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PAPER

Heterogeneous diffusion in an harmonic potential: the role of the interpretation

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Abstract

Diffusion in heterogeneous energy and diffusivity landscapes is widespread in biological systems. However, solving the Langevin equation in such environments introduces ambiguity due to the interpretation parameter α, which depends on the underlying physics and can take values in the range $0 < \alpha < 1$. The typical interpretations are Itô ($\alpha = 0$), Stratonovich ($\alpha = 1/2$), and Hänggi-Klimontovich (HK) ($\alpha = 1$). Here, we analyse the motion of a particle in an harmonic potential—modelled as an Ornstein–Uhlenbeck process—with diffusivity that varies in space. Our focus is on two-phase systems with a discontinuity in environmental properties at $x = 0$. We derive the probability density of the particle position for the process, and consider two paradigmatic situations. In the first one, the damping coefficient remains constant, and fluctuation-dissipation relations are not satisfied. In the second one, these relations are enforced, leading to a position-dependent damping coefficient. In both cases, we provide solutions as a function of the interpretation parameter α, with particular attention to the Itô, Stratonovich, and HK interpretations, revealing fundamentally different behaviours, in particular with respect to an interface located at the potential minimum.

1. Introduction

Understanding the erratic motion of a particle in complex environments is a problem that has attracted a great deal of attention over the last decade [1]. One of the typical tools used to study the diffusion of particles is the Langevin equation, where the interaction between the particle of interest and the environment is modelled via a random force [2–4]. The Langevin description can naturally incorporate an external force acting on the tracer particle. A key distinction between the random and external forces lies in their timescales: the random force arises from rapid molecular collisions and fluctuates on very short timescales, while the external force is typically deterministic and varies more slowly. Of particular interest is the case of a particle subjected to a restoring force, as that produced by optical [5–8] and magnetic tweezers [9–11], and tethered particle motion [12–14]. The stochastic process that describes the motion of a Brownian particle in such a trapping potential is known as the Ornstein–Uhlenbeck (OU) process [15–17]. This process is also widespread beyond single-molecule biophysics and it is applied, for example, in finance [18, 19], evolution [20], and chemical kinetics [21].

The Langevin equation provides a framework for modelling the diffusion of particles in complex, heterogeneous media. In such environments, the strength of the random force may be time- [22–24] and/or space-dependent [25–34], as opposed to being constant. The solution of the Langevin equation involves a stochastic integral, which is well-defined if the strength of the random force is constant or depends solely on time [35]. However, when the strength depends on the position, the stochastic integral becomes ill-defined

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due to the extra freedom in choosing how to evaluate the noise at each infinitesimal random increment [26, 32, 35–42]. To address this issue, a rule (interpretation) must be provided *a priori* on where to evaluate the noise strength. Due to their practical usefulness, three particular interpretations are typically considered, the initial-point Itô interpretation [43], the mid-point Stratonovich interpretation [44, 45], and the final-point Hänggi-Klimontovich (HK) interpretation [46–49]. It is now accepted [35] that there is no universal correct interpretation; rather, the choice depends on the modelled system. For example, it was shown experimentally that the HK interpretation is the most appropriate for modelling colloidal particles near a wall [50], while the Itô interpretation is necessary for modelling Brownian yet non-Gaussian diffusion [51].

Although the question of a correct interpretation sometimes arises for homogeneous systems (e.g. in a magnetic field [52]), it is always an issue for heterogeneous ones. Here the disordered situations are the most complex ones. Disordered systems may be classified as annealed or quenched. Annealed disorder refers to temporal changes and a particle that returns to a previously visited site does not necessarily experience the same interactions [22, 53–55]. In contrast, quenched disorder refers to heterogeneities that are static in time and depend solely on the position within the medium. Quenched disorder is often more complicated to treat analytically since returns to already visited locations introduce correlations in the particle motion. Hence, numerical approximations are usually employed to study such systems. Among the quenched disorder models, the quenched trap model has been employed broadly [56–62]. This model is related to the continuous-time random walk [63–65] and has proven to be powerful from both theoretical and experimental perspectives. To consider the effects of a force in quenched systems, one usually use the Langevin equation. However, in this case, the role of the interpretation remains unresolved.

In order to gain insight into quenched heterogeneous systems, in this article, we focus on a simple class of heterogeneity, represented by a position-dependent diffusion coefficient. We study the effect of a linear restoring force, i.e. an OU process, in a heterogeneous environment by employing the Langevin equation. In this sense, we consider the problem of the motion of a particle under the action of a restoring force in a landscape characterised by a position-dependent diffusion coefficient. We first consider the general problem for any given diffusion landscape as a function of the interpretation parameter. Then, we focus on the case where the diffusion coefficient is a piecewise-constant function, a simple heterogeneous system, with a single interface. Despite its simplicity, this system yields surprising results. We consider the interpretation as a parameter of our model instead of choosing an *a priori* interpretation. Particular attention is paid to the Itô, Stratonovich, and HK interpretations and the evolution of the system in time in these three classical interpretations. Finally, we discuss conditions under which this heterogeneous system obeys the fluctuation-dissipation relation with constant temperature [66].

2. Homogeneous OU process

We first consider the diffusion of a particle in a homogeneous environment subjected to a harmonic potential in which the force varies linearly with the distance from the origin, i.e. $F(x) = -kx$, with k being the restoring force constant (Hooke coefficient). The equation describing the motion of a particle in such a system is the one-dimensional Langevin equation of the OU process [67], namely,

$$\dot{x} = -\frac{x}{\tau} + \sqrt{2D}\,\xi(t), \tag{1}$$

where τ is the correlation time, D is the diffusion coefficient, and $\xi(t)$ is a zero-mean Gaussian white noise with δ-correlations. The correlation time is related to the constant k via the damping coefficient γ by $\tau = \gamma/k$. The solution of this equation for the initial condition $x(0) = 0$ is given by

$$x(t) = \sqrt{2D}\int_0^t \mathrm{e}^{-(t-t')/\tau}\,\xi(t')\,\mathrm{d}t'. \tag{2}$$

From this solution, it can be easily verified that the mean is zero ($\langle x(t)\rangle = 0$) and the covariance function takes the form

$$\langle x(t)\,x(t')\rangle = D\tau\left[\mathrm{e}^{-|t-t'|/\tau} - \mathrm{e}^{-(t+t')/\tau}\right], \tag{3}$$

from which the second moment (MSD) is $\langle x^2(t)\rangle = D\tau\left[1-\mathrm{e}^{-2t/\tau}\right]$. As the process approaches thermal equilibrium, the MSD converges to $\langle x^2(t)\rangle = D\tau$. In the limit $\tau\to\infty$, i.e. a vanishing potential, the OU process reduces to standard Brownian motion, being the solution of the over-damped Langevin equation.

