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Fractional diffusion in periodic potentials

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Abstract

Fractional, anomalous diffusion in space-periodic potentials is investigated. The analytical solution for the effective fractional diffusion coefficient in an arbitrary periodic potential is obtained in closed form in terms of two quadratures. This theoretical result is corroborated by numerical simulations for different shapes of the periodic potential. Normal and fractional spreading processes are contrasted via the time evolution of the corresponding probability densities in state space. While there are distinct differences occurring at small evolution times, a re-scaling of time yields a mutual matching between the long-time behaviours of normal and fractional diffusion.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

In 1905 Pearson proposed what we now know as a random walk [1]. For a one-dimensional system the problem can be formulated in the following way: a particle jumps at each point of time from its current position x to the position $x + \Delta x$ with probability p, or $x - \Delta x$ with probability $1 - p$. The approach towards diffusion theory, pioneered by Einstein, relies on postulates very similar to the ones for the random walk, leading to the same results when the jump width $\Delta x \to 0$ [2]. However, in many situations the assumptions used by Einstein and Pearson do not hold; one such example is the transport of charge carriers in amorphous semiconductors when exposed to an electric field.

Sixty years after Pearson, in 1965, Montroll and Weiss introduced the theory of continuous time random walks (CTRW) [3, 4]. It was applied to transport in semiconductors in works by Scher and Lax [5], and Scher and Montroll [6]. Due to its historical importance and vivid clarity we recall here the definition of the CTRW as given by Scher and Montroll [6]: *In our model we postulate our material to be divided into a regular lattice of equivalent cells, with each cell containing many randomly distributed localized sites available for hopping carriers. Carrier transport is a succession of carrier hops from one localized site to another and finally from one cell to another. We define the hopping time to be the time interval between the moment of arrival*

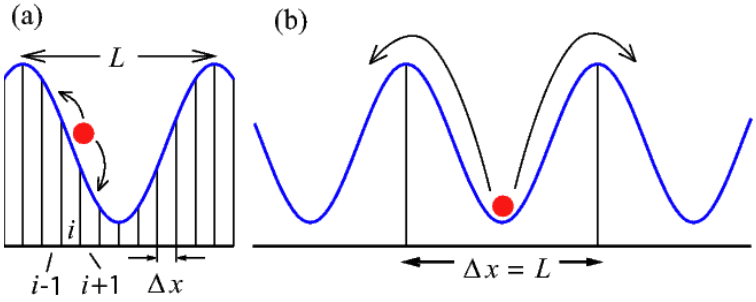

Figure 1. CTRW in a periodic cosine potential. Two different possibilities for introducing the one-dimensional lattice: (a) the lattice period Δx is much smaller than the potential period L. The particle at site i hops to site $i+1$, or $i-1$, respectively. (b) The lattice step size Δx is equal to the potential period L and the lattice sites are centred at the potential minima. The particle performs hops from one potential minimum to one of the neighbouring ones.

of a carrier into one cell and the moment of arrival into the next cell into which it lands. The random distribution of sites and hence the disorder of an amorphous material is incorporated into a hopping-time distribution function $\psi(\tau)$. The appropriate distribution $\psi(\tau)$, leading to the agreement with the experiments, was shown to possess the power-law form $\psi(\tau) \propto \tau^{-1-\alpha}$ with $\alpha \in (0, 1)$ [6–8]. For this range of the fractional exponent α all the moments of the distribution $\psi(\tau)$ diverge and the corresponding process has no characteristic timescale, thus exhibiting the phenomenon of *ageing*. As a result, the process undergoes subdiffusion [9–11], i.e. the mean square displacement grows in the absence of an external force slower than linearly in time, $\langle \delta r^2(t) \rangle \sim t^\alpha$ $(0 < \alpha < 1)$.

In the original study of fractional transport in the context of anomalous transport in semiconductors, an ensemble of carriers executing a random walk, when biased by an electric field, was studied [6, 5]. In the present paper our focus is different: We instead address the problem of the carriers executing a random walk in a spatially varying periodic potential. This situation is representative of many applications occurring in areas such as in condensed matter physics, chemical physics, nanotechnology, and molecular biology, to name but a few. For those applications it is of the utmost importance to account for the spatial variation of the transport process [12–17].

