Ergodic criterion of a random diffusivity model

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The random diffusivity, initially proposed to explain Brownian yet non-Gaussian diffusion, has garnered significant attention due to its capacity not only for elucidating the internal physical mechanism of non-Gaussian diffusion, but also for establishing an analytical framework to characterize particle motion in complex environments. In this paper, based on the correlation function $\mathcal{C}(t_1, t_2) = \langle D(t_1)D(t_2)\rangle$ of random diffusivity $D(t)$, we quantitatively propose a general criterion of determining the ergodic property of the Langevin equation with the arbitrary random diffusivity $D(t)$. Due to the critical role of correlation function $\mathcal{C}(t_1, t_2)$, we derive the criterion for the two cases with stationary diffusivity or nonstationary diffusivity, respectively. By utilizing the quantitative criterion, we can directly judge the ergodic properties of the random diffusivity model based on the correlation function $\mathcal{C}(t_1, t_2)$ of random diffusivity $D(t)$. Several typical diffusivities, including the common square of the Brownian motion and of the (fractional) Ornstein-Uhlenbeck process, are found to contribute to different ergodic properties, which validates our proposed criterion built on the correlation function $\mathcal{C}(t_1, t_2)$.

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I. INTRODUCTION

Anomalous diffusion is now generally considered to be a more common phenomenon in nature than normal diffusion [1–4]. It has been widely observed in both the microscopic motion of molecules [5–7] and the macroscopic world [8–10]. The essential physical mechanisms as the underlying causes of anomalous diffusion have been widely studied in recent years [11,12], including long-range correlations (the Joseph effect), fat-tailed probability density of increments (the Noah effect), and nonstationarity (the Moses effect) [13]. These different effects lead to deviations from normal diffusion, resulting in anomalous diffusion characterized by the nonlinear evolution of ensemble-averaged mean-squared displacement (EAMSD), i.e.,

$$\langle x^2(t)\rangle \propto t^{\mu}, \tag{1}$$

with the anomalous exponent $\mu \neq 1$ [14,15]. The identification of the effects that give rise to anomalous diffusion holds significant importance, e.g., to determine the system's expansion rate [16], rare event statistics [17,18], and crowding features in the diffusion medium [19–22]. These factors are crucial for analyzing the statistical properties associated with the anomalous diffusion processes.

In complex systems, the long-range correlation of one physical observable, usually characterized by the correlation function $C(t_1, t_2)$, is a common tool for analyzing the anomalous dynamics. Based on the character of the correlation function, the observable can be divided into two categories, namely the stationary process and the nonstationary process. The latter is also known as an aging phenomenon [23]. For stationary processes, its correlation function is a function of the time difference, i.e., $C(t_1, t_2) = \hat{C}(|t_2 - t_1|)$, and the fundamental theorems show that the stationary correlation function $C(t_1, t_2)$ contains some important dynamical information about the physical observables [24]. For example, the fluctuation-dissipation theorem [25] establishes a connection between the correlation function of the observable being studied and the imaginary part of the response function in the frequency domain. The Wiener-Khinchin theorem [26] states that the autocorrelation function of a wide-sense stationary random process has a spectral decomposition given by the corresponding power spectral density. Khinchin's theorem [27] provides the criterion of ergodicity of the process based on the corresponding stationary correlation function. However, the nonstationary correlation function $C(t_1, t_2)$ of the aging system is more difficult to characterize than the stationary one, which complicates the theoretical analyses of the aging system. Based on some specific scaling forms of the nonstationary correlation function, an extension of Khinchin's theorem and the generalized Green-Kubo formula are given in Refs. [28,29].

Recently, a new class of diffusion dynamics, known as the Brownian yet non-Gaussian process with the coexistence of the linear EAMSD and the non-Gaussian probability density function (PDF), has been discovered in a wide variety of complex systems [30–32]. This novel family of diffusion processes has a PDF that is exponentially distributed [33] rather than Gaussian, and a superstatistical technique [34–36] was used to reveal the physical interpretations of the non-Gaussian PDF [37]. After that, Chubynsky and Slater proposed a diffusing diffusivity model with diffusivity undergoing a random walk [38], and Chechkin *et al.* established a minimal model with diffusing diffusivity [39] under the framework of the Langevin equation to explain the PDF's transition from exponential distribution to Gaussian distribution.

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As a generalization of the superstatistical approach, the idea of random diffusivity has been applied to analyze the anomalous diffusion behaviors in complex environments, e.g., generalized gray Brownian motion [40], the generalized Langevin equation [41], and fractional Brownian motion [42,43]. The physical implication of the diffusivity is that it exhibits a gradual change in response to slow environmental variations over an extended timescale [38]. In addition, the ergodic properties of a general Langevin equation,

$$\frac{d}{dt}x(t) = \sqrt{2D(t)}\xi(t), \tag{2}$$

are investigated for superstatistical, uncorrelated, or correlated diffusivity $D(t)$ [44,45], where $x(t)$ represents the position of the particle, and $\xi(t)$ is Gaussian white noise with mean $\langle\xi(t)\rangle = 0$ and correlation function $\langle\xi(t_1)\xi(t_2)\rangle = \delta(t_1 - t_2)$. In particular, the ergodic properties of the random diffusivity model in a harmonic potential have also been investigated [46].

In fact, the discussions in Ref. [44] are concentrated only on several specific categories of diffusivity $D(t)$, without giving a general conclusion on how the diffusivity influences the ergodic properties of the random diffusivity model in Eq. (2). Hence, considering the importance of the correlation function in analyzing the anomalous diffusion in a nonequilibrium system, this paper explores the general criteria of determining the ergodicity of the random diffusivity model in Eq. (2) through the correlation function of diffusivity,

$$\mathcal{C}(t_1, t_2) := \langle D(t_1)D(t_2)\rangle. \tag{3}$$

Based on the explicit form of correlation function $\mathcal{C}(t_1, t_2)$, the diffusivity $D(t)$ is classified into two categories, namely a stationary process and a nonstationary process, in detailed analyses.

To investigate the ergodic property of the anomalous diffusion process, time-averaged mean-squared displacement (TAMSD) is one of the most widely used quantities, precisely defined as [47–49]

$$\overline{\delta^2(\Delta)} = \frac{1}{T-\Delta}\int_0^{T-\Delta}[x(t+\Delta) - x(t)]^2 dt, \tag{4}$$

where the lag time Δ is much smaller than the total measurement time T for obtaining a good statistical property. The system is called ergodic if the TAMSD and EAMSD are equivalent, i.e., $\overline{\delta^2(\Delta)} = \langle x^2(\Delta)\rangle$ as $T \to \infty$, such as Brownian motion and (tempered) fractional Brownian motion [50–52]. The scatter of the amplitude of TAMSD is another main quantity to characterize the ergodic property, which is denoted by $\phi(\eta)$ with the dimensionless random variable η defined as [47,48]

$$\eta := \frac{\overline{\delta^2(\Delta)}}{\langle\overline{\delta^2(\Delta)}\rangle}. \tag{5}$$

The PDF $\phi(\eta)$ and the variance of η [namely, the ergodicity breaking (EB) parameter] are the common indicators to classify numerous anomalous diffusion processes in complex environments.

The structure of this paper is as follows. In Sec. II, we show the expressions of some basis statistics, such as the EAMSD and TAMSD, of the random diffusivity model in Eq. (2). Then we derive the general criteria of determining the ergodicity of the random diffusivity model in Sec. III. By taking three specific types of diffusivity $D(t)$, we verify the general criteria in Sec. IV. Some discussions and summaries are put in Sec. V. Finally, we provide some mathematical details in the Appendixes.

II. STATISTICS OF RANDOM DIFFUSIVITY MODEL

The model studied in this paper is the Langevin equation with random diffusivity $D(t)$ in Eq. (2), based on which some basic quantities have been derived in Ref. [44], such as the EAMSD,

$$\begin{aligned}\langle x^2(t)\rangle &= 2\int_0^t dt_1'\int_0^t dt_2'\langle\sqrt{D(t_1')D(t_2')}\xi(t_1')\xi(t_2')\rangle\\ &= 2\int_0^t dt_1'\int_0^t dt_2'\langle\sqrt{D(t_1')D(t_2')}\rangle\delta(t_1'-t_2')\\ &= 2\int_0^t\langle D(t')\rangle dt',\end{aligned} \tag{6}$$

the correlation function of the displacement $x(t)$,

$$\langle x(t)x(t+\Delta)\rangle = \langle x^2(t)\rangle = 2\int_0^t\langle D(t')\rangle dt', \tag{7}$$

and the ensemble-averaged time-averaged mean-squared displacement (EATAMSD),

$$\begin{aligned}\langle\overline{\delta^2(\Delta)}\rangle &= \frac{1}{T-\Delta}\int_0^{T-\Delta}\langle x^2(t+\Delta)\rangle - \langle x^2(t)\rangle dt\\ &= \frac{2}{T-\Delta}\int_0^{T-\Delta}\int_t^{t+\Delta}\langle D(t')\rangle dt'dt.\end{aligned} \tag{8}$$

Considering the condition $\Delta \ll T$, the EATAMSD exhibits the asymptotic behavior [44]

$$\langle\overline{\delta^2(\Delta)}\rangle \simeq \frac{2\Delta}{T}\int_0^T\langle D(t')\rangle dt' = 2\Delta\langle\overline{D}(T)\rangle, \tag{9}$$

with $\overline{D}(T) := \frac{1}{T}\int_0^T D(t)dt$ representing the time average of diffusivity $D(t)$ throughout the entire observation period $[0, T]$.

It can be found that although the diffusivity $D(t)$ is random in the Langevin equation (2), the basic quantities, such as the EAMSD and EATAMSD, depend only on the mean diffusivity $\langle D(t)\rangle$, rather than the specific distribution of $D(t)$. In other words, taking the EAMSD and EATAMSD as the research objects of the overdamped Langevin equation (2), the random diffusivity with a finite mean would yield the same diffusion behavior as a fixed diffusivity. Therefore, in addition to the EAMSD and EATAMSD, the potential influences of the random diffusivity $D(t)$ would be uncovered through an investigation on more detailed quantities, such as the distribution of the TAMSD or the ergodic properties of the Langevin equation (2). Another view of research on the potential influences of the random diffusivity $D(t)$ is conducted on an underdamped Langevin equation [53,54].

