

# Modeling of subdiffusion in space-time-dependent force fields beyond the fractional Fokker-Planck equation

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In this paper we attack the challenging problem of modeling subdiffusion with an arbitrary space-time-dependent driving. Our method is based on a combination of the Langevin-type dynamics with subordination techniques. For the case of a purely time-dependent force, we recover the death of linear response and field-induced dispersion—two significant physical properties well-known from the studies based on the fractional Fokker-Planck equation. However, our approach allows us to study subdiffusive dynamics without referring to this equation.

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## I. INTRODUCTION

In recent years, systems exhibiting anomalous subdiffusive behavior attracted growing attention in the various fields of physics and related sciences. The list of systems displaying subdiffusive dynamics is diverse and very extensive. It encompasses, among others, charge carrier transport in amorphous semiconductors, nuclear magnetic resonance, diffusion in percolative and porous systems, transport on fractal geometries and dynamics of a bead in a polymeric network, as well as protein conformational dynamics, see [1] and references therein. Many physical systems subjected to the external potential varying in time exhibit various significant properties. Therefore, it is a challenging and fundamental task to investigate the properties of ultraslow diffusion in time-dependent force fields.

The study of subdiffusive dynamics in the case of a purely time-dependent force was presented in detail in [2], giving rise to the modified fractional Fokker-Planck equation (FFPE). A similar equation was derived in [3] for the class of dichotomously alternating force fields. However, a model describing subdiffusion in an arbitrary space-time-dependent field  $F(x, t)$  is still missing. In this paper, we overcome this gap by proposing another model based on the Langevin equation and subordination technique without using the FFPEs. This is a main departure from recent papers [2,3]. Our approach establishes a general link between fractional subdiffusion and Langevin-type dynamics. Therefore, it provides good physical insight through the trajectories and allows us to analyze them using Monte-Carlo simulations [4–7]. The introduced model, describing subdiffusion in a space-time-dependent potential, recovers exactly the same physical properties as the ones obtained in [2,3] from the generalized FFPE, namely death of linear response and field-induced dispersion.

A widely accepted approach to study subdiffusive dynamics in the presence of a time-independent force field  $F(x)$  is based on the FFPE, see [8]:

$$\frac{\partial w(x, t)}{\partial t} = {}_0D_t^{1-\alpha} \left[ -\frac{\partial F(x)}{\partial x} \frac{1}{\eta} + K \frac{\partial^2}{\partial x^2} \right] w(x, t). \quad (1)$$

The above equation, in the continuous-time random walk (CTRW) framework, was derived explicitly in [9], see also [1,10]. Here, the operator  ${}_0D_t^{1-\alpha}$ ,  $\alpha \in (0, 1)$ , is the fractional derivative of the Riemann-Liouville type [11]. It introduces memory effects to the system. The constant  $K$  denotes the anomalous diffusion coefficient, whereas  $\eta$  is the generalized friction coefficient.

As shown in [4], the solution  $w(x, t)$  of Eq. (1) is equal to the probability density function (PDF) of the subordinated process

$$Y(t) = X(S_t), \quad (2)$$

where the process  $X(\tau)$  is the solution of the following Itô stochastic differential equation

$$dX(\tau) = F[X(\tau)] \eta^{-1} d\tau + (2K)^{1/2} dB(\tau), \quad (3)$$

driven by the standard Brownian motion  $B(\tau)$ . The subordinator  $S_t$  is termed as the inverse-time  $\alpha$ -stable subordinator. It is defined [12,13] as

$$S_t = \inf\{\tau: U(\tau) > t\},$$

where  $U(\tau)$  denotes a strictly increasing  $\alpha$ -stable Lévy motion [14], i.e., an  $\alpha$ -stable process with Laplace transform  $\langle e^{-kU(\tau)} \rangle = e^{-\tau k^\alpha}$ . Moreover,  $B(\tau)$  and  $S_t$  are assumed to be independent. Physical properties and methods of numerical approximation of the subordinator  $S_t$  as well as the interpretation of the subordination techniques have been discussed in detail in recent papers [4,5,10,12,13,15–18].

