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The Green–Kubo formula for general Markov processes with a continuous time parameter

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Abstract

For general Markov processes, the Green–Kubo formula is shown to be valid under a mild condition. A class of stochastic evolution equations on a separable Hilbert space and three typical infinite systems of locally interacting diffusions on $\mathbb{Z}^d$ (irreversible in most cases) are shown to satisfy the Green–Kubo formula, and the Einstein relations for these stochastic evolution equations are shown explicitly as a corollary.

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1. Introduction

The Green–Kubo formula is a fundamental law in nonequilibrium statistical physics [22, 24–26]. It relates the diffusion coefficient to the time integral of the velocity (i.e. derivative) autocorrelation function, and has been explored by many authors such as [1, 2, 12, 14, 15, 20, 22–25, 30, 32–34, 37, 38, 41]. Stochastic processes and deterministic or random dynamical systems are considered as two of the most important mathematical approaches dealing with the problems in nonequilibrium statistical physics [22, 25]. Ruelle [37] shows that the Green–Kubo formula holds for smooth dynamical systems. Qian *et al* [34] derive the formula for ergodic reversible Markov chains with finite states and a continuous time parameter. Jiang and Zhang [23] show that the formula holds for general reversible Markov processes based on the spectral representation theory. For finite Markov chains with a continuous time parameter, Chen *et al* [2] deduce the formula without restriction of reversibility and ergodicity. In [41], Spohn presents the Green–Kubo formula for several models with a strong physical

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background, such as some linearized hydrodynamic equations added to fluctuating currents, and the hard core lattice gas in thermal equilibrium. In particular, he explains this famous relationship from the physical view, and connects it with some interesting physical quantities.

For the purpose of applying the approach of stochastic processes to more extensive fields, and more importantly, from Jiang, Qian and Qian's view in [22] that for systems modeled by stochastic processes, irreversible stationary processes can be taken as the mathematical correspondent of nonequilibrium steady states in statistical physics; the question naturally arises whether the Green–Kubo formula is still valid for general Markov processes, in particular, stochastic evolution equations in infinite-dimensional spaces, without restriction of reversibility. Since the Einstein relation is a special case of this formula, what is the Einstein relation of infinite systems? In this paper, we attempt to investigate these questions in a rigorous mathematical way.

This paper is organized as follows. In section 2, we first work with general Markov processes on Polish spaces to obtain the Green–Kubo formula (see theorem 2.5). In section 3, we apply these results to two classes of stochastic evolution equations in infinite dimensional spaces, stochastic PDEs on a separable Hilbert space H (see equation (3.1)) and critical interacting diffusions on $\mathbb{Z}^d$ (see equation (3.9)).

In most cases, they are irreversible. On the one hand, it is a reasonable requirement that some deterministic equations are subject to random external influences. On the other hand, some stochastic equations, for example equation (3.1), are considered as the description of an intermediate (mesoscopic) level, derived from the hydrodynamic limit [18]. The noise term naturally appears in the fluctuation problem. So, it is interesting to consider the Green–Kubo formula for the above equations, in particular, some exact relationships between the diffusion coefficients (or diffusion operators) and the mobility (or drift terms) with respect to their stationary distribution. In section 3, with some mild assumptions, we verify that equations (3.1) and (3.9) satisfy the conditions in theorem 2.5. And then, using theorem 2.5 for some special functionals, we obtain the equalities relating diffusion coefficients (or diffusion operators) to the mobility (or drift terms) (see corollaries 3.3, 3.4, 3.6), which can be regarded as the Einstein relation for equations (3.1) and (3.9) [25, 29].

Since there are some different definitions of diffusion coefficients, such as the asymptotic diffusion coefficient in [1, 25] and the conditional diffusion coefficient in [2, 23, 28] or this paper, the difference in these definitions leads to some different Green–Kubo formulas. We attempt to clarify the difference and connection of these formulas by two examples (the A-Langevin equations and the harmonic oscillator) in section 4.

Finally, some technical settings of stochastic evolution equations in infinite dimensional spaces are presented in the appendix for the reader's convenience.

2. The Green–Kubo formula for general Markov processes

Let Ξ be a Polish space (complete separable metric space) and $\{X_t\}_{t\geqslant 0}$ be a stationary Markov process on a probability space $(\Omega, \mathcal{F}, P)$, with state space Ξ and initial distribution μ. Let $L^2(\Xi, \mu) = \{f : \Xi \to \mathbb{R} : \int |f(x)|^2\mu(\mathrm{d}x) < \infty\}$. Then $L^2(\Xi, \mu)$ is a separable Hilbert space with inner product $\langle \cdot, \cdot\rangle_\mu$, where for any $f, g \in L^2(\Xi, \mu)$,

$$\langle f, g\rangle_\mu = \int f(x)g(x)\mu(\mathrm{d}x), \qquad \|f\|^2_{L^2(\mu)} = \langle f, f\rangle_\mu. \tag{2.1}$$

Denote by $\{P_t\}_{t\geqslant 0}$ the transition semigroup of $\{X_t\}_{t\geqslant 0}$, that is, P_t satisfies $P_t f(x) = E[f(X_t)|X_0 = x]$. It is well known that $\{P_t\}_{t\geqslant 0}$ is a contraction semigroup on $L^2(\Xi, \mu)$.

Assume that $\{P_t\}_{t\geqslant 0}$ is strongly continuous on $L^2(\Xi, \mu)$. Let $\mathcal{A}$ be the infinitesimal generator of $\{P_t\}_{t\geqslant 0}$ on $L^2(\Xi, \mu)$, i.e.

$$\begin{aligned} \mathcal{D}(\mathcal{A}) &= \left\{ f \in L^2(\Xi, \mu) : \lim_{t\downarrow 0} \frac{P_t f - f}{t} \text{ exists in } L^2(\Xi, \mu) \right\}, \\ \mathcal{A} f &= \lim_{t\downarrow 0} \frac{P_t f - f}{t}. \end{aligned} \tag{2.2}$$

In [23, theorem 2.3], it is shown that the Markov process $\{X_t\}_{t\geqslant 0}$ is reversible if and only if $\mathcal{A}$ is symmetric on $L^2(\Xi, \mu)$.

Let $\mathcal{P}_t$ be the σ-algebra generated by $\{X_s : s \leqslant t\}$ (the process before time t). For any positive integer m, set an m-dimensional vector-valued observable $\varphi = (\varphi_1, \varphi_2, \ldots, \varphi_m)$, where $\varphi_i \in \mathcal{D}(\mathcal{A})$, $i = 1, 2, \ldots, m$. Similar to [2], we give the following definitions by using the original idea in [28].

Definition 2.1. *For any $t \geqslant 0$, if the limit*

$$D\varphi(X_t) = \lim_{\Delta t\downarrow 0} E\left[\left. \frac{\varphi(X_{t+\Delta t}) - \varphi(X_t)}{\Delta t} \right| \mathcal{P}_t \right] \tag{2.3}$$

exists as limits in $L^1(\Xi, \mu)$, then $D\varphi(X_t)$ is called the mean forward derivative.

Proposition 2.2. *For any $f \in \mathcal{D}(\mathcal{A})$,*

$$\lim_{\Delta t\downarrow 0} \frac{1}{\Delta t} E[f(X_{t+\Delta t}) - f(X_t) | X_t = x] = \mathcal{A} f(x). \tag{2.4}$$

It is just the definition of the infinitesimal generator. Please refer to equation (4) in [23].