Associated to the Langevin equation of the OU process is a Fokker–Planck equation for the probability density function (PDF) $p(x,t)$ of the form

$$\frac{\partial}{\partial t}p(x,t) = \frac{1}{\tau}\frac{\partial}{\partial x}\left[xp(x,t)\right] + D\frac{\partial^2}{\partial x^2}p(x,t). \tag{4}$$

The solution of this Fokker–Planck equation is [68–70]

$$p(x,t) = \frac{1}{\sqrt{2\pi D\tau S(t)}}\exp\left(-\frac{x^2}{2D\tau S(t)}\right), \tag{5}$$

where $S(t) = 1 - \mathrm{e}^{-2t/\tau}$. In the limit $t \to \infty$, the system equilibrates and the steady state PDF takes the form

$$p(x) = \frac{1}{(2\pi D\tau)^{1/2}}\exp\left(-\frac{x^2}{2D\tau}\right), \tag{6}$$

which is the Boltzmann distribution with

$$D\tau = \frac{k_{\mathrm{B}}T}{k}, \tag{7}$$

where T is the temperature and k_{B} is the Boltzmann constant. Equation (7) is equivalent to the Einstein–Smoluchowski relation, a special case of the fluctuation-dissipation theorem of the second kind, $D = \mu k_{\mathrm{B}}T$ with the mobility $\mu = (\tau k)^{-1}$.

3. Heterogeneous OU process

We now consider the case when the diffusion coefficient depends on the position, i.e. $D(x)$. Analogously, in the context of annealed disorder, a time-dependent diffusivity $D(t)$ was considered by Lanoiselée *et al* for the motion of a particle in a harmonic potential (OU process) [71]. The Langevin equation (1) for the *homogeneous* OU process needs to be modified, leading to the Langevin equation for the *heterogeneous* OU process

$$\dot{x} = -\frac{x}{\tau} + \sqrt{2D(x)}\,\xi(t). \tag{8}$$

While the diffusion coefficient possesses a spatial dependence, the correlation time τ is kept constant. A constant correlation time implies that either the fluctuation-dissipation relation (equation (7)) breaks down or that the effective temperature depends on position. The former case is relevant to non-physical systems such as fluctuations in financial data [72]. In the latter case, a position-dependent temperature $T(x)$ can reach a steady state in systems away from equilibrium. For example, the local temperature increases when a laser heats up a fluid, leading to significant temperature gradients and, in turn, effects changes in the transport properties [73]. Another case in which a constant τ is relevant involves light-driven active colloids. In these systems, the intensity and/or wavelength of the incident light control the local stochastic driving force, and therefore the diffusion coefficient, while not considerably influencing the mobility [74–76]. The constant-temperature situation in which the fluctuation-dissipation relation holds and the correlation time depends on position, $\tau(x)$, is explicitly discussed in section 5.

Given the position dependence of the diffusivity, the integral that solves this stochastic differential equation (SDE) is ill-defined due to the inherent freedom in evaluating it. This ambiguity arises in Langevin equations with a position-dependent noise term, also known as multiplicative noise, as opposed to additive noise where it does not depend on the position. One thus needs to provide a rule, or interpretation, to solve the above stochastic integral [32, 35, 37, 41]. In this work, we treat the interpretation as a variable, maintaining generality, and without focusing on any specific physical system, as doing so would require selecting a particular interpretation [32].

The interpretation explicitly appears in the corresponding Fokker–Planck equation. In the heterogeneous OU process, the Fokker–Planck equation reads [40, 41]

$$\frac{\partial}{\partial t}p(x,t) = \frac{\partial}{\partial x}\left\{\frac{x}{\tau}p(x,t) + D^{\alpha}(x)\frac{\partial}{\partial x}\left[D^{1-\alpha}(x)\,p(x,t)\right]\right\}, \tag{9}$$

where $\alpha \in [0,1]$ is the interpretation parameter. For the three typical interpretations mentioned in the introduction the interpretation parameters are $\alpha = 0$, $1/2$, and 1 for Itô, Stratonovich and HK, respectively

[37]. Moreover, in the case when both the position-dependent diffusion coefficient and the PDF are differentiable functions with respect to the position, then the Fokker–Planck reduces to

$$\frac{\partial}{\partial t}p(x,t) = \frac{\partial}{\partial x}\left[\frac{x}{\tau} + (1-\alpha)\frac{\partial D(x)}{\partial x} + D(x)\frac{\partial}{\partial x}\right]p(x,t), \tag{10}$$

where one can define an effective potential $V_{\rm eff}(x)$ so as to rewrite it in the form [40, 41]

$$\frac{\partial}{\partial t}p(x,t) = \frac{\partial}{\partial x}\left[\frac{\partial V_{\rm eff}(x)}{\partial x} + D(x)\frac{\partial}{\partial x}\right]p(x,t), \tag{11}$$

where α modifies the effective potential,

$$V_{\rm eff}(x) = \frac{x^2}{2\tau} + (1-\alpha)D(x). \tag{12}$$

The contribution $(1-\alpha)D(x)$ is sometimes called the spurious drift. If the diffusion coefficient $D(x)$ is constant, the spurious drift is zero and the Fokker–Planck equation becomes independent of α. Interestingly, when the interpretation is HK ($\alpha = 1$), the effective potential reduces to the harmonic one.

The stationary solution $p_{\rm st}(x)$ follows by taking the limit $t \to \infty$ in the above Fokker–Planck equation (equation (9)),

$$\frac{\rm d}{{\rm d}x}\left\{\frac{x}{\tau}p_{\rm st}(x) + D^{\alpha}(x)\frac{\rm d}{{\rm d}x}\left[D^{1-\alpha}(x)p_{\rm st}(x)\right]\right\} = 0, \tag{13}$$

from which,

$$\frac{x}{\tau}p_{\rm st}(x) + D^{\alpha}(x)\frac{\rm d}{{\rm d}x}\left[D^{1-\alpha}(x)p_{\rm st}(x)\right] = -\mathcal{J}, \tag{14}$$

where $\mathcal{J}$ is a constant flux that must vanish in the absence of sources and sinks. Then, the solution is [41]

$$p_{\rm st}(x) = \mathcal{N}D^{\alpha-1}(x)\exp\left[-\frac{1}{\tau}\int^{x}\frac{x'}{D(x')}{\rm d}x'\right], \tag{15}$$

where $\int^x$ denotes the indefinite integral and $\mathcal{N}$ is a normalisation constant.