Our work is set up as follows: in section 2 we propose the model and define the theoretical and numerical problem. In section 3 we recall some prior results about the biased CTRW [18] and a CTRW proceeding in a washboard potential [19]. In section 4 the formula for the effective fractional diffusion coefficient in a periodic potential $U_0(x) = U_0(x + L)$ with period L is derived and the theoretical result is corroborated by numerical simulations of the CTRW for different shapes of periodic potential. Finally, we address the problem of particles spreading anomalously in a periodic potential also in the light of the time evolution of the space probability density, as compared to the case with normal diffusion.

2. Set-up of the model

Following the general picture of the CTRW we introduce a one-dimensional lattice $\{x_i = i\Delta x\}$ with a lattice period Δx and $i = 0, \pm 1, \pm 2, \ldots$. After a random residence time τ a particle at site i hops to site $i \pm 1$ with a probability $q_i^{\pm}$ (see figure 1(a)): the sites here correspond to the cells in [6]. The random time τ is extracted from a residence time distribution $\psi(\tau)$. A suitable

possible choice for $\psi(\tau)$ is a Mittag–Leffler distribution defined by

$$\psi_i(\tau) = -\frac{\mathrm{d}}{\mathrm{d}\tau} E_\alpha(-(\nu_i\tau)^\alpha), \qquad \text{with } E_\alpha(-(\nu_i\tau)^\alpha) = \sum_{n=0}^{\infty} \frac{[-(\nu_i\tau)^\alpha]^n}{\Gamma(n\alpha+1)}. \tag{1}$$

The quantity ν_i is the time-scaling parameter at lattice site i.

The CTRW with the Mittag–Leffler residence time density can be described through a fractional master equation for the site populations $P_i(t)$ [19, 20]; i.e.

$$D_*^\alpha P_i(t) = f_{i-1}P_{i-1}(t) + g_{i+1}P_{i+1}(t) - (f_i + g_i)P_i(t), \tag{2}$$

with the Caputo fractional derivative D_*^α [21] on the left-hand side defined by

$$D_*^\alpha \chi(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \mathrm{d}t' \frac{1}{(t-t')^\alpha} \frac{\partial}{\partial t'} \chi(t'). \tag{3}$$

The quantities $f_i = q_i^+ \nu_i^\alpha$ and $g_i = q_i^- \nu_i^\alpha$ in the fractional master equation (2) are referred to as the fractional forward and backward rates. Using the normalization condition for the splitting probabilities, i.e. $q_i^+ + q_i^- = 1$, one obtains that

$$q_i^+ = f_i/(f_i + g_i), \qquad q_i^- = g_i/(f_i + g_i), \tag{4}$$

$$\nu_i = (f_i + g_i)^{1/\alpha}. \tag{5}$$

For an arbitrarily shaped potential landscape $U(x)$ the fractional rates can be chosen as

$$f_i = (\kappa_\alpha/\Delta x^2) \exp[-\beta(U_{i+1} - U_i)/2], \tag{6}$$

$$g_i = (\kappa_\alpha/\Delta x^2) \exp[-\beta(U_{i-1} - U_i)/2]. \tag{7}$$

Here $U_i \equiv U(i\Delta x)$ and $\beta = 1/k_\mathrm{B}T$ is the inverse temperature; κ_α is the fractional free diffusion coefficient with dimension $\mathrm{cm}^2\ \mathrm{s}^{-\alpha}$. The form (6) and (7) of the fractional rates ensures that the Boltzmann detailed balance relation is satisfied, i.e. $f_{i-1}/g_i = \exp[\beta(U_{i-1} - U_i)]$. The lattice period Δx must fulfil the condition $U''(x)\Delta x \ll 2U'(x)$ in order to ensure the smoothness of the potential. In the case of a periodic potential this implies in particular that the lattice step size Δx is much smaller than the potential period L, $\Delta x \ll L$. Furthermore, in order to recover the continuous limit addressed below, the condition $|\beta(U_{i\pm1} - U_i)| \ll 1$ must be obeyed.

In the space-continuous limit the CTRW with the Mittag–Leffler residence time density can be described through the fractional Fokker–Planck equation [10, 19, 22, 23],

$$D_*^\alpha P(x,t) = \left[\frac{\partial}{\partial x}\frac{U'(x)}{\eta_\alpha} + \kappa_\alpha \frac{\partial^2}{\partial x^2}\right] P(x,t). \tag{8}$$

Here, $P(x,t)$ is the probability density and a prime stands for the derivative with respect to the space coordinate. The quantity η_α denotes the generalized friction coefficient, possessing the dimension $\mathrm{kg\ s}^{\alpha-2}$. It is related to the bare fractional anomalous diffusion coefficient κ_α through $\eta_\alpha\kappa_\alpha = k_\mathrm{B}T$.