Definition 2.3. *For any $t \geqslant 0$, we define the conditional diffusion coefficient for $\varphi(X_t)$,*

$$G\varphi(X_t) = \lim_{\Delta t\downarrow 0} \mathrm{E}\left[\left. \frac{(\varphi(X_{t+\Delta t}) - \varphi(X_t))^T (\varphi(X_{t+\Delta t}) - \varphi(X_t))}{\Delta t} \right| \mathcal{P}_t \right], \tag{2.5}$$

if each element of the matrix exists in $L^1(\Xi, \mu)$.

$G\varphi(X_t)$ is a positive semidefinite matrix. Denote its (i, j) entry by $G_{ij}\varphi(X_t)$. We write $\langle f \rangle_\mu = \int f(x)\mu(\mathrm{d}x)$. Let $\langle\cdot\rangle$ stand for the ensemble average, i.e. for any random variable X on probability space $(\Omega, \mathcal{F}, P)$, $\langle X \rangle = E(X)$. Since $\{X_t\}_{t\geqslant 0}$ is a stationary Markov process with initial distribution μ, then for any $i, j = 1, \ldots, m$, $\langle G_{ij}\varphi(X_t)\rangle$ is independent of t.

Proposition 2.4. *If $\varphi_i, \varphi_j \in \mathcal{D}(\mathcal{A})$, then*

$$\langle G_{ij}\varphi(X_t)\rangle = -\langle \mathcal{A}\varphi_i, \varphi_j\rangle_\mu - \langle \mathcal{A}\varphi_j, \varphi_i\rangle_\mu. \tag{2.6}$$

The proof of proposition 2.4 is presented in subsection 2.1.

Remark 1. The existence of $G_{ij}\varphi$ is implicitly assumed in the present paper, and it is natural to assume $\phi_i\phi_j \in \mathcal{D}(\mathcal{A})$ to guarantee this as presented in definition 3.3 of [23].

Our main result is as follows.

Theorem 2.5 (Green–Kubo formula). *For the stationary Markov process $\{X_t\}_{t\geqslant 0}$, let*

$$\mathcal{J} = \left\{ f \in L^2(\Xi, \mu) : \lim_{t\to\infty} \| P_t f - \langle f \rangle_\mu \|_{L^2(\mu)} = 0 \right\}. \tag{2.7}$$

Then for any $\varphi_i,\ \varphi_j \in \mathcal{D}(\mathcal{A}) \cap \mathcal{J}$,

$$\langle G_{ij}\varphi(X_t)\rangle = \int_0^\infty \langle D\varphi_i(X_0)D\varphi_j(X_t)\rangle\,\mathrm{d}t + \int_0^\infty \langle D\varphi_j(X_0)D\varphi_i(X_t)\rangle\,\mathrm{d}t. \tag{2.8}$$

Corollary 2.6. *If* $\varphi_i \in \mathcal{D}(\mathcal{A}) \cap \mathcal{J},\quad i = 1, 2, \ldots, m$, *then*

$$\frac{1}{2}\langle trG\varphi(X_t)\rangle = \int_0^\infty \langle (D\varphi)^T(X_0)D\varphi(X_t)\rangle\,\mathrm{d}t, \tag{2.9}$$

where $\langle (D\varphi)^T(X_0)D\varphi(X_t)\rangle = \sum_{i=1}^m \langle D\varphi_i(X_0)D\varphi_i(X_t)\rangle$.

The proofs of theorem 2.5, corollary 2.6 are presented in subsection 2.1.

Remark 2. Let $\mathcal{I}$ be the set of stationary distribution of $\{P_t\}_{t\geqslant 0}$, and $\mathcal{I}_{\mathrm{ext}}$ be the set of extremal points of $\mathcal{I}$, i.e. the elements of $\mathcal{I}_{\mathrm{ext}}$ are ergodic probability measures for $\{P_t\}_{t\geqslant 0}$.

(1) In fact, by the ergodic decomposition theorem (see [19]), for $f \in \mathcal{J}$, there must be an ergodic measure $\nu \in \mathcal{I}_{\mathrm{ext}}$ such that $\langle f\rangle_\mu = \langle f\rangle_\nu$.

(2) If μ is an ergodic measure of finite Markov chains with continuous time, then it is clear that $\mathcal{J} = L^2(\Xi, \mu)$. That is to say, theorem 2.5 implies theorem 1.4 of [2].

(3) Suppose that μ is an ergodic measure, and $\{X_t\}_{t\geqslant 0}$ is reversible with respect to μ. By the spectral theorem (see [27, P937] and remark IV.2 of [23]), it is easy to show that $\mathcal{J} = L^2(\Xi, \mu)$. Thus (2.8) holds by theorem 2.5, and we have that

$$\frac{1}{2}\langle G_{ij}\varphi(X_t)\rangle = \int_0^\infty \langle D\varphi_i(X_0)D\varphi_j(X_t)\rangle\,\mathrm{d}t. \tag{2.10}$$

That is to say, theorem 2.5 implies theorem III.4 of [23].

(4) However, for an ergodic measure μ, if $\{X_t\}_{t\geqslant 0}$ is irreversible with respect to μ, it is not clear for us whether $\mathcal{J} = L^2(\Xi, \mu)$ or not. But the examples given in section 3 satisfy this condition.

Before we give some applications of theorem 2.5 to stochastic evolution equations on Hilbert spaces and infinite interacting diffusions in section 3, we would like to apply theorem 2.5 to finite-dimensional diffusions without assuming reversibility. Although the example is simple, it makes readers understand more easily the meaning of the Green–Kubo formula in a nonequilibrium case.

Example 1. Assume that $X = \{X_t\}_{t\geqslant 0}$ is a stationary diffusion on $\mathbb{R}^d$ with an infinitesimal generator

$$\mathcal{A} = \frac{1}{2}\nabla\cdot(A(x)\nabla) + b(x)\cdot\nabla = \frac{1}{2}\sum_{i,j=1}^d \frac{\partial}{\partial x_i}a_{ij}(x)\frac{\partial}{\partial x_j} + \sum_{i=1}^d b_i(x)\frac{\partial}{\partial x_i}, \tag{2.11}$$

where $A(x) = (a_{ij}(x))_{1\leqslant i\leqslant d, 1\leqslant j\leqslant d}$, $b(x) = (b_1(x), b_2(x), \ldots, b_d(x))^T$ and the components of $a_{ij}(x)$ and $b_i(x)$ are smooth functions on $\mathbb{R}^d$. Moreover, we assume that the invariant distribution of $\{X_t\}_{t\geqslant 0}$ has a positive smooth density $\rho(x)$, and its transition semigroup is strongly continuous on $L^2(\mathbb{R}^d, \rho)$ (see [17, 42–44] for the conditions guaranteeing these assumptions).