4. OU with piecewise-constant diffusion coefficient

Let us now consider a piecewise constant diffusion coefficient of the form

$$D(x) = \begin{cases} D_+ & \text{for } x \geqslant 0, \\ D_- & \text{for } x < 0, \end{cases} \tag{16}$$

with $D_\pm > 0$. Note that, due to the discontinuity at $x = 0$, the position-dependent diffusion coefficient is not differentiable everywhere. As a result, we cannot directly use the Fokker–Planck in the form of equation (10), which assumes differentiability. Instead, we must use the form of equation (9). This form of position-dependent diffusion coefficient was previously used to find the solution of the Langevin equation in an open system, without a trapping potential [32]. For such a diffusion landscape, the steady-state PDF in equation (15) takes the form

$$p_{\rm st}(x) = \begin{cases} \dfrac{2\beta(\alpha)}{\sqrt{2\pi D_-\tau}}\exp\left(-\dfrac{x^2}{2D_-\tau}\right), & \text{for } x < 0, \\ \dfrac{2[1-\beta(\alpha)]}{\sqrt{2\pi D_+\tau}}\exp\left(-\dfrac{x^2}{2D_+\tau}\right), & \text{for } x \geqslant 0, \end{cases} \tag{17}$$

where

$$\beta(\alpha) = \left[1 + \left(\frac{D_-}{D_+}\right)^{(1/2-\alpha)}\right]^{-1} \tag{18}$$

is the probability of finding a particle on the negative side of the x-axis [32]. The stationary solution $p_{\rm st}(x)$ is a generalised two-piece Gaussian distribution, similar to the time-dependent PDF obtained without a trapping potential [32]. The absence of a trapping potential corresponds, in the OU process, to the limit $\tau \to \infty$. In such a case, the time-dependent PDF is [32]

$$p_{\tau\to\infty}(x,t) = \begin{cases} \dfrac{2\beta(\alpha)}{\sqrt{4\pi D_- t}} \exp\left(-\dfrac{x^2}{4D_- t}\right), & \text{for } x<0, \\ \dfrac{2[1-\beta(\alpha)]}{\sqrt{4\pi D_+ t}} \exp\left(-\dfrac{x^2}{4D_+ t}\right), & \text{for } x \geqslant 0, \end{cases} \quad (19)$$

with the same $\beta(\alpha)$ as in equation (18). The overall solution for $t \ll \tau$ must have the form of equation (19) because the trapping potential does not play any role at short times, and for $t \gg \tau$ must converge to the steady state solution (equation (17)). Given the PDF of the homogeneous OU process, the solution of the Fokker–Planck equation (equation (9)) for the heterogeneous OU process with piecewise diffusion coefficient for a particle starting at $x = 0$ has the form

$$p_{x_0=0}(x,t) = \begin{cases} \dfrac{2\beta(\alpha)}{\sqrt{2\pi D_- \tau S(t)}} \exp\left[-\dfrac{x^2}{2D_- \tau S(t)}\right], & x<0, \\ \dfrac{2[1-\beta(\alpha)]}{\sqrt{2\pi D_+ \tau S(t)}} \exp\left[-\dfrac{x^2}{2D_+ \tau S(t)}\right], & x \geqslant 0. \end{cases} \quad (20)$$

Here, analogous to the homogeneous OU process, $S(t) = 1 - \mathrm{e}^{-2t/\tau}$. The situation with a different initial condition is discussed below. The term $\beta(\alpha)$ is obtained from the continuity of the flux (particles conservation) [32] and has the same form as in equation (18) (see appendix A for the full proof). Indeed, since the probability $\beta(\alpha)$ of finding a particle on the negative x-axis does not depend on the magnitude of the restoring force (i.e. it is independent of τ), we conclude that the presence of a restoring potential does not affect the probability of finding a particle on the negative half-axis. Furthermore, for a particle that starts at the origin, this probability does not depend on time. Later in the article, we discuss a particle starting away from the origin, in which case this probability is not stationary.

To validate our solution, we numerically simulate trajectories according to the Langevin equation (equation (8)) for the piecewise diffusion coefficient for three interpretations: Itô, Stratonovich, and HK. We modified the Heun algorithm [77, 78], which implies the Stratonovich interpretation, to solve the Langevin equations with any interpretation. This generalised Heun algorithm is presented in appendix B. Using this generalised algorithm, we simulate 10^4 trajectories on a diffusivity landscape with $D_- = 2$ and $D_+ = 1$ with an integration step of $\Delta t = 10^{-2}$ and a correlation time $\tau = 25$. These trajectories are then used to construct the position PDF of the particles at different times t. Figure 1 shows the PDFs obtained via numerical simulations together with the analytical solutions for the Itô, Stratonovich, and HK interpretations (equation (20)). Figures 1(a)–(c) show the PDFs at time $t = 1$ such that $t/\tau = 0.04 \ll 1$. The dotted lines in these figures correspond to the PDFs of Brownian motion without a trapping potential (equation (19)). Figures 1(d)–(f) present the PDFs at time $t = 25$, for which $t/\tau = 1$. The dashed lines correspond to the analytical solutions given by equation (20). Finally, figures 1(g)–(i) display the steady state PDFs at time $t = 1000$ such that $t/\tau = 40 \gg 1$. The solid lines correspond to the steady state solutions of equation (17). Perfect agreement is observed between the numerical simulations and the analytical solutions. The discontinuity in the PDF for $\alpha < 1$ is a consequence of the discontinuity of $D(x)$. This observation is further addressed in appendix C, where we examine the effect of smoothing the step function with a continuous approximation.

From the PDF in equation (20), the mean and the MSD can be computed,

$$\langle x(t)\rangle_{x_0=0} = A(\alpha)\left[\tau\left(1-\mathrm{e}^{-2t/\tau}\right)\right]^{1/2}, \quad (21)$$

and

$$\langle x^2(t)\rangle_{x_0=0} = B(\alpha)\,\tau\left(1-\mathrm{e}^{-2t/\tau}\right), \quad (22)$$

with

$$A(\alpha) = \sqrt{\frac{2}{\pi}}\left[\sqrt{D_+} - \beta(\alpha)\left(\sqrt{D_+}+\sqrt{D_-}\right)\right] \quad (23)$$

