)| \xi^2 \geq (\eta(t, x) - L\|h\|)\|\xi\|^2 \geq \frac{1}{2} \eta(t, x)|\xi|^2.
$$

This shows that $X^h$ satisfies the regular condition (b) and the constant $\lambda$ can be chosen to be independent of $h$. By using similar techniques, it is easy to prove that $X^h$ satisfies the regular condition (c)-(e) and the constant $C$ can be chosen to be independent of $h$. \qed
2.3 Response function

In order to give the rigorous definition for the response function, we recall the definition of the functional derivative.

**Definition 2.9.** Fix $t > 0$. Let $F$ be a functional on $C[0, t]$ and let $h \in C[0, t]$. Then the functional derivative of $F$ with respect to $h$ is a functional $\frac{\delta F}{\delta h}$ on $C_c^\infty(0, t)$ defined as

$$\langle \frac{\delta F}{\delta h}, \phi \rangle = \frac{d}{d\epsilon} \bigg|_{\epsilon=0} F(h + \epsilon \phi) = \lim_{\epsilon \to 0} \frac{1}{\epsilon} (F(h + \epsilon \phi) - F(h)),$$

whenever the limit exists for any $\phi \in C_c^\infty(0, t)$.

We next define the response function of an observable.

**Definition 2.10.** Let $f : \mathbb{R}^d \to \mathbb{R}$ be an observable. For any $0 \leq t \leq T$, let $F_t$ be a functional on $C[0, T]$ defined as

$$F_t(h) = \mathbb{E} f(X_t^h).$$

If for any $0 \leq t \leq T$, there exists a locally integrable function $R_f(\cdot, t)$ on $(0, t)$ such that

$$\langle \frac{\delta F_t}{\delta h} \bigg|_{h=0}, \phi \rangle = \int_0^t R_f(s, t) \phi(s) ds, \quad \forall \phi \in C_c^\infty(0, t),$$

then $R_f(s, t)$ is called the *response function* of the observable $f$.

The physical implication of the response function $R_f(s, t)$ can be understood as follows. Formally, if we take $\phi(x) = \delta_s(x) = \delta(x - s)$ in (4), then we have

$$R_f(s, t) = \int_0^t R_f(u, t) \delta_s(u) du = \langle \frac{\delta F_t}{\delta h} \bigg|_{h=0}, \delta_s \rangle = \lim_{\epsilon \to 0} \frac{1}{\epsilon} (F_t(\epsilon \delta_s) - F_t(0)).$$

This suggests that if we add a small impulsive perturbation $\epsilon \delta_s$ to $X$ at time $s$, then the rate of change for the ensemble average at time $t$ is exactly $R_f(s, t)$.

3 The Agarwal-type FDT

We first study the Agarwal-type FDT. Some of the lemmas in the following two sections are well known in the case of homogeneous or bounded coefficients, while they are nontrivial in the case of inhomogeneous and unbounded coefficients. Unless otherwise specified, we always assume the regular conditions (a)-(e) and Assumption 2.7 are satisfied. The following lemma characterizes the evolution of $X$.

**Lemma 3.1.** For any $f \in C_b(\mathbb{R}^d)$ and $0 \leq s \leq t \leq T$, the function $v(s, x) = P_{s,t} f(x)$ is the unique bounded classic solution to the following parabolic equation, which is also called the Kolmogorov backward equation:

$$\begin{aligned}
\partial_s v &= -\mathcal{A}_s v, \quad 0 \leq s < t, \\
v(t, x) &= f(x).
\end{aligned}$$

Theorem 3.4. Fix $K \in C([0, t] \times \mathbb{R}^d) \cap C^{1,2}([0, t] \times \mathbb{R}^d)$. It follows from Ito’s formula that
\[
dv(u, X_u) = [\partial_u v(u, X_u) + A_u v(u, X_u)] du + \nabla v(u, X_u)^T \sigma(u, X_u) dW_u = \nabla v(u, X_u)^T \sigma(u, X_u) dW_u.
\]

For any $|x| < R$ and $s < r < t$, we have
\[
v(s, x) = \mathbb{E}_{s,x} v(r \land T, A_{r \land T} r) - \mathbb{E}_{s,x} \int_s^r \nabla v(u, X_u)^T \sigma(u, X_u) I_{(u \leq \tau_R)} dW_u.
\]

The fact that $v \in C^{1,2}([0, t] \times \mathbb{R}^d)$ and the regular condition (a) indicate that $\nabla v$ and $a$ are continuous function on $[0, r] \times B_R$, which suggests that
\[
\mathbb{E}_{s,x} \int_s^r \nabla v(u, X_u)^T \sigma(u, X_u) I_{(u \leq \tau_R)} dW_u = 0.
\]

Since $X$ is nonexplosive up to time $T$ and $v \in C_b([0, t] \times \mathbb{R}^d)$, we have
\[
v(s, x) = \lim_{r \to t} \lim_{R \to \infty} \mathbb{E}_{s,x} v(r \land T, X_{r \land T}) = \lim_{r \to t} \mathbb{E}_{s,x} v(r, X_r) = \mathbb{E}_{s,x} v(t, X_t) = \mathbb{E}_{s,x} f(X_t),
\]

which gives the desired result. \qed

Remark 3.2. If $f \in C_b^{2+\theta}([0, t] \times \mathbb{R}^d)$ for some $0 < \theta < 1$, then it can be proved that the function $v(s, x) = P_{s,t} f(x)$ is the unique bounded classic solution to the Kolmogorov backward equation:
\[
\begin{cases}
\partial_s v = -A_s v, & 0 \leq s \leq t, \\
v(t, x) = f(x),
\end{cases}
\]

where $s = t$ is included. In this case, we have $v \in C^{1,2}([0, t] \times \mathbb{R}^d)$ [36, Theorems 2.7 and Remark 2.8].

The following lemma gives the semigroup estimates for $X$.

Lemma 3.3. For any $0 \leq \gamma \leq 3$, there exists a constant $K = K(d, T, \gamma, \lambda, C) > 0$ such that
\[
\|P_{s,t} f\|_{C^\gamma_b(\mathbb{R}^d)} \leq K \|f\|_{C^\gamma_b(\mathbb{R}^d)}, \quad \forall f \in C^\gamma_b(\mathbb{R}^d), \quad 0 \leq s \leq t \leq T.
\]

Proof. Since $v(s, x) = P_{s,t} f(x)$ satisfies the Kolmogorov backward equation (5), the desired result follows from [36, Theorem 2.4]. \qed

The following theorem is interesting in its own right.

Theorem 3.4. Fix $0 \leq t \leq T$, $h \in C[0, T]$, and $f \in C_b^2(\mathbb{R}^d)$. Let $g$ be a function on $[0, t] \times \mathbb{R}^d$ defined by
\[
g(s, x) = L^h_s P_{s,t}^h f(x).
\]

Then there exists a constant $K = K(d, T, \theta, \lambda, C) > 0$ such that the following two statements hold when $\|h\|$ is sufficiently small.
(a) For any \( f \in C_b^2(\mathbb{R}^d) \), we have \( g \in C_b([0, t] \times \mathbb{R}^d) \) and
\[
\|g\|_{C_b([0, t] \times \mathbb{R}^d)} \leq 2KL\|f\|_{C_b^2(\mathbb{R}^d)}.
\]
(b) For any \( f \in C_b^{2+\theta}(\mathbb{R}^d) \), we have \( g \in C_b^{0,\theta}([0, t] \times \mathbb{R}^d) \) and
\[
\|g\|_{C_b^{0,\theta}([0, t] \times \mathbb{R}^d)} \leq 4KL\|f\|_{C_b^{2+\theta}(\mathbb{R}^d)}.
\]

