Anomalous transport in external fields: Continuous time random walks and fractional diffusion equations extended

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(Received 9 April 1998)

The continuous time random walk (CTRW) in a homogeneous velocity field and in arbitrary force fields is studied. Within the extended CTRW scheme, anomalous transport properties due to long-tailed waiting time or jump length distributions are consistently introduced. The connections with generalised diffusion equations in a potential field are discussed, these equations being of fractional order. In particular, the problems of a constant and a Hookean (linear) force, i.e., of a linear and a parabolic potential, are worked out. [S1063-651X(98)12108-6]

PACS number(s): 05.40.+j, 05.60.+w

I. INTRODUCTION

In connection with the growing interest in the physics of complex systems, anomalous transport properties and their description have received considerable interest. They find application in a wide field ranging from physics and chemistry to biology and medicine [1–4]. Among others, two powerful schemes have been established to account for the typical features of transport in complex systems: Lévy statistics, and non-Gaussian propagators, i.e., processes where Fick's second law is no longer valid. On the one hand, dating back to the 1960s, there is the continuous time random walk (CTRW) theory, which allows one to extend classical Brownian random walks to variable jump lengths and waiting times between successive jumps, both drawn from appropriate probability density functions (PDF's), that may belong to Lévy stable laws and therefore do not possess a finite variance or even a first moment [5–8]. The CTRW with long-tailed waiting time PDF's had originally been launched for the description of anomalous charge carrier transport in semiconductors [6,9]. On the other hand, there have been generalizations of the diffusion equation including derivatives of arbitrary order, so-called fractional diffusion equations [10]. In particular, the careful study of fractional relaxation equations [11] was a considerable initiator in the promotion of fractional equations. Whereas the CTRW theory has the clear advantage of being based directly on physically motivated random walk schemes, the fractional equation is often introduced *ad hoc* and is thus of a phenomenological character. Fractional equations can often be solved analytically in a closed form, thus also enabling one to calculate the spectral functions [12,13] which are, e.g., important in NMR or dynamic scattering. Here we will investigate the interrelation between CTRW processes and generalized fractional equations in a comparative sense, the meaning of which will be explained below.

Anomalous diffusion is characterized by a mean squared displacement (MSD)

$$\langle(\Delta x)^2\rangle(t)\equiv\langle x^2\rangle(t)-\langle x\rangle^2(t)\sim Dt^{\gamma}, \tag{1}$$

with $\gamma\neq 1$, deviating from the linear Fickean MSD. Note that we use $\langle(\Delta x)^2\rangle$ instead of $\langle x^2\rangle$, as we will encounter cases where the first moment does not vanish. D is a generalized diffusion coefficient of the dimension length^2/time$^{\gamma}$. Such a scaling of $\langle(\Delta x)^2\rangle$ as given in Eq. (1) can be found in a rich variety of physical cases [1–3]. Here we restrict ourselves to one dimension. Similar considerations, however, can easily be used to generalize our approach to higher dimensions.

The CTRW scheme is characterised by a jump PDF for a random walker on a regular lattice. This jump PDF $\psi(x,t)$ is the probability density that the walker makes a jump after some waiting time t of the length x. Here we mainly consider the case where the jump length and the waiting time PDF are decoupled, $\psi(x,t)=\psi(t)\lambda(x)$. The coupled case $\psi(x,t)=\lambda(x)p(t|x)$ is applied in Sec. II. For a detailed discussion of both cases, see Refs. [8,14,15]. Here $\psi(t)$ is the waiting time PDF and $\lambda(x)$ is referred to as the jump length PDF. $p(t|x)$ denotes a conditional probability relating the jump length and waiting time. One can then show that, in Fourier-Laplace space, the PDF $\varrho(x,t)$, to find the walker at a given place x at time t, is given by [8]

$$\varrho(k,u)=\frac{1-\psi(u)}{u}\frac{1}{1-\psi(k,u)}, \tag{2}$$

where here and in the following we indicate transforms by their explicit dependence on the appropriate variables, these being k for the wave variable in Fourier space, and u for the Laplace variable corresponding to the time. The simplest choice of a Poissonian waiting time and a Gaussian jump length distribution leads directly back to Fick's second law, the standard diffusion equation. In Eq. (2), the term $[1-\psi(u)]/u$ is the Laplace transformed sticking probability

$$\Phi(t)=1-\int_0^t dt'\,\psi(t'), \tag{3}$$

the probability of not having made a jump until time t. CTRW processes are characterized by the existence, or nonexistence, of a characteristic time

$$\langle \tau \rangle = \int dt \; t\psi(t), \tag{4}$$

and the second moment

$$\sigma^2 = \int dt \int dx \; x^2 \psi(x,t). \tag{5}$$

Diverging $\langle \tau \rangle$ or σ^2 comes about due to the introduction of broad distributions of either the waiting time or the jump length distributions. Especially the divergence of $\langle \tau \rangle$, intimately related to the asymptotic behavior $\psi(t) \sim (t/\tau)^{-1-\gamma}$, $0<\gamma<1$ [2,3,8,9], leads to memory effects in time, characterized through the temporal fractional differential operator in the corresponding generalized diffusion equations. The notion of memory effects is widespread in complex systems; see, e.g., Refs. [3,16,17] and references therein.

The CTRW theory was developed for regular lattices, sometimes augmented with a boundary condition [6–8]. There has been little attempt to generalize it to the case where the random walk takes place under the influence of an external potential. Here we develop an extended CTRW scheme and investigate several special cases, these being a homogeneous velocity field, a constant force, and a Hookean force (harmonic potential). The consequences of the occurring biases are discussed through the shape of the distribution function in Fourier-Laplace space, $\varrho(k,u)$, and the moments $\langle x \rangle$ and $\langle x^2 \rangle$. We find interesting dependencies of the moments on time. Especially in the harmonic potential case, the results elucidate the competition of the diffusive spreading and the restoring force, trying to confine the motion.

There has also been a recent effort to investigate the relationship between the CTRW and the fractional diffusion equation approaches [18–21,50]. Here we use the CTRW scheme, in order to establish fractional order diffusion equations consistently in a potential field. The equations we find are unique, as via the derivation the Riemann Liouville calculus in the integral form is determined. Also, each term of the equations has a fixed fractional order. In this sense the fractional equations may be viewed as extensions of the CTRW approach for small x and t [18].

The paper is organized as follows. In Sec. II we discuss the CTRW process in a homogeneous and uniform velocity field. The case of a constant force acting upon the random walk is shown to differ from this case in the anomalous regimes. Here we also introduce the concepts of different weights moving to the left or to the right, which we will use in Sec. IV to introduce nonconstant forces. The Fourier-Laplace representation turns out to be operator valued. In Sec. V we deal with the special and physically important case of an harmonic potential field, i.e., a linear Hookean force. Finally, we draw our conclusions, and summarize fractional calculus and the estimation of a summation, in the Appendices.

II. CONSTANT VELOCITY: DIFFUSION-ADVECTION PROBLEM

A modified CTRW scheme in a velocity field $v(x)$ was introduced in Ref. [22], and applied to an extended Taylor flow picture in Ref. [23]. In this modified version, the particles get stuck while they await the next jump. This may be reasonable in a flow through a porous medium where the particles can be trapped in pores. However, in the physical problem of a freely moving fluid, one would expect that the particles should be dragged along the velocity field while they wait. In this section, we present an exact model within the framework of the CTRW, and also discuss two different cases of partial sticking in a laboratory matrix.