As for the distribution of the TAMSD, an intuitive physical explanation between a random walk and the Langevin equation shows that the number of jumps between a time interval $(t, t+\Delta)$ is in proportion to the integral of diffusivity $2\int_t^{t+\Delta} D(t')dt'$ [44,45]. Considering that the TAMSD has the same distribution as that of the total number of jumps [55] and the corresponding expression of the EATAMSD in Eq. (8), the TAMSD behaves like [44]

$$\overline{\delta^2(\Delta)} \simeq \frac{2}{T-\Delta}\int_0^{T-\Delta}\int_t^{t+\Delta} D(t')dt'dt. \tag{10}$$

Furthermore, considering the condition $\Delta \ll T$, we have a simpler form for TAMSD, i.e. [44],

$$\overline{\delta^2(\Delta)} \simeq \frac{2\Delta}{T}\int_0^T D(t)dt = 2\Delta\overline{D}(T), \tag{11}$$

which is consistent with Eq. (9) by taking the ensemble average on both sides. It can be found that the TAMSD in Eq. (11) depends on the random diffusivity $D(t)$ itself, rather than the mean diffusivity $\langle D(t)\rangle$.

To explicitly evaluate the TAMSD $\overline{\delta^2(\Delta)}$, one can investigate another two common quantities, namely the scatter PDF $\phi(\eta)$ quantifying the stochasticity of TAMSD, and the ergodicity breaking (EB) parameter characterizing the variance of the TAMSD [44,47,48]. For the random diffusivity model in Eq. (2), the scatter PDF $\phi(\eta)$ is the distribution of the dimensionless random variable η,

$$\eta = \frac{\overline{\delta^2(\Delta)}}{\langle\overline{\delta^2(\Delta)}\rangle} \simeq \frac{\overline{D}(T)}{\langle\overline{D}(T)\rangle}, \tag{12}$$

for large T, where the asymptotics can be easily obtained from Eq. (11). Specifically, it holds that $\phi(\eta) = \delta(\eta - 1)$ for an ergodic process, while a nonergodic process has a broad distribution of η. The scatter of TAMSD can be measured by the variance of the dimensionless random variable η, which is also referred to as the EB parameter:

$$\mathrm{EB} = \langle\eta^2\rangle - \langle\eta\rangle^2 = \frac{\langle[\overline{\delta^2(\Delta)}]^2\rangle - \langle\overline{\delta^2(\Delta)}\rangle^2}{\langle\overline{\delta^2(\Delta)}\rangle^2}. \tag{13}$$

By substituting Eq. (12) into Eq. (13) under the condition $\Delta \ll T$, we obtain the EB parameter for the random diffusivity model, i.e.,

$$\mathrm{EB} \simeq \frac{\langle[\overline{D}(T)]^2\rangle - \langle\overline{D}(T)\rangle^2}{\langle\overline{D}(T)\rangle^2}. \tag{14}$$

If the EB parameter tends to zero as $T \to \infty$, then η converges to the distribution $\delta(\eta - 1)$ centering on its mean $\langle\eta\rangle = 1$.

Although Eq. (11) has been obtained in Ref. [44], it only shows several kinds of diffusivity $D(t)$ to verify Eq. (11), without giving a general criterion on diffusivity that shows the kind of property of diffusivity $D(t)$ and how it influences the ergodic properties of the random diffusivity model in Eq. (2). Hence this paper fills this gap by giving such a criterion.

III. ERGODICITY RELATED TO DIFFUSIVITY

Before giving the general ergodicity condition of the random diffusivity model in Eq. (2), we first present a basic hypothesis that

$$\langle D(t)\rangle \gg t^{-1} \tag{15}$$

for large t, which implies that the integral $\int_0^t \langle D(t')\rangle dt'$ increases over t. This hypothesis guarantees the increase of the EAMSD $\langle x^2(t)\rangle$ in Eq. (6). That is to say, the particles keep diffusing even for the large-time limit. Otherwise, the EAMSD converges to a positive constant in Eq. (6) and the EATAMSD converges to zero as $T \to \infty$ in Eq. (9), which yields an obvious ergodicity breaking. In addition, when $D(t)$ recovers to a deterministic function, e.g., a power-law one, $D(t) = t^{\alpha-1}$, then Eq. (2) recovers to the scaled Brownian motion, and the condition $\langle D(t)\rangle \gg t^{-1}$ is equivalent to the assumption $\alpha > 0$ in the discussions of scaled Brownian motion [56–58].

If the random diffusivity model in Eq. (2) is ergodic, then the EAMSD and TAMSD are consistent, i.e., $\langle x^2(\Delta)\rangle \simeq \overline{\delta^2(\Delta)}$ for the large-time limit $T \to \infty$. Based on the results in Sec. II, however, the EAMSD is a deterministic quantity in Eq. (6), while the TAMSD remains a random variable depending on $D(t)$ in Eq. (11). Therefore, the ergodicity implies two equalities: (i) the TAMSD $\overline{\delta^2(\Delta)}$ converges to the EATAMSD as the measurement $T \to \infty$, i.e.,

$$\overline{\delta^2(\Delta)} \simeq \langle\overline{\delta^2(\Delta)}\rangle, \tag{16}$$

and (ii) the EATAMSD should have the same asymptotic behavior as the EAMSD for large lag time Δ, i.e.,

$$\langle\overline{\delta^2(\Delta)}\rangle \simeq \langle x^2(\Delta)\rangle. \tag{17}$$

Let us first check the second equality in Eq. (17). Substituting Eqs. (6) and (9) into Eq. (17) yields

$$\int_0^\Delta \langle D(t)\rangle dt \simeq \Delta\langle\overline{D}(T)\rangle, \tag{18}$$

which can be rewritten as

$$\frac{1}{\Delta}\int_0^\Delta \langle D(t)\rangle dt \simeq \frac{1}{T}\int_0^T \langle D(t)\rangle dt. \tag{19}$$

The asymptotics "$\simeq$" above is for large lag time Δ, large measurement time T, and $\Delta \ll T$. Considering the hypothesis in Eq. (15) that the integral of $\langle D(t)\rangle$ increases over time, L'Hospital's rule can be applied on both sides of Eq. (19), which yields

$$\langle D(\Delta)\rangle \simeq \langle D(T)\rangle. \tag{20}$$

Due to the precondition $\Delta \ll T$ when investigating the TAMSD, Eq. (20) implies that the mean diffusivity $\langle D(t)\rangle$ converges to a constant value for large time.

Compared with the second equality in Eq. (17), the first equality in Eq. (16) implies that the TAMSD $\overline{\delta^2(\Delta)}$ has the property of self-averaging. On the other hand, the asymptotic behavior of the TAMSD $\overline{\delta^2(\Delta)}$ in Eq. (11) implies that $\overline{\delta^2(\Delta)}$ has the same distribution as $\overline{D}(T)$. Therefore, the equivalent condition of Eq. (16) is that the time average of the diffusivity $\overline{D}(T)$ is also self-averaging, which implies the variance of $\overline{D}(T)$ tends to zero, i.e.,

$$\langle\overline{D}(T)^2\rangle \simeq \langle\overline{D}(T)\rangle^2. \tag{21}$$

Similar to the procedure of applying L'Hospital's rule in Eq. (19), it holds that $\langle\overline{D}(T)\rangle \simeq \langle D(T)\rangle$. Hence, Eq. (21) can be rewritten as

$$\langle \overline{D}(T)^2 \rangle \simeq \langle D(T) \rangle^2. \tag{22}$$

Now we have transformed the first equality in Eq. (16) into a direct expression of diffusivity $D(T)$ in Eq. (22). With a careful observation of Eq. (22), the right-hand side depends on the mean diffusivity $\langle D(T)\rangle$, and the left-hand side depends on the correlation function of diffusivity $\mathcal{C}(t_1, t_2)$ defined in Eq. (3). Therefore, the subsequent detailed discussions are divided into two cases, one for stationary diffusivity where the correlation function $\mathcal{C}(t_1, t_2)$ only depends on the time difference $|t_1 - t_2|$, and another for nonstationary diffusivity where $\mathcal{C}(t_1, t_2)$ depends on both t_1 and t_2.

A. Stationary diffusivity

The well-known Khinchin theorem [27] provides a criterion for the ergodicity of a process in terms of the corresponding stationary correlation function. To keep this section self-contained, we present the conclusion of Khinchin's theorem together with some basic notations.

Denote the state of some system as x, representing a general point in the phase space whose dynamics is described by a one-parameter flow $\mathcal{F}_t$. Consider an observable $O(x)$ as a measurable function on the state space, which in time t is $O(\mathcal{F}_t x)$. Then we define the finite-time average of the observable as [28]

$$\overline{O}(x, T) := \frac{1}{T}\int_0^T O(\mathcal{F}_t x)dt, \tag{23}$$

and the ensemble average

$$\langle O\rangle := \int O(x)\mu(dx), \tag{24}$$

where μ is a stationary ensemble measure, as well as the correlation function of the observable $O(x)$ denoted by

$$\mathcal{C}_O(t_1, t_2) := \langle O(\mathcal{F}_{t_1}\cdot)O(\mathcal{F}_{t_2}\cdot)\rangle. \tag{25}$$

Khinchin's theorem [27,28,59] states that if the observable O is a stationary process and its correlation function $\mathcal{C}_O(t_1, t_2)$ is irreversible, i.e., satisfying

$$\lim_{|t_2-t_1|\to\infty} \mathcal{C}_O(t_1, t_2) = \langle O\rangle^2, \tag{26}$$

then the process is ergodic, i.e.,

$$\lim_{T\to\infty} \overline{O}(x, T) = \langle O\rangle, \tag{27}$$

for μ almost every x. Equation (27) demonstrates the existence of the infinite-time limit of the observable O for μ almost every x, and it indicates that the system reaches a steady state for large time.