**Proof.** It is easy to see that
\[
g(s, x) = \sum_{i=1}^{d} q_{ih}(s, x) \partial_i P_{s,t}^h f(x) + \frac{1}{2} \sum_{i,j=1}^{d} s_{ijh}(s, x) \partial_{ij} P_{s,t}^h f(x) := g_1(s, x) + g_2(s, x).
\]
It follows from Assumption 2.7(b) that
\[
\|g\|_{C_b([0, t] \times \mathbb{R}^d)} \leq 2L \sup_{0 \leq s \leq t} \|P_{s,t}^h f\|_{C_b^2(\mathbb{R}^d)}.
\]
By Lemmas 2.8 and 3.3, there exists a constant \( K = K(d, T, \lambda, C) > 0 \) such that when \( \|h\| \) is sufficiently small,
\[
\|P_{s,t}^h f\|_{C_b^2(\mathbb{R}^d)} \leq K \|f\|_{C_b^0(\mathbb{R}^d)}, \quad \forall \ 0 \leq s \leq t \leq T.
\]
Thus we have proved (a). In addition, it is easy to check that
\[
g_1(s, x) = g_1(s, y)
\]
\[
\begin{align*}
= & \sum_{i=1}^{d} q_{ih}(s, x) (\partial_i P_{s,t}^h f(x) - \partial_i P_{s,t}^h f(y)) + \sum_{i=1}^{d} (q_{ih}(s, x) - q_{ih}(s, y)) \partial_i P_{s,t}^h f(y).
\end{align*}
\]
This suggests that
\[
\|g_1(s, \cdot)\|_{C_b^0(\mathbb{R}^d)} \leq \|q_h(s, \cdot)\|_{C_b^1(\mathbb{R}^d)} \|P_{s,t}^h f\|_{C_b^1(\mathbb{R}^d)} + \|q_h(s, \cdot)\|_{C_b^0(\mathbb{R}^d)} \|P_{s,t}^h f\|_{C_b^0(\mathbb{R}^d)}.
\]
By Lemmas 2.8 and 3.3, there exists a constant \( K_1 = K_1(d, T, \lambda, C, \theta) > 0 \) such that when \( \|h\| \) is sufficiently small,
\[
\|P_{s,t}^h f\|_{C_b^{1+\theta}(\mathbb{R}^d)} \leq K_1 \|f\|_{C_b^{1+\theta}(\mathbb{R}^d)}, \quad \forall \ 0 \leq s \leq t \leq T.
\]
Recall the following interpolation inequality of Hölder spaces [37, Section 2.7.2, Theorem 1]: there exists a constant \( K_2 = K_2(\theta) > 0 \) such that
\[
\|f\|_{C_b^{1+\theta}(\mathbb{R}^d)} \leq K_2 \|f\|_{C_b^0(\mathbb{R}^d)} \|f\|_{C_b^{1+\theta}(\mathbb{R}^d)} \leq K_2 \|f\|_{C_b^{2+\theta}(\mathbb{R}^d)}.
\]
The above three inequalities, together with Assumption 2.7(b), show that there exists a constant \( K = K(d, T, \theta, \lambda, C) > 0 \) such that
\[
\|g_1\|_{C_b^{0,\theta}([0, t] \times \mathbb{R}^d)} \leq 2K \|q_h\|_{C_b^{0,\theta}([0, t] \times \mathbb{R}^d)} \|f\|_{C_b^{2+\theta}(\mathbb{R}^d)} \leq 2KL\|f\|_{C_b^{2+\theta}(\mathbb{R}^d)}.
\]
Similarly, we can prove that
\[
\|g_2\|_{C_b^{0,\theta}([0, t] \times \mathbb{R}^d)} \leq 2KL\|f\|_{C_b^{2+\theta}(\mathbb{R}^d)}.
\]
Then (b) follows from the above two inequalities. \( \square \)
Lemma 3.5. For any \( f \in C^2_b(\mathbb{R}^d) \) and \( 0 \leq s \leq t \leq T \), when \( \|h\| \) is sufficiently small,

\[
P^{h}_{s,t} f(x) - P_{s,t} f(x) = \int_s^t P_{s,u}(A^h_u - A_u) P_{u,t}^h f(x) du.
\]

Proof. Since both \( X^h \) and \( X \) satisfy the regular conditions, it follows from Lemma 3.1 that their transition semigroups satisfy the Kolmogorov backward equations (5). Therefore, the function \( u(s, x) = P^{h}_{s,t} f(x) - P_{s,t} f(x) \) is the bounded classical solution to the following parabolic equation:

\[
\begin{align*}
\partial_s u(s, x) &= -A_s u(s, x) - h(s) g(s, x), \quad 0 \leq s < t \\
u(t, x) &= 0,
\end{align*}
\]

where \( g(s, x) \) is defined in Theorem 3.4. It follows from Ito’s formula that

\[
du(s, X_s) = [\partial_s u(s, X_s) + A_s u(s, X_s)] ds + \nabla u(s, X_s) \sigma(s, X_s) dW_s
\]

\[
= -h(s) g(s, X_s) ds + \nabla u(s, X_s) \sigma(s, X_s) dW_s.
\]

If \( |x| < R \) and \( s < r < t \), we have

\[
u(s, x) = E_{s,x} u(r \wedge \tau_R, X_{r \wedge \tau_R}) + E_{s,x} \int_s^r h(u) g(u, X_u) I_{\{u \leq \tau_R\}} du.
\]

Since \( X \) is nonexplosive up to time \( T \) and \( u \in C_b([0, t] \times \mathbb{R}^d) \), we have

\[
\lim_{r \to t} \lim_{R \to \infty} E_{s,x} u(r \wedge \tau_R, X_{r \wedge \tau_R}) = \lim_{r \to t} E_{s,x} u(r, X_r) = E_{s,x} u(t, X_t) = 0.
\]

It follows from Theorem 3.4 that \( g \in C_b([0, t] \times \mathbb{R}^d) \). By the dominated convergence theorem, we finally obtain that

\[
u(s, x) = \int_s^t E_{s,x} h(u) g(u, X_u) du = \int_s^t E_{s,x} (A^h_u - A_u) P_{u,t}^h f(X_u) du,
\]

which gives the desired result. \( \square \)

The following lemma, whose proof can be found in [36, Theorem 2.7], gives the Schauder estimate of parabolic equations.

Lemma 3.6. Fix \( 0 \leq t \leq T \) and \( 0 < \gamma < 1 \). For any \( f \in C^{2+\gamma}_b(\mathbb{R}^d) \) and \( g \in C^{0,\gamma}_b([0, t] \times \mathbb{R}^d) \), the Cauchy problem of the parabolic equation

\[
\begin{align*}
\partial_s u(s, x) &= -A_s u(s, x) - g(s, x), \quad 0 \leq s \leq t \\
u(t, x) &= f(x),
\end{align*}
\]

has a unique bounded classical solution. Moreover, there exists a constant \( K = K(d, T, \gamma, \lambda, C) > 0 \) such that

\[
\|u\|_{C^{0,2+\gamma}_b([0, t] \times \mathbb{R}^d)} \leq K \left[ \|f\|_{C^{2+\gamma}_b(\mathbb{R}^d)} + \|g\|_{C^{0,\gamma}_b([0, t] \times \mathbb{R}^d)} \right].
\]

The above Schauder estimate shows that if the driving term \( g \) is of the class \( C^{0,\gamma}_b([0, t] \times \mathbb{R}^d) \), then the solution \( u \) is of the class \( C^{0,2+\gamma}_b([0, t] \times \mathbb{R}^d) \).
Lemma 3.7. For any \( f \in C^{2+\theta}_{b}(\mathbb{R}^d) \), \( \phi \in C[0, T] \), and \( 0 \leq s \leq t \leq T \),
\[
\lim_{\epsilon \to 0} \frac{1}{\epsilon} (P^{\epsilon \phi}_{0,t} f(x) - P_{0,t} f(x)) = \int_0^t \phi(s) P_{0,s} \mathcal{L}_s P_{s,t} f(x) ds.
\]

Proof. It follows from Lemma 3.5 that when \( \epsilon \) is sufficiently small,
\[
\frac{1}{\epsilon} (P^{\epsilon \phi}_{0,t} f(x) - P_{0,t} f(x)) = \frac{1}{\epsilon} \int_0^t P_{0,s} (\mathcal{A}_s \phi - \mathcal{A}_s) P^{\epsilon \phi}_{s,t} f(x) ds = \int_0^t \phi(s) \mathbb{E}_x g_\epsilon(s, X_s) ds, \tag{8}
\]
where \( g_\epsilon(s, x) = \mathcal{L}_s^{\epsilon \phi} P^{\epsilon \phi}_{s,t} f(x) \). By Theorem 3.4 we have
\[
\|g_\epsilon\|_{C^0_b([0,t] \times \mathbb{R}^d)} \leq 4KL\|f\|_{C^{2+\theta}_b(\mathbb{R}^d)}. \tag{9}
\]
Thus we obtain that
\[
\sup_{0 \leq s \leq t} \|\epsilon \phi(s) g_\epsilon(s, \cdot)\|_{C^0_b(\mathbb{R}^d)} \leq \epsilon \|\phi\| \|g_\epsilon\|_{C^0_b([0,t] \times \mathbb{R}^d)} \to 0, \quad \text{as} \; \epsilon \to 0.
\]
By (6) and Lemma 3.6, we have
\[
\sup_{0 \leq s \leq t} \|P^{\epsilon \phi}_{s,t} f - P_{s,t} f\|_{C^{2+\theta}_b(\mathbb{R}^d)} \to 0, \quad \text{as} \; \epsilon \to 0.
\]
This shows that as \( \epsilon \to 0 \),
\[
g_\epsilon(s, x) = \sum_{i=1}^d q^{i \phi}_e(s, x) \partial_i P^{\epsilon \phi}_{s,t} f(x) + \frac{1}{2} \sum_{i,j=1}^d r^{ij \phi}_e(s, x) \partial_i \partial_j P^{\epsilon \phi}_{s,t} f(x) \tag{10}
\]
\[
\to \sum_{i=1}^d q^i(s, x) \partial_i P_{s,t} f(x) + \frac{1}{2} \sum_{i,j=1}^d r^{ij}(s, x) \partial_i \partial_j P_{s,t} f(x) = \mathcal{L} P_{s,t} f(x).
\]
Thus it follows from (8), (9), (10), and the dominated convergence theorem that
\[
\lim_{\epsilon \to 0} \frac{1}{\epsilon} (P^{\epsilon \phi}_{0,t} f(x) - P_{0,t} f(x)) = \int_0^t \phi(s) \mathbb{E}_x g_\epsilon(s, X_s) ds = \int_0^t \phi(s) \mathbb{E}_x \mathcal{L}_s P_{s,t} f(X_s) ds, \tag{11}
\]
which gives the desired result. \( \square \)

The following lemma gives the regularity of the probability densities for \( X \).

Lemma 3.8. If the regular conditions (a) and (b) hold, then \( X_t \) has a positive probability density \( p_t \in H^2_{\text{loc}}(\mathbb{R}^d) \) with respect to the Lebesgue measure for almost all \( 0 \leq t \leq T \). In particular, the stationary distribution of \( X \), if it exists, must have a positive probability density \( \mu \in H^2_{\text{loc}}(\mathbb{R}^d) \).