Suppose for any i, j, x_i, x_j and $x_i x_j \in \mathcal{D}(\mathcal{A}) \cap \mathcal{J}$. For each fixed i, j, let $\varphi_i(x) = x_i$, $\varphi_j(x) = x_j$; then direct computation yields that

$$D_i(x) \equiv D\varphi_i(x) = b_i(x) + \frac{1}{2}\sum_{k=1}^{d}\frac{\partial a_{ik}}{\partial x_k}(x),$$
$$D_j(x) \equiv D\varphi_j(x) = b_j(x) + \frac{1}{2}\sum_{k=1}^{d}\frac{\partial a_{jk}}{\partial x_k}(x), \tag{2.12}$$

and $G_{ij}\varphi(x) = a_{ij}(x)$. Then, by theorem 2.5, we can obtain the following Green–Kubo formula, for any i, j:

$$\int_{\mathbb{R}^d} a_{ij}(x)\rho(x)\,\mathrm{d}x = \int_0^\infty \langle D_i(X_0)D_j(X_t)\rangle\,\mathrm{d}t + \int_0^\infty \langle(D_j(X_0)D_i(X_t)\rangle\,\mathrm{d}t. \tag{2.13}$$

Comparing (2.13) with the Green–Kubo formula of the reversible diffusion on $\mathbb{R}^d$ presented in [22] (example 4.3.9) or in [23] (example 3.5), there are some clear differences between irreversible cases and reversible ones (see also remark 2 (3)).

Furthermore, by corollary 2.6, we have for $\varphi(x) = (x_1, x_2, \ldots, x_d)^T$,

$$\frac{1}{2}\int_{\mathbb{R}^d}\sum_{i=1}^{d} a_{ii}(x)\rho(x)\,\mathrm{d}x = \int_0^\infty \left\langle \sum_{i=1}^{d} D_i(X_0)D_i(X_t)\right\rangle \mathrm{d}t. \tag{2.14}$$

2.1. Proofs of theorems

Proof of proposition 2.4. By definition 2.3, we obtain

$$\begin{aligned}
\langle G_{ij}\varphi(X_t)\rangle &= \lim_{s\downarrow 0}\frac{1}{s}E[(\varphi_i(X_{t+s}) - \varphi_i(X_t))(\varphi_j(X_{t+s}) - \varphi_j(X_t))]\\
&= \lim_{s\downarrow 0}\frac{1}{s}E[2\varphi_i(X_t)\varphi_j(X_t) - \varphi_i(X_{t+s})\varphi_j(X_t) - \varphi_j(X_{t+s})\varphi_i(X_t)]\\
&= \lim_{s\downarrow 0}\frac{1}{s}[\langle\varphi_i,\varphi_j\rangle_\mu - \langle P_s\varphi_i,\varphi_j\rangle_\mu] + \lim_{s\downarrow 0}\frac{1}{s}[\langle\varphi_j,\varphi_i\rangle_\mu - \langle P_s\varphi_j,\varphi_i\rangle_\mu]\\
&= \left\langle \lim_{s\downarrow 0}\frac{\varphi_i - P_s\varphi_i}{s},\varphi_j\right\rangle_\mu + \left\langle \lim_{s\downarrow 0}\frac{\varphi_j - P_s\varphi_j}{s},\varphi_i\right\rangle_\mu\\
&\quad \text{(by the continuity of the inner product)}\\
&= -\langle\mathcal{A}\varphi_i,\varphi_j\rangle_\mu - \langle\mathcal{A}\varphi_j,\varphi_i\rangle_\mu. \quad \text{(by } \varphi_i,\varphi_j \in \mathcal{D}(\mathcal{A}) \text{ and equation (2.2))}
\end{aligned} \tag{2.15}$$

□

Lemma 2.7. *If $f \in L^2(\Xi,\mu)$ satisfies that*

$$\lim_{t\to\infty}\|P_t f - \langle f\rangle_\mu\|_{L^2(\mu)} = 0, \tag{2.16}$$

then for any $\varphi \in \mathcal{D}(\mathcal{A})$,

$$\lim_{t\to\infty}\langle P_t f, \mathcal{A}\varphi\rangle_\mu = 0. \tag{2.17}$$

Proof. By Hölder inequality, we have

$$\begin{aligned}
|\langle P_t f - \langle f\rangle_\mu, \mathcal{A}\varphi\rangle_\mu| &\leqslant \int |(P_t f - \langle f\rangle_\mu)\mathcal{A}\varphi|\,\mathrm{d}\mu\\
&\leqslant \|P_t f - \langle f\rangle_\mu\|_{L^2(\mu)}\|\mathcal{A}\varphi\|_{L^2(\mu)}.
\end{aligned}$$

It follows from (2.16) that

$$\lim_{t\to\infty}\langle P_t f - \langle f\rangle_\mu, \mathcal{A}\varphi\rangle_\mu = 0.$$

Since μ is invariant, $\langle \mathcal{A}\varphi \rangle_\mu = 0$. Thus,

$$\begin{aligned}\lim_{t\to\infty} \langle P_t f, \mathcal{A}\varphi \rangle_\mu &= \lim_{t\to\infty} \langle P_t f - \langle f \rangle_\mu, \mathcal{A}\varphi \rangle_\mu + \langle f \rangle_\mu \langle \mathcal{A}\varphi \rangle_\mu \\ &= 0.\end{aligned}$$

□

Lemma 2.8. *Suppose that* $\varphi_i, \varphi_j \in \mathcal{D}(\mathcal{A})$, *then*

$$\int_0^\infty \langle D\varphi_i(X_0) D\varphi_j(X_t)\rangle \,\mathrm{d}t = -\langle \varphi_j, \mathcal{A}\varphi_i \rangle_\mu \tag{2.18}$$

holds if and only if

$$\lim_{t\to\infty} \langle P_t\varphi_j, \mathcal{A}\varphi_i \rangle_\mu = 0. \tag{2.19}$$

Proof. When $t \geqslant 0$, it follows from the semigroup equation[5] (i.e. the Kolmogorov forward equation) that

$$\begin{aligned} &\mathrm{d}P_t\varphi_j = P_t\mathcal{A}\varphi_j \,\mathrm{d}t, \\ &\text{and} \qquad \mathrm{d}\langle P_t\varphi_j, \mathcal{A}\varphi_i \rangle_\mu = \langle P_t\mathcal{A}\varphi_j, \mathcal{A}\varphi_i \rangle_\mu \,\mathrm{d}t. \end{aligned} \tag{2.20}$$

Thus,

$$\int_0^t \langle P_s\mathcal{A}\varphi_j, \mathcal{A}\varphi_i \rangle_\mu \,\mathrm{d}s = \langle P_t\varphi_j, \mathcal{A}\varphi_i \rangle_\mu - \langle \varphi_j, \mathcal{A}\varphi_i \rangle_\mu. \tag{2.21}$$

Taking the limitation, it yields that

$$\int_0^\infty \langle P_s\mathcal{A}\varphi_j, \mathcal{A}\varphi_i \rangle_\mu \,\mathrm{d}s = \lim_{t\to\infty} \langle P_t\varphi_j, \mathcal{A}\varphi_i \rangle_\mu - \langle \varphi_j, \mathcal{A}\varphi_i \rangle_\mu. \tag{2.22}$$

By definition 2.1 and proposition 2.2, we have

$$\int_0^\infty \langle D\varphi_i(X_0) D\varphi_j(X_t)\rangle \,\mathrm{d}t = \int_0^\infty \langle P_t\mathcal{A}\varphi_j, \mathcal{A}\varphi_i \rangle_\mu \,\mathrm{d}t \tag{2.23}$$

$$= \lim_{t\to\infty} \langle P_t\varphi_j, \mathcal{A}\varphi_i \rangle_\mu - \langle \varphi_j, \mathcal{A}\varphi_i \rangle_\mu. \tag{2.24}$$

Hence equation (2.18) holds if and only if equation (2.19) is valid. □

Proof of theorem 2.5. By proposition 2.4 we have

$$\langle G_{ij}\varphi(X_t)\rangle = -\langle \mathcal{A}\varphi_i, \varphi_j \rangle_\mu - \langle \mathcal{A}\varphi_j, \varphi_i \rangle_\mu.$$