and

$$B(\alpha) = D_+ + \beta(\alpha)(D_- - D_+). \quad (24)$$

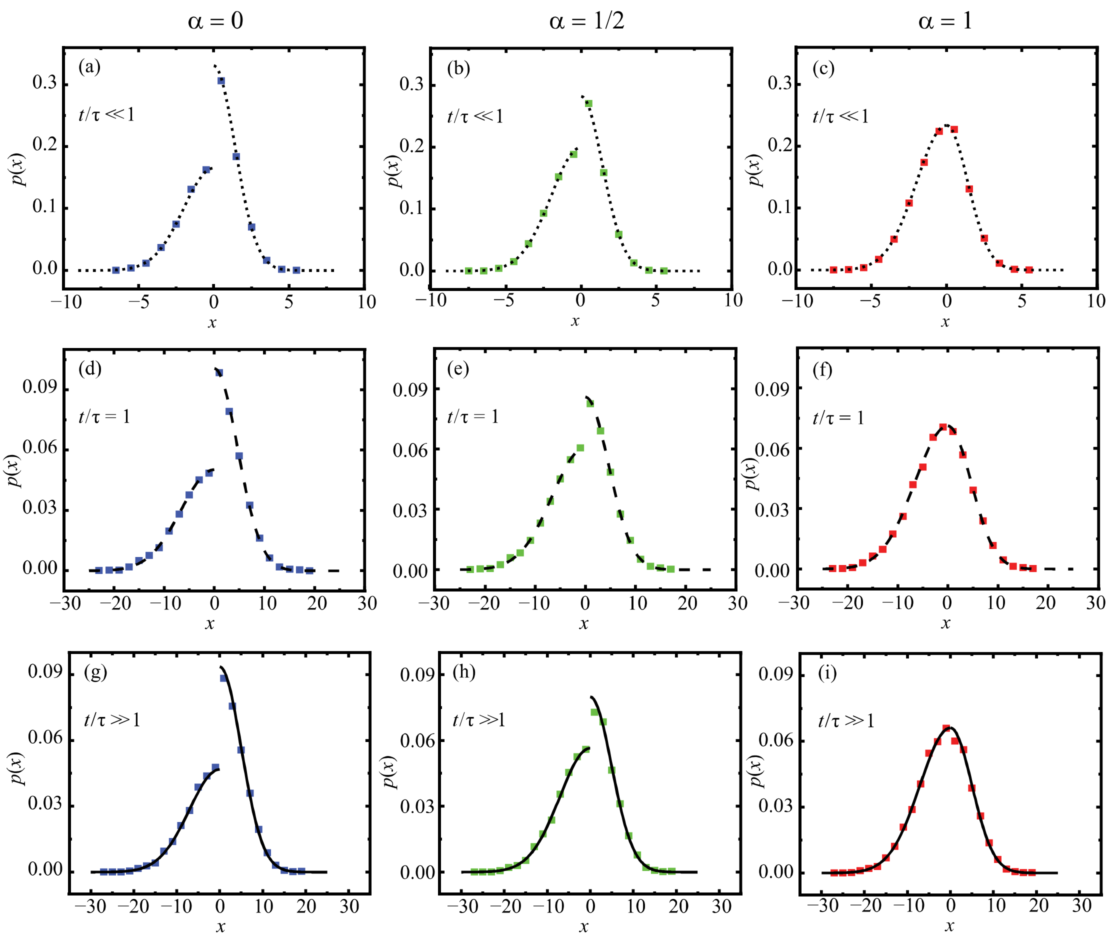

Figure 1. PDFs of the heterogeneous OU process with $\tau = 25$ and piecewise diffusion coefficient with $D_- = 2$ and $D_+ = 1$ for the interpretation parameters $\alpha = 0$, $1/2$, and 1, corresponding to the Itô, Stratonovich, and Hänggi-Klimontovich interpretations, respectively. (a)–(c) PDFs at time $t = 1$ so that $t/\tau = 0.04 \ll 1$. The dotted lines are the PDFs of Brownian motion, equation (19). (d)–(f) PDFs at time $t = 25$ so that $t/\tau = 1$. The dashed lines are analytical solutions, equation (20). (g)–(i) PDFs at time $t = 1000$ so that $t/\tau = 40 \gg 1$. The solid lines are the steady state solutions, equation (17).

For $t \to 0$, the mean and MSD reduce respectively to $\langle x(t)\rangle_{x_0=0} = A(\alpha)\sqrt{2t}$ and $\langle x^2(t)\rangle_{x_0=0} = 2B(\alpha)t$, which are the quantities obtained in the absence of a trapping potential [32]. In this case, there is an initial flux in the direction of the larger diffusivity, except when $\alpha = 0$, in which case the flux vanishes. On the other hand, for $t \to \infty$, the mean and MSD reach a steady state with $\langle x(t)\rangle_{x_0=0} = A(\alpha)\tau^{1/2}$ and $\langle x^2(t)\rangle_{x_0=0} = B(\alpha)\tau$.

We now relax the assumption that the particles start at $x_0 = 0$, where the position-dependent diffusion coefficient $D(x)$ presents a discontinuity and the potential has its minimum. Then, for short times t such that $t \ll \tau$ and $|x_0| \gg \sqrt{2D_\pm t}$, the PDF of the displacements is described by

$$p_{t\to 0}(x,t) = \frac{1}{\sqrt{2\pi D_\pm \tau S(t)}} \exp\left(-\frac{\left(x - x_0 \mathrm{e}^{-t/\tau}\right)^2}{2D_\pm \tau S(t)}\right), \tag{25}$$

for an initial condition $p(x,0) = \delta(x - x_0)$, $D_\pm = D_+$ when $x_0 > 0$, and conversely $D_\pm = D_-$ for $x_0 < 0$. This PDF is essentially a Gaussian profile centred at $x_0 \mathrm{e}^{-t/\tau}$ and corresponds to the solution of the OU process with a constant diffusion coefficient for an arbitrary initial condition. In the short time limit, the probability of finding a particle in the semi-infinite line opposite to the initial position is practically zero and can be neglected, regardless of the interpretation.

As the system evolves, the centre of the Gaussian profile moves towards $x = 0$, the potential minimum and where the diffusion coefficient has its discontinuity. Due to this discontinuity, particles on either side of $x = 0$ will move with different diffusion coefficients. As a result, a generalised two-piece Gaussian distribution forms, where the probability of being in the negative region depends on the interpretation. Furthermore, since the initial condition is not at the origin, this probability varies with time. In the long time limit, the memory of the initial condition is lost, and the PDF takes the form of equation (17).

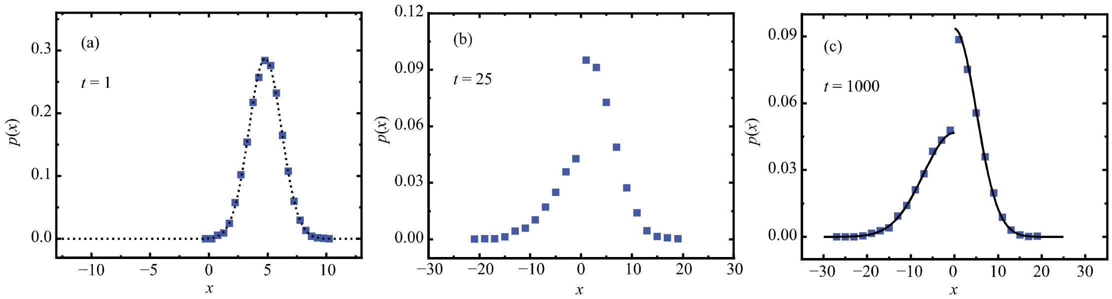

Figure 2. PDFs of the heterogeneous OU process with a piecewise diffusion coefficient with $D_- = 2$ and $D_+ = 1$ for the Itô interpretation with initial condition $x_0 = 5$. In the simulations we set $\tau = 25$. PDF at times (a) $t = 1$, (b) $t = 25$, and (c) $t = 1000$. The dotted line is the PDF of the homogeneous OU process, equation (25), with $D_+ = 1$ at $t = 1$. The solid line shows the steady state PDF, equation (17).