Let us consider our random diffusivity model in Eq. (2), where $D(t)$ is the quantity we are concerned with when checking Eq. (22). Turning the observable $O(x)$ in Khinchin's theorem to $D(t)$, we get the conclusion that if $D(t)$ is a stationary process, and its correlation function satisfies the irreversible relation

$$\lim_{|t_2-t_1|\to\infty} \mathcal{C}(t_1, t_2) = \lim_{T\to\infty} \langle D(T)\rangle^2, \tag{28}$$

then we can get

$$\overline{D}(T) \simeq \langle D(T)\rangle \tag{29}$$

for large time T. Squaring and taking the ensemble average on both sides of Eq. (29) yields Eq. (22). Note that Khinchin's theorem implies that the mean diffusivity $\langle D(t)\rangle$ on the right-hand side of Eq. (28) tends to a constant, which validates the second equality in Eq. (17). Therefore, based on Khinchin's theorem, when the stationary diffusivity $D(t)$ satisfies Eq. (28), it signifies the presence of ergodic behavior of the random diffusivity model.

B. Nonstationary diffusivity

The second type of diffusivity $D(t)$ is characterized by a nonstationary process, where the correlation function $\mathcal{C}(t_1, t_2)$ depends not only on the lag time $|t_1 - t_2|$, but also on t_1 or t_2. Assuming that $t_1 < t_2$, t_1 is also called the age of the system, and the detailed analyses are commonly conducted under the assumption that the correlation function $\mathcal{C}(t_1, t_2)$ obeys some asymptotic scaling form [28,29].

Here we assume that [29]

$$\mathcal{C}(t_1, t_2) \simeq t_1^{\nu-2}\phi\left(\frac{t_2 - t_1}{t_1}\right) \tag{30}$$

for large t_1, t_2 and $t_1 < t_2$, where the parameter ν and the scaling function $\phi(\cdot)$ vary for different diffusion processes. This scaling form is effective for the majority of the nonstationary process, and based on this scaling form, we can directly calculate the second moment of $\overline{D}(T)$:

$$\begin{aligned}\langle \overline{D}(T)^2\rangle &= \frac{1}{T^2}\int_0^T\int_0^T \mathcal{C}(t_1, t_2)dt_1dt_2\\ &= \frac{2}{T^2}\int_0^T\int_0^{t_2} \mathcal{C}(t_1, t_2)dt_1dt_2\\ &\simeq \frac{2}{T^2}\int_0^T\int_0^{t_2} {t_1}^{\nu-2}\phi\left(\frac{t_2-t_1}{t_1}\right)dt_1dt_2.\end{aligned} \tag{31}$$

After the substitution $(t_1, t_2) \to (s, t_2)$, where $s = \frac{t_2-t_1}{t_1}$, we find the result

$$\begin{aligned}\langle \overline{D}(T)^2\rangle &\simeq \frac{2}{T^2}\int_0^T {t_2}^{\nu-1}dt_2\int_0^{+\infty}(s+1)^{-\nu}\phi(s)ds\\ &= \frac{2T^{\nu-2}}{\nu}\int_0^{+\infty}(s+1)^{-\nu}\phi(s)ds,\end{aligned} \tag{32}$$

where T represents the entire observation time, the scaling function is $\phi(s)$, and the parameter ν can be obtained by comparing the correlation function of a specific diffusivity $D(t)$ with the scaling form in Eq. (30). Now we can determine the condition for Eq. (22) to be established through the correlation function of diffusivity $D(t)$, which is

$$\frac{2T^{\nu-2}}{\nu}\int_0^{+\infty}(s+1)^{-\nu}\phi(s)ds \simeq \langle D(T)\rangle^2. \tag{33}$$

Note that Eq. (33) only guarantees the first equality in Eq. (16), i.e., the TAMSD is self-averaging. Furthermore, considering the second equality in Eq. (17) requires that the mean diffusivity tends to a constant, i.e., the right-hand side of Eq. (33) is a constant. Therefore, for an ergodic process, the left-hand side is also a constant, which implies $\nu = 2$ and the integral $\int_0^{+\infty}(s+1)^{-\nu}\phi(s)ds$ converges. In other words, there is a direct way to identify the nonergodic properties of the random diffusivity model in Eq. (2). By rewriting the correlation function of the diffusivity $D(t)$ into the scaling form as Eq. (30), if $\nu \neq 2$ or the integral $\int_0^{+\infty}(s+1)^{-\nu}\phi(s)ds$ diverges, then Eq. (2) must be nonergodic.

The utilization of Eq. (28) [and Eq. (33)] as a criterion for assessing the ergodicity of a diffusion process in the presence of a stationary (and nonstationary) diffusivity $D(t)$ enables us to directly analyze the impact of the diffusivity's property of particle motion in complex environments. This innovative perspective facilitates the investigation of statistical properties related to particle motion, and it provides insights into the internal physical mechanisms underlying external diffusion behaviors.

IV. SEVERAL SPECIFIC RANDOM DIFFUSIVITIES

In this section, we take several specific stationary and nonstationary diffusivities $D(t)$ to validate the ergodic criterion given in Sec. III. Since the diffusivity $D(t)$ is non-negative in the random diffusivity model, we choose $D(t) = Y^2(t)$, with $Y(t)$ being some common diffusion process, such as the Ornstein-Uhlenbeck (OU) process [39], Brownian motion, and reflected Brownian motion [44]. In particular, to compare with the OU process, which is stationary, we also choose $Y(t)$ to be the nonstationary fractional OU process.

A. $D(t) = Y^2(t)$

The first selected diffusivity is the square of the OU process $D(t) = Y^2(t)$, where the OU process is modeled as [60–62]

$$\frac{dY(t)}{dt} = -\theta Y(t) + \sigma\omega(t), \tag{34}$$

where θ and σ are fixed parameters and $\omega(t)$ is Gaussian white noise. Assuming the initial condition is $Y(0) = 0$, we can solve Eq. (34) through the Laplace transform and obtain

$$Y(t) = \sigma \int_0^t e^{-\theta(t-u)}\omega(u)du. \tag{35}$$

The OU process $Y(t)$ tends to a steady state with a constant second moment, which is also the mean of diffusivity $D(t)$:

$$\langle D(t)\rangle = \langle Y^2(t)\rangle = \frac{\sigma^2}{2\theta}\left(1 - e^{-2\theta t}\right) \simeq \frac{\sigma^2}{2\theta}. \tag{36}$$

In fact, the diffusivity $D(t)$ also tends to be stationary as its second moment also converges to a constant, which can be found from the correlation function of the diffusivity $D(t)$:

$$\mathcal{C}_1(t_1,t_2) = \langle Y^2(t_1)Y^2(t_2)\rangle \simeq \frac{\sigma^4}{4\theta^2}\left(2e^{-2\theta(t_2-t_1)} + 1\right). \tag{37}$$

The detailed calculations are conducted by using Itô's lemma, and they are presented in Appendix A. On the other hand, from Eq. (36) we directly obtain the asymptotic behavior of the square of mean diffusivity,

$$\langle D(t)\rangle^2 \simeq \frac{\sigma^4}{4\theta^2}. \tag{38}$$

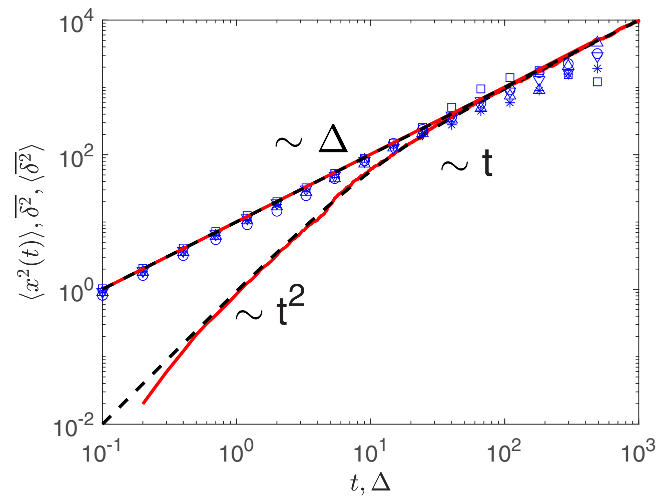

FIG. 1. EAMSD $\langle x^2(t)\rangle$ and EATAMSD $\langle\overline{\delta^2(\Delta)}\rangle$ (red solid lines) as well as five individual time traces $\overline{\delta^2(\Delta)}$ (blue markers) for the random diffusivity model in Eq. (2), plotted vs (lag) time. The physical time t corresponds to EAMSD $\langle x^2(t)\rangle$, while the lag time Δ corresponds to the time averages $\langle\overline{\delta^2(\Delta)}\rangle$ and $\overline{\delta^2(\Delta)}$. The theoretical results for $\langle x^2(t)\rangle$ in Eq. (6) and $\langle\overline{\delta^2(\Delta)}\rangle$ in Eq. (9) are shown by black dashed lines. Both of the theoretical results coincide with the simulated markers when the diffusivity $D(t)$ is taken as the square of the OU process $Y^2(t)$. Other parameters: the measurement time is $T = 10^3$, the number of trajectories used for ensemble is 10^3, and the initial position is $x_0 = 0$.

Combining Eqs. (37) and (38), we find that $D(t)$ is stationary and satisfies the irreversible condition in Eq. (28). Therefore, when the diffusivity is the square of the OU process, i.e., $D(t) = Y^2(t)$ considered in Ref. [39], the random diffusivity model in Eq. (2) is ergodic.

Further, for the stationary diffusivity $D(t)$ in this case, we can still calculate the second moment of $\overline{D}(t)$ with a similar procedure to Eq. (31). By substituting the second moment of $\overline{D}(t)$ and Eq. (38) into Eq. (14), we obtain the EB parameter

$$\mathrm{EB} \simeq \left(\frac{1}{\theta} + \frac{2}{\sigma^2}\right)T^{-1}, \tag{39}$$

which decay to zero at the rate of T^{-1}.