Since $\varphi_i,\ \varphi_j \in \mathcal{D}(\mathcal{A}) \cap \mathcal{J}$ we have by lemma 2.7

$$\lim_{t\to\infty} \langle P_t\varphi_j, \mathcal{A}\varphi_i \rangle_\mu = 0, \qquad \lim_{t\to\infty} \langle P_t\varphi_i, \mathcal{A}\varphi_j \rangle_\mu = 0. \tag{2.25}$$

From lemma 2.8 we have

$$-\langle \varphi_j, \mathcal{A}\varphi_i \rangle_\mu = \int_0^\infty \langle P_t\mathcal{A}\varphi_j, \mathcal{A}\varphi_i \rangle_\mu \,\mathrm{d}t, \tag{2.26}$$

$$-\langle \varphi_i, \mathcal{A}\varphi_j \rangle_\mu = \int_0^\infty \langle P_t\mathcal{A}\varphi_i, \mathcal{A}\varphi_j \rangle_\mu \,\mathrm{d}t. \tag{2.27}$$

This proves the expression given in equation (2.8). □

Proof of corollary 2.6. Note that $\langle tr G\varphi(X_t)\rangle = \sum_{i=1}^m \langle G_{ii}\varphi(X_t)\rangle$. Therefore, by theorem 2.5 we have

$$\langle tr G\varphi(X_t)\rangle = 2\sum_{i=1}^m \int_0^\infty \langle D\varphi_i(X_0) D\varphi_i(X_t)\rangle \,\mathrm{d}t = 2\int_0^\infty \langle (D\varphi)^T(X_0) D\varphi(X_t)\rangle \,\mathrm{d}t.$$

□

[5] The reader can refer to pp 235–9 of [35] for the semigroup equation.

3. The Green–Kubo formula for stochastic evolution equations

In fact, L^2-convergence, ergodicity and irreversibility with respect to the invariant measure for general Markov processes are sophisticated topics in probability theory (see [21] and references therein), which is not the main purpose of this paper. To illustrate the Green–Kubo formula, we present two typical classes of stochastic evolution equations in infinite dimensional spaces, of which L^2 convergence and irreversibility have been shown by Da Prato *et al* [6], Chojnowska–Michalik *et al* [3], Deuschel [11] and Feng *et al* [16]. One is a class of stochastic evolution equations in a separable Hilbert space, which has a unique invariant measure. The other is a class of critical interacting diffusions on $\mathbb{Z}^d$, which possesses infinitely many extremal invariant measures. Both of them have been motivated by describing random phenomena in physics, chemistry, and biology.

3.1. Stochastic evolution equations in Hilbert space

Let H and U be two separable Hilbert spaces (with norms $|\cdot|_H$, $|\cdot|_U$, and inner products $\langle\cdot\rangle_H$, $\langle\cdot\rangle_U$, respectively). We are concerned with the following stochastic differential equation:

$$\begin{cases} \mathrm{d}X_t = (AX_t + F(X_t))\,\mathrm{d}t + B\,\mathrm{d}W_t, & t \geqslant 0, \\ X_0 = x \in H, \end{cases} \tag{3.1}$$

where $A : \mathcal{D}(A) \subset H \to H$ and $B : U \to H$ are linear operators, $F : H \to H$ is a nonlinear function, and $W = \{W_t\}_{t\geqslant 0}$ is a cylindrical Wiener process on U (for the precise definition of the cylindrical Wiener process, please see definition 5.2 in appendix A.1).

Many kinds of dynamics in physics and chemistry can be modeled by equation (3.1), for example, stochastic reaction–diffusion equations (see [5, 6, 8, 18, 31]). More information about equation (3.1) can be found in [5–8, 31].

We assume that F is a Lipschitz function. Under hypothesis 5.4 in appendix A.1, equation (3.1) has a unique mild solution $\{X_t\}_{t\geqslant 0}$ (for the precise definition of mild solution, please see definition 5.3 in appendix A.1). Let $\{P_t\}_{t\geqslant 0}$ be the transition semigroup of $\{X_t\}_{t\geqslant 0}$, defined by $P_t f(x) = E[f(X_t)|X_0 = x]$ for any bounded Borel-measurable function f on H. Under hypotheses 5.4 and 5.5 in appendix A.1, there exists a unique invariant probability measure for $\{P_t\}_{t\geqslant 0}$, denoted by μ. By the results in [5] ([5], p 79), $\{P_t\}_{t\geqslant 0}$ can be uniquely extended to a strongly continuous contraction semigroup on $L^2(H, \mu)$, which is still denoted by $\{P_t\}_{t\geqslant 0}$. We denote by $\mathcal{A}$ the infinitesimal generator of $\{P_t\}_{t\geqslant 0}$ on $L^2(H, \mu)$. Let $L(U; H)$ be the space of all linear continuous operators from U into H, and $L(H)$ be the space of all linear continuous operators from H into H endowed with the norm

$$|\|T|\| \equiv \sup\{|Tx|_H : x \in H, |x|_H = 1\}, \qquad T \in L(H).$$

Let $C_b(H; H)$ be the space of all uniformly continuous and bounded mappings from H into H. Denote by $C_b^1(H; H)$ the space of all uniformly continuous and bounded functions $f : H \to H$ which are Fréchet differentiable on H with uniformly continuous and bounded derivative, and $C_b^2(H; H)$ the subspace of $C_b^1(H; H)$ of all functions $f : H \to H$ which are twice Fréchet differentiable on H with uniformly continuous and bounded second derivative. Denote by A^*, B^* the adjoint operators of A and B, respectively. Let $C = BB^*$ and $N(0, Q_\infty)$ be a Gaussian probability measure on H with mean $0 \in H$ and covariance operator Q_∞ in H. Here, $Q_\infty x = \int_0^\infty \mathrm{e}^{tA} C\, \mathrm{e}^{tA^*} x\,\mathrm{d}t$, $x \in H$ (for the definition of Gaussian probability measures on Hilbert space, please refer to [7, 31]).

Proposition 3.1.

(I) (Proposition 3.42 in [5]). Assume that $C = \mathbb{I}$ *(identity operator) and* $F \in C_b(H, H)$*. Then*

$$\mathcal{A} \text{ is symmetric if and only if } F = \tfrac{1}{2}\nabla \log \rho,$$

where $\rho = \frac{d\mu}{d\nu}$*, the Radon–Nikodym derivative of* μ *with respect to* ν*,* $\nu = N(0, Q_\infty)$*.*

(II) (Theorem 2.4 in [3]). Assume that $F = 0$*. The following conditions are equivalent.*

(i) The semigroup P_t *is symmetric in* $L^2(H, \mu)$*.*

(ii) If $x \in \mathcal{D}(A^*)$*, then* $Cx \in \mathcal{D}(A)$ *and*

$$ACx = CA^*x.$$

(iii) $e^{tA}C = C(e^{tA})^*$ *for all* $t \geqslant 0$*.*

Thus, from proposition 3.1, equation (3.1) is irreversible in most cases.