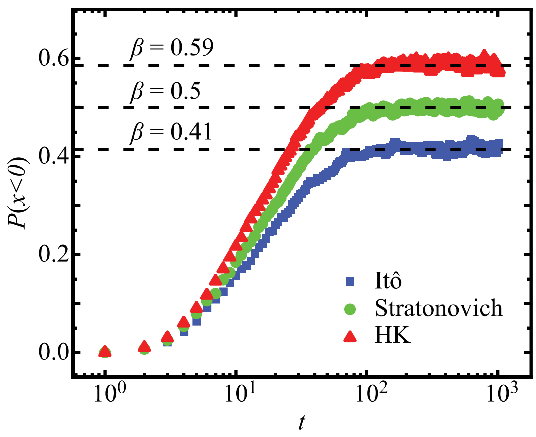

Figure 3. Temporal evolution of the probability of finding a particle in the negative part of the x-axis, $P(x < 0)$, for the heterogeneous OU process with a piecewise constant diffusion coefficient with $D_- = 2$ and $D_+ = 1$ with Itô, Stratonovich, and Hänggi-Klimontovich (HK) interpretations with initial condition $x_0 = 5$, and $\tau = 25$. The dashed lines corresponds to $\beta(\alpha)$ for $x_0 = 0$ (equation (18)) for the three interpretations.

Finding a general solution of the Fokker–Planck equation (equation (9)) for an arbitrary non-zero initial condition is beyond our abilities at the moment. However, we can perform numerical simulations to gain insight into the behaviour of the PDF. Figure 2 shows the evolution of the PDF for a system with $D_+ = 1$ and $D_- = 2$ with initial condition $x_0 = 5$ under the Itô interpretation. The behaviour we describe here is qualitatively similar to the other interpretations. In these simulations, we use the same parameters as above. Figure 2(a) shows the PDF at time $t = 1$. In this short time behaviour ($t \to 0$), the particle is found around the starting point and the probability of being in the negative part is essentially zero, i.e. $P(x < 0; t \to 0) = 0$. Figure 2(b) presents the PDF at time $t = 25$. During this intermediate time, the probability of being in the negative part of the x-axis grows with time. Finally, figure 2(c) depicts the PDF at time $t = 1000$. In this long time limit ($t \to \infty$), one sees that the initial condition is forgotten, and the PDF takes the asymptotic form of equation (17) with $\beta(\alpha)$ defined by equation (18) for $\alpha = 0$. In this asymptotic regime, the probability $P(x < 0)$ reaches a steady state equal to $\beta(\alpha)$. The evolution of the probability of finding a particle in the negative part of the x-axis is presented in figure 3.

5. Heterogeneous OU process with constant temperature

Let us now consider the case of constant temperature, for which the correlation time $\tau(x)$ is position dependent (cf section 3) and is given by

$$\tau(x) = k_B T / kD(x), \tag{26}$$

and the Langevin equation takes the form

$$\dot{x} = -\frac{kxD(x)}{k_B T} + \sqrt{2D(x)}\xi(t). \tag{27}$$

The associated Fokker–Planck equation is then

$$\frac{\partial}{\partial t}p(x,t) = \frac{\partial}{\partial x}\left(\frac{kxD(x)}{k_BT}p(x,t) + D(x)\frac{\partial}{\partial x}\left[D^{1-\alpha}(x)p(x,t)\right]\right). \tag{28}$$

Following a similar procedure as we did before, we find the steady state solution $p_{st}^{T}(x)$ in the limit $t\to\infty$,

$$p_{st}^{T}(x) = \mathcal{M}D^{\alpha-1}(x)\exp\left(-\frac{kx^2}{2k_BT}\right), \tag{29}$$

with the normalisation constant $\mathcal{M}$. The superscript T stands for fulfilment of the fluctuation-dissipation relation (26) with constant temperature.

Let us consider again the piecewise-constant diffusion coefficient of equation (16). For such a diffusion landscape, the steady state PDF (29) takes the form

$$p_{st}^{T}(x) = \begin{cases} \dfrac{2\eta(\alpha)}{\sqrt{2\pi k_BT/k}}\exp\left(-\dfrac{kx^2}{2k_BT}\right), & \text{for } x<0, \\ \dfrac{2[1-\eta(\alpha)]}{\sqrt{2\pi k_BT/k}}\exp\left(-\dfrac{kx^2}{2k_BT}\right), & \text{for } x\geqslant 0, \end{cases} \tag{30}$$

with

$$\eta(\alpha) = \left[1+\left(\frac{D_-}{D_+}\right)^{(1-\alpha)}\right]^{-1}. \tag{31}$$

Note the different α-dependence of $\eta(\alpha)$ when compared to $\beta(\alpha)$ in equation (18). Despite the presence of the heterogeneous environment, the PDF $p_{st}^{T}(x)$ is Gaussian in the HK interpretation ($\alpha=1$),

$$p_{st}^{T}(x) = \sqrt{\frac{k}{2\pi k_BT}}\exp\left(-\frac{kx^2}{2k_BT}\right), \tag{32}$$

which is the Boltzmann distribution, and not a two-piece Gaussian distribution as in the case discussed above. It is the same PDF one obtains for the steady state solution of the homogeneous OU process (6).

We now find a solution for any α and any time with $x_0=0$. Let us define $D^*\tau^*=k_BT/k$, $\tau_{min}=\min_x\{\tau(x)\}$, and $\tau_{max}=\max_x\{\tau(x)\}$. Following a similar line of thought as before, the overall solution must have the form of equation (19) for $t\ll\tau_{min}$, because the trapping potential does not play any role at short times. It must also converge to the steady state solution (equation (30)) for $t\gg\tau_{max}$. The solution of the Fokker–Planck equation (28) for a process fulfilling the fluctuation-dissipation relation, for a piecewise constant diffusion coefficient for a particle starting at $x_0=0$ is given by

$$p_{x_0=0}^{T}(x,t) = \begin{cases} \dfrac{2\eta(\alpha,t)}{\sqrt{2\pi D^*\tau^*S_-(t)}}\exp\left[-\dfrac{x^2}{2D^*\tau^*S_-(t)}\right], & x<0, \\ \dfrac{2[1-\eta(\alpha,t)]}{\sqrt{2\pi D^*\tau^*S_+(t)}}\exp\left[-\dfrac{x^2}{2D^*\tau^*S_+(t)}\right], & x\geqslant 0, \end{cases} \tag{33}$$

with

$$\eta(\alpha,t) = \left\{1+\left(\frac{D_-}{D_+}\right)^{1-\alpha}\left[\frac{S_-(t)}{S_+(t)}\right]^{-1/2}\right\}^{-1}, \tag{34}$$

and $S_\pm(t) = 1-\exp(-2D_\pm t/D^*\tau^*)$. This form of $\eta(\alpha,t)$ is obtained, as for the previous case, by the continuity of the flux (see equation (A.15) in appendix A). Note that in this case the probability of being in the negative part ($x<0$) depends on both time and the interpretation α, as opposed to the previous case in which such a probability depends only on the interpretation. The MSD of this process are presented in appendix D.