In Fig. 1, we show the simulations of the $\langle x^2(t)\rangle$, $\langle\overline{\delta^2(\Delta)}\rangle$, and five individual time traces $\overline{\delta^2(\Delta)}$ based on the random diffusivity model in Eq. (2) with diffusivity $D(t) = Y^2(t)$, together with the theoretical lines of $\langle x^2(t)\rangle$ and $\langle\overline{\delta^2(\Delta)}\rangle$ obtained by substituting $\langle D(t)\rangle$ into Eqs. (6) and (9). At the large-time limit, the two MSDs, $\langle x^2(t)\rangle$ and $\langle\overline{\delta^2(\Delta)}\rangle$, coincide with each other, and they also overlap with the simulation results. Five individual time traces $\overline{\delta^2(\Delta)}$ coincide with each other when $\Delta \ll T$, which is consistent with the theoretical ergodic behavior of this case. In Fig. 2, we show the corresponding amplitude scatter PDF $\phi(\eta)$. The dimensionless random variable η exhibits a narrow distribution similar to $\delta(\eta - 1)$, which is in accordance with the behavior of the EB parameter decaying to zero as $t \to \infty$. This also suggests that TAMSD is self-averaging and converges to its ensemble average at $T \to \infty$, providing further evidence for the validation of ergodic behavior when $Y(t)$ is an OU process.

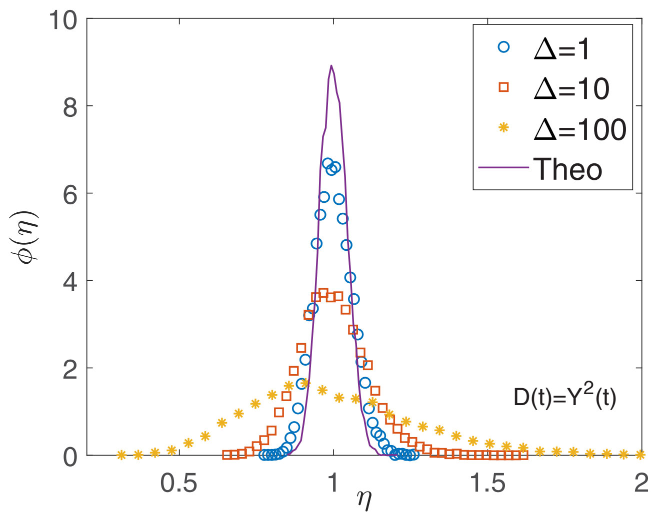

FIG. 2. Amplitude scatter PDF $\phi(\eta)$ for the random diffusivity $D(t)=Y^2(t)$, where $Y(t)$ is an OU process. The markers (circle, square, star) denote the simulations for Δ $(=1, 10, 100)$, respectively. The solid lines are obtained by making simulations directly on the trajectories of diffusivity $D(t)$ based on the theoretical result $\eta\simeq\overline{D(t)}/\langle\overline{D(t)}\rangle$ in Eq. (12). Due to the condition $\Delta\ll T$, the circle markers ($\Delta=1$) are more consistent than the star markers ($\Delta=100$) with the solid lines. Other parameters: the measurement time is $T=10^3$, the number of trajectories used for ensemble is 10^3, and the initial position is $x_0=0$.

B. $D(t)=Y^2(s(t))$

The second diffusivity $D(t)$ is the square of the fractional OU process $D(t)=Y^2(s(t))$, where the fractional OU process $Y(s(t))$ is described as [61]

$$\frac{dY(s)}{ds}=-\theta Y(s)+\sigma\zeta(s),\qquad \frac{dt(s)}{ds}=\tau(s), \tag{40}$$

where $Y(s)$ and $t(s)$ denote the position and time in physical space, and the Gaussian white noise $\zeta(s)$ and fully skewed α-stable $(0<\alpha<1)$ Lévy noise $\tau(s)$ are independent and responsible for the stochastic characters of the process $Y(s(t))$ [63,64]. We are interested in the process $Y(s(t))$, i.e., the evolution of the random variable Y with respect to the physical time t.

For the characterization of the process, we introduce the two-point joint PDFs [1,11]:

$$\begin{aligned} f_1(y_2,s_2;y_1,s_1)&=\langle\delta(y_2-Y(s_2))\delta(y_1-Y(s_1))\rangle,\\ h(s_2,t_2;s_1,t_1)&=\delta(s_2-s(t_2))\delta(s_1-s(t_1))\rangle,\\ f(y_2,t_2;y_1,t_1)&=\langle\delta(y_2-Y(s(t_2)))\delta(y_1-Y(s(t_1)))\rangle,\end{aligned} \tag{41}$$

where $f_1(y_2,s_2;y_1,s_1)$ represents the two-point PDF of the corresponding Markovian process $Y(s)$ defined in Eq. (40), $h(s_2,t_2;s_1,t_1)$ denotes the two-point PDF of the inverse subordinator $s(t)$, and $f(y_2,t_2;y_1,t_1)$ signifies the two-point PDF of the fractional OU process $Y(s(t))$. The last one can be formulated as

$$\begin{aligned} f(y_2,t_2;y_1,t_1)&=\langle\delta(y_2-Y(s_2))\delta(s_2-s(t_2))\\ &\quad\times\delta(y_1-Y(s_1))\delta(s_1-s(t_1))\rangle\\ &=\int_0^\infty\int_0^\infty ds_1ds_2h(s_2,t_2;s_1,t_1)\\ &\quad\times f_1(y_2,s_2;y_1,s_1),\end{aligned} \tag{42}$$

where the two processes $Y(s)$ and $t(s)$ are statistically independent in the relationship above. The Laplace transform ($t_1\leftrightarrow\lambda_1$ and $t_2\leftrightarrow\lambda_2$) of $h(s_2,t_2;s_1,t_1)$ is given by [65]

$$\begin{aligned}\tilde h(s_2,\lambda_2;s_1,\lambda_1)&=\delta(s_2-s_1)\frac{\lambda_1^\alpha-(\lambda_1+\lambda_2)^\alpha+\lambda_2^\alpha}{\lambda_1\lambda_2}\\ &\quad\times e^{-s_1(\lambda_1+\lambda_2)^\alpha}+\Theta(s_2-s_1)\\ &\quad\times\frac{(\lambda_2^\alpha)\big[(\lambda_1+\lambda_2)^\alpha-\lambda_2^\alpha\big]}{\lambda_1\lambda_2}\\ &\quad\times e^{-(\lambda_1+\lambda_2)^\alpha s_1}e^{-\lambda_2^\alpha(s_2-s_1)}+\Theta(s_1-s_2)\\ &\quad\times\frac{(\lambda_1^\alpha)\big[(\lambda_1+\lambda_2)^\alpha-\lambda_1^\alpha\big]}{\lambda_1\lambda_2}\\ &\quad\times e^{-(\lambda_1+\lambda_2)^\alpha s_2}e^{-\lambda_1^\alpha(s_1-s_2)},\end{aligned} \tag{43}$$

where $\Theta(\cdot)$ is the Heaviside step function.

The correlation function of the random diffusivity $D(t)$ is given by

$$\begin{aligned}\mathcal{C}_2(t_1,t_2)&=\langle Y^2(s(t_1))Y^2(s(t_2))\rangle\\ &=\int_0^\infty\int_0^\infty ds_1ds_2\langle Y^2(s_1)Y^2(s_2)\rangle h(s_2,t_2;s_1,t_1),\end{aligned} \tag{44}$$

where $\langle Y^2(s_1)Y^2(s_2)\rangle$ represents the correlation function of the square of the OU process $Y(s)$ and has been obtained in Eq. (37). Then we perform the Laplace transform on both sides, substitute Eqs. (37) and (43) into Eq. (44), and obtain (see Appendix B for the details)

$$\begin{aligned}\mathcal{L}\{\mathcal{C}_2(t_1,t_2)\}&\simeq\frac{\sigma^4}{2\theta^2}\frac{\lambda_1^\alpha}{\lambda_1\lambda_2(\lambda_1+\lambda_2)^\alpha}\\ &\quad+\frac{\sigma^4}{2\theta^2}\frac{\lambda_2^\alpha}{\lambda_1\lambda_2(\lambda_1+\lambda_2)^\alpha}-\frac{\sigma^4}{4\theta^2}\frac{1}{\lambda_1\lambda_2}.\end{aligned} \tag{45}$$

The inverse Laplace transform leads to the result with $t_1<t_2$,

$$\mathcal{C}_2(t_1,t_2)\simeq\frac{\sigma^4}{4\theta^2}+\frac{\sigma^4}{2\theta^2}I\left(\frac{t_1}{t_2};\alpha,1-\alpha\right), \tag{46}$$

where $I(z;\alpha,1-\alpha)$ is the normalized Beta function, defined as

$$I(z;a,b)=\frac{\mathcal{B}(z;a,b)}{\mathcal{B}(a,b)}, \tag{47}$$

and

$$\mathcal{B}(z;a,b)=\int_0^z y^{a-1}(1-y)^{b-1}dy \tag{48}$$

is the incomplete Beta function [66]. The correlation function in Eq. (46) implies that the diffusivity $D(t)$ is a nonstationary process. Therefore, we check the correlation function through the scaling form in Eq. (30), and we find that $\nu = 2$, and

$$\phi(s) = \frac{\sigma^4}{4\theta^2} + \frac{\sigma^4}{2\theta^2} I\left(\frac{1}{1+s}; \alpha, 1-\alpha\right). \tag{49}$$

Substituting the $\phi(s)$ above into Eq. (32) yields the second moment of time-averaged diffusivity $\overline{D}(T)$,

$$\begin{aligned}\langle \overline{D}(T)^2 \rangle &\simeq \int_0^{+\infty} (s+1)^{-2} \phi(s) ds \\ &= \frac{\sigma^4}{4\theta^2} + \frac{\sigma^4}{2\theta^2} \int_0^1 I(z; \alpha, 1-\alpha) dz.\end{aligned} \tag{50}$$

To check the ergodicity condition in Eq. (22), we also need to evaluate the first moment of diffusivity $\langle D(t) \rangle$, which can be expressed by

$$\langle D(t) \rangle = \langle Y^2(s(t)) \rangle = \int_0^{\infty} \langle Y^2(s) \rangle h(s,t) ds. \tag{51}$$

Similar to the two-point PDF $\tilde{h}(s_2, \lambda_2; s_1, \lambda_1)$ in Eq. (43), the single-point PDF in Laplace transform $\tilde{h}(s, \lambda)$ has also been given in Ref. [65]:

$$\tilde{h}(s, \lambda) = \lambda^{\alpha-1} e^{-s\lambda^{\alpha}}. \tag{52}$$

Therefore, performing the Laplace transform on Eq. (51) and utilizing the single-point PDF $\tilde{h}(s, \lambda)$ of inverse subordinator $s(t)$ yield

$$\langle D(T) \rangle \simeq \frac{\sigma^2}{2\theta}. \tag{53}$$

Combining Eqs. (50) and (53), we find

$$\langle \overline{D}(T)^2 \rangle \neq \langle D(T) \rangle^2, \tag{54}$$

which means that the condition in Eq. (33) fails. Therefore, when the diffusivity is the fractional OU process, i.e., $D(t) = Y^2(s(t))$, the random diffusivity model in Eq. (2) is nonergodic. The corresponding EB parameter is

$$\text{EB} \simeq 2 \int_0^1 I(z; \alpha, 1-\alpha) dz, \tag{55}$$

which is a nonzero constant.