Formula (2) is the stochastic representation of the FFPE (1). It describes the multiple trapping scenario, in which the consecutive trapping events induced by  $S_t$  are superimposed to the Langevin dynamics (3), [19]. The role of the subordi-

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nator  $S_t$  in this representation is analogous to the role of the fractional Riemann-Liouville derivative  ${}_0D_t^{1-\alpha}$  in the FFPE, since they both give rise to the subdiffusive behavior of the system under consideration (i.e., to power-law waiting-time distributions between consecutive jumps of a particle). Every trajectory of  $S_t$  is obtained as the right inverse of the trajectory of  $U(\tau)$ . Consequently, we have

$$U(S_t) = \begin{cases} t, & t = t_j \\ t + l_t, & t \neq t_j, \end{cases} \quad (4)$$

where  $t_j, j \in \mathbb{N}$ , is the instant of time when a test particle is released from a  $j$ th trap, and  $l_t$  is a random leapover time [20–22]. For a graphical interpretation of Eq. (4) see [22]. Observe that  $l_t$  is also known as an overshoot in mathematical literature [23]. Relation (4) will play a crucial role in our further discussion.

## II. TO UNDERSTAND SUBORDINATION

The starting point of our considerations is the process  $X(S_t)$  defined in Eqs. (2) and (3), describing subdiffusion in a time-independent force field  $F(x)$ . In order to obtain a model with a time-varying force, we have to modify the subordination  $X(S_t)$ . A first, somewhat naive, attempt to solve the problem seems to be straightforward. Let us replace the time-independent force  $F(x)$  in stochastic differential equation (3) with  $F(x, \tau)$  obtaining

$$d\tilde{X}(\tau) = F[\tilde{X}(\tau), \tau] \eta^{-1} d\tau + (2K)^{1/2} dB(\tau), \quad (5)$$

and consider the subordinated process  $\tilde{Y}(t) = \tilde{X}(S_t)$ . As a consequence, the force field  $F(x, S_t)$  corresponding to  $\tilde{Y}(t)$  varies in random time  $S_t$  but not in real time  $t$ , which cannot be physically accepted. This difficulty has been recently pointed out in [3] in the context of the generalized FFPE, but not analyzed further. To visualize this effect, let us consider the following dichotomously alternating force:

$$F(x, \tau) = -cx(-1)^{\lfloor \tau \rfloor}, \quad (6)$$

where  $c$  is a positive constant and  $\lfloor y \rfloor$  denotes the integer part of  $y$ . The exemplary trajectory of the standard Brownian particle biased by this force is presented in Fig. 1.

If the initial position of the particle is assumed  $x=0$ , then, in the first time unit, the harmonic form of the force (6) yields its oscillation around the origin. After the first time unit passes, the sign of the force alters, causing dramatic change of the motion. The particle, during the second time unit, moves either to the positive or negative direction. When the second time unit passes, the sign of the force alters again to the harmonic form. The particle moves from its earlier position towards the equilibrium point, and recovers the oscillation around the origin during the third time unit. The speed of the return to the equilibrium depends on the constant  $c$  in (6). The constant  $c=10^2$  chosen in Figs. 1–3 is relatively large for better illustration of the force-switching moments (the particle returns to the equilibrium very quickly). In general, after each time unit, the sign of the force changes, switching the motion of the particle with character-