For a uniform homogeneous velocity field v, we introduce the similarity variable $\xi = x - vt$ for the moving frame. This reduces the problem to the standard CTRW problem which simply has to be transformed to the laboratory frame.

In the rest frame of the fluid, the frame moving with velocity v relative to the laboratory frame, the jump PDF is given by the standard CTRW expression $\psi(x,t)$. Therefore, following the Galilei transformation to the laboratory frame, the jump PDF there, $\phi(x,t)$, can be expressed as

$$\phi(x,t) = \psi(x - vt, t). \tag{6}$$

To see the consequences to the CTRW process in the laboratory frame, we need to calculate the Fourier-Laplace transform of Eq. (6). Employing the standard theorems of Fourier and Laplace transforms [24], one finds

$$\phi(k,t) = e^{-ivtk} \psi(k,t) \tag{7}$$

in Fourier time space, and

$$\phi(k,u) = \psi(k, u + ivk) \tag{8}$$

in Fourier-Laplace space. Here we note the difference when compared to the approach in Refs. [22,23]. There, due to the choice of $\phi(k,u)$, the variables (k,u) remain uncoupled, whereas, in our approach, u and k are coupled via v. The meaning of the Galilei transformation in Eq. (6) within the CTRW framework is the following. After a waiting time t, drawn from the waiting time PDF $\psi(t)$, the jump length of the particle is corrected by the distance covered by the moving environment during that time. That is, the particle is effectively dragged along with the fluid.

A. Brownian motion in a constant velocity field

First, consider the case where we find a finite characteristic time τ and a finite variance σ^2. In the $(k,u) \to (0,0)$ limit, we have

$$\phi(k,\mu) = \frac{1}{1 + (u + ivk)\tau} \, e^{-\sigma^2 k^2} \sim 1 - (u + ivk)\tau - \sigma^2 k^2 \tag{9}$$

for the jump PDF, where we assumed a Gaussian jump length, and a Poissonian waiting time distribution. From Eq. (2) and $\phi(k,u)$, we obtain

$$\varrho(k,u) = \frac{1}{u + ivk + \sigma^2 \tau^{-1} k^2}, \tag{10}$$

which leads to

$$u\varrho - 1 = -ivk\varrho - Dk^2 \varrho, \tag{11}$$

with $D=\sigma^2/\tau$. Assuming the initial condition $\varrho(x,0)=\delta(x)$, the following partial differential equation is derived:

$$\dot{\varrho}(x,t)+v\varrho'=D\varrho'' \tag{12}$$

in (x,t) space, which is the diffusion-advection equation [25,26]. The moments of the PDF $\varrho(x,t)$ can be calculated directly from $\varrho(k,u)$ via the relation

$$\langle x^n\rangle(u)=i^n \lim_{k\to 0}\frac{d^n\varrho}{dk^n} \tag{13}$$

and a Laplace inversion. One thus arrives at the well-known results

$$\langle x\rangle(t)=vt, \tag{14a}$$

$$\langle x^2\rangle(t)=2Dt+v^2t^2, \tag{14b}$$

$$\langle(\Delta x)^2\rangle(t)=2Dt \tag{14c}$$

with a linear MSD. In Eq. (14b) we recognize the sum of the ''molecular'' diffusion and the contribution of the velocity field. In his notation, Lévy calls the equivalent to D the velocity of spreading (*vitesse de dispersion*), and the equivalent to v the probable velocity (*vitesse probable*) (Ref. [25], p. 66).

B. Dispersive motion in a constant velocity field

Next let us consider the case of a diverging characteristic time $\langle\tau\rangle\to\infty$ and a finite variance $\sigma^2<\infty$. This case can be modeled via a waiting time distribution $\psi(u)=1/[1+(u\tau)^\gamma]$ in Laplace space and a Gaussian jump length PDF, as before. We encounter a situation where the Laplace transform of the sticking probability, [Eq. (3)] is

$$\Phi(u)=\frac{1-\psi(u)}{u}\sim\tau(u\tau)^{\gamma-1} \tag{15}$$

in the rest frame, which is explicitly dependent on u. To preserve the Galilei invariance

$$\varrho(k,u)\to\varrho(k,u+ikv) \tag{16}$$

of the propagator which is defined through Eqs. (2) and (3), we now have to choose

$$\Phi(u)\to\Phi(u+ivk)\sim\tau^\gamma u^{\gamma-1}\times\left(1+i(\gamma-1)vu^{-1}k-\frac{(\gamma-1)(\gamma-2)}{2}v^2u^{-2}k^2\right) \tag{17}$$

for the sticking probability in the laboratory frame, expanding up to second order in k. This means that we have to assume that the particle is dragged along with the velocity field while it awaits a jump. The choice of $\Phi(u)=\phi(k,u)|_{k=0}$, in accordance with $\psi(u)=\psi(k,u)|_{k=0}$ in standard CTRW theory, would violate the Galilei invariance of the problem, leading to a partial sticking in the laboratory matrix, as we will discuss in Sec. II D.

We combine Eq. (17) with

$$\phi(k,u)=\frac{1}{1+(u\tau+iv\tau k)^\gamma}e^{-\sigma^2k^2}\sim 1-(u\tau)^\gamma\times\left(1+i\gamma vu^{-1}k-\frac{\gamma(\gamma-1)}{2}v^2u^{-2}k^2\right)-\sigma^2k^2, \tag{18}$$

and thus arrive at the Fourier-Laplace propagator

$$\varrho(k,u)=\frac{1}{u+ivk}\frac{1}{1+Dk^2u^{-\gamma}}\sim\frac{1}{u+ivk+Dk^2u^{1-\gamma}} \tag{19}$$

in the $k\to 0$ and $u\to 0$ limits.

We again compute the moments, and find

$$\langle x\rangle(t)=vt, \tag{20a}$$

$$\langle x^2\rangle(t)=\frac{2D}{\Gamma(1+\gamma)}t^\gamma+v^2t^2, \tag{20b}$$

$$\langle(\Delta x)^2\rangle(t)=\frac{2D}{\Gamma(1+\gamma)}t^\gamma. \tag{20c}$$

That is, we have the simple result that the particle moves dispersively in the rest frame and the distribution is shifted by the dragging. We will see below (Sec. II D) that this case is significantly different from the case of partial sticking in the laboratory matrix. Of course, for the limit $\gamma\to 1$, we come back to the standard diffusion-advection problem.

The corresponding generalized diffusion equation to the result in Eq. (19) can easily be established [18,20], the result being

$$\dot{\varrho}(x,t)+v\varrho'=D\frac{\partial^{1-\gamma}\varrho''}{\partial t^{1-\gamma}}. \tag{21}$$

Here, on the right-hand side, we find a fractional differentiation of order $(1-\gamma)$, whereas the left-hand side preserves the shape of the standard diffusion-advection equation. In the dispersive case underlying Eq. (21), this fractional differential equation, together with the initial condition $\varrho_0(x)=\delta(x)$, and assuming natural boundary conditions, contains the same information as the CTRW formalism, leading to Eq. (19). For both approaches we find a stretched Gaussian solution in the asymptotic limit. Note that Eq. (21) can be recast in the form [27]

$$\frac{\partial^\gamma\varrho}{\partial t^\gamma}-\frac{t^{-\gamma}\delta(x)}{\Gamma(1-\gamma)}+\frac{\partial^{\gamma-1}v\varrho'}{\partial t^{\gamma-1}}=D\varrho'', \tag{22}$$

where now the initial condition is directly incorporated. Both Eqs. (21) and (22) reduce to Eq. (12) for $\gamma\to 1$.