Proof. For any \( \phi \in C^\infty_c((0, T) \times \mathbb{R}^d) \), it follows from Ito’s formula that
\[
d\phi(t, X_t) = [\partial_t \phi(t, X_t) + \mathcal{A}_t \phi(t, X_t)] dt + \nabla \phi(t, X_t) \sigma(t, X_t) dW_t. \tag{11}
\]
Since \( \nabla \phi^T a \nabla \phi \) is bounded, we have
\[
\int_0^T \int_{\mathbb{R}^d} [\partial_t \phi(t, x) + \mathcal{A}_t \phi(t, x)] p_t(dx) dt = 0,
\]
\[

\int_0^T \int_{\mathbb{R}^d} [\partial_t \phi(t, x) + \mathcal{A}_t \phi(t, x)] p_t(dx) dt = 0,
\]
\[

\int_0^T \int_{\mathbb{R}^d} [\partial_t \phi(t, x) + \mathcal{A}_t \phi(t, x)] p_t(dx) dt = 0,
\]
\[

\int_0^T \int_{\mathbb{R}^d} [\partial_t \phi(t, x) + \mathcal{A}_t \phi(t, x)] p_t(dx) dt = 0,
\]
\[

\int_0^T \int_{\mathbb{R}^d} [\partial_t \phi(t, x) + \mathcal{A}_t \phi(t, x)] p_t(dx) dt = 0,
\]
\[

\int_0^T \int_{\mathbb{R}^d} [\partial_t \phi(t, x) + \mathcal{A}_t \phi(t, x)] p_t(dx) dt = 0,
\]
\[

\int_0^T \int_{\mathbb{R}^d} [\partial_t \phi(t, x) + \mathcal{A}_t \phi(t, x)] p_t(dx) dt = 0,
\]
\[

\int_0^T \int_{\mathbb{R}^d} [\partial_t \phi(t, x) + \mathcal{A}_t \phi(t, x)] p_t(dx) dt = 0,
\]
\[

\int_0^T \int_{\mathbb{R}^d} [\partial_t \phi(t, x) + \mathcal{A}_t \phi(t, x)] p_t(dx) dt = 0,
\]
\[

\int_0^T \int_{\mathbb{R}^d} [\partial_t \phi(t, x) + \mathcal{A}_t \phi(t, x)] p_t(dx) dt = 0,
where \( p_t(dx) \) is the probability distribution of \( X_t \). Under the regular conditions (a) and (b), by [38, Corollary 6.4.3 and Theorem 6.2.7], there exists a positive function \( \rho \in C((0, T) \times \mathbb{R}^d) \) such that

\[
p_t(dx)dt = \rho(t, x)dt \, dx.
\]

This shows that \( X_t \) has a positive probability density \( p_t = \rho(t, \cdot) \) for almost all \( 0 \leq t \leq T \). Moreover, it follows from (11) that for any \( \epsilon > 0 \) and \( \epsilon \leq t \leq T - \epsilon \),

\[
\int_{\mathbb{R}^d} \phi(t, x)p_t(x)dx - \int_{\mathbb{R}^d} \phi(\epsilon, x)p_\epsilon(x)dx - \int_{\epsilon}^{t} \int_{\mathbb{R}^d} [\partial_s \phi(s, x) + A_s \phi(s, x)]p_s(x)dxds = 0.
\]

Under the regular condition (a), it follows from the integration by parts formula that

\[
\int_{\mathbb{R}^d} p_t(x)\phi(t, x)dx - \int_{\mathbb{R}^d} p_\epsilon(x)\phi(\epsilon, x)dx - \int_{\epsilon}^{t} \int_{\mathbb{R}^d} p_s \partial_s \phi dxds
\]

\[
+ \int_{\epsilon}^{t} \int_{\mathbb{R}^d} \sum_{i,j=1}^{d} \left[ \frac{1}{2} a^{ij} \partial_i p_s \partial_j \phi + \left( b^i - \frac{1}{2} \partial_j a^{ij} \right) \partial_i p_s \phi + \left( \partial_t b^i - \frac{1}{2} \partial_j a^{ij} \right) p_s \phi \right] dxds = 0.
\]

For any bounded open subset \( U \subset \mathbb{R}^d \), it is easy to check that the above equality holds for any \( \phi \in C^1([\epsilon, T - \epsilon] \times U) \) with \( \phi \) vanishing on \([\epsilon, T - \epsilon] \times \partial U\). This shows that \( p_t(x) \) is a classical weak solution [39, Chapter VI, Section 1] of the parabolic equation

\[
\partial_t p_t - \frac{1}{2} \sum_{i,j=1}^{d} \partial_j (a^{ij} \partial_i p_t) + \sum_{i,j=1}^{d} \left( b^i - \frac{1}{2} \partial_j a^{ij} \right) \partial_i p_t
\]

\[
+ \sum_{i,j=1}^{d} \left( \partial_t b^i - \frac{1}{2} \partial_j a^{ij} \right) p_t = 0 \quad \text{in} \quad [\epsilon, T - \epsilon] \times U.
\]

By [38, Corollary 6.4.3], the initial value \( p_\epsilon \) of the above parabolic equation satisfies \( p_\epsilon \in H^1(U) \). In terms of [39, Theorem 6.6], the weak solution must satisfy \( p_t \in H^2_{loc}(U) \) for almost all \( \epsilon \leq t \leq T - \epsilon \). By the arbitrariness of \( \epsilon > 0 \) and the bounded open subset \( U \), we have \( p_t \in H^2_{loc}(\mathbb{R}^d) \) for almost all \( 0 \leq t \leq T \). \( \square \)

For any \( t > 0 \), let \( p_t \) denote the probability density of \( X_t \). The following theorem gives an explicit expression for the response function of an observable.

**Theorem 3.9.** Let \( f \in C_b^{2+\theta}(\mathbb{R}^d) \) be an observable and let \( R_f \) be the response function of \( f \). Then for any \( 0 \leq s \leq t \leq T \),

\[
R_f(s, t) = \mathbb{E} \mathcal{L}_s P_{s,t} f(X_s) = \int_{\mathbb{R}^d} \mathcal{L}_s P_{s,t} f(x)p_s(x)dx.
\]

**Proof.** For any \( 0 \leq t \leq T \), it is easy to see that

\[
\mathbb{E} f(X_t) = \int_{\mathbb{R}^d} \mathbb{E}_x f(X_t)p_0(dx) = \int_{\mathbb{R}^d} P_{0,t} f(x)p_0(dx) = \mathbb{E} P_{0,t} f(X_0).
\]
Thus it follows from Lemma[3,7] that for any \( 0 \leq t \leq T \) and \( \phi \in C^\infty_c(0, t) \),
\[
\left< \frac{\delta F_t}{\delta h} \bigg|_{h=0}, \phi \right> = \lim_{\epsilon \rightarrow 0^+} \frac{1}{\epsilon} (F_t(\epsilon \phi) - F_t(0)) = \lim_{\epsilon \rightarrow 0^-} \frac{1}{\epsilon} (\mathbb{E} f(X_t^{\epsilon \phi}) - \mathbb{E} f(X_t))
\]
\[
= \lim_{\epsilon \rightarrow 0^-} \mathbb{E} \left[ \frac{1}{\epsilon} (P_{0,t}^\epsilon f(X_0) - P_{0,t} f(X_0)) \right]
\]
\[
= \int_0^t \phi(s) \mathbb{E} P_{0,s} \mathcal{L}_s P_{s,t} f(X_0) ds
\]
\[
= \int_0^t \phi(s) \mathbb{E} \mathcal{L}_s P_{s,t} f(X_s) ds,
\]
which gives the desired result. \( \square \)

We are now in a position to prove the Agarwal-type FDT.

**Theorem 3.10.** Fix \( 0 \leq s \leq t \leq T \) such that \( X_s \) has a positive probability density \( p_s \in H^2_{\text{loc}}(\mathbb{R}^d) \). Assume that \( q(s, \cdot) \in C^1_{c}(\mathbb{R}^d) \) and \( r(s, \cdot) \in C^2_{c}(\mathbb{R}^d) \). Let \( v_s \) be a function on \( \mathbb{R}^d \) defined by
\[
v_s(x) = \frac{\mathcal{L}^*_s p_s(x)}{p_s(x)},
\]
where
\[
\mathcal{L}^*_s f(x) = - \sum_{i=1}^d \partial_i (q_i(s, x) f(x)) + \frac{1}{2} \sum_{i,j=1}^d \partial_{ij} (r_{ij}(s, x) f(x)), \quad f \in W^2_{\text{loc}}(\mathbb{R}^d)
\]
is the adjoint operator of \( \mathcal{L}_s \). Then for any \( f \in C^{2+\theta}(\mathbb{R}^d) \),
\[
R_f(s, t) = \mathbb{E} f(X_t) v_s(X_s).
\]