With this material at hand we have defined our theoretical problem as well as the numerical procedure. In the simulations of the CTRW we use for $\alpha \in (0, 0.8]$ a Pareto residence time distribution, i.e.

$$\psi_i(\tau) = -\frac{\mathrm{d}}{\mathrm{d}\tau} P_\alpha(\nu_i\tau), \qquad \text{with } P_\alpha(\nu_i\tau) = \frac{1}{\left[1 + \Gamma(1-\alpha)^{1/\alpha}\nu_i\tau\right]^\alpha}, \tag{9}$$

instead of the Mittag–Leffler one, as for every $0 < \alpha < 1$ the long-time behaviour of the system is determined solely by the tail of the residence time distribution [24]. For $\alpha > 0.8$ the Mittag–Leffler density (1) is employed. For $\alpha = 1$ the Mittag–Leffler density transforms into the exponential distribution, covering the regime of normal overdamped Brownian motion. The

spatial lattice step in our simulations is $\Delta x = 0.001$, measured in units of the spatial period L. The energy is measured in units of the potential amplitude A, and the time unit is set as $\tau_0 = (\eta_\alpha L^2/A)^{1/\alpha}$. For a detailed description of the algorithm for the numerical simulations and of the employment of the Pareto or Mittag–Leffler distribution, we refer readers to the comprehensive work in [25].

3. Biased CTRW and CTRW in a washboard potential

3.1. Biased CTRW

The anomalous diffusion that is biased by a constant external force F is a well established phenomenon found in many different systems. For the biased CTRW the fractional rates (6) and (7) become site-independent, $f_i \equiv f$ and $g_i \equiv g$, as $U_{i\pm1} - U_i = \pm F\Delta x$. From the fractional master equation (2) one finds then the solutions for the mean particle position and for the mean square displacement [18],

$$\langle x(t)\rangle = \langle x(0)\rangle + \frac{\Delta x(f-g)}{\Gamma(\alpha+1)}t^\alpha, \tag{10}$$

$$\langle \delta x^2(t)\rangle = \langle \delta x^2(0)\rangle + \frac{\Delta x^2(f+g)}{\Gamma(\alpha+1)}t^\alpha + \left[\frac{2}{\Gamma(2\alpha+1)} - \frac{1}{\Gamma^2(\alpha+1)}\right]\Delta x^2(f-g)^2 t^{2\alpha}. \tag{11}$$

The solutions of the corresponding fractional Fokker–Planck equation are in the same form as the ones for the fractional master equation; i.e.

$$\langle x(t)\rangle = \langle x(0)\rangle + \frac{F}{\eta_\alpha}\frac{t^\alpha}{\Gamma(\alpha+1)}, \tag{12}$$

$$\langle \delta x^2(t)\rangle = \langle \delta x^2(0)\rangle + 2\kappa_\alpha\frac{t^\alpha}{\Gamma(\alpha+1)} + \frac{F^2}{\eta_\alpha^2}\left[\frac{2}{\Gamma(2\alpha+1)} - \frac{1}{\Gamma^2(\alpha+1)}\right]t^{2\alpha}. \tag{13}$$

The comparison of the solutions (10)–(12) and (11)–(13) gives

$$\Delta x(f-g) = F/\eta_\alpha \qquad \text{and} \qquad \Delta x^2(f+g)/2 = \kappa_\alpha. \tag{14}$$

The latter equations define the anomalous current and the anomalous diffusion coefficient through the fractional rates f and g, and are of the same form as the corresponding relations for normal Brownian diffusion, determined through the corresponding escape rates.

If at a given temperature T the system is close to thermal equilibrium, the mean square displacement in the absence of an external force and the average displacement induced by a bias $F \neq 0$ are related through the *generalized Einstein relation* [9, 26, 27],

$$\langle \delta x^2(t)\rangle\big|_{F=0} = \frac{2}{\beta F}\,\langle x(t) - x(0)\rangle|_F\,. \tag{15}$$