C. Enhanced motion in a constant velocity field

Let us now come to the case of finite $\tau<\infty$ and diverging $\sigma^2=\infty$. Here we take a Poissonian waiting time and Lévy jump length distribution which we write in Fourier space in the form $\lambda(k)=e^{-\sigma^\beta|k|^\beta}$. In the same spirit as before, we are led to the result

$$\varrho(k,u)=\frac{1}{u+ivk+D|k|^{\beta}}, \tag{23}$$

with the generalized diffusion constant σ^{β}/τ. The divergence of the second moment underlying Eq. (23) is due to the possible occurrence of very long jumps which are so characteristic for *Lévy flights*. In (x,t) space, the fractional diffusion equation [18]

$$\dot{\varrho}+v\varrho'=D\mathcal{R}^{\beta}\varrho, \tag{24}$$

is found corresponding to Eq. (23), where $\mathcal{R}^{\beta}$ is the Riesz derivative defined via

$$\mathcal{F}[\mathcal{R}^{\beta}f(x);k]=i^{[\beta]+1}|k|^{\beta}f(k), \tag{25}$$

see Ref. [28]. Here, we choose the $i^{[\beta]+1}$ prefactor to preserve the standard differentiation theorem of the Fourier transform. $[\cdot]\equiv\mathrm{int}(\cdot)$ denotes the Landau bracket taking the integer value of its argument.

Dealing with these kinds of stable distributions, one often calculates the fractional (lower order) moments [29]. Restricting ourselves, for example, to the range $1<\beta<2$, however we can calculate the mean

$$\langle x\rangle(t)=vt, \tag{26}$$

which turns out to be the same as in the normal diffusion advection case. Thus $\langle x\rangle(t)$ describes the dragging along v. The random motion is symmetric and thus cannot affect the first moment. Again, choosing $\beta\to 2$, the normal diffusion-advection equation is recovered.

The diverging MSD, as seen from Eq. (23), makes the calculation of transport properties problematic. This can be overcome by introducing finite velocities of the walkers [8,30]. To account for a finite speed of propagation, one often introduces the *Lévy walk* model with a coupling of waiting time and jump length PDF leading to a time ''cost'' of long jumps. A usual choice is [8]

$$\psi(x,t)=C|x|^{-\mu}\delta(|x|-t^{\nu}). \tag{27}$$

Three interesting cases that stem from the choice of Eq. (27) can be distinguished.

The first case involves a finite $\langle\tau\rangle$ caused by the inequality $\nu\mu>2$. Assuming further $\nu(\mu-2)<1$, one arrives at the jump PDF

$$\psi(k,u)\sim 1-\tau u-\sigma^2k^2u^{\nu(\mu-2)-1}. \tag{28}$$

Following the above procedure, we calculate the propagator

$$\varrho(k,u)=\frac{1}{u+ivk+Dk^2u^{\nu(\mu-2)-1}}, \tag{29}$$

which is to be compared with Eq. (38) in Ref. [8]. From Eq. (29), we deduce the moments

$$\langle x\rangle(t)=vt, \tag{30a}$$

$$\langle x^2\rangle(t)=2D\,\frac{t^{2+\nu(2-\mu)}}{\Gamma(3+\nu[2-\mu])}+v^2t^2, \tag{30b}$$

$$\langle(\Delta x)^2\rangle(t)=2D\,\frac{t^{2+\nu(2-\mu)}}{\Gamma(3+\nu[2-\mu])} \tag{30c}$$

describing enhanced transport between the linear and ballistic cases. The corresponding fractional equation takes on the form

$$\dot{\varrho}+v\varrho'=D\,\frac{\partial^{-[1-\nu(\mu-2)]}\varrho''}{\partial t^{-[1-\nu(\mu-2)]}}, \tag{31}$$

where the fractional operator on the right-hand side represents an integral operation; see Appendix A. The fractional diffusion equation (31) leads to a modified Gaussian PDF in the long distance long time limit [19,20]. The CTRW scheme, however, leads to a power law behavior, and to peaks at $|x|=t^{\nu}$ [31–33].

The second and third cases refer to an infinite characteristic time, i.e., $1<\nu\mu<2$. The first possible choice $\nu(\mu-2)>1$ leads to the dispersive case

$$\psi(k,u)=1-(u\tau)^{\nu\mu-1}-\sigma^2k^2, \tag{32}$$

matching the problem already discussed in Eqs. (19)ff. The third and last case follows from $\nu(\mu-2)<1$. This choice leads to the jump PDF

$$\psi(k,u)=1-(u\tau)^{\nu\mu-1}-Dk^2(u\tau)^{\nu(\mu-2)-1}, \tag{33}$$

and consequently to the propagator in Fourier-Laplace space:

$$\varrho=\frac{1}{u+ivk}\,\frac{1}{1+Dk^2u^{-2\nu}}\sim\frac{1}{u+ivk+Dk^2u^{1-2\nu}}, \tag{34}$$

which is to be compared with Eq. (43) in Ref. [8]. For the moments we end up with

$$\langle x\rangle(t)=vt, \tag{35a}$$

$$\langle x^2\rangle(t)=\frac{2Dt^{2\nu}}{\Gamma(1+2\nu)}+v^2t^2, \tag{35b}$$

$$\langle(\Delta x)^2\rangle(t)=\frac{2Dt^{2\nu}}{\Gamma(1+2\nu)}, \tag{35c}$$

so that in this case we again have a part ballistic for the MSD as in the dispersive case (19)ff. Now, however, 2ν can be larger or smaller than 1, describing enhanced or dispersive motion, respectively. Finally, the corresponding fractional equation is of the form

$$\dot{\varrho}(x,t)+v\varrho'=D\,\frac{\partial^{1-2\nu}\varrho''}{\partial t^{1-2\nu}}, \tag{36}$$

similar to Eq. (21), where now the right-hand side can either be a fractional integration or differentiation, according to the value of ν.

D. Partial sticking in the dispersive case

In the above discussion we have seen that, for diverging $\langle\tau\rangle$, we have to be careful preserving the Galilei invariance when we write down the sticking probability $\Phi(u)$ in the laboratory frame. On the other hand, if we consider a case where the diffusing particle becomes temporarily stuck in the laboratory matrix, we should observe deviations from the moments in Eqs. (20a)–(20c).

We can model partial sticking in such a way that, while the particle awaits its next jump, it is not to be moved along with the velocity v, but instead is trapped in the laboratory matrix. This means that, unlike Eq. (17), we have to choose $\Phi(u)$ according to Eq. (15), which leads to a Galilei variant propagator

$$\varrho(k,u)=u^{-1}\frac{1}{1+\gamma ivku^{-1}-\frac{\gamma(\gamma-1)}{2}v^2u^{-2}k^2+Du^{-\gamma}k^2}. \tag{37}$$

The results for the moments are now

$$\langle x\rangle(t)=\gamma vt, \tag{38a}$$

$$\langle x^2\rangle(t)=\frac{2D}{\Gamma(1+\gamma)}t^{\gamma}+\frac{\gamma(\gamma+1)}{2}v^2t^2, \tag{38b}$$

$$\langle(\Delta x)^2\rangle(t)=\frac{2D}{\Gamma(1+\gamma)}t^{\gamma}+\frac{\gamma(1-\gamma)}{2}v^2t^2. \tag{38c}$$

In this case, the velocity dependence does not cancel out, quite similar to the results in Ref. [23]. Here, a ballistic behavior is found, in contrast to the result $\propto t^{2\gamma}$ in [23]. However, the velocity is scaled by the factor $0<\gamma<1$.