**Proof.** For any \( 0 \leq s \leq t \) and any measurable function \( u \) on \( \mathbb{R}^d \) such that \( \mathbb{E}|u(X_s)| < \infty \), we have
\[
\mathbb{E} f(X_t) u(X_s) = \mathbb{E} u(X_s) \mathbb{E}\{ f(X_t) | X_s \} = \mathbb{E} P_{s,t} f(X_s) u(X_s).
\] (12)
Since \( q(s, \cdot) \in C^1_{c}(\mathbb{R}^d), r(s, \cdot) \in C^2_{c}(\mathbb{R}^d), \) and \( p_s \in W^2_{\text{loc}}(\mathbb{R}^d) \), we have \( q(s, \cdot)p_s \in W^{1,1}_{\text{loc}}(\mathbb{R}^d) \) and \( r(s, \cdot)p_s \in W^2_{\text{loc}}(\mathbb{R}^d) \) \[40, \text{Section 5.2.3, Theorem 1}\]. Thus it follows from Theorem[3,9] and the integration by parts formula that
\[
R_f(s, t) = \int_{\mathbb{R}^d} \mathcal{L}_s p_s(x) P_{s,t} f(x) p_s(x) dx
\]
\[
= \sum_{i=1}^d \int_{\mathbb{R}^d} q_i(s, x) p_s(x) \partial_i P_{s,t} f(x) dx + \frac{1}{2} \sum_{i,j=1}^d \int_{\mathbb{R}^d} r_{ij}(s, x) p_s(x) \partial_{ij} P_{s,t} f(x) dx
\]
\[
= - \sum_{i=1}^d \int_{\mathbb{R}^d} \partial_i (q_i(s, x) p_s(x)) P_{s,t} f(x) dx + \frac{1}{2} \sum_{i,j=1}^d \int_{\mathbb{R}^d} \partial_{ij} (r_{ij}(s, x) p_s(x)) P_{s,t} f(x) dx
\]
\[
= \int_{\mathbb{R}^d} \mathcal{L}^*_s p_s(x) P_{s,t} f(x) dx = \int_{\mathbb{R}^d} P_{s,t} f(x) v_s(x) p_s(x) dx = \mathbb{E} P_{s,t} f(X_s) v_s(X_s),
\]
which gives the desired result. \( \square \)
Remark 3.11. The above theorem indicates that for inhomogeneous diffusion processes, the response of an observable \( f \) to a small external perturbation can be represented as the correlation function of this observable and the conjugate observable \( v_s = \mathcal{L}_s^* p_s / p_s \), which generally depends on the early time \( s \). If \( X \) is inhomogeneous, then the generator \( \mathcal{L}_s \) will depend on \( s \). If \( X \) is nonstationary, then the probability distribution \( p_s \) will depend on \( s \). If we hope the conjugate observable \( v_s \) to be independent of \( s \), the diffusion process must be both homogeneous and stationary.

The following theorem shows that the conjugate observable in the Aargwal-type FDT is unique.

**Theorem 3.12.** Fix \( 0 \leq s < T \) such that \( X_s \) has a positive probability density \( p_s \). Assume that there exists another function \( \tilde{v}_s \in L^1(p_s) \) on \( \mathbb{R}^d \) such that

\[
\mathbb{E} f(X_t) v_s(X_s) = \mathbb{E} f(X_t) \tilde{v}_s(X_s), \quad \forall f \in C_c^\infty(\mathbb{R}^d), \ s < t \leq T.
\]

Then \( v_s = \tilde{v}_s \) almost everywhere.

**Proof.** From (12), it is easy to check that

\[
\int_{\mathbb{R}^d} P_{s,t} f(x)(v_s(x) - \tilde{v}_s(x)) p_s(x) dx = 0.
\]

Since \( f \in C_c^\infty(\mathbb{R}^d) \), taking \( t \to s \) in the above equation and applying the dominated convergence theorem give rise to

\[
\int_{\mathbb{R}^d} f(x)(v_s(x) - \tilde{v}_s(x)) p_s(x) dx = 0,
\]

By the arbitrariness of \( f \), we obtain the desired result. \( \square \)

Let us recall the following important definition from stochastic thermodynamics.

**Definition 3.13.** Let \( X \) be homogenous and stationary. Then \( X \) is said to be in an equilibrium state if \( X \) is symmetric with respect to its stationary distribution and \( X \) is said to be in an NESS if \( X \) is nonsymmetric with respect to its stationary distribution.

If \( X \) is homogeneous and stationary, then the generator \( \mathcal{A} \), the operator \( \mathcal{L} \), and the functions \( b, a, q, \) and \( r \) are all independent of the time variable \( t \). Moreover, the transition semigroup \( P_{s,t} \) only depends on the time difference \( t - s \) and can be formally represented as \( P_{s,t} = e^{\mathcal{A}(t-s)} \). In this case, the above result reduces to the Agarwal-type FDT for an NESS.

**Theorem 3.14.** Let \( X \) be homogeneous and stationary with \( \mu \in H^2_{\text{loc}}(\mathbb{R}^d) \) being the positive stationary density. Assume that \( q \in C_c^1(\mathbb{R}^d) \) and \( r \in C_c^2(\mathbb{R}^d) \). Let \( v \) be a function on \( \mathbb{R}^d \) defined by

\[
v(x) = \frac{\mathcal{L}^* \mu(x)}{\mu(x)}.
\]

Then for any \( f \in C_b^{2+\theta}(\mathbb{R}^d) \) and \( 0 \leq s \leq t \),

\[
R_f(s, t) = \mathbb{E} f(X_t) v(X_s) = \int_{\mathbb{R}^d} \mathcal{L} e^{\mathcal{A}(t-s)} f(x) \mu(dx).
\]
Proof. The desired result follows directly from Theorems 3.9 and 3.10.

According to the above theorem, if $X$ is in an NESS, then the conjugate observable $v$ does not depend on the early time $s$ and the response function $R_f(s, t)$ only depends on the time difference $t - s$.

Lemma 3.8 shows that the stationary distribution of $X$, if it exists, must have a positive probability density $\mu \in H_{\text{loc}}^2(\mathbb{R}^d)$. Theoretical physicists may be particularly interested in the following proposition, which contains very weak conditions for the higher-order regularity of the stationary density and generalizes the classical results on NESS [27, Theorem 3.2.5] to a large extent. We do not assume the regular conditions (a)-(e) in the following proposition.

**Proposition 3.15.** Let $X$ be homogenous. Assume that $a$ satisfies the following locally elliptic condition: there exists a positive function $\eta : \mathbb{R}^d \to \mathbb{R}$ such that

$$\xi^T a(x) \xi \geq \eta(x) |\xi|^2. \quad (13)$$

Then the following five statements hold.

(a) If $b$ is locally bounded and $a \in W_{\text{loc}}^{1,p}(\mathbb{R}^d)$ for some $p > d$, then the stationary distribution of $X$, if it exists, has a positive probability density $\mu \in C_{\text{loc}}^{1-d/p}(\mathbb{R}^d) \cap W_{\text{loc}}^{1,p}(\mathbb{R}^d)$.

(b) If $b, a \in C_{\text{loc}}^\alpha(\mathbb{R}^d)$ for some $0 < \alpha < 1$, then the stationary distribution of $X$, if it exists, must be unique.

(c) If $b \in C^1(\mathbb{R}^d)$ and $a \in C^2(\mathbb{R}^d)$, then $\mu \in H_{\text{loc}}^2(\mathbb{R}^d)$.

(d) If $b \in C^m(\mathbb{R}^d)$ and $a \in C^{m+1}(\mathbb{R}^d)$ for some integer $m \geq 2$, then $\mu \in H_{\text{loc}}^m(\mathbb{R}^d)$.

(e) If $b, a \in C^\infty(\mathbb{R}^d)$, then $\mu \in C^\infty(\mathbb{R}^d)$.

Proof. The first part of (a) follows from [38, Corollaries 1.6.9 and 1.7.2] and the Sobolev embedding theorem, which claims that $W^{1,p}(U)$ with $p > d$ can be embedded into $C_b^{1-d/p}(U)$ for any open ball $U \subset \mathbb{R}^d$. The second part of (a) follows from Ito’s formula and [38, Theorem 5.3.3]. Moreover, (b) follows from [41, Theorem 8.1.15].

We next prove (c). For any $\phi \in C^2(\mathbb{R}^d)$, it follows from Ito’s formula that

$$d\phi(X_t) = A\phi(X_t)dt + \nabla \phi(X_t)^T \sigma(X_t)dW_t.$$

Since $\nabla \phi^T a \nabla \phi$ is bounded, we have

$$\int_0^t ds \int_{\mathbb{R}^d} A\phi(x) \mu(dx) = \int_0^t \mathbb{E}_\mu A\phi(X_s)ds = \mathbb{E}_\mu \phi(X_t) - \mathbb{E}_\mu \phi(X_0) = 0,$$

which suggests that

$$\int_{\mathbb{R}^d} A\phi(x) \mu(dx) = 0.$$

Since $b \in C^1(\mathbb{R}^d)$ and $a \in C^2(\mathbb{R}^d)$, it follows from (a) that $\mu \in H_{\text{loc}}^1(\mathbb{R}^d)$. By the integration by parts formula, it is easy to check that

$$\int_{\mathbb{R}^d} \sum_{i,j=1}^d \left[ \frac{1}{2} a^{ij} \partial_i \mu \partial_j \phi + \left( b^i - \frac{1}{2} \partial_j a^{ij} \right) \partial_i \mu \phi + \left( \partial_i b^i - \frac{1}{2} \partial_j a^{ij} \right) \mu \phi \right] dx = 0.$$
For any bounded open subsets \( U \subset \mathbb{R}^d \), since \( C_c^2(U) \) is dense in \( H^1_0(U) \), it is easy to check that the above equality holds for any \( \phi \in H^1_0(U) \). This suggests that \( \mu \) is a classical weak solution \([40, \text{Section 6.1}]\) for the following elliptic equation of the divergence form:

\[
-\frac{1}{2} \sum_{i,j=1}^d \partial_j (a^{ij} \partial_i \mu) + \sum_{i,j=1}^d \left( b^i - \frac{1}{2} \partial_j a^{ij} \right) \partial_i \mu + \sum_{i,j=1}^d \left( \partial_i b^j - \frac{1}{2} \partial_{ij} a^{ij} \right) \mu = 0 \quad \text{in} \ U.
\]

By \([40, \text{Section 6.3.1. Theorem 1}]\), the weak solution must satisfy \( \mu \in H^2_{\text{loc}}(U) \). By the arbitrariness of the bounded open subsets \( U \), we have \( \mu \in H^2_{\text{loc}}(\mathbb{R}^d) \).