To validate our solution, we numerically solved equation (27) for the piecewise diffusion coefficient using the modified Heun algorithm (see appendix B) to obtain trajectories of the process $x(t)$ in three interpretations: Itô, Stratonovich and HK. In the simulations we, $\tau_{min}=50$, $\tau_{max}=100$, set $D^*\tau^*=100$ and $\Delta t=5\times10^{-3}$. We simulate 10^4 trajectories on a diffusivity landscape with $D_-=2$ and $D_+=1$. Using these

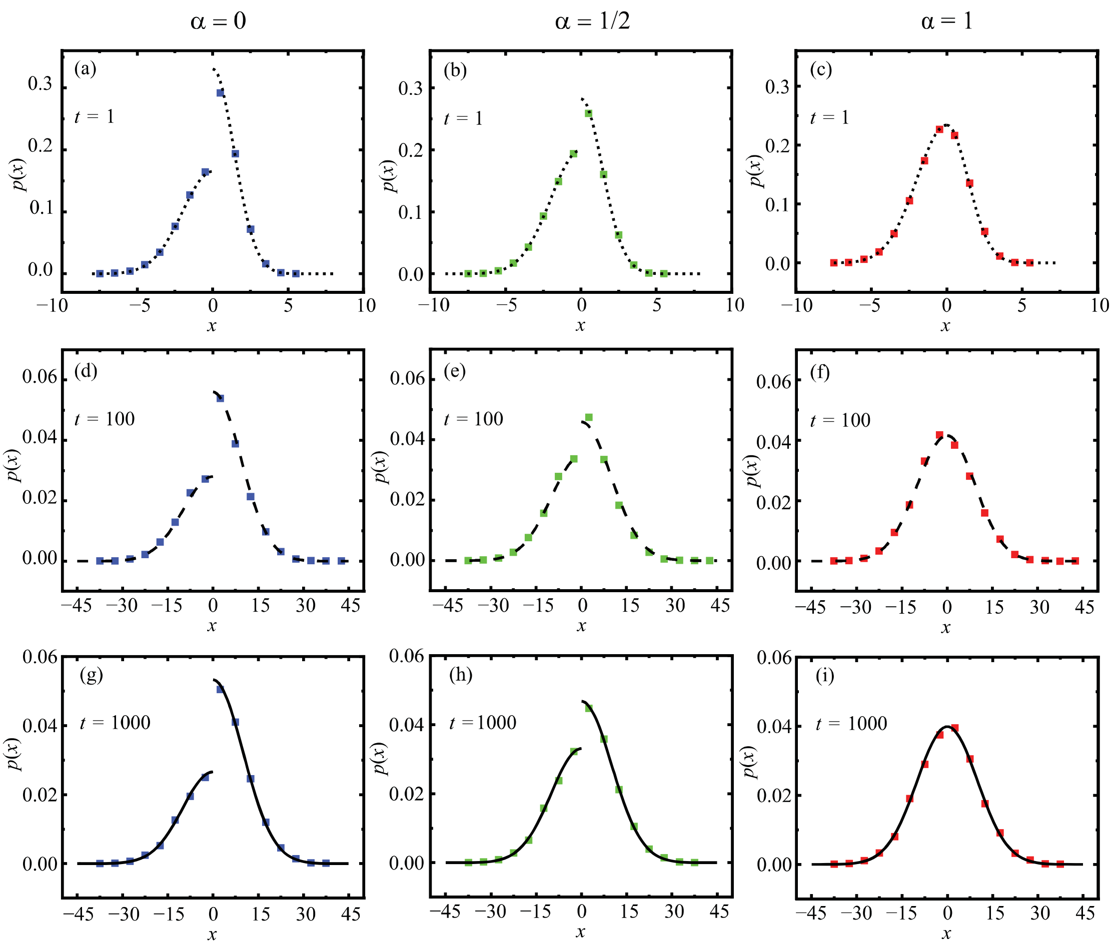

Figure 4. PDFs of the heterogeneous OU process with a piecewise diffusion coefficient, constant temperature, and fluctuation-dissipation relations. The diffusivities are $D_- = 2$ and $D_+ = 1$. In the simulations, we set $D^*\tau^* = k_BT/k = 100$. (a)–(c) PDFs at time $t = 1$ so that $t \ll \tau_{\rm min}$. The dotted lines are the PDF (19) of Brownian motion. (d)–(f) PDFs at time $t = 100$ so that $t \gg \tau_{\rm max}$. The dashed lines are the analytical solutions, equation (33). (g)–(i) PDFs at time $t = 1000$ so that $t/D^*\tau^* = 10 > 1$. The solid lines represent the steady state PDF (32).

trajectories, we construct the PDF with the position of the particles at a given time t. Figure 4 shows the PDFs obtained via numerical simulations at different times along with the corresponding analytical solutions. Figures 4(a)–(c) show the PDFs at time $t = 1$ such that $t \ll \tau_{\rm min}$. The dotted lines are the PDFs of Brownian motion, equation (19). Figures 4(d)–(f) present the PDFs at time $t = 100$. The dashed lines are the analytical solution, equation (33). Finally, figures 4(g)–(i) display the PDFs at time $t = 1000$ such that $t \gg \tau_{\rm max}$. The solid lines are the PDF of the steady state solution, equation (32). Excellent agreement is again observed.

6. Discussion and conclusions

In this work, we studied the motion of a particle in a harmonic potential within a heterogeneous environment modelled by a position-dependent diffusion coefficient. To account for the heterogeneous landscape, we modified the Langevin equation of the homogeneous OU process so that the diffusion coefficient depends on position, i.e. $D(x)$. We first consider the problem for a general landscape $D(x)$ with constant correlation time τ, i.e. constant damping coefficient. Then, within the assumption of a constant correlation time, we turned our attention to the case of a piecewise constant diffusion coefficient (equation (16)) with a discontinuity at $x = 0$, which is also the point of the minimum of the potential. We first considered the situation where the particle's initial position coincides with this discontinuity, i.e. $x_0 = 0$. This situation is particularly interesting since it allows us to find an exact solution to the Fokker–Planck equation. Remarkably, the obtained PDF has a similar form as the PDF obtained without a harmonic potential [32], namely, a generalised two-piece Gaussian distribution. Moreover, while in the presence of the potential, the probability of finding a particle in the negative part ($x < 0$) depends on α, it does not change with time. This probability is also not affected by the potential [32]. We corroborated our analytical solutions by numerically solving the corresponding Langevin equation for the Itô, Stratonovich, and HK interpretations.

We further considered the solution where the initial condition is not at the origin. We performed numerical simulations to obtain the PDF. It was found that at short times, the PDF is described by the homogeneous OU process. On the other hand, at large times, the PDF shows the same asymptotic behaviour as in the case with the initial condition at $x_0 = 0$.

In the second part of this work, we consider the scenario in which the fluctuation-dissipation relation is fulfilled under constant temperature, which is the case for most single-molecule experiments. Thus, we analysed the case where the damping coefficient depends on the position and is inversely proportional to the diffusion coefficient. We found the exact PDF that solves the Fokker–Planck equation for an initial condition at the origin, $x_0 = 0$. Similar to the previous situation, the time-dependent solution for this case also has the form of a generalised two-piece Gaussian distribution. However, the probability of being in the negative part of the x-axis is not constant but a time-dependent quantity that depends on the interpretation parameter. Interestingly, the PDF convergences to a normal distribution for the HK interpretation ($\alpha = 1$). Again, we corroborated our solutions with numerical simulations of the Langevin equation.