Regarding the generalized equation corresponding to Eq. (37),

$$\dot{\varrho}+v\varrho'=\frac{\gamma(1-\gamma)}{2}v^2\frac{\partial^{-1}\varrho''}{\partial t^{-1}}+D\frac{\partial^{1-\gamma}\varrho''}{\partial t^{1-\gamma}}, \tag{39}$$

we recognize the division of the transport process into two different mechanisms: a dispersive part characterized by D, and a ''ballistic'' part. In this process, the particles that jump often are separated more efficiently from those which are stuck.

The consequences of a comparison of the results in Eqs. (20a) and (20c) with Eqs. (38a) and (38c) is interesting in respect to experimental measurements. Consider, for example, the measurement of the moments in a ground water flow or the flow through a porous system. Our calculation shows explicitly that a distinction between free dragging and partial sticking is, at least in principle, easily possible by the measurement of the MSD of the quantity of interest.

Similarly, corresponding to the model of Eq. (33), we calculate the moments

$$\langle x\rangle(t)=(\nu\mu-1)vt, \tag{40a}$$

$$\langle x^2\rangle(t)=\frac{2Dt^{2\nu}}{\Gamma(1+2\nu)}+\frac{\nu\mu(\nu\mu-1)}{2}v^2t^2, \tag{40b}$$

$$\langle(\Delta x)^2\rangle(t)=\frac{2Dt^{2\nu}}{\Gamma(1+2\nu)}+\frac{3\mu\nu-(\mu\nu)^2-2}{2}v^2t^2, \tag{40c}$$

again reducing to the standard case for $\mu\nu\to 2$.

Let us discuss the differences to the model in Refs. [22, 23]]. Starting off from the diffusion-advection equation (12), an extended jump length PDF of the form $\lambda(k)=1-i\tau kv-\tau Dk^2$, $k\to 0$ is assumed, which takes into account the shift due to the velocity v in an effective way, via the mean time τ of the Brownian process. For the generalized model, a finite ''advection time scale'' τ_a is assumed, leading to a modified jump PDF $\phi(x,t)=\psi(x-v\tau_a,t)$, which clearly differs from our approach [Eq. (6)]. In the Brownian case both models lead back to the diffusion-advection problem. For a case with diverging $\langle\tau\rangle$, however, we encounter the temporal evolution of the moments according to

$$\langle x\rangle(t)=\frac{Avt^{\gamma}}{\Gamma(1+\gamma)}, \tag{41a}$$

$$\langle x^2\rangle(t)=\frac{2Dt^{\gamma}}{\Gamma(1+\gamma)}+\frac{2A^2v^2t^{2\gamma}}{\Gamma(1+2\gamma)}, \tag{41b}$$

$$\langle(\Delta x)^2\rangle(t)=\frac{2Dt^{\gamma}}{\Gamma(1+\gamma)}+A^2v^2t^{2\gamma}\left(\frac{2}{\Gamma(1+2\gamma)}-\frac{1}{\Gamma(1+\gamma)^2}\right), \tag{41c}$$

with $A=\tau_a/\tau^{\gamma}$. The introduction of the microscopic advection time scale τ_a in Refs. [22,23], the physical mechanism of which is unclear, causes a sublinear dependence of the mean $\langle x\rangle$ on t. This might imply some kind of countermotion, which might be of relevance for molecular machines moving actively against the velocity.

In this section we have shown that the diffusion-advection problem with a homogeneous velocity field can be treated in the same way as a standard CTRW problem in the rest frame, and can be exactly mapped back to the laboratory frame. Via this method, a straightforward generalization to anomalous transport is possible. The walkers are dragged along the velocity field while awaiting their next jump, and thus we have found a more direct generalization in comparison to the extension presented in Refs. [22,23].

III. CONSTANT FORCE PROBLEM

Here we start off from a different point of view. Let us regard the master equation approach [7,8] in a biased environment. By this we mean that for each step we have a different probability to go left or right, that is, a constant force. Similar considerations may be found in Refs. [26,29,30,34]. We will see that this approach leads, in general, to a different result than the constant velocity problem in Sec. II, as we expect. In the constant v case the system is already in a stationary state, whereas, for a constant force, the particle is accelerated before reaching a steady state. This difference will in the fractional case lead to results where memory effects are important, and stationarity is only reached for very long times.

Let us assume a process with a nondiverging variance, so that we can write the jump PDF in the form

$$\psi(x,t)=\psi(t)\lambda^{\pm}(x), \tag{42}$$

with

$$\lambda^{\pm}=[\lambda^{+}(x)\Theta(x)+\lambda^{-}(x)\Theta(-x)], \tag{43}$$

where $\Theta(x)$ is Heaviside's jump function. For a constant bias, let us choose $\lambda^{+}=\sqrt{a/\pi}\exp\{-ax^2\}$ and $\lambda^{-}=\sqrt{b/\pi}\exp\{-bx^2\}$. The choice of Eq. (43) becomes clear when we regard the master equation in its integral form

$$\varrho(x,t)=\int dx'\int_0^t d\tau\varrho(x',\tau)\psi(x-x',t-\tau)+\phi(t)\delta(x), \tag{44}$$

the continuum version of Eq. (19) in Ref. [7]. If x', the starting point of the jump leading to x, lies to the left of x, then of course $x-x'>0$; thus λ^{+} determines the jump length for a jump to the right, and vice versa. λ^{+} and λ^{-} have different widths. This means that the probability to jump to the left is weighted differently from that to jump to the right, and so each jump is biased.

To calculate the Fourier-Laplace transform $\psi(k,u)$, we have to compute the Fourier transforms of $\lambda^{\pm}$. Due to the Heaviside functions, this becomes

$$\lambda^{\pm}(k)=[\lambda_{\mathcal{C}}^{+}(k)+\lambda_{\mathcal{C}}^{-}(k)]+i[\lambda_{\mathcal{S}}^{+}(k)-\lambda_{\mathcal{S}}^{-}(k)], \tag{45}$$

the indices $\mathcal{C}/\mathcal{S}$ denoting the Fourier cosine and sine transforms [24].