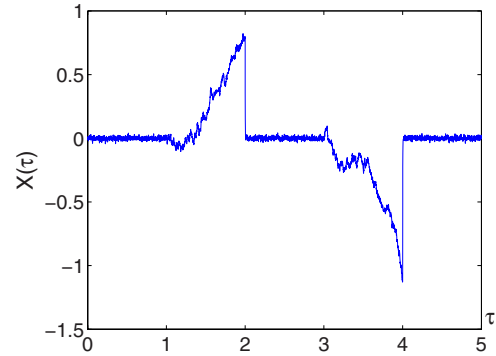


FIG. 1. (Color online) An exemplary sample path of the standard Brownian particle biased by the dichotomously alternating force (6). After each time unit the sign of the force changes, switching the motion of the particle. The particle either oscillates around zero or moves left/right. Note that only in the case of standard Brownian diffusion  $\tau=t$ . The parameters are  $c=10^2$  and  $\eta=K=1$ .

istic moves towards origin, when the force (6) takes the harmonic form.

Now, let us analyze the trajectory of the introduced process  $\tilde{Y}(t) = \tilde{X}(S_t)$  with the alternating force (6). An exemplary sample path of  $\tilde{Y}(t)$  is presented in Fig. 2. The constant intervals of the trajectory correspond to the heavy-tailed waiting time between consecutive jumps of a particle in the underlying continuous-time random walk scenario. Such constant intervals are typical for subdiffusion [4,5]. However, the shape of the trajectory confirms that the force  $F$  varies in a random time. We observe the changes of particle motion in random instants of time and not after each time unit, which is the consequence of the subordination procedure. This confirms our previous statement about the failure of such an approach.

The above considerations show that the process  $\tilde{Y}(t) = \tilde{X}(S_t)$  is not the correct model for describing subdiffusion in

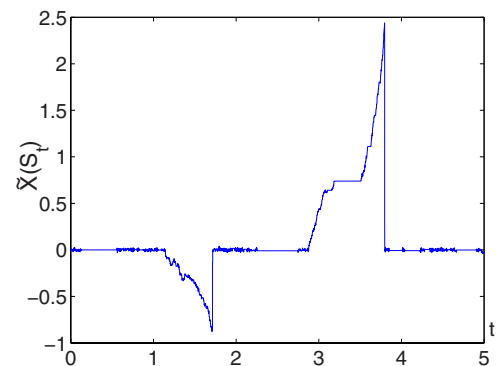


FIG. 2. (Color online) An exemplary sample path of the process  $\tilde{Y}(t) = \tilde{X}(S_t)$  with the dichotomously alternating force (6). The constant intervals of the trajectory are typical for subdiffusion. However, the shape of the trajectory indicates that the force  $F$  varies in random time, which is physically not acceptable. We observe the changes of particle motion in some random time points and not after each time unit, cf. Fig. 1. This is the consequence of the subordination procedure. The parameters are  $\alpha=0.9$ ,  $c=10^2$ , and  $\eta=K=1$ .

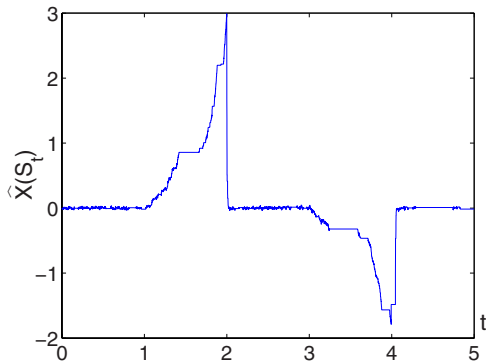


FIG. 3. (Color online) An exemplary trajectory of the process  $\hat{Y}(t)=\hat{X}(S_t)$  describing subdiffusion in a space-time-dependent potential with the dichotomously alternating force  $F(x,t)$  given by (6). The shape of the trajectory confirms that the force  $F$  varies in the real time  $t$ , since, by (4),  $U(S_t)=t$ . Note that the change of the particle motion is observed after each time unit, cf. Figs. 1 and 2. The constant intervals of the trajectory are typical for subdiffusion and represent the heavy-tailed rests of the test particle. The parameters are  $\alpha=0.9$ ,  $c=10^2$ , and  $\eta=K=1$ .