Similarly, if \( b \in C^m(\mathbb{R}^d) \) and \( a \in C^{m+1}(\mathbb{R}^d) \) for some integer \( m \geq 2 \), the weak solution must satisfy \( \mu \in H^m_{\text{loc}}(U) \) \([40, \text{Section 6.3.1. Theorem 2}]\). Finally, if \( b, a \in C^\infty(\mathbb{R}^d) \), the weak solution must satisfy \( \mu \in C^\infty(\mathbb{R}^d) \) \([40, \text{Section 6.3.1. Theorem 3}]\). Thus we have proved (d) and (e).

\[\square\]

4 The Seifert-Speck-type FDT

In fact, the Seifert-Speck-type FDT only holds for an NESS and does not hold for general nonequilibrium states. Therefore, we always assume that \( X \) is homogeneous and stationary in this section and we shall use the semigroup theory of homogenous Markov processes to study this type of FDT. If \( X \) is homogenous, the transition semigroup \( \{P_t\} \) of \( X \) is defined as

\[
P_t f(x) = \mathbb{E}_x f(X_t) := \mathbb{E}\{f(X_t)|X_0 = x\}, \quad f \in B(\mathbb{R}^d).
\]

**Lemma 4.1.** If the regular conditions (a) and (b) hold, then \( \{P_t\} \) is a contractive semigroup on \( C_b(\mathbb{R}^d) \).

**Proof.** By \([42, \text{Corollary 4.7}]\), the regular conditions (a) and (b) imply that \( X \) is strong Feller, that is, \( P_t f \in C_b(\mathbb{R}^d) \) for any bounded measurable function \( f \) and \( t > 0 \). Therefore, \( P_t \) is a bounded linear operator on \( C_b(\mathbb{R}^d) \). The semigroup property and contractive property are obvious. \[\square\]

We stress here that if \( b \) or \( a \) is unbounded, then \( \{P_t\} \) may not be a strongly continuous semigroup on \( C_b(\mathbb{R}^d) \) and thus the classical semigroup theory is not applicable. Even for the OU process, \( \{P_t\} \) is not strongly continuous on \( C_b(\mathbb{R}^d) \) \([43]\) and we cannot define the generator in the usual sense. Fortunately, \( \{P_t\} \) is a weakly continuous semigroup and we can define the generator in the weak sense \([41, \text{Section 2.4}]\).

**Definition 4.2.** For any \( f \in C_b(\mathbb{R}^d) \), we say that \( f \in D(A) \) if

\[
\sup_{\epsilon > 0} \left\| \frac{1}{\epsilon} (P_\epsilon f - f) \right\| < \infty \tag{14}
\]

and there exists \( u \in C_b(\mathbb{R}^d) \) such that as \( \epsilon \downarrow 0 \),

\[
\frac{1}{\epsilon} (P_\epsilon f(x) - f(x)) \to u(x), \quad \forall \ x \in \mathbb{R}^d.
\]

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Let $A : D(A) \to C_b(\mathbb{R}^d)$ be a linear operator defined by

$$Af(x) = \lim_{\epsilon \to 0} \frac{1}{\epsilon} (P_\epsilon f(x) - f(x)).$$

Then $A$ is called the weak generator of the semigroup $\{P_t\}$.

In fact, it can be proved that $D(A)$ is a dense subset of $C_b(\mathbb{R}^d)$ in the following sense: for any $f \in C_b(\mathbb{R}^d)$, there exists a sequence $\{f_n\} \subset D(A)$ such that $f_n \to f$ uniformly on every compact subsets of $\mathbb{R}^d$ [41, Proposition 2.3.5]. Specifically, under the regular conditions, $D(A)$ can be characterized explicitly as follows [41, Propositions 2.3.6 and 4.1.1]:

$$D(A) = \{ u \in C_b(\mathbb{R}^d) \cap \bigcap_{1 \leq p < \infty} H^p_{\text{loc}}(\mathbb{R}^d) : Au \in C_b(\mathbb{R}^d) \}.$$

From the above characterization, it is easy to see that $C^2_c(\mathbb{R}^d) \subset D(A)$. Moreover, if $b$ and $a$ are bounded, then $C^2_b(\mathbb{R}^d) \subset D(A)$.

Since $X$ is homogeneous, the trivariate functions defined in (3) do not depend on the time variable $t$ and reduce to

$$\bar{b} : [-1, 1] \times \mathbb{R}^d \to \mathbb{R}^d, \quad \bar{a} : [-1, 1] \times \mathbb{R}^d \to M_{d \times d}(\mathbb{R}).$$

For any $-1 \leq h \leq 1$, we define an auxiliary diffusion process $\tilde{X}^h = \{\tilde{X}^h_t : t \geq 0\}$ with perturbed drift $\tilde{b}_h(x) = \bar{b}(h, x)$ and diffusion coefficient $\tilde{a}_h(x) = \bar{a}(h, x)$. We stress here that the perturbed process $X^h$ and the auxiliary process $\tilde{X}^h$ are different. The perturbed process $X^h$ is an inhomogeneous diffusion process with generator

$$A^h_t f = \sum_{i=1}^d \tilde{b}^i(h(t), x) \partial_i f + \sum_{i,j=1}^d \tilde{a}^{ij}(h(t), x) \partial_{ij} f, \quad f \in W^{2,1}_{\text{loc}}(\mathbb{R}^d),$$

where $h = h(t)$ is a continuous function. However, the auxiliary process is a homogeneous diffusion process with generator

$$\bar{A}^h f = \sum_{i=1}^d \bar{b}^i(h, x) \partial_i f + \sum_{i,j=1}^d \bar{a}^{ij}(h, x) \partial_{ij} f, \quad f \in W^{2,1}_{\text{loc}}(\mathbb{R}^d).$$

where $h$ is taken as a constant. In the following, we do not distinguish $b_h(x)$ and $\bar{b}(h, x)$ and do not distinguish $a_h(x)$ and $\bar{a}(h, x)$. The notations should be clear from the context. It is easy to see that when $h$ is sufficiently small, the auxiliary process $\tilde{X}^h$ also satisfies the regular conditions.

**Assumption 4.3.** In the following, we assume that the auxiliary diffusion process $\tilde{X}^h$ satisfies the following two conditions.

(a) When $h$ is sufficiently small, $\tilde{X}^h$ has a stationary density $\mu_h$. The stationary density of $X$ is denoted by $\mu$.  

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(b) The stationary density \( \mu_h \) is differentiable in \( L^1(\mathbb{R}^d) \) at \( h = 0 \). In other words, there exists \( \nu \in L^1(\mathbb{R}^d) \) such that

\[
\frac{1}{h}(\mu_h - \mu) \xrightarrow{L^1(\mathbb{R}^d)} \nu, \quad \text{as } h \to 0.
\]

There are many verifiable conditions which can guarantee (b). For example, we have the following lemma, whose proof can be found in [44].

**Lemma 4.4.** Assume that \( b_h, a_h, \) and \( \partial_i a_h \) are continuously differentiable with respect to \( h \) for any \( 1 \leq i \leq d \). Assume that \( a_h, a_h^{-1}, \) and \( \partial_i a_h \) are uniformly bounded and there exists two constants \( C, k > 0 \) such that

\[
|\partial_i a_h(x)| + |\partial_i \partial_j a_h(x)| + |b_h(x)| + |\partial_i b_h(x)| \leq C(1 + |x|^k), \quad \forall 1 \leq i \leq d, h \in [-1, 1], x \in \mathbb{R}^d.
\]

Assume also that

\[
\lim_{|x| \to \infty} \sup_{h \in [-1, 1]} b_h(x)^T x = -\infty.
\]

Then Assumption 4.3(b) holds.

The following lemma characterizes the weak generator of the auxiliary process.

**Lemma 4.5.** If \( f \in D(A) \cap C_b^2(\mathbb{R}^d) \), then \( f \in D(\tilde{A}^h) \) when \( h \) is sufficiently small. In this case, we have

\[
\tilde{A}^h f = h\mathcal{L}^h f + Af.
\]

**Proof.** Let \( \{\tilde{P}^h_t\} \) denote the transition semigroup of the auxiliary process \( \tilde{X}^h \). Then we have

\[
\frac{1}{\epsilon}(\tilde{P}^h_{\epsilon} f(x) - f(x)) = \frac{1}{\epsilon}(\tilde{P}^h_{\epsilon} f(x) - P^h f(x)) + \frac{1}{\epsilon}(P^h f(x) - f(x)).
\]

When \( h \) sufficiently small, it follows from Lemma 3.5 and Theorem 3.4 that

\[
\tilde{P}^h_{\epsilon} f(x) - P^h f(x) = \int_0^{\epsilon} P_{\epsilon-s}(A^h - A)\tilde{P}^h_s f(x)ds + h \int_0^{\epsilon} \mathbb{E}xg(s, X_{\epsilon-s})ds.
\]

where \( g(s, x) = \mathcal{L}^h \tilde{P}^h_s f(x) \in C_b([0, T] \times \mathbb{R}^d) \). This suggests that \( \mathbb{E}xg(s, X_{\epsilon-s}) \) as a function of \( s \) and \( \epsilon \) is continuous on \( 0 \leq s \leq \epsilon \leq T \). Thus we obtain that

\[
\lim_{\epsilon \to 0} \frac{1}{\epsilon}(\tilde{P}^h_{\epsilon} f(x) - P^h f(x)) = h \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_0^{\epsilon} \mathbb{E}xg(s, X_{\epsilon-s})ds = h\mathbb{E}xg(0, X_0) = h\mathcal{L}^h f(x).
\]

Moreover, it follows from Theorem 3.4 that

\[
\sup_{0 < \epsilon \leq T} \left\| \frac{1}{\epsilon}(\tilde{P}^h_{\epsilon} f - P^h f) \right\| \leq \|h\|\|g\|_{C_b([0, T] \times \mathbb{R}^d)} \leq 2KL\|h\|\|f\|_{C_b^2(\mathbb{R}^d)}.
\]

This suggests that \( f \in D(\tilde{A}^h) \) and \( \tilde{A}^h f = h\mathcal{L}^h f + Af \).