In addition, assume that $C^{-1} \in L(H)$ and $F \in C_b^2(H; H)$, by proposition 3.29 in [5], then we have for any $f \in L^2(H, \mu)$,

$$\lim_{t\to\infty} \|P_t f - \langle f\rangle_\mu\|_{L^2(\mu)} = 0. \tag{3.2}$$

That is to say, it is the same as $\mathcal{J} = L^2(H, \mu)$ for use in theorem 2.5. Therefore,

Corollary 3.2. *The Green–Kubo formula is valid in theorem 2.5 for the stochastic evolution equation (3.1).*

Now, for some special observable φ, we give the explicit form of the Green–Kubo formula for equation (3.1). Let φ_i, φ_j be bounded linear functionals on H. More precisely, we set $\varphi_i(x) = \langle \xi, x\rangle_H$ and $\varphi_j(x) = \langle \eta, x\rangle_H$, where $\xi, \eta \in \mathcal{D}(A^*) \subset H$. Then direct computation yields that

$$D\varphi_i(x) = \langle x, A^*\xi\rangle_H + \langle F(x), \xi\rangle_H, \qquad D\varphi_j(x) = \langle x, A^*\eta\rangle_H + \langle F(x), \eta\rangle_H.$$

We have the following result.

Corollary 3.3.

$$\begin{aligned}\langle C\eta, \xi\rangle_H = {} & \int_0^\infty \langle D\varphi_i(X_0)D\varphi_j(X_t)\rangle\,dt + \int_0^\infty \langle D\varphi_j(X_0)D\varphi_i(X_t)\rangle\,dt \\ & + \int (\langle F(x), \xi\rangle_H \langle \eta, x\rangle_H + \langle F(x), \eta\rangle_H \langle \xi, x\rangle_H)\,d\mu \\ & + \int \langle Q_\infty \nabla \log \rho, A^*\nabla(\varphi_i\varphi_j)\rangle_H\,d\mu.\end{aligned} \tag{3.3}$$

Proof. From lemma 2.45 in [5], one has

$$\langle Q_\infty \xi, A^*\eta\rangle_H + \langle Q_\infty \eta, A^*\xi\rangle_H = -\langle C\eta, \xi\rangle_H. \tag{3.4}$$

Recalling that $\rho = \frac{d\mu}{d\nu}$ and $\nu = N(0, Q_\infty)$, it follows from proposition 2.46 in [5], proposition 2.4 and (3.4) that

$$\begin{aligned}\langle G_{ij}\varphi(X_t)\rangle &= -\langle \varphi_j, \mathcal{A}\varphi_i\rangle_\mu - \langle \varphi_i, \mathcal{A}\varphi_j\rangle_\mu \\ &= -\int \langle x, A^*\xi\rangle_H \langle \eta, x\rangle_H \rho\,d\nu - \int \langle x, A^*\eta\rangle_H \langle \xi, x\rangle_H \rho\,d\nu \\ &\quad - \int \big(\langle F(x), \xi\rangle_H \langle \eta, x\rangle_H + \langle F(x), \eta\rangle_H \langle \xi, x\rangle_H\big)\rho\,d\nu\end{aligned}$$

$$
\begin{aligned}
&= -\int (\langle Q_\infty \nabla(\varphi_j \rho), A^*\xi\rangle_H + \langle Q_\infty \nabla(\varphi_i \rho), A^*\eta\rangle_H)\,\mathrm{d}\nu \\
&\quad - \int (\langle F(x), \xi\rangle_H \langle \eta, x\rangle_H + \langle F(x), \eta\rangle_H \langle \xi, x\rangle_H)\rho\,\mathrm{d}\nu \\
&= -\int (\langle Q_\infty \xi, A^*\eta\rangle_H + \langle Q_\infty \eta, A^*\xi\rangle_H)\rho\,\mathrm{d}\nu - \int \langle Q_\infty \nabla\rho, A^*\nabla(\varphi_i\varphi_j)\rangle_H\,\mathrm{d}\nu \\
&\quad - \int (\langle F(x), \xi\rangle_H \langle \eta, x\rangle_H + \langle F(x), \eta\rangle_H \langle \xi, x\rangle_H)\rho\,\mathrm{d}\nu \\
&= \langle C\eta, \xi\rangle_H - \int \langle Q_\infty \nabla \log\rho, A^*\nabla(\varphi_i\varphi_j)\rangle_H\,\mathrm{d}\mu \\
&\quad - \int (\langle F(x), \xi\rangle_H \langle \eta, x\rangle_H + \langle F(x), \eta\rangle_H \langle \xi, x\rangle_H)\,\mathrm{d}\mu. \qquad (3.5)
\end{aligned}
$$

Therefore, corollary 3.3 follows from theorem 2.5 and (3.5). □

In particular, if $F = 0$, the process $\{X_t\}_{t\geqslant 0}$ is called Ornstein–Uhlenbeck process. Here, $\mu = N(0, Q_\infty)$ is the unique invariant probability measure for $\{X_t\}_{t\geqslant 0}$. In this case, it is clear that both the second term and the third term on the right-hand side of (3.5) vanish. Thus,

$$
\langle G_{ij}\varphi(X_t)\rangle = \langle C\eta, \xi\rangle_H. \qquad (3.6)
$$

On the other hand,

$$
\begin{aligned}
&\int_0^\infty \langle D\varphi_i(X_0) D\varphi_j(X_t)\rangle\,\mathrm{d}t + \int_0^\infty \langle D\varphi_j(X_0) D\varphi_i(X_t)\rangle\,\mathrm{d}t \\
&\quad = \int_0^\infty E^\mu[\langle X_0, A^*\xi\rangle_H \langle X_t, A^*\eta\rangle_H]\,\mathrm{d}t + \int_0^\infty E^\mu[\langle X_0, A^*\eta\rangle_H \langle X_t, A^*\xi\rangle_H]\,\mathrm{d}t \\
&\quad = \int_0^\infty \left[\int \langle x, A^*\xi\rangle_H \langle x, (\mathrm{e}^{tA})^* A^*\eta\rangle_H\,\mathrm{d}\mu\right]\mathrm{d}t \\
&\qquad + \int_0^\infty \left[\int \langle x, A^*\eta\rangle_H \langle x, (\mathrm{e}^{tA})^* A^*\xi\rangle_H\,\mathrm{d}\mu\right]\mathrm{d}t \\
&\quad = \int_0^\infty \langle \mathrm{e}^{tA} Q_\infty A^*\xi, A^*\eta\rangle_H\,\mathrm{d}t + \int_0^\infty \langle \mathrm{e}^{tA} Q_\infty A^*\eta, A^*\xi\rangle_H\,\mathrm{d}t. \qquad (3.7)
\end{aligned}
$$

Therefore, from (3.6) and (3.7), we obtain the following result.

Corollary 3.4. *Suppose that $F = 0$; then the Green–Kubo formula for the Ornstein–Uhlenbeck process $\{X_t\}_{t\geqslant 0}$ is*

$$
\langle C\eta, \xi\rangle_H = \int_0^\infty \langle \mathrm{e}^{tA} Q_\infty A^*\xi, A^*\eta\rangle_H\,\mathrm{d}t + \int_0^\infty \langle \mathrm{e}^{tA} Q_\infty A^*\eta, A^*\xi\rangle_H\,\mathrm{d}t. \qquad (3.8)
$$

In fact, (3.3) and (3.8) can be regarded as the Einstein relation for stochastic evolution equations (3.1).

3.2. Critical interacting diffusion processes

In this subsection, three examples of critical interacting diffusion processes are shown to satisfy the Green–Kubo formula.

Let I be a closed interval of $\mathbb{R}$, and set $\Xi = I^{\mathbb{Z}^d} \cap \mathscr{J}'(\mathbb{Z}^d)$, where $\mathscr{J}'(\mathbb{Z}^d)$ denotes the set of tempered configurations $x \in \mathbb{R}^{\mathbb{Z}^d}$ with $\sum_i (1+|i|)^{-2p}|x(i)|^2 < \infty$, for some $p \geqslant 1$.