Note that equation (15) is strictly valid only in the linear response regime, which is approached when $F \to 0$. It then leads to the generalized fluctuation-dissipation theorem

$$\kappa_\alpha = (\beta\eta_\alpha)^{-1}. \tag{16}$$

3.2. CTRW in a washboard potential

Solving in the stationary limit the fractional Fokker–Planck equation (8) for a biased periodic potential $U(x) = U_0(x) - Fx$, one finds for the mean particle position [19],

$$\langle x(t)\rangle = \langle x(0)\rangle + \frac{v_\alpha(F)}{\Gamma(\alpha+1)}t^\alpha. \tag{17}$$

The anomalous current $v_\alpha(F)$ in the washboard potential is then given by a generalized Stratonovich formula, put forward in [19], i.e.

$$v_\alpha(F) = \frac{\kappa_\alpha L[1 - \exp(-\beta F L)]}{\int_0^L \mathrm{d}x \int_x^{x+L} \mathrm{d}y \exp(-\beta[U(x) - U(y)])}. \tag{18}$$

In analogy to the case with normal Brownian motion, in order to study the fractional diffusion in a periodic or washboard potential it would seem natural to choose the lattice period Δx to be equal to the space period L and the sites to be centred at minima, as illustrated in figure 1(b). In this case the fractional rates, that we mark for such a lattice with f_j and g_j, are independent of the site j, $f_j \equiv \hat{f}$ and $g_j \equiv \hat{g}$. It was proved in [19] that considering the CTRW in the lattice $\{x_j = jL\}$, the asymptotic solution ($t \to \infty$) for the mean square displacement in a tilted periodic potential is of the same form as the solution (11) for the biased CTRW, as the equation (17) is of the same form as equation (10). The fractional rates $\hat{f}$ and $\hat{g}$, however, are no longer given by equations (6) and (7) and the model does not provide their explicit dependence on the potential.

Whereas in the washboard potential $\Delta x(\hat{f} - \hat{g})$ is equal to the generalized Stratonovich current v_α, one could expect that $\Delta x^2(\hat{f} + \hat{g})/2$ follows a generalized formula for the effective diffusion coefficient in a tilted periodic potential [28, 29], in correspondence to equations (14), because the problem can be mapped onto the case with a constant bias. However, in the long-time limit the ballistic term $\propto t^{2\alpha}$ prevails over the term proportional to t^α and the effect of the latter term is negligible: the ratio between the mean square displacement and squared average coordinate depends in the asymptotic limit only on the fractional exponent α and obeys the same result as for the biased CTRW [6, 19]. The term proportional to t^α becomes relevant for $t \to \infty$ only in the limit $\alpha \to 1$, leading to the normal diffusive behaviour, or for $F \to 0$ as $\hat{f} - \hat{g} \to 0$, i.e. for a periodic potential.

4. Fractional diffusion in a periodic potential

4.1. The mean square displacement

In this section we present our results for fractional diffusion in spatially varying, periodic potentials. We start from the expression of the mean square displacement for the particle in the periodic potential $U_0(x)$. For zero tilting the fractional rates $\hat{f}$ and $\hat{g}$ become equal and the ballistic term occurring in equation (11), reformulated for a washboard potential, thus disappears. Therefore, the asymptotic mean square displacement now reads

$$\langle \delta x^2(t) \rangle = \langle \delta x^2(0) \rangle + \Delta x^2(\hat{f} + \hat{g}) \frac{t^\alpha}{\Gamma(\alpha + 1)}. \tag{19}$$

This equation is confirmed by the numerical results, depicted in figure 2 for various values of the fractional exponent α, which is equal to the slope of the numerically evaluated curves on the logarithmic scale.

Correspondingly, the asymptotic solution of the fractional Fokker–Planck equation for the periodic potential $U_0(x)$ can be written in the form analogous to the case of the fractional diffusion in the absence of force, i.e.

$$\langle \delta x^2(t) \rangle = \langle \delta x^2(0) \rangle + 2\kappa_\alpha^{(\mathrm{eff})} \frac{t^\alpha}{\Gamma(\alpha + 1)}, \tag{20}$$

This equation defines the *effective fractional diffusion coefficient* $\kappa_\alpha^{(\mathrm{eff})}$,

$$\kappa_\alpha^{(\mathrm{eff})} = \Gamma(\alpha + 1) \lim_{t \to \infty} \frac{\langle \delta x^2(t) \rangle - \langle \delta x^2(0) \rangle}{2t^\alpha}. \tag{21}$$