The following lemma shows that formally, the stationary density \( \mu \) satisfies \( A^* \mu = 0 \).

**Lemma 4.6.** For any \( f \in D(A) \),

\[
\int_{\mathbb{R}^d} \mu(x)Af(x)dx = 0.
\]
Proof. By the dominated convergence theorem, we have
\[
\int_{\mathbb{R}^d} \mu(x) A f(x) dx = \int_{\mathbb{R}^d} \mu(x) \lim_{\epsilon \to 0} \frac{1}{\epsilon} (P_\epsilon f(x) - f(x)) dx
= \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_{\mathbb{R}^d} \mu(x) (P_\epsilon f(x) - f(x)) dx
= \lim_{\epsilon \to 0} \frac{1}{\epsilon} (\mathbb{E} f(X_\epsilon) - \mathbb{E} f(X_0)).
\]
The fact that $X$ is stationary gives the desired result. \(\square\)

The following lemma shows that the weak generator $A$ and the operator $L$ are formally related by $A^* \nu = -L^* \mu$.

**Lemma 4.7.** For any $f \in \mathcal{D}(A) \cap C^2_b(\mathbb{R}^d)$,
\[
\int_{\mathbb{R}^d} \nu(x) A f(x) dx = -\int_{\mathbb{R}^d} \mu(x) L f(x) dx.
\]

**Proof.** It follows from Lemmas 4.5 and 4.6 that
\[
\int_{\mathbb{R}^d} \mu(x) A f(x) dx = \int_{\mathbb{R}^d} \mu_h(x) \bar{A} f(x) dx = 0.
\]
This fact, together with Assumption 4.3 and Lemma 4.5, shows that
\[
\int_{\mathbb{R}^d} \nu(x) A f(x) dx = \int_{\mathbb{R}^d} \mu_h(x) \bar{A} f(x) dx = 0.
\]

This fact, together with Assumption 4.3 and Lemma 4.5, shows that
\[
\int_{\mathbb{R}^d} \nu(x) A f(x) dx = \lim_{h \to 0} \int_{\mathbb{R}^d} \mu_h(x) (\bar{A} - A) f(x) dx = \lim_{h \to 0} \int_{\mathbb{R}^d} \mu_h(x) L_h f(x) dx.
\]
It is easy to see that
\[
\int_{\mathbb{R}^d} \mu_h(x) L_h f(x) dx = \int_{\mathbb{R}^d} (\mu_h(x) - \mu(x)) L_h f(x) dx + \int_{\mathbb{R}^d} \mu(x) L_h f(x) dx := I + II.
\]
By Assumptions 2.7 and 4.3 we have
\[
I \leq \| \mu_h - \mu \|_{L^1(\mathbb{R}^d)} \| L_h f \| \to 0, \quad \text{as} \; h \to 0.
\]

On the other hand, it follows from the dominated convergence theorem that
\[
II \to \int_{\mathbb{R}^d} \mu(x) L f(x) dx, \quad \text{as} \; h \to 0,
\]
which gives the desired result. \(\square\)

We are now in a position to prove the Seifert-Speck-type FDT.

**Theorem 4.8.** Let $w$ be a function on $\mathbb{R}^d$ defined by
\[
w(x) = \frac{\nu(x)}{\mu(x)}.
\]
Then for any $f \in \mathcal{D}(A) \cap C^2_b(\mathbb{R}^d)$ and $0 \leq s \leq t$,
\[
R_f(s, t) = \frac{\partial}{\partial s} \mathbb{E} f(X_t) w(X_s).
\]
Proof. By the definition of \( w(x) \), we have
\[
\mathbb{E} f(X_t)w(X_s) = \mathbb{E} w(X_s)\mathbb{E}_{X_t} f(X_{t-s}) = \int_{\mathbb{R}^d} \mathbb{E}_x f(X_{t-s})w(x)\mu(x)dx = \int_{\mathbb{R}^d} P_{t-s}f(x)\nu(x)dx.
\]
Recall the following property of the weak generator [41, Lemma 2.3.3]: for any \( f \in D(A) \), we have \( P_tf \in D(A) \) and
\[
\frac{d}{dt} P_tf(x) = AP_tf(x) = P_tA f(x), \quad \forall \ t \geq 0, x \in \mathbb{R}^d.
\tag{17}
\]
By the dominated convergence theorem, we have
\[
\frac{\partial}{\partial s} \mathbb{E} f(X_t)w(X_s) = \int_{\mathbb{R}^d} \frac{\partial}{\partial s} P_{t-s}f(x)\nu(x)dx = -\int_{\mathbb{R}^d} AP_{t-s}f(x)\nu(x)dx.
\]
It follows from Lemma 3.3 that \( P_{t-s}f \in D(A) \cap C_b^0(\mathbb{R}^d) \). This fact, together with Theorem 3.9 and Lemma 4.7, shows that
\[
\frac{\partial}{\partial s} \mathbb{E} f(X_t)w(X_s) = \int_{\mathbb{R}^d} \mathcal{L} P_{t-s}f(x)\mu(x)dx = R_f(s,t),
\]
which gives the desired result. \( \square \)

The following theorem shows that under mild conditions, the conjugate observable in the Seifert-Speck-type FDT is unique up to a constant.

**Theorem 4.9.** Assume that there exists \( K > 0 \) such that
\[
|b(x)| \leq K(1+|x|), \quad |a(x)| \leq K(1+|x|^2), \quad \forall \ x \in \mathbb{R}^d.
\]
Assume that there exists another function \( \hat{w} \in L^1(\mu) \) on \( \mathbb{R}^d \) such that
\[
\frac{\partial}{\partial s} \mathbb{E} f(X_t)w(X_s) = \frac{\partial}{\partial s} \mathbb{E} f(X_t)\hat{w}(X_s), \quad \forall \ f \in C_c^\infty(\mathbb{R}^d), 0 \leq s < t \leq T. \tag{18}
\]
Then \( w - \hat{w} \) must be a constant almost everywhere.

**Proof.** From (18), it is easy to check that
\[
\frac{\partial}{\partial s} \int_{\mathbb{R}^d} P_{t-s}f(x)(w(x) - \hat{w}(x))\mu(x)dx = 0.
\]
Since \( f \in C_c^\infty(\mathbb{R}^d) \subset D(A) \), it follows from the dominated convergence theorem that
\[
\int_{\mathbb{R}^d} \mathcal{A} f(x)(w(x) - \hat{w}(x))\mu(x)dx = 0.
\]
Since \( w - w \in L^1(\mu) \), it follows from [38, Proposition 4.3.6 and Theorem 4.3.3] that \( w - \hat{w} \) is a constant almost everywhere. \( \square \)

**Remark 4.10.** In the Seifert-Speck-type FDT, if we allow the conjugate observable \( w_s \) to depend on the early time \( s \), then it can be proved that there will be infinite number of conjugate observables satisfying (16) and thus the uniqueness will be broken. However, according to Theorem 3.12, the Agarwal-type FDT has a unique conjugate observable \( v_s \) even if we allow it to depend on \( s \). This is an important difference between the two types of FDTs.
To understand the physical implication of the Seifert-Speck-type FDT, let us recall the following concept from stochastic thermodynamics [19].

**Definition 4.11.** The stochastic entropy of the stationary density $\mu_h$ is an observable $s_h : \mathbb{R}^d \to \mathbb{R}$ defined as
\[
s_h(x) = -\log \mu_h(x).
\]

**Remark 4.12.** If $\mu_h$ is differentiable with respect to $h$ in the usual sense, then $\nu = \partial_h |_{h=0} \mu_h$ almost everywhere and
\[
w(x) = \partial_h |_{h=0} \frac{\mu_h(x)}{\mu(x)} = -\partial_h |_{h=0} s_h(x).
\]

Therefore, the Seifert-Speck-type FDT shows that for homogeneous and stationary diffusion processes, the response of an observable to a small external perturbation can be expressed as the correlation function of this observable and another one that is conjugate to the perturbation with respect to the stochastic entropy.