Assume $d \geqslant 3$. Let $X_t = \{X_t(i),\ i \in \mathbb{Z}^d\}$ be the system on I defined by the following stochastic differential equations:

$$dX_t(i) = \sum_{j\in\mathbb{Z}^d} q_{ij} X_t(i)\,dt + \sqrt{a(X_t(i))}\,dB_t(i), \qquad i \in \mathbb{Z}^d, \tag{3.9}$$

where $\{B_t(i)\}_{i\in\mathbb{Z}^d}$ is an independent system of one-dimensional standard Brownian motions, and $Q = \{q_{ij}\}$ is an irreducible $\mathbb{Z}^d \times \mathbb{Z}^d$ real matrix satisfying the following:

(H1) $q_{ij} \geqslant 0, i \neq j$, and $Q = \{q_{ij}\}$ is of finite range, that is $q_{ij} > 0$ $(i \neq j)$ for only finitely many $i, j \in \mathbb{Z}^d$.
(H2) $-q_{ii} = \sum_{j\neq i} q_{ij} = 1$.
(H3) $q_{ij} = q_{0(j-i)}$.

Then it was shown by Shiga and Shimizu [40] that the system (3.9) has a unique Ξ-valued strong solution $\{X_t\}_{t\geqslant 0}$.

Denote by $\mathcal{L}(\Xi)$ the set of Lipschitz continuous functions on Ξ. (For the precise definition of $\mathcal{L}(\Xi)$, please see appendix A.2.) Then let $\mathcal{L}_0(\Xi)$ be the set of local Lipschitz functions depending on finitely many coordinates, and $C_0^2(\Xi)$ be the set of all bounded functions $f : \Xi \to \mathbb{R}$ depending on finitely many coordinates with bounded partial derivatives of first and second order. We define $\{P_t\}_{t\geqslant 0}$ to be the transition semigroup of $\{X_t\}_{t\geqslant 0}$, and set $P_t f(x) = E[f(X_t)|X_0 = x]$ for any bounded Borel-measurable function f on Ξ. Here $\{P_t\}_{t\geqslant 0}$ satisfies

$$P_t f - f = \int_0^t P_s \mathcal{A} f\,ds \qquad \text{for} \quad f \in C_0^2(\Xi),$$

where $\mathcal{A}$ is the generator of $\{P_t\}_{t\geqslant 0}$, and

$$\mathcal{A}f(x) = \frac{1}{2}\sum_{i\in\mathbb{Z}^d} a(x(i)) \frac{\partial^2}{\partial x(i)^2} f(x) + \sum_{i\in\mathbb{Z}^d}\left(\sum_{j\in\mathbb{Z}^d} q_{ij} x(j)\right)\frac{\partial}{\partial x(i)} f(x). \tag{3.10}$$

In this paper, we are interested in the following three concrete examples which have physics and biology background.

(1) *The critical Ornstein–Uhlenbeck process (see [10, 11]).* In the system (3.9), we set

$$I = \mathbb{R} \quad \text{and} \quad a(y) \equiv 1, \qquad y \in \mathbb{R}.$$

As pointed by Deuschel in [11], for each $\tau \in \mathbb{R}$, there exists an extremal $\{P_t\}_{t\geqslant 0}$-invariant measure $\mu = \mu(\tau)$ (Gaussian measure) on Ξ with constant mean $\tau \in \mathbb{R}$ and covariances

$$\mathrm{cov}_\mu(x(i), x(j)) = \int_0^\infty e^{tQ}(i, j)\,dt, \qquad i, j \in \mathbb{Z}^d.$$

In fact, from proposition 3.1, the critical Ornstein–Uhlenbeck process $\{X_t\}_{t\geqslant 0}$ is irreversible in most cases.

(2) *The continuous time stepping stone model* (see [11, 39]). Set

$$I = [0, 1] \qquad \text{and} \qquad a(y) = y(1 - y), \qquad y \in [0, 1].$$

Such a system is called a continuous time stepping stone model which comes from population biology. By the results in [16] (see example 1 in [16]), the stepping stone model is irreversible. Shiga [39] has shown that there exists an extremal $\{P_t\}_{t\geqslant 0}$-invariant measure μ on Ξ for each $\tau \in [0.1]$ such that, each $f \in \mathcal{L}_0(\Xi)$

$$\lim_{t\to\infty} P_t f(\tau) = \langle f\rangle_\mu \qquad \text{and} \qquad \langle x(i)\rangle_\mu = \tau, \qquad i \in \mathbb{Z}^d. \tag{3.11}$$

(3) *The measure-valued critical branching random walk (see [9, 11, 13]).* Set

$$I = \mathbb{R}^+ \qquad \text{and} \qquad a(y) = y, \qquad y \in \mathbb{R}^+.$$

As pointed by Deuschel in [11], for each $\tau \in \mathbb{R}^+$, there exists an extremal $\{P_t\}_{t\geqslant 0}$-invariant measure μ on Ξ satisfying (3.11). However, we do not know the irreversibility of the measure-valued critical branching random walk. Although we think it is irreversible, we cannot give a proof immediately.

It is shown that $\{P_t\}_{t\geqslant 0}$ simply has a unique extension to a strongly continuous contraction semigroup on $L^2(\Xi, \mu)$ (which is still denoted by $\{P_t\}_{t\geqslant 0}$) in appendix A.2. If μ is an extremal invariant measure of $\{P_t\}_{t\geqslant 0}$, then due to the results in [11], for any $f \in \mathcal{L}(\Xi)$, $\lim_{t\to\infty} \|P_t f - \langle f\rangle_\mu\|_{L^2(\mu)} = 0$. Since $\mathcal{L}(\Xi)$ is a dense subset of $L^2(\Xi, \mu)$, then for any $f \in L^2(\Xi, \mu)$,

$$\lim_{t\to\infty} \|P_t f - \langle f\rangle_\mu\|_{L^2(\mu)} = 0.$$

That is to say, it is the same as $\mathcal{J} = L^2(\Xi, \mu)$ for use in theorem 2.5. Thus,

Corollary 3.5. *The Green–Kubo formula is valid in theorem 2.5 for the above three processes.*

Furthermore, for fixed $i, j \in \mathbb{Z}^d$, let $\varphi_i(x) = x(i)$, $\varphi_j(x) = x(j)$. For $\beta : \mathbb{Z}^d \to \mathbb{R}$, set $Q\beta(i) = \sum_k q_{ik}\beta(k)$ and $\mathrm{e}^{tQ}\beta(j) = \sum_k \mathrm{e}^{tQ}(j,k)\beta(k)$, respectively. Then, we obtain the following Green–Kubo formula from equation (3.9).

Corollary 3.6.

$$\delta(i,j)\sigma^2(\mu) = \int_0^\infty \int (Qx(i))(\mathrm{e}^{tQ}Qx(j))\,\mathrm{d}\mu\,\mathrm{d}t + \int_0^\infty \int (Qx(j))(\mathrm{e}^{tQ}Qx(i))\,\mathrm{d}\mu\,\mathrm{d}t, \tag{3.12}$$

where $\delta(i,j) = 1$, *if* $i = j$; $\delta(i,j) = 0$, *if* $i \neq j$, *and* $\sigma^2(\mu) = \int a(x(i))\,\mathrm{d}\mu$, *which is a constant independent of* i.