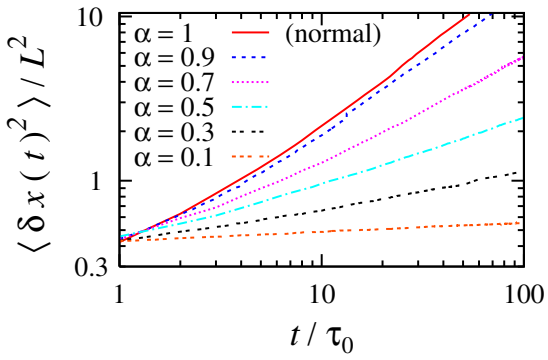

Figure 2. The mean square displacement computed numerically for the CTRW in the cosine potential $U_0(x) = A\cos(2\pi x/L)$ for different values of the fractional exponent α. The re-scaled temperature is set at $k_B T/A = 0.5$.

Also the explicit expression for the fractional rates to hop from one minimum to one of the neighbouring minima follows from equations (19) and (20), as for $\hat{f} \equiv \hat{g}$

$$\kappa_\alpha^{(\mathrm{eff})} = \frac{\Delta x^2(\hat{f}+\hat{g})}{2} \equiv \Delta x^2 \hat{f} \equiv \Delta x^2 \hat{g}. \tag{22}$$

4.2. Effective fractional diffusion coefficient

Next, a useful analytical expression for $\kappa_\alpha^{(\mathrm{eff})}$ in a periodic potential can be derived from a generalized Einstein relation. Equation (15) is valid in the linear response regime also for any periodic potential $U_0(x)$, as the problem of fractional diffusion in a periodic potential can be mapped onto the force-free case [19]. In doing so we can write

$$\kappa_\alpha^{(\mathrm{eff})} = \frac{1}{\beta}\lim_{F\to 0}\frac{v_\alpha(F)}{F} = \frac{1}{\beta}\frac{\mathrm{d}v_\alpha(F)}{\mathrm{d}F}\bigg|_{F=0}, \tag{23}$$

where $v_\alpha(F)$ is given by the generalized Stratonovich formula (18). As a central result we thus obtain the following closed, exact analytical expression for the effective fractional diffusion coefficient, reading

$$\kappa_\alpha^{(\mathrm{eff})} = \frac{\kappa_\alpha}{L^{-2}\int_0^L \mathrm{d}x \exp\left[\beta U_0(x)\right]\int_0^L \mathrm{d}y \exp\left[-\beta U_0(y)\right]}. \tag{24}$$

This expression is valid for an arbitrarily shaped, unbiased periodic potential $U_0(x)$. It reduces for $\alpha = 1$ to the corresponding formula for the normal diffusion in a periodic potential, first derived by Lifson and Jackson in [30] and independently again in [31, 32]. Our new result therefore provides the generalization for fractional diffusion processes which are anomalous.

The behaviour of equation (24) versus re-scaled temperature $k_B T/A$ is illustrated in figure 3(a) for the following periodic potentials, depicted in figure 3(b):