a space-time-dependent potential. However, this first attempt presented above is a step towards the right direction. We need only to eliminate the obvious drawback of the model, which is the force varying in the random time  $S_t$  but not in the real time  $t$ . To do so, we take advantage of relation (4) and modify equation (5) in the following way:

$$d\hat{X}(\tau) = F[\hat{X}(\tau), U(\tau)]\eta^{-1}d\tau + (2K)^{1/2}dB(\tau). \quad (7)$$

Next, we consider the subordinated process

$$\hat{Y}(t) = \hat{X}(S_t). \quad (8)$$

We claim that the process  $\hat{Y}(t)$  describes subdiffusion driven by the space-time-dependent force  $F(x,t)$ . Indeed, after the subordination  $\hat{X}(S_t)$ , the actual force is given by  $F[x, U(S_t)]$ . Therefore, using relation (4), we obtain that in every release moment  $t=t_j$ , the particle is biased by the force  $F(x,t)$ . In other words, we subordinate the process without subordinating the time-dependent force. So, the force corresponding to  $\hat{Y}(t)$  varies in the real time  $t$ . Additionally, the subordinator  $S_t$  introduces heavy-tailed rests of the particle, which are characteristic for subdiffusion. Thus,  $\hat{Y}(t)$  describes subdiffusion in the time-varying force field  $F(x,t)$ . As a confirmation of our result, in Fig. 3, we present an exemplary trajectory of the process  $\hat{Y}(t)=\hat{X}(S_t)$  with the dichotomously alternating force  $F(x,t)$  given by (6). The physical requirement that the force varies in the real time  $t$  is evidently fulfilled. We observe that changes of the particle motion appear exactly after each time unit. The particle, alternatively, oscillates around zero or moves towards positive/negative directions of the  $x$  axis. Observe that the motion does not have periodic character. The particle can move either to the left or to the right with the same probability, as it follows from the symmetry of the statistical picture presented in Figs. 4 and 5. The constant

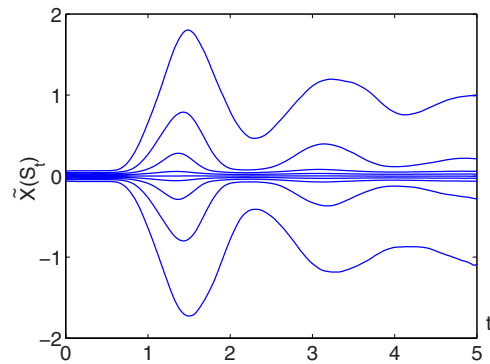


FIG. 4. (Color online) Quantile lines (10%, 20%, ..., 90%) corresponding to the process  $\tilde{Y}(t)=\tilde{X}(S_t)$  in the presence of the dichotomously alternating force (6). The lowest line is the 10%-quantile line, the second line from the bottom corresponds to the 20%-quantile line, etc. The shape of the lines indicates that the force does not switch after each time unit, thus  $F$  does not vary in the real time  $t$ . This is the consequence of the random time change after subordination. The parameters as in Fig. 2. The quantile lines were estimated by Monte-Carlo methods [4,5].

intervals of the trajectory indicate the subdiffusive character of the motion.

As an additional statistical argument in our discussion we present nine estimated quantile lines (10%, 20%, ..., 90%) corresponding to the processes  $\tilde{Y}(t)=\tilde{X}(S_t)$  and  $\hat{Y}(t)=\hat{X}(S_t)$ . The shape of the quantile lines of  $\tilde{Y}(t)=\tilde{X}(S_t)$  (Fig. 4) clearly indicates that the force does not switch after each time unit. On the contrary, the quantile lines of  $\hat{Y}(t)=\hat{X}(S_t)$  (Fig. 5) are typical for the dichotomously alternating force (6). Evidently, their shape changes after each time unit, which is another confirmation that the force varies in the real time  $t$ . Although the trajectories in Figs. 2 and 3 are similar, the corresponding quantile-line picture does not preserve these similarities. The reason for this is the fact that, contrary to