## 5 Relationship between the two types of FDTs

When $X$ is homogeneous and stationary, we have proved two types of FDTs as stated in Theorems 3.14 and 4.8
\[
R_f(s, t) = \mathbb{E} f(X_t) v(X_s) = \frac{\partial}{\partial s} \mathbb{E} f(X_t) w(X_s). \tag{19}
\]

Readers may ask what is the connection between the conjugate observables $v$ and $w$. Assume that the conditions of the two types of FDTs are both satisfied. Then Lemma 4.7 shows that for any $f \in D(A) \cap C^2_b(\mathbb{R}^d)$,
\[
\int_{\mathbb{R}^d} v(x) A f(x) dx = -\int_{\mathbb{R}^d} \mu(x) L f(x) dx = -\int_{\mathbb{R}^d} \mu^* \mu(x) f(x) dx.
\]

By the definitions of $v$ and $w$, we have
\[
(A f, w)_\mu = \int_{\mathbb{R}^d} \mu(x) w(x) A f(x) dx = -\int_{\mathbb{R}^d} \mu(x) v(x) f(x) dx = -(f, v)_\mu,
\]

where $(\cdot, \cdot)_\mu$ is the inner product of two functions with respect to the stationary density $\mu$. This shows that the conjugate observables $v$ and $w$ are formally related by
\[
v = -A^\dagger w, \tag{20}
\]

where $A^\dagger$ is the adjoint operator of $A$ with respect to the inner product $(\cdot, \cdot)_\mu$.

The operator $A^\dagger$ can be understood in two different ways. Under mild conditions, it can be proved that the time-reversed process of $X$ is also a homogenous and stationary diffusion process with drift $b^\dagger = -b + \nabla a + a \nabla \log \mu$ and diffusion coefficient $a^\dagger = a$ [27, Theorem...
3.3.5]. In fact, the generator of the time-reversed process is exactly the operator $A^\dagger$, which can be written as

$$A^\dagger = \sum_{i=1}^{d} (-b^i + \partial_j a^{ij} + a^{ij} \partial_j \log \mu) \partial_i + \frac{1}{2} \sum_{i,j=1}^{d} a^{ij} \partial_i.$$ 

From the perspective of Nelson’s stochastic mechanics [45], the mean backward velocity of an observable $f$ is another observable $V_{\text{backward}} f$ defined as

$$V_{\text{backward}} f(x) = \lim_{h \to 0} \frac{1}{h} \mathbb{E}\{f(X_t) - f(X_{t-h})|X_t = x\}.$$ 

Under mild conditions, the mean backward velocity of $f$ can be written as [27, Section 4.2.1]

$$V_{\text{backward}} f = -A^\dagger f.$$ 

Therefore, it follows from (20) that the conjugate observable in the Agarwal-type FDT is exactly the mean backward velocity of that in the Seifert-Speck-type FDT. This builds up a bridge between the two types of FDTs.

6 Examples

The classical theory of parabolic equations can only deal with the case of bounded drift and diffusion coefficients. Here we show that how our theory can be applied to diffusion processes with unbounded drift or diffusion coefficients.

6.1 Agarwal-type FDT for inhomogeneous OU processes

The classical OU process describes the velocity of an underdamped Brownian particle or the position of an overdamped Brownian particle driven by the harmonic potential [46]. Here we consider the following $d$-dimensional inhomogeneous OU process $X = \{X_t : t \geq 0\}$, which is the solution to the following SDE:

$$dX_t = (B(t)X_t + g(t))dt + A(t)dW_t, \quad X_0 = x_0, \quad (21)$$

whose drift $b = b(t, x)$ and diffusion coefficient $a = a(t)$ are given by

$$b(t, x) = B(t)x + g(t), \quad a(t) = A(t)A(t)^T,$$

where $g : \mathbb{R}^+ \to \mathbb{R}^d$, $B : \mathbb{R}^+ \to M_{d \times d}(\mathbb{R})$, and $A : \mathbb{R}^+ \to M_{d \times n}(\mathbb{R})$ are continuous. We further assume that $a$ satisfies the following strictly elliptic condition: there exists $\lambda > 0$ such that

$$\xi^T a(t) \xi \geq \lambda |\xi|^2, \quad \forall t \geq 0, \xi \in \mathbb{R}^d. \quad (22)$$

The inhomogeneous OU processes are also important models in statistical physics [47, 48].

Lemma 6.1. $X$ satisfies the regular conditions.
Proof. The regular condition (b) follows from the strictly elliptic condition with \( \eta(t, x) = \lambda \). Since \( b \) is linear with respect to \( x \) and \( a \) is independent of \( x \), it is easy to check that the regular conditions (a), (c), and (d) hold. If we take \( \phi(x) = 1 + |x|^2 \), then for any \( 0 \leq t \leq T \),

\[
A_t \phi(x) = 2b(t, x)^T x + \text{tr}(a(t)) = 2x^T B(t)x + 2g(t)^T x + \text{tr}(a(t)) \\
\leq 2\|B\|_{C[0,T]}|x|^2 + 2\|g\|_{C[0,T]}|x| + \|a\|_{C[0,T]}.
\]

Since \( |x| \leq \max\{1, |x|^2\} \), the regular condition (e) also holds.

For the inhomogeneous OU process, it is convenient to introduce the following notations. For any \( s, t \in \mathbb{R} \), let \( T(s, t) \in M_{d \times d}(\mathbb{R}) \) denote the solution to the following matrix-valued ordinary differential equation (ODE):

\[
\dot{x} = B(t)x, \quad x(s) = I. \tag{23}
\]

Then the solution of (21) can be calculated explicitly as [49]

\[
X_t = T(0, t)x_0 + \int_0^t T(s, t)g(s)ds + \int_0^t T(s, t)A(s)dW_s.
\]

This indicates that \( X_t \) is a Gaussian random variable for any \( t > 0 \) with mean

\[
m(t) = T(0, t)x_0 + \int_0^t T(s, t)g(s)ds
\]

and covariance matrix

\[
\Sigma(t) = \int_0^t T(s, t)a(s)T(s, t)^T ds.
\]

Therefore, \( X_t \) has a probability density \( p_t \in C_b^\infty(\mathbb{R}^d) \) which is given by

\[
p_t(x) = \left[2\pi \det(\Sigma(t))\right]^{-\frac{1}{2}} e^{-\frac{1}{2}(x-m(t))\Sigma(t)^{-1}(x-m(t))}. \tag{24}
\]

We next consider the perturbed process \( X^h = \{X^h_t : t \geq 0\} \) whose drift \( b_h = b_h(t, x) \) and diffusion coefficient \( a_h = a_h(t) \) are given by

\[
b_h(t, x) = b(t, x) + hq_h(t, x), \quad a_h(t, x) = a(t) + hr_h(t, x),
\]

where \( q_h \) and \( r_h \) satisfy Assumption 2.7. We assume that \( b_h \) and \( a_h \) are differentiable with respect to \( h \) and write

\[
q(t, x) = \partial_h|_{h=0} b_h(t, x), \quad r(t, x) = \partial_h|_{h=0} a_h(t, x).
\]

For convenience, set \( m(s) = (m^i(s)) \) and \( \Sigma^{-1}(s) = (\sigma_{ij}(s)) \) for any \( s \geq 0 \). The following theorem gives the Agarwal-type FDT for inhomogeneous OU processes.
**Theorem 6.2.** Fix $0 < s \leq t \leq T$. Assume $q(s, \cdot) \in C^1_b(\mathbb{R}^d)$ and $r(s, \cdot) \in C^2_b(\mathbb{R}^d)$. Let $v_s$ be a function on $\mathbb{R}^d$ defined by

$$v_s(x) = -\sum_{i=1}^{d} \partial_i q^i(s, x) + \frac{1}{2} \sum_{i,j=1}^{d} \partial_{ij} r^{ij}(s, x) - r^{ij}(s, x) \sigma_{ij}(s)$$

$$+ \sum_{i,j,k=1}^{d} (q^i(s, x) - \partial_i r^{ij}(s, x)) \sigma_{ik}(s)(x^k - m^k(s))$$

$$+ \frac{1}{2} \sum_{i,j,k,l=1}^{d} r^{ij}(s, x) \sigma_{ik}(s) \sigma_{jl}(s)(x^k - m^k(s))(x^l - m^l(s)).$$

Then for any $f \in C^{2+\theta}_b(\mathbb{R}^d)$,

$$R_f(s, t) = \mathbb{E} f(X_t)v_s(X_s).$$

**Proof.** Since the probability density $p_s$ exponentially decays with respect to $x$, it is easy to check that the assumptions of Theorem 3.10 can be weakened as $q(s, \cdot) \in C^1_b(\mathbb{R}^d)$ and $r(s, \cdot) \in C^2_b(\mathbb{R}^d)$. By Theorem 3.10 we have $R_f(s, t) = \mathbb{E} f(X_t)v_s(X_s)$, where $v_s = \mathcal{L}_s^* p_s / p_s$. It is easy to see that

$$\mathcal{L}_s^* p_s = -\partial_i (q^i p_s) + \frac{1}{2} \partial_{ij} (r^{ij} p_s) = -(\partial_i q^i - \frac{1}{2} \partial_{ij} r^{ij}) p_s - (q^i - \partial_i r^{ij}) \partial_i p_s + \frac{1}{2} r^{ij} \partial_{ij} p_s,$$

where we have used Einstein’s summation convention: if the same index appears twice in any term, once as an upper index and once as a lower index, that term is understood to be summed over all possible values of that index. From (24), it is easy to check that

$$\partial_i p_s = -\sigma_{ik}(x^k - m^k)p_s,$$

$$\partial_{ij} p_s = [-\sigma_{ij} + \sigma_{ik}\sigma_{jl}(x^k - m^k)(x^l - m^l)]p_s.$$

Thus we finally obtain that

$$v_s = - (\partial_i q^i - \frac{1}{2} \partial_{ij} r^{ij}) + (q^i - \partial_i r^{ij}) \sigma_{ik}(x^k - m^k)$$

$$+ \frac{1}{2} r^{ij}[-\sigma_{ij} + \sigma_{ik}\sigma_{jl}(x^k - m^k)(x^l - m^l)]$$

$$= - \partial_i q^i + \frac{1}{2} \partial_{ij} r^{ij} - \frac{1}{2} r^{ij} \sigma_{ij} + (q^i - \partial_i r^{ij}) \sigma_{ik}(x^k - m^k)$$

$$+ \frac{1}{2} r^{ij} \sigma_{ik}\sigma_{jl}(x^k - m^k)(x^l - m^l),$$

which gives the desired result. 