We show the simulation of MSDs, the amplitude scatter PDF $\phi(\eta)$, and corresponding EB parameters for the random diffusivity model with diffusivity $D(t) = Y^2(s(t))$ in Figs. 3–6. In Fig. 3, the simulations of EAMSD and EATAMSD deviate in a short time but coincide at a long time, which is consistent with the theoretical results of Eqs. (6) and (9). The five individual time averages $\overline{\delta^2(\Delta)}$ from different trajectories show a near-parallel relationship, which implies the nonergodic behavior of the model, consistent with the conclusion in Eq. (54). On the other hand, the broad distribution of $\phi(\eta)$ in Figs. 4 and 5 and the convergence of the EB parameter to a nonzero constant in Fig. 6 also imply the ergodicity breaking.

The case with the fractional OU process $Y(t)$ provides a stark contrast to the case with the OU process $Y(t)$ discussed in Sec. IV A. More precisely, for the OU process $Y(t)$, the diffusivity $D(t)$ is stationary, and the two equalities in Eqs. (16) and (17) are both valid so that the random diffusivity model is ergodic, while for the fractional OU process $Y(t)$, the

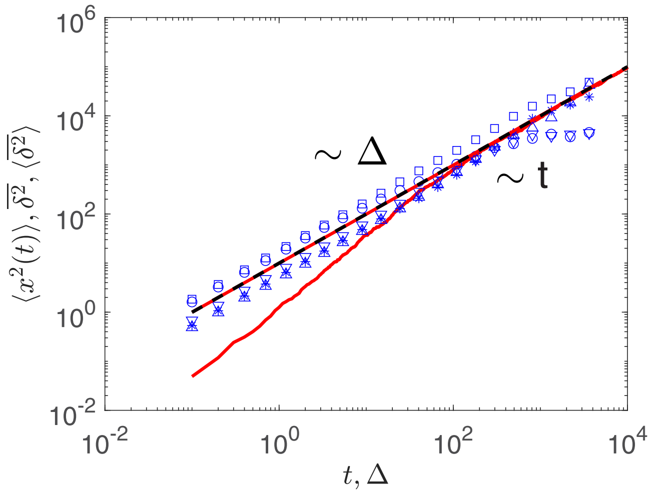

FIG. 3. EAMSD $\langle x^2(t) \rangle$ and EATAMSD $\langle \overline{\delta^2(\Delta)} \rangle$ (red solid lines) as well as five individual time traces $\overline{\delta^2(\Delta)}$ (blue markers) for the random diffusivity model in Eq. (2), plotted vs (lag) time. The physical time t corresponds to EAMSD $\langle x^2(t) \rangle$, while the lag time Δ corresponds to the time averages $\langle \overline{\delta^2(\Delta)} \rangle$ and $\overline{\delta^2(\Delta)}$. The theoretical results for $\langle x^2(t) \rangle$ in Eq. (6) and $\langle \overline{\delta^2(\Delta)} \rangle$ in Eq. (9) are shown by black dashed lines. When the diffusivity $D(t)$ is taken as the square of the fractional OU process $Y^2(s(t))$, the theoretical results of $\langle \overline{\delta^2(\Delta)} \rangle$ coincide with the simulated markers. The long-term consistency between the theoretical value of $\langle x^2(t) \rangle$ and $\langle \overline{\delta^2(\Delta)} \rangle$ corresponds to the tendency to a constant of the mean diffusivity $\langle D(t) \rangle$ in Eq. (53). Other parameters: the measurement time is $T = 10^4$, the number of trajectories used for ensemble is 10^3, and the initial position is $x_0 = 0$.

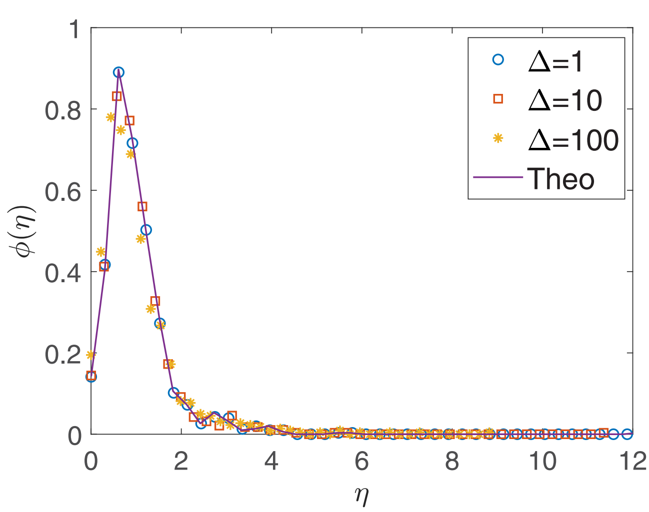

FIG. 4. Amplitude scatter PDF $\phi(\eta)$ for diffusing diffusivity: $D(t) = Y^2(s(t))$, where $Y(s(t))$ is the fractional OU process. The markers (circle, square, star) denote the simulations for Δ (= 1, 10, 100), respectively. The solid lines are obtained by making simulations directly on the trajectories of diffusivity $D(t)$ based on the theoretical result $\eta \simeq \overline{D(t)}/\langle \overline{D(t)} \rangle$ in Eq. (12). Due to the condition $\Delta \ll T$, the circle markers ($\Delta = 1$) are more consistent than the star markers ($\Delta = 100$) with the solid lines. Other parameters: the measurement time is $T = 10^3$, the number of trajectories used for ensemble is 10^3, and the initial position is $x_0 = 0$.

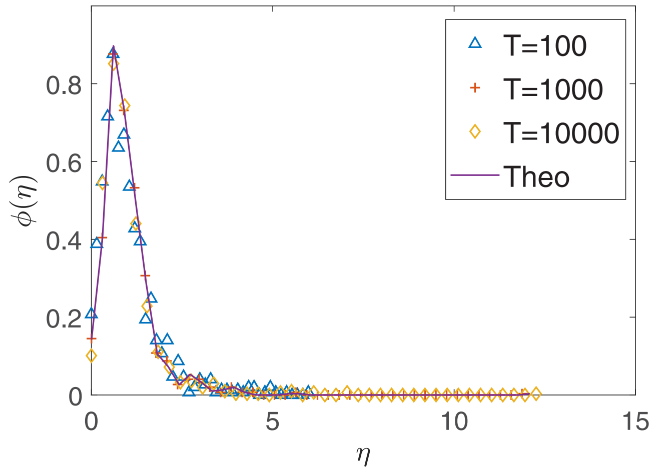

FIG. 5. Amplitude scatter PDF $\phi(\eta)$ for diffusing diffusivity: $D(t) = Y^2(s(t))$, where $Y(s(t))$ is the fractional OU process. The markers (triangle, cross, rhombus) denote the simulations for T (= 100, 10 000, 10 000), respectively. The solid lines are obtained by making simulations directly on the trajectories of diffusivity $D(t)$ based on the theoretical result $\eta \simeq \overline{D(t)}/\langle \overline{D(t)}\rangle$ in Eq. (12). Other parameters: the lag time is $\Delta = 1$, the number of trajectories used for ensemble is 10^3, and the initial position is $x_0 = 0$.

diffusivity $D(t)$ is nonstationary. The mean diffusivity tends to a constant in Eq. (53), which guarantees the second equality in Eq. (17). However, the condition in Eq. (33) fails so that the first equality in Eq. (16) breaks. Thus the TAMSD is not self-averaging even for large measurement time T, and the random diffusivity model is nonergodic.

C. $D(t) = |B(t)|$ and $D(t) = B^2(t)$

The last category of diffusivity $D(t)$ is the reflected Brownian motion [67–69] and the squared of Brownian motion [70–72]. Since the standard Brownian motion $B(t)$ has stationary and independent increments, the two-point joint PDF of $(B(t_1), B(t_2))$ is

$$g(x_2, t_2; x_1, t_1) = p(x_1, t_1)p(x_2 - x_1, t_2 - t_1) \tag{56}$$

for $t_1 < t_2$, where

$$p(x;t) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{x^2}{2t}\right). \tag{57}$$

When diffusivity $D(t)$ is the reflected Brownian motion, i.e., $D(t) = |B(t)|$, based on Eq. (56), we get the correlation function

$$\begin{aligned}\mathcal{C}_3(t_1, t_2) &= \langle |B(t_1)B(t_2)| \rangle \\ &= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} |x_1 x_2| g(x_2, t_2; x_1, t_1)dx_1 dx_2 \\ &= \frac{2t_1}{\pi}\left[\sqrt{\frac{t_2 - t_1}{t_1}} + \operatorname{arccot}\left(\sqrt{\frac{t_2 - t_1}{t_1}}\right)\right],\end{aligned} \tag{58}$$

which indicates that $\nu = 3$ in Eq. (30) and

$$\phi(s) = \frac{2}{\pi}(\sqrt{s} + \operatorname{arccot}(\sqrt{s})). \tag{59}$$

Then we substitute ν and $\phi(s)$ into Eq. (32), and we obtain the second moment of $\overline{D}(T)$, i.e.,

$$\langle \overline{D}(T)^2 \rangle = \frac{2T}{3}\int_0^{+\infty}(s+1)^{-3}\phi(s)ds = \frac{3T}{8}. \tag{60}$$