This work presents the analysis of the heterogeneous OU process where the interpretation is considered as a parameter throughout the analysis. Finally, this study paves the way for a possible generalisation to any potential, or even, for cases where the system presents correlations, like in the case of fractional Brownian motion.

Data availability statement

No new data were created or analysed in this study.

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Appendix A. Probability of being in $x < 0$

Let us start from the Fokker–Planck equation (9) which we rewrite in the form

$$\frac{\partial}{\partial t}p(x,t) = \frac{\partial}{\partial x}\left[\frac{x}{\tau}p(x,t)\right] + \frac{\partial}{\partial x}\left\{D^{\alpha}(x)\frac{\partial}{\partial x}\left[D^{1-\alpha}(x)p(x,t)\right]\right\}, \tag{A.1}$$

which is essentially a continuity equation and can be rewritten as

$$\frac{\partial}{\partial t}p(x,t) = -\frac{\partial}{\partial x}\mathcal{J}(x,t), \tag{A.2}$$

with $\mathcal{J}(x,t)$ being the diffusive flux defined as

$$\mathcal{J}(x,t) = -\frac{x}{\tau}p(x,t) - D^{\alpha}(x)\frac{\partial}{\partial x}\left[D^{1-\alpha}(x)p(x,t)\right]. \tag{A.3}$$

This is essentially a generalised form of Fick's first law that includes the potential.

Given that the transport equation (in our case, the Fokker–Planck equation) appears as a combination of a generalised continuity equation (possibly, with sources), and a constitutive equation for the flux (equation (A.3)), the discontinuity of the flux would imply the existence of a point source at the point of discontinuity. In our setup the sources are, however, absent. Therefore, the flux is continuous and differentiable with respect to x. Moreover, the definition of the flux (equation (A.3)) implies that the product $D^{1-\alpha}(x)p(x,t)$ must itself be differentiable with respect to position. With these considerations in place, we proceed to determine the probability $\beta(\alpha)$ of finding a particle on the negative side of the x-axis. Since the diffusion coefficient $D(x)$ is strictly positive, we can divide both sides of equation (A.3) by $D^{\alpha}(x)$, which yields

$$-\frac{\mathcal{J}(x,t)}{D^{\alpha}(x)} = \frac{x}{\tau}\frac{p(x,t)}{D^{\alpha}(x)} + \frac{\partial}{\partial x}\left[D^{1-\alpha}(x)p(x,t)\right]. \tag{A.4}$$

Next, we integrate both sides of this expression in a vicinity of the origin, from $-\epsilon$ to ϵ, and obtain

$$-\int_{-\epsilon}^{\epsilon}\frac{\mathcal{J}(x,t)}{D^{\alpha}(x)}\mathrm{d}x = \int_{-\epsilon}^{\epsilon}\frac{x}{\tau}\frac{p(x,t)}{D^{\alpha}(x)}\mathrm{d}x + \int_{-\epsilon}^{\epsilon}\frac{\partial}{\partial x}\left[D^{1-\alpha}(x)p(x,t)\right]\mathrm{d}x. \tag{A.5}$$

The last integral on the right-hand side can be readily computed since $D^{1-\alpha}(x)p(x,t)$ is differentiable, therefore

$$-\int_{-\epsilon}^{\epsilon}\frac{\mathcal{J}(x,t)}{D^{\alpha}(x)}\mathrm{d}x=\int_{-\epsilon}^{\epsilon}\frac{x}{\tau}\frac{p(x,t)}{D^{\alpha}(x)}\mathrm{d}x+\left[D^{1-\alpha}(\epsilon)\,p(\epsilon,t)-D^{1-\alpha}(-\epsilon)\,p(-\epsilon,t)\right]. \tag{A.6}$$

The remaining two integrals can be solved by means of the mean-value theorem: let $f(x)$ be a continuous function on $[a,b]$, and let $g(x)$ be integrable and non-negative on $[a,b]$. Then, there exist some $c\in[a,b]$ such that

$$\int_a^b f(x)\,g(x)\,\mathrm{d}x=f(c)\int_a^b g(x)\,\mathrm{d}x. \tag{A.7}$$

We can apply the mean-value theorem to the integrals in equation (A.6) since both $\mathcal{J}(x,t)$ and x are continuous functions, and $1/D^{\alpha}(x)$ and $p(x,t)/D^{\alpha}(x)$ are integrable, non-negative functions. Thus, for some x' and $x''\in(-\epsilon,\epsilon)$, we have

$$-\mathcal{J}(x',t)\left(\frac{\epsilon}{D_+^{\alpha}}+\frac{\epsilon}{D_-^{\alpha}}\right)=\frac{x''}{\tau}\int_{-\epsilon}^{\epsilon}\frac{p(x,t)}{D^{\alpha}(x)}\mathrm{d}x+\left[D^{1-\alpha}(\epsilon)\,p(\epsilon,t)-D^{1-\alpha}(-\epsilon)\,p(-\epsilon,t)\right]. \tag{A.8}$$

Then, in the limit $\epsilon\to0$, the l.h.s. vanishes. In this limit, the first term on the r.h.s. also vanishes since $x''\to0$. Hence,

$$D_+^{1-\alpha}p(0_+,t)=D_-^{1-\alpha}p(0_-,t). \tag{A.9}$$

This shows that there is a discontinuity in the PDF for any $\alpha\neq1$. The same expression holds if one starts from the Fokker–Planck equation (28). However, in this case the PDF is different. Let us then treat these two cases separately:

(i) Let us first consider the PDF in equation (20). This PDF at $x=0_\pm$ reads

$$p(0_-,t)=\frac{2\beta(\alpha)}{\sqrt{2\pi D_-\tau S(t)}} \tag{A.10}$$

and

$$p(0_+,t)=\frac{2[1-\beta(\alpha)]}{\sqrt{2\pi D_-\tau S(t)}}. \tag{A.11}$$

Then, substituting these two expressions into equation (A.9), we obtain

$$\beta(\alpha)=\left[1+\left(\frac{D_-}{D_+}\right)^{1/2-\alpha}\right]^{-1}. \tag{A.12}$$

(ii) Next, let us consider the PDF in equation (33). This PDF at $x=0_\pm$ has the form

$$p(0_-,t)=\frac{2\beta(\alpha)}{\sqrt{2\pi D^*\tau^*S_-(t)}} \tag{A.13}$$

and

$$p(0_+,t)=\frac{2[1-\beta(\alpha)]}{\sqrt{2\pi D^*\tau^*S_+(t)}}. \tag{A.14}$$

Next, we substitute these two expression into equation (A.9) and obtain

$$\eta(\alpha,t)=\left[1+\left(\frac{D_-}{D_+}\right)^{1-\alpha}\left(\frac{S_-(t)}{S_+(t)}\right)^{-1/2}\right]^{-1}. \tag{A.15}$$