In the above case, we calculate

$$\begin{aligned}\psi(k,u)&=[1-(u\tau)^{\gamma}+O(u^2)]\\&\quad\times\left(\left[\frac{1}{2}-\frac{k^2}{8a}+\frac{1}{2}-\frac{k^2}{8b}+O(k^4)\right]\right.\\&\quad\left.+i\left[\frac{k}{2\sqrt{a\pi}}-\frac{k}{2\sqrt{b\pi}}+O(k^3)\right]\right)\\&\sim[1-(u\tau)^{\gamma}]\left(\left[1-\frac{k^2}{8}\left(\frac{a+b}{ab}\right)\right]\right.\\&\quad\left.+i\left[\frac{k}{2\sqrt{\pi}}\frac{\sqrt{b}-\sqrt{a}}{\sqrt{ab}}\right]\right)\\&\sim 1-(u\tau)^{\gamma}-\frac{k^2}{8}\frac{a+b}{ab}-i\frac{k}{2\sqrt{\pi}}\frac{\sqrt{a}-\sqrt{b}}{\sqrt{ab}}.\end{aligned} \tag{46}$$

Thus we end up with

$$\varrho=\frac{(u\tau)^{\gamma}}{u}\frac{1}{(u\tau)^{\gamma}+i\dfrac{k}{2\sqrt{\pi}}\dfrac{\sqrt{a}-\sqrt{b}}{\sqrt{ab}}+\dfrac{k^2}{8}\dfrac{a+b}{ab}} \tag{47}$$

for the PDF, from which we can calculate the moments

$$\langle x\rangle(t)=\frac{\sqrt{a}-\sqrt{b}}{2\sqrt{\pi}\sqrt{ab}}\frac{(t/\tau)^{\gamma}}{\Gamma(1+\gamma)} \tag{48a}$$

$$\langle x^2\rangle(t)=\frac{a+b}{4ab}\frac{(t/\tau)^{\gamma}}{\Gamma(1+\gamma)}+\frac{(\sqrt{a}-\sqrt{b})^2}{2\pi ab}\frac{(t/\tau)^{2\gamma}}{\Gamma(1+2\gamma)}, \tag{48b}$$

$$\langle(\Delta x)^2\rangle(t)=\frac{(\sqrt{a}-\sqrt{b})^2}{4\pi ab}\frac{2\Gamma^2(1+\gamma)-\Gamma(1+2\gamma)}{\Gamma(1+2\gamma)\Gamma^2(1+\gamma)}\left(\frac{t}{\tau}\right)^{2\gamma}+\frac{a+b}{4ab}\frac{(t/\tau)^{\gamma}}{\Gamma(1+\gamma)}. \tag{48c}$$

Note the transition from the anomalous behavior proportional t^{γ} to the $t^{2\gamma}$ régime. This result differs from Eqs. (20a)–(20c), but is very similar to Eqs. (41a)–(41c). Whereas we find some kind of stationary problem in the constant velocity model, here we have an accelerating force. In the standard case $\gamma=1$, both results become the same. In the fractional case, however, the memory effects in the force term do not allow us to reach a truly stationary velocity case; also see the discussions in Refs. [35,36]. This may also be seen in the corresponding fractional diffusion equation in a field:

$$\frac{\partial^{\gamma}\varrho}{\partial t^{\gamma}}-\frac{t^{-\gamma}\delta(x)}{\Gamma(1-\gamma)}+\frac{\partial F\varrho}{\partial x}=\frac{\partial^2 D\varrho}{\partial x^2}, \tag{49}$$

with the force term

$$F=\frac{\sqrt{a}-\sqrt{b}}{2\tau^{\gamma}\sqrt{\pi}\sqrt{ab}}, \tag{50}$$

and the generalized diffusion constant

$$D=\frac{a+b}{8\tau^{\gamma}ab}. \tag{51}$$

Compare this result to Eq. (21). Here there is no fractional integral operator acting upon the advection term. This causes the first moment to scale like t^{γ} instead linearly in time, as in Eq. (21). Clearly, for the symmetric walk, i.e., $a=b$, we are led back to the fractional diffusion equation, or Fick's second law $(\gamma=1)$, respectively.

Let us now regard a generalization for a finite characteristic time $\langle\tau\rangle$, but a Lévy-type jump length PDF. We choose

$$\lambda^{+}(x)=\frac{N_a}{1+ax^{\alpha+1}}, \tag{52}$$

$$\lambda^{-}(x)=\frac{N_b}{1+bx^{\alpha+1}}, \tag{53}$$

with $\alpha\in(0,2)$, and where

$$N_a=\frac{(1+\alpha)\sin\dfrac{\pi}{1+\alpha}}{2\pi}a^{1/(1+\alpha)}, \tag{54}$$

and an analogous expression for N_b, are the normalization constants. In the following we give the results of the intermediate steps only in terms of λ^{+}. The Fourier sine and cosine transforms of $\lambda^{\pm}$ can be calculated exactly in terms of Fox functions [37–39]:

$$\lambda_{\mathcal{C}}^{+}=\frac{N_a\pi}{1+\alpha}\,k^{-1}H_{2,3}^{2,1}\left[\frac{k}{a^{1/(1+\alpha)}}\middle|\begin{matrix}(1,1/[1+\alpha]),(1,\frac{1}{2})\\(1,1),(1,1/[1+\alpha]),(1,\frac{1}{2})\end{matrix}\right] \tag{55}$$

$$\sim\frac{1}{2}-a^{1/(1+\alpha)-1}\underbrace{\frac{\Gamma(-\alpha)}{2\pi}\left|\sin\pi\frac{1+\alpha}{2}\right|}_{\Omega^{+}}k^{\alpha}, \tag{56}$$

where the expansion is valid in the small k limit, and

$$\lambda_{\mathcal{S}}^{+}=\frac{N_a\pi}{1+\alpha}\,k^{-1}H_{2,3}^{2,1}\left[\frac{k}{a^{1/(1+\alpha)}}\middle|\begin{matrix}(1,1/[1+\alpha]),(\frac{1}{2},\frac{1}{2})\\(1,1),(1,1/[1+\alpha]),(\frac{1}{2},\frac{1}{2})\end{matrix}\right] \tag{57}$$

$$\sim a^{-1/(1+\alpha)}\underbrace{\frac{1}{2}\frac{\sin\frac{\pi}{1+\alpha}}{\sin\frac{2\pi}{1+\alpha}}}_{\Omega^{-}}k. \tag{58}$$

Thus, we end up with the PDF in Fourier-Laplace space (assuming a Poissonian waiting time PDF),

$$\varrho=\frac{1}{u-iFk-Dk^{\alpha}}, \tag{59}$$

with the force term

$$F=\Omega^{-}(a^{-1/(1+\alpha)}-b^{-1/(1+\alpha)}) \tag{60}$$

and the diffusion constant

$$D=\Omega^{+}(a^{1/(1+\alpha)-1}+b^{1/(1+\alpha)-1}). \tag{61}$$

Equation (59) refers again to a Lévy flight. With the Riesz fractional operator $\mathcal{R}^{\alpha}$ [28], the corresponding fractional diffusion equation can be written as follows:

$$\dot{\varrho}+\frac{\partial F\varrho}{\partial x}=D\mathcal{R}^{\alpha}\varrho \tag{62}$$

where we find that only the diffusive part of the spatial derivatives is affected by the procedure of introducing a Lévy-type jump length PDF, and thus we end up with the same equation as in Sec. II, Eq. (24). The reason stems from the difference of Fourier sine and cosine transforms. The sine transformation turns the even PDF into an odd function where the small k expansion starts with a power k^1; under the cosine transformation it stays even, and the lowest order term in k is constant. As in both cases, the zeroth term does not show a dependence of the power of k on the Lévy index α; there is no influence of it on the Fourier sine transform. For a discussion of the coupled CTRW mechanism, we refer to Sec. II.