(i) a cosine potential,

$$U_0^{(1)}(x) = A\cos(2\pi x/L), \tag{25}$$

(ii) a double hump potential,

$$U_0^{(2)}(x) = Aa_1[\cos(2\pi x/L) + \cos(4\pi x/L)], \tag{26}$$

with the coefficient $a_1 = 16/25$, and

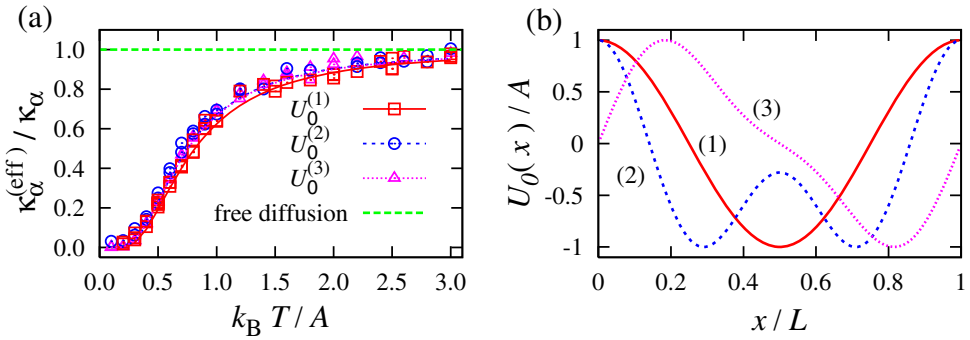

Figure 3. (a) Effective anomalous diffusion coefficient $\kappa_\alpha^{(\mathrm{eff})}$ in a periodic potential versus the re-scaled temperature $k_B T/A$. The quantity $\kappa_\alpha^{(\mathrm{eff})}$ is re-scaled by the corresponding free fractional diffusion coefficient κ_α. The theoretical curves obtained from equation (24) (lines) are compared to the numerical results (symbols). The different periodic potentials used are given by equations (25)–(27). For each potential and at given temperature the numerical points are computed for some values of α within the interval $\alpha \in [0.1, 0.9]$. (b) A comparison among the different periodic potentials (25)–(27) used for the numerics: (1) the cosine potential $U_0^{(1)}(x)$; (2) the double hump potential $U_0^{(2)}(x) - (2a_1 - 1)$; (3) the ratchet potential $U_0^{(3)}(x)$.

(iii) a ratchet potential,

$$U_0^{(3)}(x) = A[a_2 \sin(2\pi x/L) + a_3 \sin(4\pi x/L)], \tag{27}$$

with $a_2 = 85/(21\sqrt{21})$, $a_3 = 25/(21\sqrt{21})$. The coefficients a_1, a_2, a_3 are chosen such that the potentials (25)–(27) have the same amplitude A. The theoretical curves are confirmed by numerical results, depicted in figure 3 with symbols. The anomalous diffusion coefficient is computed as defined by equation (21). As the ratio $\kappa_\alpha^{(\mathrm{eff})}/\kappa_\alpha < 1$, one can conclude that, analogously to the normal case, the effect of any one-dimensional non-biased periodic field is to *suppress* the macroscopic anomalous diffusion coefficient compared to the value in the absence of force [30]. A possible enhancement may be expected in the presence of time-dependent, periodic landscape modulations as demonstrated for normal diffusion in [33–35]. Furthermore, it is to be noticed that the ratio $\kappa_\alpha^{(\mathrm{eff})}/\kappa_\alpha$ does *not* depend on the fractional exponent α and, moreover, the shape of the periodic potential $U_0(x)$ has only a small influence, as one can see by comparing the theoretical curves in figure 3(a) (note also [36, 37]).

4.3. Probability density: anomalous versus normal

In the previous section it was demonstrated that the effective fractional diffusion coefficient in a periodic potential is of the same form as the Lifson–Jackson formula for normal diffusion. This represents a further element of the formal analogy between fractional and normal diffusion, besides, for example, the validity of the generalized Stratonovich formula (18) [19] and the fact that the stationary reduced probability density is the same for both cases [25]. Here, we present additional results which support and corroborate this formal analogy further. We notice that in the absence of a bias, all the odd moments of the probability density are identically zero for both normal and fractional diffusion. As for the second moment, upon introducing the re-scaled time,

$$t' = \frac{(t/\tau_0)^\alpha}{\Gamma(1+\alpha)}, \tag{28}$$

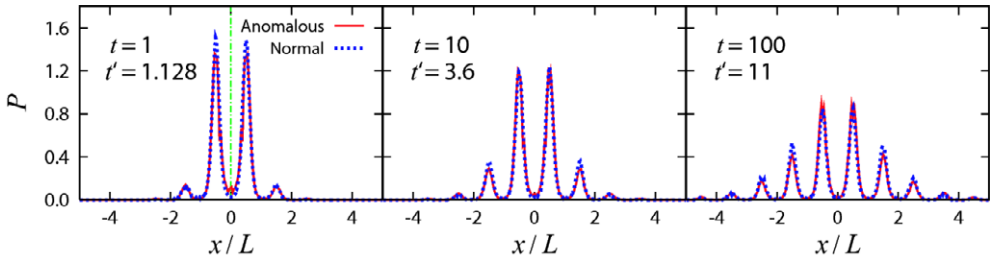

Figure 4. The time evolutions of the probability densities characterizing the anomalous and normal diffusion processes in the periodic cosine potential (25). The re-scaled temperature is $k_B T/A = 0.5$ and the fractional exponent is $\alpha = 0.5$. The anomalous probability density $P(x, t)$ cannot be distinguished from that of the normal case, $P(x, t')$, once the time has been re-scaled according to equation (28). Similar results are obtained for other values of $\alpha \in (0, 1)$ (not depicted).