On the other hand, based on Eq. (57), the first moment of diffusivity $D(t)$ is

$$\langle D(T) \rangle = \langle |B(T)| \rangle = \sqrt{\frac{2T}{\pi}}, \tag{61}$$

which implies that

$$\langle \overline{D}(T)^2 \rangle \neq \langle D(T) \rangle^2. \tag{62}$$

Consequently, when $D(t) = |B(t)|$, the random diffusivity model in Eq. (2) is nonergodic. The corresponding EB parameter can also be obtained as

$$\mathrm{EB} = \frac{27\pi}{64} - 1. \tag{63}$$

Similarly, when the diffusivity $D(t)$ is the square of Brownian motion, i.e., $D(t) = B^2(t)$, by assuming $t_1 < t_2$ and using the independent and stationary increments of Brownian motion $B(t)$, we have

$$\begin{aligned}\mathcal{C}_4(t_1, t_2) &= \langle B^2(t_1)B^2(t_2) \rangle \\ &= \langle B^2(t_1)[B(t_2) - B(t_1) + B(t_1)]^2 \rangle \\ &= \langle B^4(t_1) + B^2(t_1)[B(t_2) - B(t_1)]^2 \rangle \\ &= 2t_1^2 + t_1 t_2,\end{aligned} \tag{64}$$

which indicates that diffusivity $D(t)$ is a nonstationary process. From the asymptotic scaling form of Eq. (30), we can get $\nu = 4$ and

$$\phi(s) = 3 + s. \tag{65}$$

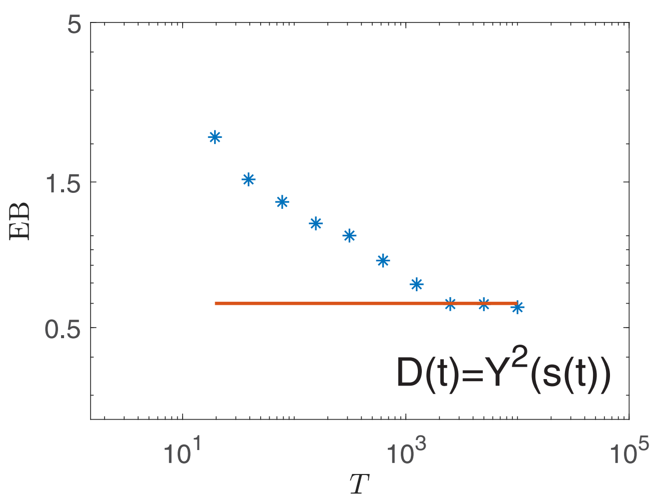

FIG. 6. EB parameter vs entire observation time T with diffusivity $D(t) = Y^2(s(t))$. The star markers converge to a nonzero constant for a long time, and this constant agrees with the theoretical result in Eq. (55). Other parameters: the lag time is $\Delta = 1$, the number of trajectories used for ensemble is 10^4, and the initial position is $x_0 = 0$.

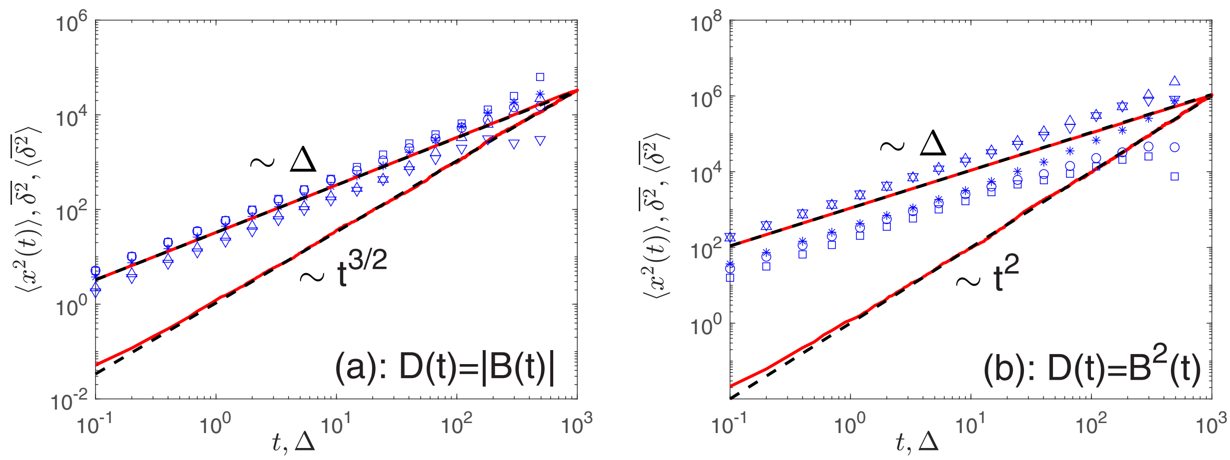

FIG. 7. EAMSD $\langle x^2(t)\rangle$ and EATAMSD $\langle\overline{\delta^2(\Delta)}\rangle$ (red solid lines) as well as five individual time traces $\overline{\delta^2(\Delta)}$ (blue markers) for the random diffusivity model in Eq. (2), plotted vs (lag) time. The physical time t corresponds to EAMSD $\langle x^2(t)\rangle$, while the lag time Δ corresponds to the time averages $\langle\overline{\delta^2(\Delta)}\rangle$ and $\overline{\delta^2}(\Delta)$. The theoretical results for $\langle x^2(t)\rangle$ in Eq. (6) and $\langle\overline{\delta^2(\Delta)}\rangle$ in Eq. (9) are shown by black dashed lines. Both of these theoretical results coincide with the simulated values when the diffusivity $D(t)$ is taken as $|B(t)|$ in (a) and $B^2(t)$ in (b), where $B(t)$ is the Brownian motion. Other parameters: the measurement time is $T = 10^3$, the number of trajectories used for ensemble is 10^3, and the initial position is $x_0 = 0$.

Substituting the above results into Eq. (32) yields

$$\langle\overline{D}(T)^2\rangle = \frac{T^2}{2}\int_0^{+\infty}(s+1)^{-4}\phi(s)ds = \frac{7T^2}{12}. \tag{66}$$

However, the first moment of $D(T)$ is

$$\langle D(T)\rangle = \langle B^2(T)\rangle = T, \tag{67}$$

which also shows that $\langle\overline{D}(T)^2\rangle \neq \langle D(T)\rangle^2$. Therefore, the random diffusivity model in Eq. (2) with the diffusivity $D(t) = B^2(t)$ is also nonergodic. The corresponding EB parameter is also nonzero, which is

$$\mathrm{EB} = \tfrac{4}{3}. \tag{68}$$

We show the simulation of MSDs, the amplitude scatter PDF $\phi(\eta)$, and the EB parameters for the random diffusivity model with diffusivity $D(t) = |B(t)|$ [in (a)] and $D(t) = B^2(t)$ [in (b)] in Figs. 7–10, respectively. In Fig. 7, the discrepancy between the EAMSD and TAMSD implies nonergodic behavior. Furthermore, the five individual times $\overline{\delta^2(\Delta)}$ in both (a) and (b) remain parallel for $\Delta \ll T$, which indicates that the TAMSD is not self-averaging and has a broad distribution, as shown in Figs. 8 and 9. The theoretical lines in Figs. 8 and 9 are obtained by using Eq. (12) and making simulations directly on the trajectories of diffusivity $D(t)$ without simulating the Langevin equation (2). In Fig. 10, the EB parameter tends towards nonzero constants as $T \to \infty$, thereby corroborating the findings of the broad distribution $\phi(\eta)$ in Figs. 8 and 9.

Although the direct way of finding the ergodicity breaking of the random diffusivity model in Eq. (2), i.e., whether the parameter ν is equal to 2, can be applied for the cases $D(t) = |B(t)|$ and $D(t) = B^2(t)$, we evaluate all the related quantities, including the second moment of $\overline{D}(T)$, mean diffusivity $\langle D(T)\rangle$, and EB parameter for a comprehensive understanding of the diffusion behavior of the diffusivity $D(t)$. It can be found that $\nu \neq 2$, and the mean diffusivity $\langle D(T)\rangle$ does not tend to a constant for both cases here, which implies that neither of the two equalities in Eqs. (16) and (17) works, in contrast with the examples in Secs. IV A and IV B.

In addition to the MSDs analyzed above, we show some sample trajectories with four kinds of diffusivities $D(t)$ in Fig. 11 to enhance the intuitive understanding of the random diffusivity processes. Based on the mean diffusivity $\langle D(t)\rangle$ in Eqs. (36), (53), (61), and (67), the larger $\langle D(t)\rangle$ implies greater fluctuations, which can be found by comparing the vertical coordinates of the four graphs in Fig. 11. Although the trajectories exhibit similar fluctuations in (a) and (b) resulting from the same value of $\langle D(t)\rangle$, some segments of the trajectories in (b) are almost flat due to the presence of the inverse subordinate $s(t)$ in the fractional OU process $Y(s(t))$.

V. CONCLUSION

The application of random diffusivity $D(t)$ to the physical models describing the particle's motion in complex systems offers us a broader perspective for comprehending stochastic dynamics. When investigating the ergodic property of the random diffusivity model in Eq. (2), we found that the EAMSD and EATAMSD depend only on the mean diffusivity $\langle D(t)\rangle$, and the specific distribution of $D(t)$ might determine the distribution of the TAMSD in Refs. [44,45]. Therefore, for a deeper examination of the ergodic property of the random diffusivity processes, we propose in this paper a general ergodic criterion for determining the ergodic property of the Langevin equation with an arbitrary random diffusivity $D(t)$.