Proof. Note that $\mathcal{A}\varphi_i(x) = \sum_l q_{il}x(l)$ and $\mathcal{A}\varphi_j(x) = \sum_l q_{jl}x(l)$. Therefore, proposition 2.4 implies

$$\langle G_{ij}\varphi(X_t)\rangle = -\sum_l q_{il}\int x(j)x(l)\,\mathrm{d}\mu - \sum_l q_{jl}\int x(i)x(l)\,\mathrm{d}\mu. \tag{3.13}$$

From the proof of lemma 2.3 in [11], we have

$$\sum_l q_{il}\int x(j)x(l)\,\mathrm{d}\mu + \sum_l q_{jl}\int x(i)x(l)\,\mathrm{d}\mu = -\delta(i,j)\sigma^2(\mu),$$

where $\sigma^2(\mu) = \int a(x(i))\,\mathrm{d}\mu$ is a constant independent of $i \in \mathbb{Z}^d$ because of the shift invariance of μ. Substituting in (3.13), it yields

$$\langle G_{ij}\varphi(X_t)\rangle = \delta(i,j)\sigma^2(\mu). \tag{3.14}$$

On the other hand,

$$D\varphi_i(x) = \mathcal{A}\varphi_i(x) = \sum_k q_{ik}x(k), \qquad D\varphi_j(x) = \mathcal{A}\varphi_j(x) = \sum_l q_{jl}x(l).$$

In fact, they are just the drift coefficients of $\{X_t\}_{t\geqslant 0}$. By lemma 1 in [4], we have

$$E^x X_t(l) = \sum_m \mathrm{e}^{tQ}(l,m)x(m). \tag{3.15}$$

Taking (3.15) into account it follows that

$$\begin{aligned}\int_0^\infty E^\mu\left[\sum_k q_{ik}X_0(k)\sum_l q_{jl}X_t(l)\right]\mathrm{d}t &= \int_0^\infty\int\sum_k q_{ik}x(k)\sum_l q_{jl}E^x X_t(l)\,\mathrm{d}\mu\,\mathrm{d}t\\ &= \int_0^\infty\int\sum_k q_{ik}x(k)\sum_l q_{jl}\sum_m \mathrm{e}^{tQ}(l,m)x(m)\,\mathrm{d}\mu\,\mathrm{d}t\\ &= \int_0^\infty\int(Qx(i))(Q\,\mathrm{e}^{tQ}x(j))\,\mathrm{d}\mu\,\mathrm{d}t\\ &= \int_0^\infty\int(Qx(i))(\mathrm{e}^{tQ}Qx(j))\,\mathrm{d}\mu\,\mathrm{d}t.\end{aligned}$$

By a similar argument, we obtain

$$\int_0^\infty E^\mu\left[\sum_l q_{jl}X_0(l)\sum_k q_{ik}X_t(k)\right]\mathrm{d}t = \int_0^\infty\int(Qx(j))(\mathrm{e}^{tQ}Qx(i))\,\mathrm{d}\mu\,\mathrm{d}t.$$

Therefore, the conclusion follows from theorem 2.5. □

4. A comparison between two types of diffusion coefficients

Besides the conditional diffusion coefficient (see definition 2.3 in section 2), there is an asymptotic diffusion coefficient given in [1, 25]. We compare two types of diffusion coefficients through two examples in this section.

Suppose that $(v_x(t), v_y(t))$ is the velocity. Let the instantaneous position be

$$x(t) = x(0) + \int_0^t v_x(s)\,\mathrm{d}s \equiv x(0) + \delta x(t). \tag{4.1}$$

$y(t)$ is similar.

Definition 4.1. *(See equation (11.8) in [1]) The asymptotic diffusion coefficient is defined by* $\lim_{t\to\infty}\frac{\mathrm{d}}{\mathrm{d}t}\langle\delta x^2(t)\rangle$.[6]

Example 2. For the A-Langevin equations [1, pp 181–6]

$$\begin{bmatrix}\mathrm{d}v_x(t)\\ \mathrm{d}v_y(t)\end{bmatrix} = \begin{bmatrix}-r & \Omega\\ -\Omega & -r\end{bmatrix}\begin{bmatrix}v_x(t)\\ v_y(t)\end{bmatrix}\mathrm{d}t + \sigma\begin{bmatrix}\mathrm{d}B_1(t)\\ \mathrm{d}B_2(t)\end{bmatrix}, \tag{4.2}$$

where $r > 0$, $\Omega > 0$, and $(B_1(t), B_2(t))$ is the standard two-dimensional Wiener process. Clearly, $(v_x(t), v_y(t))$ has an invariant distribution. It is shown in [1, p 186] that

$$\lim_{t\to\infty}\frac{\mathrm{d}}{\mathrm{d}t}\langle\delta x^2(t)\rangle = 2\int_0^\infty\langle v_x(t)v_x(0)\rangle\,\mathrm{d}t. \tag{4.3}$$

Equation (4.3) is also named as the Green–Kubo formula.

The process associated with a complete set of variables $\{\xi_t = (x(t), y(t), v_x(t), v_y(t))\}$ is the Markov process. The mean forward derivative of $x(t)$ is exactly $v_x(t)$. However, the process $\{\xi_t\}_{t\geqslant 0}$ has no invariant distribution, which prevents equation (2.8) from being used.

[6] The $\frac{1}{2}$ is elided here.

Example 3. Suppose $p(t)$ is the momentum. For the harmonic oscillator [36, 45], the explicit equations of motions are

$$\begin{cases} \mathrm{d}x = \dfrac{p}{m}\,\mathrm{d}t \\ \mathrm{d}p = \left(-m\omega_0^2 x - \gamma p\right)\mathrm{d}t + \sqrt{2kTm\gamma}\,\mathrm{d}B(t), \end{cases} \tag{4.4}$$

where $B(t)$ is the standard Brownian motion on the real line. $\{\xi_t = (x(t), p(t))\}_{t\geqslant 0}$ is a two-dimensional Markov diffusion with invariant distribution

$$\begin{aligned} \rho(x, p) &= \frac{\omega_0}{2\pi kT}\exp\left\{-\frac{m\omega_0^2 x^2}{2kT} - \frac{p^2}{2mkT}\right\} \\ &= \frac{\omega_0\sqrt{m}}{\sqrt{2\pi KT}}\exp\left\{-\frac{m\omega_0^2 x^2}{2kT}\right\}\cdot\frac{1}{\sqrt{2\pi mKT}}\exp\left\{-\frac{p^2}{2mkT}\right\}, \end{aligned} \tag{4.5}$$

and $Dx(t) = \frac{p(t)}{m}$. By theorem 2.5, definition 4.1 and direct computation, we have that

$$\langle Gx(t)\rangle = \lim_{t\to\infty}\frac{\mathrm{d}}{\mathrm{d}t}\langle\delta x^2(t)\rangle = 2\int_0^\infty\left\langle\frac{p(t)}{m}\frac{p(0)}{m}\right\rangle\mathrm{d}t. \tag{4.6}$$

The asymptotic diffusion coefficient and the expectation of the conditional diffusion coefficient are identical now. This means that these two different diffusion coefficients lead to the same Green–Kubo formula for this example.

Remark 3. Although we obtain equation (4.6), we have to employ the special form of $\rho(x, p)$. At present, it is not clear to us whether this equality always holds for general Hamiltonian systems perturbed by random force with stationary distribution. This is an interesting problem in our future research.