**6.2 Agarwal-type FDT for homogeneous OU processes**

As a special case, we consider the following $d$-dimensional homogeneous OU process $X = \{X_t : t \geq 0\}$, which is the solution to the following SDE:

$$dX_t = (BX_t + g)dt + dW_t,$$
whose drift \( b = b(x) \) and diffusion coefficient \( a \) are given by
\[
b(x) = Bx + g, \quad a = AA^T,
\]
where \( g \in \mathbb{R}^d, B \in M_{d \times d}(\mathbb{R}), \) and \( A \in M_{d \times n}(\mathbb{R}) . \) The following lemma gives the sufficient and necessary condition for the existence of a stationary distribution.

**Lemma 6.3.** The stationary distribution of \( X \) exists if and only if all the eigenvalues of \( B \) have negative real parts. The stationary distribution of \( X \), if it exists, must be a Gaussian distribution with mean \( m = -B^{-1}g \) and covariance matrix
\[
\Sigma = \int_0^\infty e^{sB} ae^{sB^T} ds.
\]
In other words, the stationary density \( \mu \) of \( X \) is given by
\[
\mu(x) = \left[2\pi \det(\Sigma)\right]^{-\frac{1}{2}} e^{-\frac{1}{2}(x-m)^T \Sigma^{-1}(x-m)}.
\]

**Proof.** It is a classical result that the lemma holds when \( g = 0 \) [41, Proposition 9.3.1 and Remark 9.3.2]. The proof in general case of \( g \neq 0 \) is straightforward by using the method of translation. \( \square \)

For convenience, set \( m = (m^i) \) and \( \Sigma^{-1} = (\sigma_{ij}) \). The following theorem, which is a direct corollary of Theorem 6.2, gives the Agarwal-type FDT for homogeneous OU processes.

**Theorem 6.4.** Assume \( q \in C^1_b(\mathbb{R}^d) \) and \( r \in C^2_b(\mathbb{R}^d) \). Let \( v \) be a function on \( \mathbb{R}^d \) defined by
\[
v(x) = \sum_{i=1}^d \partial_i q^i(x) + \frac{1}{2} \sum_{i,j=1}^d \partial_{ij} r^{ij}(x) - r^{ij}(x) \sigma_{ij} + \sum_{i,j,k=1}^d (q^i(x) - \partial_j r^{ij}(x)) \sigma_{ik} (x^k - m^k)
\]
\[
+ \frac{1}{2} \sum_{i,j,k,l=1}^d r^{ij}(x) \sigma_{ik} \sigma_{jl} (x^k - m^k)(x^l - m^l).
\]
Then for any \( 0 \leq s \leq t \) and \( f \in C_{b}^{2+\theta}(\mathbb{R}^d) \),
\[
R_f(s, t) = E f(X_t) v(X_s).
\]

### 6.3 Seifert-Speck-type FDT for homogeneous OU processes

In this section, we still focus on the homogenous OU process \( X \). For simplicity of calculation, we assume that \( B \) is a symmetric matrix whose all eigenvalues are negative. Moreover, we assume that the perturbed drift \( b_h \) and diffusion coefficient \( a_h \) have the form of
\[
b_h(x) = Bx + g + h\tilde{g}, \quad a_h(x) = a + h\tilde{a},
\]
where \( \tilde{g} \in \mathbb{R}^d \) and \( \tilde{a} \in M_{d \times d}(\mathbb{R}) . \) If \( h = h(t) \) is taken as a continuous function, then \( b_h \) and \( a_h \) correspond to the perturbed process \( X^h \). If \( h \) is taken as a constant, then \( b_h \) and \( a_h \) correspond to the auxiliary process \( \bar{X}^h \).
It is easy to see that the auxiliary process $\tilde{X}^h$ is also a homogenous OU process whose stationary distribution is a Gaussian distribution with mean $m_h = -B^{-1}(g + \tilde{g}h)$ and covariance matrix
\[
\Sigma_h = \int_0^\infty e^{sB}(a + h\tilde{a})e^{sB^T}ds.
\]
Thus the stationary density $\mu_h$ of $\tilde{X}^h$ is given by
\[
\mu_h(x) = [2\pi \det(\Sigma_h)]^{-\frac{1}{2}} e^{-\frac{1}{2}(x-m_h)^T\Sigma_h^{-1}(x-m_h)}.
\]

**Lemma 6.5.** When $h$ is sufficiently small, the auxiliary processes $\tilde{X}_h$ satisfies Assumptions 2.7 and 4.3.

**Proof.** Since $q_h = \tilde{g}$ and $r_h = \tilde{a}$ do not depend on $x$, it is easy to check that Assumptions 2.7 and 4.3(a) hold. We next use Lemma 4.4 to verify Assumption 4.3(b). When $h$ is sufficiently small, we have
\[
a_h^{-1} = (I + ha^{-1}\tilde{a})^{-1}a^{-1} = \sum_{n=0}^\infty (-ha^{-1}\tilde{a})^na^{-1},
\]
which implies that
\[
|a_h^{-1}| \leq \frac{|a^{-1}|}{1 - |h||a^{-1}\tilde{a}|} \leq \frac{1}{2}|a^{-1}|.
\]
This shows that $a_h$, $a_h^{-1}$, and $\partial_h a_h$ are locally bounded. Moreover, it is easy to see that
\[
|b_h(x)| + |\partial_h b_h(x)| \leq |B||x| + |g| + 2|\tilde{g}|, \quad \forall h \in [-1, 1], x \in \mathbb{R}^d.
\]
Since $B$ is a symmetric matrix whose all eigenvalues are negative, we have
\[
b_h(x)^T x = x^T B x + g^T x + h\tilde{g}^T x \leq -\gamma |x|^2 + (|g| + |\tilde{g}|)|x|, \quad \forall h \in [-1, 1], x \in \mathbb{R}^d,
\]
where $-\gamma$ is the maximum eigenvalue of $B$. Thus all the conditions of Lemma 4.4 are satisfied, which shows that Assumption 4.3(b) holds.

The following theorem gives the Seifert-Speck-type FDT for homogeneous OU processes.

**Theorem 6.6.** Let $w$ be a function on $\mathbb{R}^d$ defined by
\[
w(x) = -\pi(2\pi \det(\Sigma))^{-1}\partial_h|_{h=0}\det(\Sigma_h) - \tilde{g}^T B^{-T}\Sigma^{-1}(x-m)
- \frac{1}{2}(x-m)^T\partial_h|_{h=0}\Sigma_h^{-1}(x-m).
\]
Then for any $0 \leq s \leq t$ and $f \in D(A) \cap C^{2+\theta}_b(\mathbb{R}^d)$,
\[
R_f(s,t) = \frac{\partial}{\partial s}\mathbb{E}f(X_t)w(X_s).
\]

**Proof.** Since Assumptions 2.7 and 4.3 are satisfied, it is easy to check that
\[
\nu(x) = \partial_h|_{h=0}\mu_h = \left[-\pi(2\pi \det(\Sigma))^{-1}\partial_h|_{h=0}\det(\Sigma_h) + \partial_h|_{h=0}m_h^T\Sigma_h^{-1}(x-m)
- \frac{1}{2}(x-m)^T\partial_h|_{h=0}\Sigma_h^{-1}(x-m)\right]\mu(x).
\]
Since $\partial_h|_{h=0}m_h = -B^{-1}\tilde{g}$, the desired result follows from Theorem 4.8.
7 Conclusions and discussion

In this work, we provide a rigorous mathematical theory of two types of nonequilibrium FDTs for general inhomogeneous diffusion processes with weak and unbounded coefficients. In fact, the Kolmogorov backward equation of a diffusion process is a partial differential equation of parabolic type. However, the classical parabolic equation theory assumed that both the drift and diffusion coefficients are bounded and all their spatial partial derivatives are bounded. Moreover, when the drift and diffusion coefficients are unbounded, the transition semigroup of a diffusion process may not be strongly continuous on $C_b(\mathbb{R}^d)$ and the classical semigroup theory is not applicable. Here we overcome these difficulties and give rigorous proofs of the FDTs when the drift and diffusion coefficients are unbounded. There are two key mathematical tools during the proofs: the first one is the Schauder estimates for parabolic equations and the second one is the theory of weak generators.

Under the regular conditions, we derive an explicit formula of the response function which applies to any forms of nonlinear external perturbations, rather than merely linear perturbations as in most previous papers. We further express the response function as the correlation function of the original and conjugate observables in two different ways. The conjugate observable in the Agarwal-type FDT is always unique, while the conjugate observable in the Seifert-Speck-type FDT is unique only when it does not depend on the early time $s$. When the diffusion process is homogeneous and stationary, we build up a bridge between the two types of FDTs using concepts in stochastic mechanics [45]. We show that the conjugate observable in the Agarwal-type FDT is exactly the mean backward velocity of that in the Seifert-Speck-type FDT.

We anticipate that our theory could promote the development of the mathematical foundation for nonequilibrium stochastic thermodynamics.

Acknowledgments

The authors are grateful to Prof. M. Röckner for pointing out the reference [38] and for stimulating discussions. X. Chen was supported by the Fundamental Research Funds for the Central Universities, Xiamen University (Grant No.20720170008).

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