Since the ergodicity implies consistency between the EAMSD and TAMSD, i.e., $\langle x^2(\Delta)\rangle \simeq \overline{\delta^2(\Delta)}$, both equalities in Eqs. (16) and (17) should be satisfied. The same diffusion behavior of the EAMSD and EATAMSD in Eq. (17) is found to be equivalent to the tendency to zero of the mean diffusivity $\langle D(t)\rangle$ in Eq. (20). As for Eq. (16), which implies the self-averaging property of the TAMSD, it is not easy to interpret directly. Inspired by Khinchin's theorem, which provides

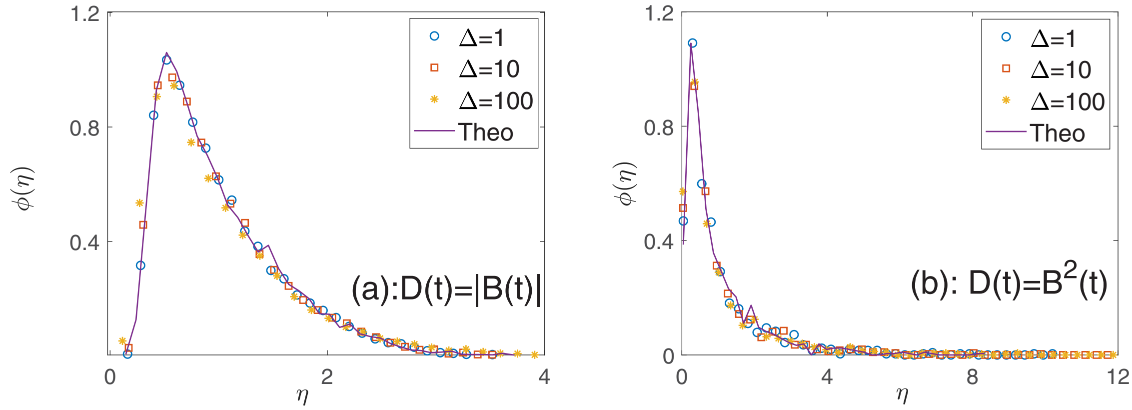

FIG. 8. Amplitude scatter PDF $\phi(\eta)$ for two kinds of diffusivity: the diffusivity $D(t)$ is taken as $|B(t)|$ in (a) and $B^2(t)$ in (b), where $B(t)$ is the Brownian motion. The markers (circle, square, star) denote the simulations for Δ (= 1, 10, 100), respectively. The solid lines are obtained by making simulations directly on the trajectories of diffusivity $D(t)$ based on the theoretical result $\eta \simeq \overline{D(t)}/\langle\overline{D(t)}\rangle$ in Eq. (12). Due to the condition $\Delta \ll T$, the circle markers ($\Delta = 1$) are more consistent than the star markers ($\Delta = 100$) with the solid lines. Other parameters: the measurement time is $T = 10^3$, the number of trajectories used for ensemble is 10^3, and the initial position is $x_0 = 0$.

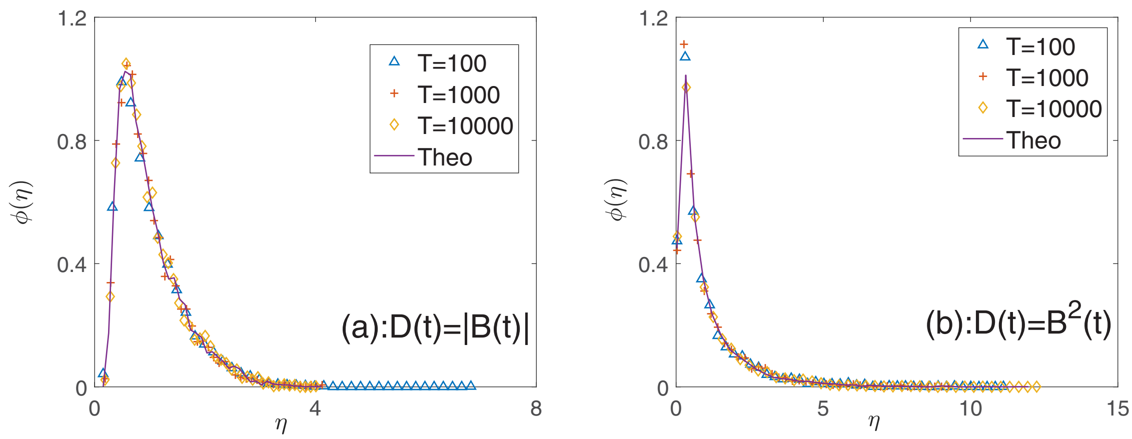

FIG. 9. Amplitude scatter PDF $\phi(\eta)$ for two kinds of diffusivity: the diffusivity $D(t)$ is taken as $|B(t)|$ in (a) and $B^2(t)$ in (b), where $B(t)$ is the Brownian motion. The markers (triangle, cross, rhombus) denote the simulations for T (= 100, 10 000, 10 000), respectively. The solid lines are obtained by making simulations directly on the trajectories of diffusivity $D(t)$ based on the theoretical result $\eta \simeq \overline{D(t)}/\langle\overline{D(t)}\rangle$ in Eq. (12). Other parameters: the lag time is $\Delta = 1$, the number of trajectories used for ensemble is 10^3, and the initial position is $x_0 = 0$.

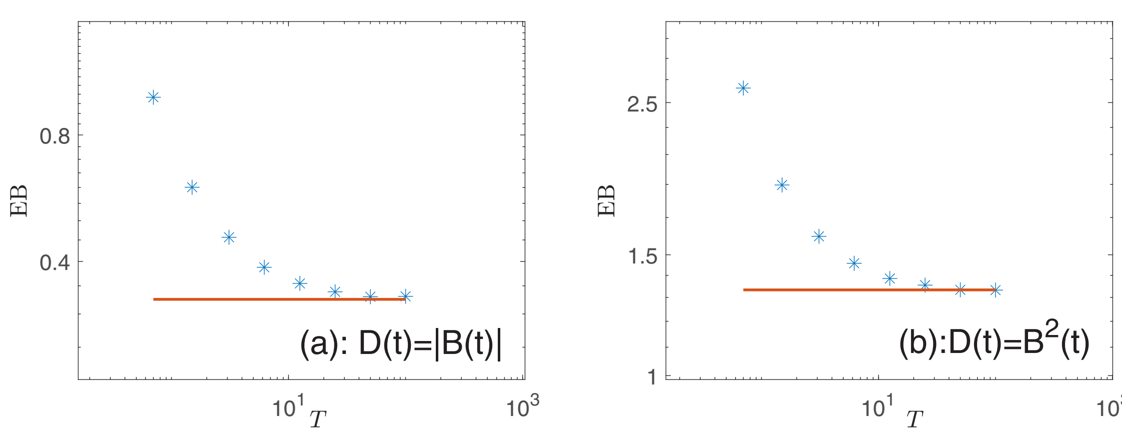

FIG. 10. EB parameter vs entire observation time T with two kinds of diffusivity: $D(t) = |B(t)|$ in (a) and $D(t) = B^2(t)$ in (b). Instead of decaying to zero, the star markers converge to a constant for a long time. This constant agrees with the theoretical result in Eq. (63) in (a) and Eq. (68) in (b). Other parameters: the lag time is $\Delta = 1$, the number of trajectories used for ensemble is 10^4, and the initial position is $x_0 = 0$.

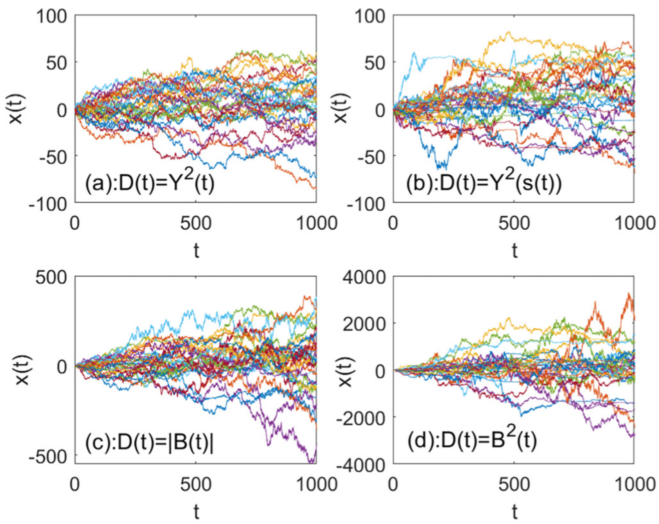

FIG. 11. Sample trajectories with different diffusivity $D(t)$, which is $Y^2(t)$ in (a), $Y^2(s(t))$ in (b), $|B(t)|$ in (c), and $B^2(t)$ in (d). Here, $Y(t)$ is the OU process, $Y(s(t))$ is the fractional OU process, and $B(t)$ is the Brownian motion. Other parameters: the measurement time is $T = 10^3$, the number of trajectories in each graph is 30, and the initial position is $x_0 = 0$.

the criterion of ergodicity based on the stationary correlation function of the concerned observable, we find the correlation function $\mathcal{C}(t_1, t_2)$ of the diffusivity $D(t)$ plays the dominating role in the statistical property of the TAMSD in the random diffusivity model. Therefore, the detailed theoretical analyses are divided into two cases distinguished by whether the diffusivity $D(t)$ is stationary or not. Further, we propose the criteria in Eq. (28) for the stationary diffusivity and in Eq. (33) for the nonstationary diffusivity, respectively.

To verify our proposed criteria, we choose three categories of diffusivity $D(t)$ in Sec. IV: the two equalities in Eqs. (16) and (17) are satisfied and the system is ergodic in Sec. IV A, the second equality is satisfied but the first equality fails so that the system is nonergodic in Sec. IV B, and both equalities fails and the system is obviously nonergodic in Sec. IV C. The separate discussions of the two equalities and the carefully selected examples help us to understand more thoroughly the statistical property of the TAMSD. Actually, we have omitted another typical anomalous diffusion process, namely scaled Brownian motion with a deterministic diffusivity $D(t) = t^{\alpha-1}$. The investigation of the ergodic property of the scaled Brownian motion implies that the first equality is satisfied but the second equality fails for $\alpha \neq 1$ [44,56–58]. Since this paper aims to propose the general criterion of the ergodic property for arbitrary random diffusivity $D(t)$, we omit the example of scaled Brownian motion in Sec. IV.

For the nonergodic cases in Sec. IV, the TAMSD is not self-averaging and it has a broad distribution $\phi(\eta)$, which shows a great similarity with the heterogeneous diffusion processes with a space-dependent diffusivity $D(x)$ discussed in Ref. [73]. This might reveal some commonalities of the anomalous diffusion phenomena in complex heterogenous environments. In addition, since the value of the diffusivity $D(t)$ can be regarded as the degree of diffusion at a physical time t, the results in this paper are also instructive in the investigation of the ergodic properties of correlated random walks where the correlation of the jump lengths can be characterized similarly to $C(t_1, t_2) = \langle D(t_1)D(t_2)\rangle$ here.