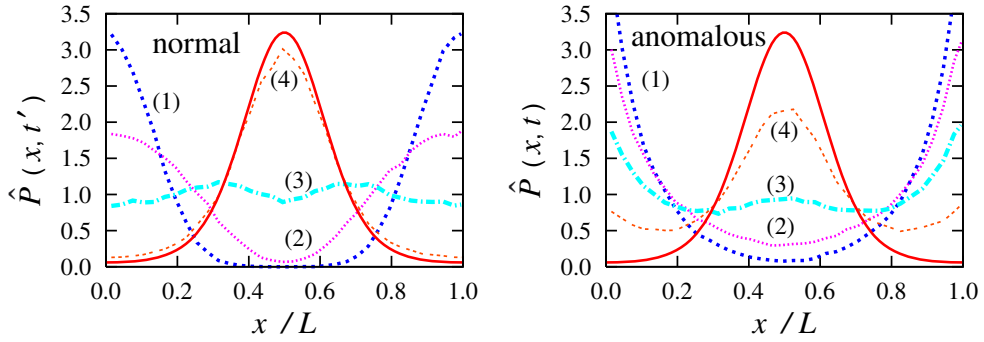

Figure 5. The different small-time evolutions of the normal (left) and anomalous (right) reduced probability densities $\hat{P}(x, t)$ and $\hat{P}(x, t')$ defined by equation (29), in the cosine potential (25). Curve labels (1)–(4) represent increasing values of re-scaled time $t' = 0.01, 0.02, 0.04, 0.11$ for the normal case and of time t for the anomalous case, related to t' through equation (28). The solid line represents the theoretical stationary solution. The re-scaled temperature is $k_B T/A = 0.5$ and $\alpha = 0.5$ for the anomalous process, as in figure 4.

it follows from equation (20) that the mean square displacement (in units of L^2) formally coincides with that of the normal diffusion case, $[\langle \delta x^2(t') \rangle - \langle \delta x^2(0) \rangle]/L^2 = 2T't'$, independently of the fractional exponent α, wherein $T' = k_B T/A$, with A the potential amplitude, is the re-scaled temperature. The study of the time evolution of the probability density is illustrated with the example in figure 4, choosing the times t for the anomalous diffusion process and the corresponding times t' for normal diffusion so that they satisfy equation (28): the probability densities for anomalous diffusion (continuous lines) and normal diffusion (dashed lines) processes are barely distinguishable from each other for sufficiently long evolution times.

In clear contrast, however, appreciable differences between the normal diffusion coordinate density $P(x, t')$ and the anomalous coordinate density $P(x, t)$ emerge for small times. This is best detected by comparing the reduced probability density, mapped onto a single spatial period

$$\hat{P}(x, t) = \sum_n P(nL + x, t), \quad n \in \mathbb{Z}, \tag{29}$$

as done in figure 5. In the normal case (figure 5 left) the two initial maxima at $x = 0$ and $x/L = 1$, due to the initial conditions $\hat{P}(x, 0) = \delta(x)$, move toward the centre and finally