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Appendix

A.1. Setting of stochastic PDE (3.1)

Denote by $L(U)$ the space of all linear continuous operators from U into U. Let e_k, $k \in \mathbb{N}$, be an orthonormal basis of U and $Q \in L(U)$ be nonnegative, symmetric and with finite trace, i.e. $\mathrm{tr}Q < \infty$, where $\mathrm{tr}Q \equiv \sum_{k\in\mathbb{N}}\langle Qe_k, e_k\rangle_U$, if the series is convergent.

Definition 5.1. *(Q-Wiener process, see [7, 31]). A stochastic process $W(t)$, $t \in [0, T]$ (where T is a positive real number), on a probability space $(\Omega, \mathcal{F}, P)$ is called a (standard) Q-Wiener process on U if*

(1) $W(0) = 0$,

(2) W has P-a.s. continuous trajectories,

(3) W has independent increments, i.e. the random variables

$$W(t_1), W(t_2) - W(t_1), \ldots, W(t_n) - W(t_{n-1})$$

are independent for all $0 \leqslant t_1 \leqslant \cdots \leqslant t_n \leqslant T,\ n \in \mathbb{N}$,

(4) the increments have the following Gaussian law:

$$P \circ (W(t) - W(s))^{-1} = N(0, (t-s)Q) \quad \textit{for all} \quad 0 \leqslant s \leqslant t \leqslant T,$$

where $N(0, (t-s)Q)$ is a Gaussian probability measure on U with mean 0 and covariance operator $(t-s)Q$ on U.

In fact, Q is not necessarily of finite trace. In the case that $\mathrm{tr}Q = +\infty$, we will give the definition of cylindrical Wiener processes. Let $U_0 = Q^{\frac{1}{2}}(U)$ and U_1 be an arbitrary Hilbert space such that U_0 is embedded continuously into U_1 and the embedding (denoted by J) is Hilbert–Schmidt. A bounded linear operator $K : U \to H$ is called Hilbert–Schmidt if

$$\sum_{k\in\mathbb{N}} |Ke_k|_H^2 < \infty,$$

where $e_k,\ k \in \mathbb{N}$, is an orthonormal basis of U.

Definition 5.2. *(Cylindrical Wiener processes, see [7, 31]). Let $\tilde{e}_k,\ k \in \mathbb{N}$ be an orthonormal basis of U_0 and $\beta_k,\ k \in \mathbb{N}$, be a family of independent real-valued Brownian motions. The formula*

$$W(t) = \sum_{j=1}^{\infty} \beta_k(t) J\tilde{e}_k, \qquad t \in [0, T],$$

defines a Q_1-Wiener process on U_1 with $\mathrm{tr}Q_1 < +\infty$, where $Q_1 \equiv JJ^*$. The process $W(t),\ t \geqslant 0$, is called a cylindrical Wiener process on U.

Let $C_W([0, T]; H)$ be the space of all continuous mappings $f : [0, T] \to L^2(\Omega, \mathcal{F}, P; H)$ which are adapted to W, that is $f(t)$ is $\mathcal{F}_t$-measurable for any $s \in [0, T]$, where $\mathcal{F}_t$ is the σ-algebra generated by all $\beta_k(s)$ with $s \leqslant t$ and $k \in \mathbb{N}$. Now let us introduce the notion of mild solution.

Definition 5.3. *(Mild solution, see [5, 7, 31]). A stochastic process $X \in C_W([0, T]; H)$ is called a mild solution of problem (3.1) if*

$$X(t) = \mathrm{e}^{tA}x + \int_0^t \mathrm{e}^{(t-s)A} F(X(s))ds + \int_0^t \mathrm{e}^{(t-s)A} B\,\mathrm{d}W(s),$$

where the appearing integrals have to be well defined, and e^{tA} is the strongly continuous semigroup generated by A.

To show the existence and uniqueness of mild solution of problem (3.1), it is convenient to introduce the following assumptions.

Hypothesis 5.4.

(i) $A : \mathcal{D}(A) \subset H \to H$ is the infinitesimal generator of a strongly continuous semigroup e^{tA}.

(ii) $B \in L(U; H)$.

(iii) For any $t > 0$ the linear operator Q_t is of trace class, which is defined as

$$Q_t x = \int_0^t \mathrm{e}^{sA} C\, \mathrm{e}^{sA^*} x ds, \qquad x \in H, \quad t \geqslant 0,$$

where $C = BB^*$, and A^* and B^* are the adjoint operators of A and B respectively.

(iv) There exists $K > 0$ *such that*

$$|F(x) - F(y)|_H \leqslant K|x - y|_H, \qquad x, y \in H.$$

By the Hille–Yosida theorem, there exist $M \geqslant 0$ *and* $w \in \mathbb{R}$ *such that*

$$|||e^{tA}||| \leqslant M\, e^{\omega t}, \qquad t \geqslant 0. \tag{A.1}$$

By theorem 3.2 in [5], equation (3.1) has a unique mild solution $\{X_t\}_{t\geqslant 0}$. Let $\{P_t\}_{t\geqslant 0}$ be the transition semigroup of $\{X_t\}_{t\geqslant 0}$, defined by $P_t f(x) = E[f(X_t)|X_0 = x]$ for any bounded Borel-measurable function f on H. In order to show the existence and uniqueness of invariant probability measure, we need the following additional assumptions:

Hypothesis 5.5.

(i) (5.1) *holds with* $M = 1$.
(ii) $\omega + \kappa < 0$, *where*

$$\kappa \equiv \inf\left\{\frac{\langle F(x) - F(y), x - y\rangle_H}{|x - y|_H^2} : x, y \in H\right\}.$$

It follows from theorem 3.17 in [5] that there exists a unique invariant probability measure for $\{P_t\}_{t\geqslant 0}$, denoted by μ.

A.2. Setting of critical interacting diffusion processes

Let $C(\Xi)$ be the set of all bounded continuous functions on Ξ and $\mathcal{L}(\Xi)$ be the set of Lipschitz continuous functions $f : \Xi \to \mathbb{R}$ satisfying

$$|f(x) - f(y)| \leqslant \sum_{i\in\mathbb{Z}^d} \delta_i(f)|x_i - y_i|,$$

where $\delta(f) = \{\delta_i(f) :\ i \in \mathbb{Z}^d\}$ denotes the oscillation of f:

$$\delta_i(f) \equiv \sup\left\{\frac{|f(x) - f(y)|}{x_i - y_i} : x_i > y_i \text{ and } x_j = y_j \text{ for } j \neq i\right\},$$

and $\|\delta(f)\|_1 \equiv \sum_{i\in\mathbb{Z}^d} \delta_i(f) < \infty$.

On the one hand, for any $f \in C(\Xi)$

$$\int |P_t f|^2\, d\mu \leqslant \int P_t f^2\, d\mu = \int f^2\, d\mu. \tag{A.2}$$

On the other hand, for any $f \in C(\Xi)$, by the dominated convergence theorem,

$$\lim_{t\downarrow 0} \int |P_t f - f|^2\, d\mu = \int \lim_{t\downarrow 0} |P_t f - f|^2\, d\mu = 0. \tag{A.3}$$

Since $C(\Xi)$ is dense in $L^2(\Xi, \mu)$, $\{P_t\}_{t\geqslant 0}$ has a unique extension to a strongly continuous contraction semigroup on $L^2(\Xi, \mu)$ (which is still denoted by $\{P_t\}_{t\geqslant 0}$).

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