Appendix B. Generalised Heun algorithm

The Heun algorithm [77, 78] is a *predictor-corrector* method that is used to numerically integrate a SDE in the Stratonovich interpretation. The Heun algorithm for a general SDE of the form

$$\mathrm{d}X(t) = f[X(t), t]\,\mathrm{d}t + g[X(t), t]\,\mathrm{d}B(t), \tag{B.1}$$

is a two-step process: first, one *predicts* the next value using an Euler scheme [78],

$$\overline{X}_{i+1} = X_i + f(X_i, t_i)\,\Delta t + g(X_i, t_i)\,\xi_i, \tag{B.2}$$

where $X_i = X(t_i)$, and $t_{i+1} = t_i + \Delta t$. Then, one *corrects* this value for the Stratonovich interpretation using

$$X_{i+1} = X_i + \frac{1}{2}\left[f(X_i, t_i) + f\left(\overline{X}_{i+1}, t_{i+1}\right)\right]\Delta t + \frac{1}{2}\left[g(X_i, t_i) + g\left(\overline{X}_{i+1}, t_{i+1}\right)\right]\xi_i. \tag{B.3}$$

The proposed modified Heun algorithm is again a two part process: first, using the same Euler scheme in equation (B.2), we predict the value $\overline{X}_{i+1}$ after one time-step $t_{i+1} = t_i + \Delta t$. Then, we modify the correction part of the standard Heun method to account for the different interpretations as follows

$$X_{i+1} = X_i + \left\{f(X_i, t_i) + \alpha\left[f\left(\overline{X}_{i+1}, t_{i+1}\right) - f(X_i, t_i)\right]\right\}\Delta t + \left\{g(X_i, t_i) + \alpha\left[g\left(\overline{X}_{i+1}, t_{i+1}\right) - g(X_i, t_i)\right]\right\}\xi_i. \tag{B.4}$$

For the Itô interpretation with $\alpha = 0$, the correction step is redundant and thus our modified Heun algorithm reduces to the standard Euler scheme. For the Stratonovich case with $\alpha = 1/2$, our modified scheme reduces to the standard Heun algorithm. For the HK with $\alpha = 1$, the new algorithm takes the form

$$X_{i+1} = X_i + f\left(\overline{X}_{i+1}, t_{i+1}\right)\Delta t + g\left(\overline{X}_{i+1}, t_{i+1}\right)\xi_i. \tag{B.5}$$

Appendix C. Continuity of the PDF for smooth diffusion coefficient

To better understand the origin of the discontinuity in $p(x,t)$, we examine whether it arises from the discontinuity in the space-dependent diffusion coefficient $D(x)$. Although this analysis can be carried out for both versions of the heterogeneous OU process, we consider only the first case for simplicity. We begin by rewriting the piecewise-constant diffusion coefficient in equation (16) as

$$D(x) = (D_+ - D_-)\,U(x) + D_-, \tag{C.1}$$

where $U(x)$ is the Heaviside step function. Then, we consider a smooth approximation of the Heaviside function in the form of a logistic function

$$\mathcal{U}(x) = \frac{1}{1 + \exp(-kx)}, \tag{C.2}$$

which converges to $U(x)$ as $k \to \infty$. We then define the continuous diffusion coefficient as

$$D(x) = (D_+ - D_-)\,\mathcal{U}(x) + D_-. \tag{C.3}$$

Using the generalised Heun algorithm, we computed 10^4 trajectories for three values of $k = 0.5$, 1, and 10 under the Itô interpretation, as this is the case in which the PDF shows the greatest discontinuity for the piecewise-constant diffusion coefficient (see figure 1). From these trajectories, we calculate the PDF at time $t = 1000$ for each value of k and display it in figure C1, along with corresponding continuous diffusion coefficient used in the simulations. As shown in the figure, the PDF remains continuous when the diffusion coefficient is continuous (see figures C1(a) and (b) for $k = 0, 5$, and 1, respectively). However, when the smooth diffusion coefficient begins to closely resemble the discontinuous, as is already the case at $k = 10$, the PDF also becomes visibly discontinuous, as illustrated in figure C1(c).

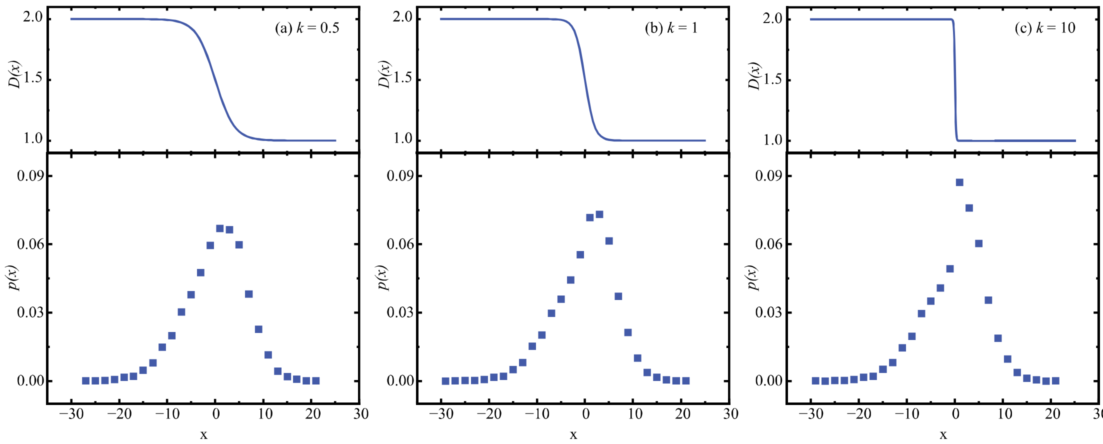

Figure C1. PDFs of the heterogeneous OU process with continuous diffusion coefficient defined in equation (C.3), shown for three values of the parameter k: 0.5, 1, and 10 corresponding to panels (a), (b), and (c), respectively. Each panel also displays the corresponding diffusion coefficient used in the simulations.

Appendix D. Mean and MSD of the PDF in equation (33)

From the PDF in equation (33), the first two moments can be computed. Then, the mean is

$$\langle x(t)\rangle = \sqrt{\frac{2D^*\tau^*}{\pi}}\,\frac{D_-^{1-\alpha}\left(1-\mathrm{e}^{-2D_+t/D^*\tau^*}\right) - D_+^{1-\alpha}\left(1-\mathrm{e}^{-2D_-t/D^*\tau^*}\right)}{D_+^{1-\alpha}\left(1-\mathrm{e}^{-2D_-t/D^*\tau^*}\right)^{1/2} + D_-^{1-\alpha}\left(1-\mathrm{e}^{-2D_+t/D^*\tau^*}\right)^{1/2}}, \tag{D.1}$$

and the MSD is

$$\langle x^2(t)\rangle = D^*\tau^*\frac{D_-^{1-\alpha}\left(1-\mathrm{e}^{-2D_+t/D^*\tau^*}\right)^{3/2} + D_+^{1-\alpha}\left(1-\mathrm{e}^{-2D_-t/D^*\tau^*}\right)^{3/2}}{D_+^{1-\alpha}\left(1-\mathrm{e}^{-2D_-t/D^*\tau^*}\right)^{1/2} + D_-^{1-\alpha}\left(1-\mathrm{e}^{-2D_+t/D^*\tau^*}\right)^{1/2}}. \tag{D.2}$$

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