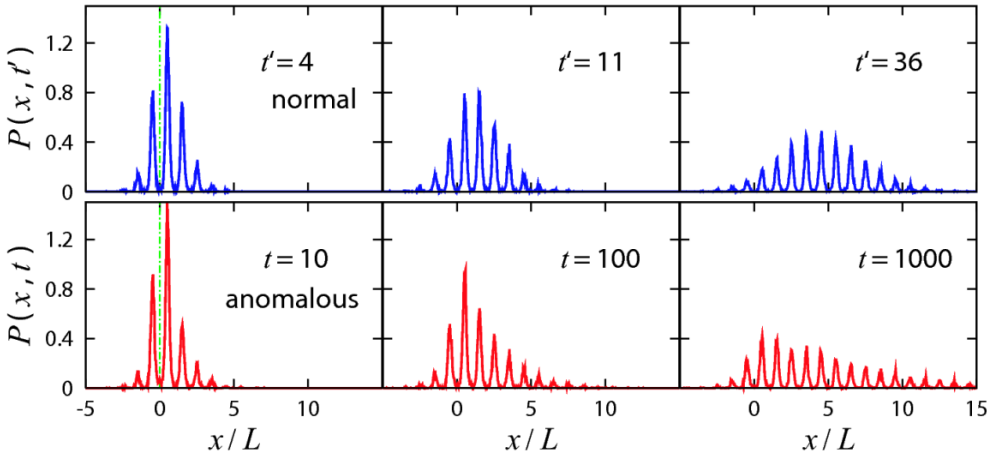

Figure 6. The time evolutions of the probability densities characterizing the normal (above) and anomalous (below) diffusion processes in a tilted cosine potential $U(x) = A\cos(2\pi x/L) - Fx$. The re-scaled temperature is $k_{\mathrm{B}}T/A = 0.5$ and the fractional exponent is $\alpha = 0.5$, as in figure 4. The tilting force is $F = 0.1 \times F_{\mathrm{cr}}$, where $F_{\mathrm{cr}} = 2\pi A/L$ is the re-scaled critical bias, corresponding to the disappearance of potential minima. For sufficiently small times the probability densities of the normal and anomalous processes are very similar. However, at larger times (in the long-time limit) the maximum of the density for normal diffusion moves with the directed current. In contrast, the mean square displacement of an ensemble of particles undergoing fractional diffusion is dominated by the ballistic contribution and the typical stretched spreading in the direction of bias is observed, while leaving the maximum of the density near the origin.

merge into the asymptotic stationary density (solid line) $\hat{P}_{\mathrm{st}}(x) = \mathcal{N}^{-1}\exp[-\beta U_o(x)]$, where $\mathcal{N} = \int_0^1 \mathrm{d}x' \exp[-\beta U_o(x')]$ is a normalization factor and $U_0(x) = A\cos(2\pi x/L)$. On the other hand, in the anomalous case the two initial maxima gradually disappear while a new peak grows at $x/L = 0.5$ and evolves into the stationary density $\hat{P}_{\mathrm{st}}(x)$.

Moreover, as soon as the process is biased by an external finite force, $F \neq 0$, a qualitative difference arises in the time evolution of the probability densities of the anomalous and the normal processes in the long-time limit as well, see also [25]. This is true even for small values of F in the linear response regime, as one can defer from figure 6. All this indicates a profound difference between a fractal diffusion dynamics that is based on the fractal Brownian motion introduced by Mandelbrot and van Ness [38] and the fractional diffusion based on the CTRW [3]. The time evolution of the density of an ensemble of particles undergoing normal diffusion can be interpreted as a superposition of a translational motion and a spreading of the initially localized density. In this case one observes the global maximum of the probability density moving in the direction of the external bias (figure 6 (above)). Instead, in the anomalous case, only a spreading of the initial density takes place, resulting in a long tail in the direction of the bias. The global maximum of the density remains close, however, to its initial position (figure 6 (below)) [25]. This intriguing behaviour is related to the presence of a ballistic contribution proportional to $t^{2\alpha}$ in the mean square displacement (see equation (11)). We remark that for α close to 1 and for small values of external bias F, at small times the term $\propto t^{\alpha}$ can prevail over the ballistic term. However, in the long-time limit the ballistic term takes over and always dominates. The latter remark may be relevant for experimental studies. It in addition also provides a crucial test that allows one to distinguish between fractal and fractional Brownian motion on a practical level.

5. Conclusion

In this work we investigated anomalous diffusion whose dynamics is governed by a fractional Fokker–Planck equation with a spatially varying, periodic potential. As a main result we derive a generalization of the celebrated Lifson–Jackson result for normal diffusion [30–32] to our case with anomalous fractional diffusion: it relates the effective fractional diffusion coefficient $\kappa_\alpha^{(\mathrm{eff})}$ in equation (24) to the bare fractional diffusion coefficient in terms of two inverse quadratures of the periodic potential only. This result is consistent with a general integral transformation connecting the solutions of normal and fractional Fokker–Planck equations in the same potential with natural, or free, boundaries [23, 39]. As a consequence, we find that as in the case with normal diffusion the effective anomalous diffusion always becomes suppressed over the bare value. This result may find ample application in diverse areas where anomalous diffusion occurs; typical examples are the case of superionic conductors [40] or for Josephson junction dynamics [17, 41] when the role of disorder may change normal diffusion into anomalous diffusion.

In addition, we contrasted the time evolution for normal diffusion with anomalous, fractional diffusion. In doing so, we find that after a proper re-scaling of time the corresponding asymptotic densities $P(x, t)$ for the coordinate x match each other. Distinct differences occur, however, at small evolution times. This time evolution of the densities drastically changes upon the application of a finite bias F. Now, the long-time evolution between normal diffusion and anomalous diffusion becomes markedly distinct as well: while the maximum of the biased normal diffusion moves with the normal, directed current, the anomalous case is dominated by a ballistic spreading that leaves the maximum of the density around the origin. Moreover, this characteristic difference can be put to work to differentiate between fractional and fractal Brownian diffusion.

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