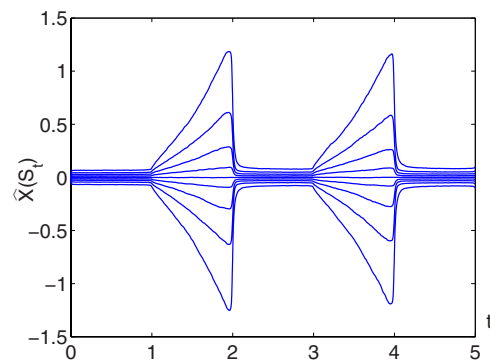


FIG. 5. (Color online) Quantile lines (10%, 20%, ..., 90%) corresponding to the process  $\hat{Y}(t)=\hat{X}(S_t)$  in the presence of the dichotomously alternating force (6). The lowest line is the 10%-quantile line, the second line from the bottom corresponds to the 20%-quantile line, etc. The shape of the lines confirms that the force  $F$  varies in the real time  $t$ . The change of their shape is observed after each time unit, cf. Fig. 4. The parameters as in Fig. 3. The quantile lines were estimated by Monte Carlo methods [4,5].

the case of  $\hat{Y}(t)=\hat{X}(S_t)$ , each trajectory of  $\tilde{Y}(t)=\tilde{X}(S_t)$  is qualitatively different, since the random moments of force switching are different for every realization. The symmetry of the quantile lines wrt.  $t$  axis in Figs. 4 and 5 is physically justified by the fact that both noise and potential in the models are symmetric. Recall that a  $p$ -quantile line,  $p \in (0, 1)$ , for a stochastic process  $Y(t)$  is a function  $q_p(t)$  given by the relationship  $\text{Pr}[Y(t) \leq q_p(t)] = p$  [14]. The Monte-Carlo methods of the presented numerical results are based on the classical Euler scheme applied for subordinators [4].

### III. DEATH OF LINEAR RESPONSE AND FIELD-INDUCED DISPERSION

The validity and usefulness of the introduced model  $\hat{Y}(t)$  can be verified now by considering some special cases of a space-time-dependent force  $F(x, t)$ . The first special case is the time-independent force  $F(x, t) = F(x)$ . In such a setting,  $\hat{Y}(t)$  reduces to the process defined by Eqs. (2) and (3). Therefore, the PDF of  $\hat{Y}(t) = Y(t)$  obeys the dynamics of the FFPE (1).

More interesting results are obtained in the case of a purely time-dependent force  $F(x, t) = F(t)$ . Then, by Eqs. (7) and (8),  $\hat{Y}(t)$  takes the form

$$\hat{Y}(t) = \eta^{-1} \int_0^{S_t} F[U(\tau)] d\tau + (2K)^{1/2} B(S_t). \quad (9)$$

It can be shown that the integral in the above formula is equal to

$$\int_0^{S_t} F[U(\tau)] d\tau = \int_0^t F(u) dS_u = S_t F(t) - \int_0^t S_u F'(u) du. \quad (10)$$

Using this result and methods of calculating integrals of inverse subordinators [24], we calculate moments of the process  $\hat{Y}(t)$ . For the first moment  $m_1(t) = \langle \hat{Y}(t) \rangle$  we have

$$\dot{m}_1(t) = [\Gamma(\alpha) \eta]^{-1} F(t) t^{\alpha-1},$$

which gives

$$m_1(t) = \frac{1}{\Gamma(\alpha) \eta} \int_0^t F(u) u^{\alpha-1} du. \quad (11)$$

For the second moment  $m_2(t) = \langle \hat{Y}^2(t) \rangle$  we get

$$\dot{m}_2(t) = 2[\Gamma(\alpha) \eta]^{-1} F(t) \frac{d}{dt} \int_0^t (t-u)^{\alpha-1} m_1(u) du + \frac{2K}{\Gamma(\alpha)} t^{\alpha-1}.$$