IV. NONCONSTANT FORCE

Problems involving external force fields are usually formulated in terms of a Fokker-Planck approach [40,41]. Within this framework, however, the generalization to anomalous transport properties remains equivocal. Here we develop a generalized picture within the CTRW scheme. Let us recall the diffusion equation in a potential $V(x)$ [40],

$$\dot{\varrho}=\frac{\partial V'(x)\varrho}{\partial x}+\frac{\partial^2 D(x)\varrho}{\partial x^2}, \tag{63}$$

which leads back to our previous problem for a linear potential, i.e., a constant force and a constant diffusion coefficient D. It can be seen, expanding the force $F(x)=-V'(x)$ in a Taylor series [and similarly for $D(x)$],

$$F(x)=\sum_{n=0}^{\infty}\frac{1}{n!}f_n x^n:., \quad f_n=F^{(n)}(0), \tag{64}$$

that the corresponding equation in Fourier-Laplace space takes on the form

$$u\varrho-1=-ik\hat{F}(k)\varrho-k^2\hat{D}(k)\varrho \tag{65}$$

$$=-ik\sum_{n=0}^{\infty}\frac{(i)^n}{n!}f_n\varrho^{(n)}-k^2\sum_{n=0}^{\infty}\frac{(i)^n}{n!}d_n\varrho^{(n)}. \tag{66}$$

Thus the Fourier transform of the jump PDF becomes an operator valued function.

To see a possible generalization of this problem, we start by introducing a waiting time distribution, and avoid going to Fourier space. In the same spirit as in Weiss' treatise [29], we start off from the master equation (19) introduced in Ref. [8], and restrict ourselves to nearest neighbor jumps, but with a waiting time distribution $\psi(t)$:

$$p_j(t)=\int_0^t d\tau[A_{j-1}p_{j-1}(\tau)+B_{j+1}p_{j+1}(\tau)]\times\psi(t-\tau)+\delta_{x,0}\Phi(t), \tag{67}$$

where A_{j-1} (B_{j+1}) is the probability to jump from site $j-1$ ($j+1$) to site j, and $\Phi(t)=1-\int_0^t dt'\psi(t')$ is the sticking probability [Eq. (3)]. A and B fulfill the local condition $A(j)=1-B(j)$. Introducing the expansions

$$A_{j-1}p_{j-1}(t)\sim A(x)p(x,t)-\Delta x\,\frac{\partial A(x)p(x,t)}{\partial x}+\frac{(\Delta x)^2}{2}\frac{\partial^2 A(x)p(x,t)}{\partial x^2} \tag{68}$$

and Laplace transforming Eq. (67), we arrive at

$$\frac{1}{\psi(u)}\left(p(x,u)-\delta_{x,0}\,\frac{1-\psi(u)}{u}\right)=p(x,u)-\Delta x\,\frac{\partial[A(x)-B(x)]p(x,u)}{\partial x}+\frac{(\Delta x)^2}{2}\frac{\partial^2[A(x)+B(x)]p(x,u)}{\partial x^2}, \tag{69}$$

which can be recast to give

$$\frac{1-\psi(u)}{\psi(u)}\,p(x,u)-\delta(x)\,\frac{1-\psi(u)}{u\psi(u)}=-\tau^\gamma\,\frac{\partial F(x)p(x,u)}{\partial x}+\tau^\gamma\,\frac{\partial^2 D(x)p(x,u)}{\partial x^2} \tag{70}$$

in the continuum limit. We have assumed a waiting time distribution of the form $\psi(u)\sim 1-(u\tau)^\gamma$ for $u\to 0$. For the limit we have considered the expressions $\Delta x/\tau^\gamma$ and $(\Delta x)^2/\tau^\gamma$ [29]. Thus

$$F(x)=\lim_{\Delta x\to 0}\frac{\Delta x}{\tau^\gamma}[A(x)-B(x)] \tag{71}$$

and

$$D(x)=\lim_{\Delta x\to 0}\frac{(\Delta x)^2}{2\tau^\gamma}[A(x)+B(x)]. \tag{72}$$

Returning to time space, after choosing an appropriate waiting time distribution, results in a generalized diffusion equation in a potential field. Especially for the choice of a long-tailed distribution for ψ, $\psi(u)\sim 1-(u\tau)^\gamma$ for $u\to 0$, we find, the fractional generalized diffusion equation,

$$\frac{\partial^\gamma \varrho}{\partial t^\gamma}-\frac{t^{-\gamma}\delta(x)}{\Gamma(1-\gamma)}=-\frac{\partial F(x)\varrho}{\partial x}+\frac{\partial^2 D(x)\varrho}{\partial x^2}, \tag{73}$$

which reduces to the result in Ref. [29] for $\gamma\to 1$. Actually, the force F is normalized in such a way that it has the dimension of a generalized velocity, length/time$^\gamma$, similar to the introduction of mass forces in hydrodynamics.

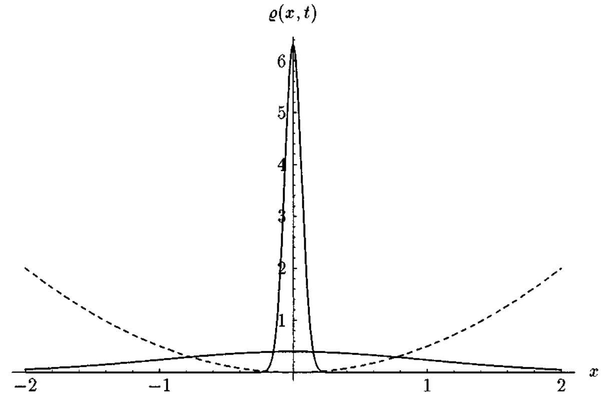

FIG. 1. Sketch of the random walk problem in a harmonic potential $V(x)=V_0/2x^2$ (dashed line). The peak is approximately a Gaussian, whereas the flat curve is the stationary solution for a Brownian random walk in the potential V.

Of course, we could also have used the direct generalization of our procedure in Sec. III. That is, the direct assumption of a continuous $\lambda^{\pm}(x)$ as in Eq. (43), and knowing that the Fourier sine transformation will always deliver a first order term proportional to k. The result is the same, and therefore we do not explicitly give the derivation. We also note in passing that with higher order terms in k, we would end up with higher order derivatives in the corresponding generalised diffusion equation, thus reaching some kind of Kramers-Moyal expansion [40,41].

V. SPECIAL CASE: HARMONIC POTENTIAL

In this section we consider the potential $V(x)=V_0x^2/2$, leading to a linear force field $F(x)=-V_0x$ directed at the origin. We would thus expect to find a MSD growing in time very slowly. Especially interesting will be to see the changes due to generalized transport mechanisms, i.e., $\langle\tau\rangle\to\infty$ or $\sigma^2\to\infty$. A schematic picture is drawn in Fig. 1. The model developed herein is not only of relevance in random walk theory. It is closely related to the problem of a molecule trapped in the cul-de-sac-like structure of a large protein molecule, where an escape is only possible through a fluctuating bottleneck [42]. There is also an intimate relation to a problem where the movement is confined by reflecting walls, and a trap is centered in between these walls [43]. It may also be interesting for reaction kinetics.