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APPENDIX A: THE CORRELATION FUNCTION OF $Y^2(t)$ IN EQ. (37)

Following Eq. (35), $Y(t)$ can be rewritten as

$$Y(t) = \sigma \int_0^t e^{-\theta(t-u)}\omega(u)du := \sigma e^{-\theta t} Z(t). \tag{A1}$$

Based on Eq. (A1), we can calculate the moments of $Y(t)$ as

$$\langle Y(t)\rangle = 0, \quad \langle Y^2(t)\rangle = \frac{\sigma^2}{2\theta}(1 - e^{-2\theta t}). \tag{A2}$$

So the correlation function of $Y^2(t)$ when $t < s$ is

$$\begin{aligned}
\langle Y^2(t)Y^2(s)\rangle &= \sigma^4 e^{-2\theta(t+s)}\langle Z^2(t)Z^2(s)\rangle \\
&= \sigma^4 e^{-2\theta(t+s)}\langle Z^2(t)[Z(s) - Z(t) + Z(t)]^2\rangle \\
&= \sigma^4 e^{-2\theta(t+s)}(\langle Z^4(t)\rangle + 2\langle Z^3(t)[Z(s) - Z(t)]\rangle + \langle Z^2(t)[Z(s) - Z(t)]^2\rangle) \\
&= \sigma^4 e^{-2\theta(t+s)}(\langle Z^4(t)\rangle + \langle Z^2(t)\rangle\langle [Z(s) - Z(t)]^2\rangle) \\
&= \sigma^4 e^{-2\theta(t+s)}\left(\left\langle\left(\int_0^t e^{\theta u}\omega(u)du\right)^4\right\rangle + \left\langle\left(\int_0^t e^{\theta u}\omega(u)du\right)^2\right\rangle\left\langle\left(\int_t^s e^{\theta v}\omega(v)dv\right)^2\right\rangle\right).
\end{aligned} \tag{A3}$$

To simplify the calculation, we define $I_t = \int_0^t e^{\theta u}\omega(u)du$. From Itô's lemma, we can get

$$d\left(I_t^4\right) = 4I_t^3 e^{\theta t}\omega(t)dt + 6I_t^2 e^{2\theta t}dt, \tag{A4}$$

and then we know

$$\begin{aligned}\left\langle\left(\int_0^t e^{\theta u}\omega(u)du\right)^4\right\rangle = \left\langle\int_0^t d\left(I_t^4\right)\right\rangle = \left\langle\int_0^t 4I_u^3 e^{\theta u}\omega(u)du\right\rangle + \left\langle\int_0^t 6I_u^2 e^{2\theta u}du\right\rangle \\ = 6\int_0^t \langle I_u^2\rangle e^{2\theta u}du \\ = 6\int_0^t \frac{(e^{2\theta u}-1)}{2\theta}e^{2\theta u}du \\ = \frac{3e^{4\theta t}}{4\theta^2} - \frac{3e^{2\theta t}}{2\theta^2} + \frac{3}{4\theta^2}.\end{aligned} \tag{A5}$$

For the other one, we can directly calculate

$$\left\langle\left(\int_0^t e^{\theta u}\omega(u)du\right)^2\right\rangle\left\langle\left(\int_t^s e^{\theta v}\omega(v)dv\right)^2\right\rangle = \int_0^t e^{2\theta u}du\int_t^s e^{2\theta v}dv = \frac{(e^{2\theta t}-1)}{2\theta}\frac{(e^{2\theta s}-e^{2\theta t})}{2\theta}. \tag{A6}$$

Combining the results of Eq. (A5) and (A6), we can get the value of Eq. (A3):

$$\begin{aligned}\langle Y^2(t)Y^2(s)\rangle &= \sigma^4 e^{-2\theta(t+s)}\left(\frac{3e^{4\theta t}}{4\theta^2} - \frac{3e^{2\theta t}}{2\theta^2} + \frac{3}{4\theta^2} + \frac{(e^{2\theta t}-1)}{2\theta}\frac{(e^{2\theta s}-e^{2\theta t})}{2\theta}\right) \\ &= \frac{\sigma^4}{4\theta^2}(1 - e^{-2\theta t} - 5e^{-2\theta s} + 2e^{-2\theta(s-t)} + 3e^{-2\theta(t+s)}) \simeq \frac{\sigma^4}{4\theta^2}(1 + 2e^{-2\theta(s-t)})\end{aligned} \tag{A7}$$

for large t and s.

APPENDIX B: THE CORRELATION FUNCTION OF $Y^2(s(t))$ IN EQ. (45)

Based on Eq. (A7) in the case of the OU process $Y(t)$, we can write the correlation function of the square of the OU process $Y(s)$ as

$$\langle Y^2(s_1)Y^2(s_2)\rangle = \frac{\sigma^4}{4\theta^2}\left(1 - e^{-2\theta s_1} - 5e^{-2\theta s_2} + 2e^{-2\theta|s_2-s_1|} + 3e^{-2\theta(s_1+s_2)}\right). \tag{B1}$$

Then we combine Eqs. (43) and (B1) and get the correlation function of the square of the fractional OU process $Y(s(t))$ in Laplace space as

$$\begin{aligned}\mathcal{L}\{\langle Y^2(t_1)Y^2(t_2)\rangle\} &= \int_0^\infty\int_0^\infty \tilde{h}(s_2,\lambda_2;s_1,\lambda_1)\langle Y^2(s_1)Y^2(s_2)\rangle ds_1 ds_2 \\ &= \frac{3\sigma^4}{4\theta^2}\frac{\left[\lambda_1^\alpha - (\lambda_1+\lambda_2)^\alpha + \lambda_2^\alpha\right]}{\lambda_1\lambda_2}\left[\frac{1}{(\lambda_1+\lambda_2)^\alpha} - \frac{2}{2\theta+(\lambda_1+\lambda_2)^\alpha} + \frac{1}{4\theta+(\lambda_1+\lambda_2)^\alpha}\right] \\ &\quad + \frac{\sigma^4}{4\theta^2}\frac{\left(\lambda_2^\alpha\right)\left[(\lambda_1+\lambda_2)^\alpha - \lambda_2^\alpha\right]}{\lambda_1\lambda_2}\left[\frac{1}{\lambda_2^\alpha-(\lambda_1+\lambda_2)^\alpha}\left(\frac{1}{(\lambda_1+\lambda_2)^\alpha} - \frac{1}{\lambda_2^\alpha} - \frac{5}{2\theta+(\lambda_1+\lambda_2)^\alpha} + \frac{5}{2\theta+\lambda_2^\alpha}\right)\right. \\ &\quad - \frac{1}{\lambda_2^\alpha-2\theta-(\lambda_1+\lambda_2)^\alpha}\left(\frac{1}{2\theta+(\lambda_1+\lambda_2)^\alpha} - \frac{1}{\lambda_2^\alpha}\right) + \frac{2}{\lambda_2^\alpha+2\theta-(\lambda_1+\lambda_2)^\alpha}\left(\frac{1}{(\lambda_1+\lambda_2)^\alpha} - \frac{1}{2\theta+\lambda_2^\alpha}\right) \\ &\quad \left. + \frac{3}{\lambda_2^\alpha-2\theta-(\lambda_1+\lambda_2)^\alpha}\left(\frac{1}{4\theta+(\lambda_1+\lambda_2)^\alpha} - \frac{1}{2\theta+\lambda_2^\alpha}\right)\right] \\ &\quad + \frac{\sigma^4}{4\theta^2}\frac{\left(\lambda_1^\alpha\right)\left[(\lambda_1+\lambda_2)^\alpha - \lambda_1^\alpha\right]}{\lambda_1\lambda_2}\left[\frac{1}{\lambda_1^\alpha-(\lambda_1+\lambda_2)^\alpha}\left(\frac{1}{(\lambda_1+\lambda_2)^\alpha} - \frac{1}{\lambda_1^\alpha} - \frac{5}{2\theta+(\lambda_1+\lambda_2)^\alpha} + \frac{5}{2\theta+\lambda_1^\alpha}\right)\right. \\ &\quad - \frac{1}{\lambda_1^\alpha-2\theta-(\lambda_1+\lambda_2)^\alpha}\left(\frac{1}{2\theta+(\lambda_1+\lambda_2)^\alpha} - \frac{1}{\lambda_1^\alpha}\right) + \frac{2}{\lambda_1^\alpha+2\theta-(\lambda_1+\lambda_2)^\alpha}\left(\frac{1}{(\lambda_1+\lambda_2)^\alpha} - \frac{1}{2\theta+\lambda_1^\alpha}\right) \\ &\quad \left. + \frac{3}{\lambda_1^\alpha-2\theta-(\lambda_1+\lambda_2)^\alpha}\left(\frac{1}{4\theta+(\lambda_1+\lambda_2)^\alpha} - \frac{1}{2\theta+\lambda_1^\alpha}\right)\right].\end{aligned} \tag{B2}$$

Considering the asymptotic behavior $\lambda_1, \lambda_2 \to 0$ and keeping the leading terms yields

$$\begin{aligned}\mathcal{L}\{\langle Y^2(t_1)Y^2(t_2)\rangle\} &\simeq \frac{3\sigma^4}{4\theta^2}\frac{\left[\lambda_1^\alpha-(\lambda_1+\lambda_2)^\alpha+\lambda_2^\alpha\right]}{\lambda_1\lambda_2}\frac{1}{(\lambda_1+\lambda_2)^\alpha}\\ &\quad+\frac{\sigma^4}{4\theta^2}\frac{\lambda_2^\alpha}{\lambda_1\lambda_2}\left(\frac{1}{\lambda_2^\alpha}-\frac{1}{(\lambda_1+\lambda_2)^\alpha}\right)+\frac{\sigma^4}{4\theta^2}\frac{\lambda_1^\alpha}{\lambda_1\lambda_2}\left(\frac{1}{\lambda_1^\alpha}-\frac{1}{(\lambda_1+\lambda_2)^\alpha}\right)\\ &=\frac{\sigma^4}{2\theta^2}\frac{\lambda_1^\alpha}{\lambda_1\lambda_2(\lambda_1+\lambda_2)^\alpha}+\frac{\sigma^4}{2\theta^2}\frac{\lambda_2^\alpha}{\lambda_1\lambda_2(\lambda_1+\lambda_2)^\alpha}-\frac{\sigma^4}{4\theta^2}\frac{1}{\lambda_1\lambda_2}.\end{aligned}\tag{B3}$$

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