Therefore,

$$m_2(t) = \sigma_1(t) + \sigma_2(t) \quad (12)$$

with

$$\sigma_1(t) = 2[\Gamma(\alpha) \eta]^{-1} \int_0^t ds F(s) \frac{d}{ds} \int_0^s (s-u)^{\alpha-1} m_1(u) du$$

and

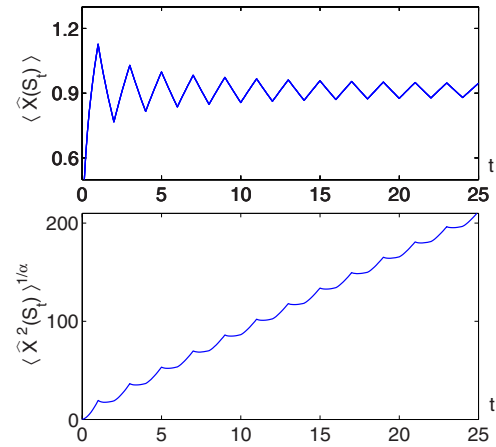


FIG. 6. (Color online) The first two moments of the process  $\hat{Y}(t) = \hat{X}(S_t)$  with periodic rectangular driving force, evaluated using expressions (14) and (15). In the top panel the mean particle position stagnates. This effect is termed “death of linear response” [2]. The linear growth of  $\langle \hat{X}^2(S_t) \rangle^{1/\alpha}$  in the bottom panel means that the asymptotic growth of the field-dependent second moment is given by  $t^\alpha$ . This is the manifestation of the effect called “field-induced dispersion” [2,3]. The parameters are  $\alpha=0.4$ ,  $\eta=f_0=1$ , and  $K=1/2$ .

$$\sigma_2(t) = \frac{2K}{\Gamma(\alpha)} \int_0^t u^{\alpha-1} du = \frac{2K}{\Gamma(\alpha+1)} t^\alpha.$$

Surprisingly, nontrivial expressions (11) and (12) for the first two moments of  $\hat{Y}(t)$  are exactly the same as the ones obtained in [2] for the generalized FFPE

$$\frac{\partial w(x, t)}{\partial t} = \left[ -\frac{F(t)}{\eta} \frac{\partial}{\partial x} + K \frac{\partial^2}{\partial x^2} \right] {}_0 D_t^{1-\alpha} w(x, t). \quad (13)$$

Moreover, in the presence of the periodic force  $F(t) = f_0 \sin(\omega t)$ , the process  $\hat{Y}(t)$  displays two significant properties, namely, “death of linear response” and “field-induced dispersion” (see [2,17,25] for the details). These properties evidently justify physically our approach, cf. Fig. 6. Let us emphasize that by the Monte Carlo methods from explicit integral representation (9) one can numerically calculate all the moments of  $\hat{Y}(t)$ .

For the periodic rectangular driving force (6) studied in [3], using (10), we obtain the following elegant and useful representation:

$$\hat{Y}(t) = \eta^{-1} f_0 (-1)^N S_t - 2 \eta^{-1} f_0 \sum_{i=1}^N (-1)^i S_i + (2K)^{1/2} B(S_t),$$

where  $N < t \leq N+1$ . The above formula immediately implies that the explicit form of the first moment reads

$$\langle \hat{Y}(t) \rangle = \frac{\eta^{-1} f_0}{\Gamma(\alpha+1)} (-1)^N t^\alpha - \frac{2 \eta^{-1} f_0}{\Gamma(\alpha+1)} \sum_{i=1}^N (-1)^i i^\alpha. \quad (14)$$