The paralleling diffusion equation

$$\dot{\varrho}=\frac{\partial V_0 x\varrho}{\partial x}+D\varrho'' \tag{74}$$

shows that the underlying process corresponds to a competition between a part responsible for the spreading of an initial population, characterized by the diffusion constant D, and a part of strength V_0 which tends to confine it. For very small D, the equation can be viewed as an inhomogeneous relaxation equation with a parametric dependence on x. Loosely speaking, this energy-entropy competition, characterized by the relation D/V_0, can also be thought of as a temperature-controlled process. It is here where we profit from our discussion involving the connections of the CTRW scheme and fractional equations, as the operator-valued expression

$\lambda^{\pm}(k)$ makes the treatment in Fourier-Laplace space intricate. Let us therefore start with the diffusion equation in an harmonic potential [Eq. (74)]. The fractional generalization of Eq. (74) is, in analogy to the preceding cases,

$$\frac{\partial^\gamma \varrho}{\partial t^\gamma}-\frac{t^{-\gamma}\delta(x)}{\Gamma(1-\gamma)}=\frac{\partial V_0 x\varrho}{\partial x}+D\varrho''. \tag{75}$$

The solution is obtained via a separation ansatz [44] (a different method is shown in Ref. [26]), i.e., $\varrho(x,t)=T(t)X(x)$. Introducing the rescaled time $\tilde{t}=V_0 t$ and coordinate $\tilde{x}=\sqrt{V_0/Dx}$, this gives the two ordinary differential equations (for simplicity, we drop the tildes)

$$\frac{\partial^\gamma T}{\partial t^\gamma}-\frac{t^{-\gamma}}{\Gamma(1-\gamma)}+\lambda T=0, \tag{76}$$

$$X''+xX'+(\lambda+1)X=0 \tag{77}$$

as $\varrho(x,0)=X(x)T(0)=X(x)$ for $T(0)=1$. The solution of Eq. (76) is well known, and given by the Mittag-Leffler function [24]:

$$T(t)=E_\gamma(-\lambda t^\gamma), \tag{78}$$

which reduces to the exponential for $\gamma\rightarrow 1$, $E_1(-\lambda t)=\exp(-\lambda t)$, as it should. The asymptotic properties are

$$E_\gamma(-\lambda t^\gamma)\sim\begin{cases}1, & t\ll\lambda^{1/\gamma}\\ \lambda^{-1}t^{-\gamma}, & t\gg\lambda^{1/\gamma},\end{cases} \tag{79}$$

and the series expansion reads [24]

$$E_\gamma(z)=\sum_{k=0}^{\infty}\frac{z^k}{\Gamma(\gamma k+1)}. \tag{80}$$

For the solution of Eq. (77) we introduce the ansatz

$$X(x)=e^{-x^2/4}Y(x), \tag{81}$$

which is well known from the harmonic oscillator problem in quantum mechanics. This leads to an equation for $Y(x)$ as follows:

$$Y''+\left(\lambda+\frac{1}{2}-\frac{x^2}{4}\right)Y=0. \tag{82}$$

Here we find the differential equation defining the Hermite polynomials [45]

$$Y_n(x)=e^{-x^2/4}H_n\left(\frac{x}{\sqrt{2}}\right), \tag{83}$$

with the corresponding eigenvalues $\lambda_n=n$. Thus we end up with the solution for the spatial part,

$$X(x)=e^{-x^2/2}H_n\left(\frac{x}{\sqrt{2}}\right), \tag{84}$$

so that the general solution of Eq. (75) is given via the summation of independent solutions [44]:

$$\varrho=\frac{1}{\sqrt{2\pi}}\sum_{n=0}^{\infty}\frac{1}{2^n n!}E_\gamma(-nt^\gamma)H_n(0)H_n\left(\frac{x}{\sqrt{2}}\right)e^{-x^2/2}. \tag{85}$$

The factor $H_n(0)$ refers to the initial condition of starting in the origin [44]. In the case of $\gamma=1$, it is possible to rewrite Eq. (85) using Mehler's summation formula [46]:

$$\varrho=\sqrt{2\pi(1-e^{-2t})}^{\,-1}\exp\left(-\frac{x^2}{4}(1+\coth t)\right). \tag{86}$$

For very short times we would expect the potential to influence the diffusion process weakly, as it has a zero derivative at the origin. This can be seen directly from Eq. (86), from which we find

$$\varrho\sim\frac{1}{\sqrt{4\pi t}}\exp\left(-\frac{x^2}{4t}\right),\quad t\ll 1, \tag{87}$$

the standard Gaussian. At long times, the potential should dominate, trying to confine the random motion. To see this, let us calculate the moments. From the symmetry of the problem it is clear that this time there is no first moment. A closed expression can be found for the case $\gamma=1$:

$$\langle x^2\rangle(t)=\frac{2}{1+\coth t}\sim\begin{cases}2t, & t\ll 1\\ 1, & t\gg 1,\end{cases} \tag{88}$$

which states that the variance cannot grow larger than a given threshold. Note that the result is still written in the reduced variables. In the original variables this result reads

$$\langle x^2\rangle(t)\sim\begin{cases}2Dt, & t\ll V_0\\ D/V_0, & t\gg V_0.\end{cases} \tag{89}$$

The steeper the potential in comparison to the diffusivity, the more hindered the random walk process becomes.

In the case of $0<\gamma<1$ the sum cannot be expressed in a closed form. The convergence makes it possible to exchange integration and summation, so that we can calculate a summation representation for $\langle x^2\rangle$ in this case [24,47]. For short times we have to use a trick to evaluate the summation, as we cannot simply take the expansion $E_\gamma(-t)\sim 1$, $t\ll 1$, due to the occurrence of the summation index n in the argument of the Mittag-Leffler function. With a small error, however, we evaluate $E_\gamma(-t)\sim e^{-t}$ in the initial region. On the other hand, for long times, we have to take care that the first summand $(n=0)$ is independent of time. The remaining summation can then be approximated numerically, and reveals a negative term, so that we end up with the limiting cases for the MSD:

$$\langle x^2\rangle(t)\sim\begin{cases}2t^\gamma, & t\ll 1\\ 1-dt^{-\gamma}, & t\gg 1,\end{cases} \tag{90}$$

where the constant $d=|2\sqrt{\pi}\Sigma_{n=2}^{\infty}(n\Gamma([1-n]/2))^{-1}|$ is positive (see Appendix B). Again, we find that in the fractional case the limit is only reached asymptotically via a power law. In the original variables, we find the limiting behavior

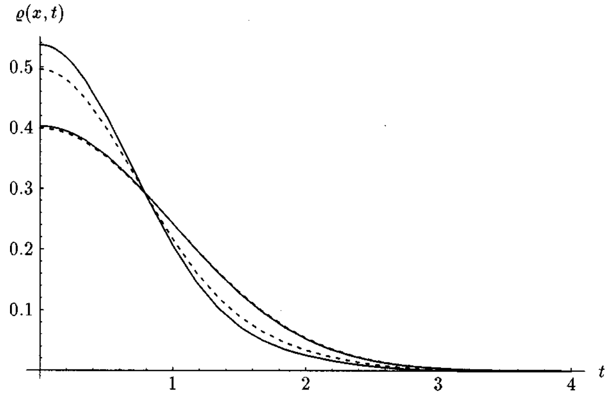

FIG. 2. Probability density function $\varrho(x,t)$ for the times $t=2$(—) and $t=4$(– – –). The upper line in both cases corresponds to the dispersive random walker, with $\gamma=\frac{1}{2}$. Note that for the Brownian walker we are almost in the stationary regime.