This result agrees with the one derived by a different method in [3], where it was also shown that the mean square dis-



placement grows as  $t^\alpha$ . Moreover, we get the exact result for the second moment,

$$\langle \hat{Y}^2(t) \rangle = \frac{2(\eta^{-1}f_0)^2}{\Gamma(2\alpha+1)} t^{2\alpha} - 4(\eta^{-1}f_0)^2 (-1)^N \sum_{i=1}^N (-1)^i \langle S_i S_t \rangle + 4(\eta^{-1}f_0)^2 \sum_{i,j=1}^N (-1)^{i+j} \langle S_i S_j \rangle + \frac{2K}{\Gamma(\alpha+1)} t^\alpha, \quad (15)$$

where

$$\langle S_u S_t \rangle = \frac{u^{2\alpha}}{\Gamma(2\alpha+1)} + \frac{\alpha}{\Gamma^2(\alpha+1)} \int_0^u (t-y)^\alpha y^{\alpha-1} dy$$

for  $u \leq t$ . Using (14) and (15) one verifies that the properties “death of linear response” and “field-induced dispersion” are present also in the case of a periodic rectangular driving force, see Fig. 6, without referring to the FFPE methodology.

#### IV. CONCLUSIONS

The paper introduces an approach to studying of subdiffusion without referring to the FFPE. It is based on the Langevin-type equation and subordination, therefore it provides good physical insight through the trajectories of the studied process. We have proposed a general model (7) and (8) describing subdiffusion in a space-time-dependent potential, which recovers exactly the same physical properties as the ones obtained in [2,3] from the generalized FFPE (13). Additionally, an extension of the model to a more general class of noises (e.g. Lévy noise), is straightforward by the method of [5], see also [26–28]. Namely, Eq. (7) is replaced by

$$d\hat{X}(\tau) = F[\hat{X}(\tau), U(\tau)] \eta^{-1} d\tau + K^{1/\mu} dL_\mu(\tau), \quad (16)$$

where  $L_\mu$ ,  $0 < \mu \leq 2$ , is a  $\mu$ -stable Lévy motion [14]. This suggests the following modified FFPE with Lévy flights and space-time-dependent force  $F(x, t)$ :

$$\frac{\partial w(x, t)}{\partial t} = \left[ -\frac{\partial}{\partial x} \frac{F(x, t)}{\eta} + K \nabla^\mu \right] {}_0 D_t^{1-\alpha} w(x, t), \quad (17)$$

where  $\nabla^\mu$  is the Riesz fractional derivative. The occurrence of the operator  ${}_0 D_t^{1-\alpha}$  is induced by the heavy-tailed waiting times between successive jumps of the particle, whereas  $\nabla^\mu$  is related to the heavy-tailed distributions of the jumps. Let us note that a crucial point in the justification of the above claim is the fact shown in this paper that the force  $F(x, t)$  should not be subordinated (compare the discussion of Figs. 1–3), meaning that it must appear to the left of the fractional derivative  $D_t^{1-\alpha}$ , but to the right of the partial derivative  $\frac{\partial}{\partial x}$ . For a special case  $\mu=2$  this fact was also formulated in [3]. However, our detailed analysis presented in Sec. II adds some different supporting arguments.

At this stage of understanding the problem, one does not know if modified FFPE (17) holds for arbitrary space-time-dependent force  $F(x, t)$ . For physical arguments see [3]. However, we propose here an alternative approach (7) or (16) for subdiffusive dynamics in space-time-dependent force fields. This paper demonstrates that the subordination technique is useful when applied correctly to the process, but not to the time-dependent force field. Since our model is based on the Langevin-type equation (7) or (16), it allows for both analytical and numerical study of subdiffusive dynamics [4–6] without referring to (13) and (17).

Finally, let us underline that in cases where we already know the FFPE, our approach recovers physical properties of subdiffusion. For example, it is demonstrated in Sec. III that one can derive such significant properties as “death of linear response” and “field induced dispersion” from Eq. (7) solely. This is the main difference between our approach and the recent works [2,3].

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