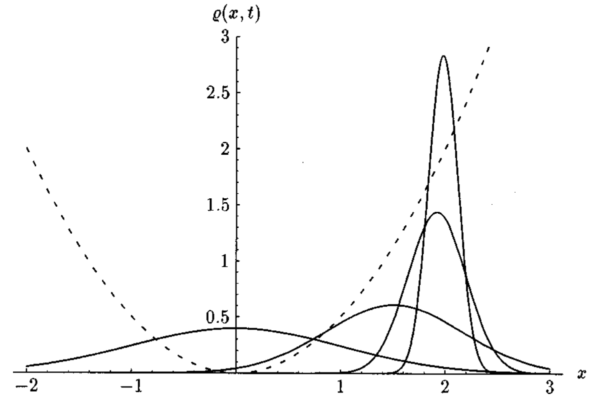

FIG. 4. Nonsymmetric case where the walker is released some distance x_0 away from the origin. The dashed line is again the potential $V(x)=V_0x^2/2$. The full lines correspond to the propagator for increasing times. The last curve is the steady state solution coinciding with the centered case.

$$\langle x^2\rangle(t)\sim\begin{cases}2DV_0^{\gamma-1}t^\gamma, & t\ll V_0^{1/\gamma}\\ D/V_0[1-d(V_0t)^{-\gamma}], & t\gg V_0^{1/\gamma}.\end{cases} \tag{91}$$

The propagators for the standard and dispersive cases are displayed in Fig. 2. Figure 3 shows the normally diffusive ($\gamma=1$) and dispersive ($\gamma=\frac{1}{2}$) results, including the asymptotic behaviors.

Finally, let us make some remarks on the nonsymmetric case, when the initial distribution of the random walk process is concentrated at some coordinate x_0 off the origin. This asymmetry in respect to the origin leads to a drift visible in a nonvanishing first moment, and driving the diffusing particle toward the origin. This situation is graphed in Fig. 4. The general solution becomes

$$\varrho=\frac{1}{\sqrt{2\pi}}\sum_{n=0}^{\infty}\frac{1}{2^nn!}H_n\left(\frac{x_0}{\sqrt{2}}\right)H_n\left(\frac{x}{\sqrt{2}}\right)E_\gamma(-nt^\gamma)e^{-x^2/2}. \tag{92}$$

For the standard case $\gamma\to 1$, one finds, with Mehler's formula [29,46],

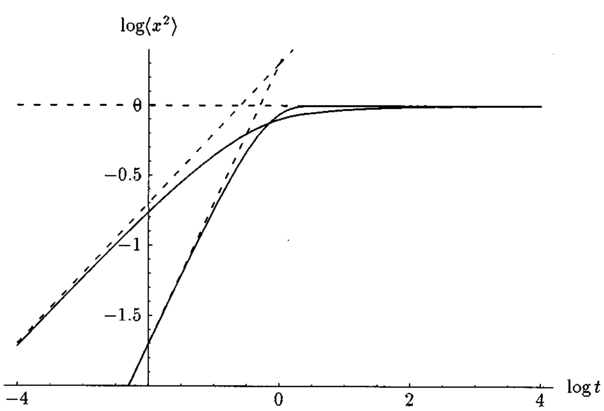

FIG. 3. Graph of the second moment (variance) of the Brownian and dispersive ($\gamma=\frac{1}{2}$) case in a decadic log-log scale. The dashed lines indicate the asymptotes $2t$ and $2t^\gamma$. The left-hand side asymptote was interpolated by 1 minus a small power of t.

$$\varrho=\frac{1}{\sqrt{2\pi(1-e^{-2t})}}\exp\left\{-\frac{(xe^{t/2}-x_0e^{-t/2})^2}{2(e^t-e^{-t})}\right\}, \tag{93}$$

which is, for short times $t\ll 1$ equivalent to the translated Gaussian

$$\varrho=\frac{1}{\sqrt{4\pi t}}e^{(x-x_0)^2/(4t)} \tag{94}$$

without a field. Calculating the moments for the solution in Eq. (93), one arrives at

$$\langle x\rangle(t)=x_0e^{-t}, \tag{95a}$$

$$\langle x^2\rangle(t)=\frac{2}{1+\coth t}+x_0^2e^{-2t}, \tag{95b}$$

$$\langle(\Delta x)^2\rangle(t)=\frac{2}{1+\coth t}. \tag{95c}$$

Thus the Hookean force field restores the equilibrium situation, pushing the PDF of the random walk back to the center where energy and entropy are balanced. For small times, we can calculate the moments for the anomalous case, resulting in

$$\langle x\rangle(t)=x_0, \tag{96a}$$

$$\langle x^2\rangle(t)=2t^\gamma+x_0^2, \tag{96b}$$

$$\langle(\Delta x)^2\rangle(t)=2t^\gamma \tag{96c}$$

for $t\ll 1$. For larger times, the integration $\int dx\ \varrho x^2$ cannot be evaluated analytically. The MSD should, however, reach the same asymptotic fractal behavior as given in Eq. (91).

VI. CONCLUSIONS

We have considered an extension of the continuous time random walk scheme to random walks in external fields, and studied the effects upon the corresponding generalized diffusion equation. For the case of transport in a homogeneous uniform velocity field, we showed a direct generalization employing the similarity variable of the wave variable type. As a consequence of the Galilei invariance condition imposed upon the propagator, the CTRW could be consistently extended. The resulting motion is a sum of an anomalous ''molecular'' diffusion and a usual drift. Two different partial sticking mechanisms were discussed in detail, offering interesting consequences for possible experimental realizations. Physically speaking, the difference between the partial sticking and the situation, where the particles are constantly dragged along the velocity field, lies in the dismissal of the Galilei invariance. This may be encountered in those situations, where the transported particles can become trapped in pores, cul-de-sac's off the main transport direction, on surfaces, or in vortices.

The problem of transport in a constant force has been calculated using the persistent random walk model. This model allows for a direct generalization in terms of a long-tailed distribution in either the waiting time or the jump length PDF. As a consequence, the probabilities to go to the left or right are different, causing a bias in the random walk. The results of the constant velocity and constant force problems do not coincide in the general case of anomalous transport. Only for the Brownian case do both models turn out to be the same.

In the same spirit as above, assuming an asymmetric jump picture, the problem of a nonconstant force has been introduced. In this generalization, the algebraic equation for ϱ in Fourier-Laplace space becomes a differential equation of the same order, as the force is expanded in powers of x. Therefore, the solution within the CTRW scheme becomes more intricate, and for certain cases the parallel approach via generalized diffusion-type equations becomes helpful, as it enables one to employ certain techniques established for the solution of partial differential equations.

The special case of a harmonic potential has been studied in some detail. It is here where we find stationary solutions. The restoring Hookean force confines the random motion, so that for long times an equilibrium between the ''entropic'' diffusive spreading and the ''energetic'' potential term is obtained. In the dispersive case, however, this stationarity behavior is reached only for very large times. The MSD consequently shows a transition from a purely diffusive regime to a constant value.

ACKNOWLEDGMENTS

We acknowledge financial support from GIF, the Gordon Center for Energy Studies, and the Deutsche Forschungsgemeinschaft. R.M. was supported by the Alexander von Humboldt Stiftung Bonn am Rhein, Germany. R.M. thanks I. Becker for stimulating discussions.

APPENDIX A: FRACTIONAL INTEGRATION AND DIFFERENTIATION

There exists a number of definitions of fractional calculi, e.g., Riemann, Erdélyi-Kobler, or the Riemann-Liouville and Riesz fractional operators we encounter in the main part. An overview over fractional calculus is the famous book by Oldham and Spanier [27], or the more mathematically oriented volume by Miller and Ross [48]. The whole entity of definitions, including applications, is collected in the compendium by Samko, Kilbas, and Marichev [28]. Here we give a short derivation of the Riemann-Liouville calculus; the basic property of the Riesz derivative was already given in Eq. (25), and we do not go into more detail here. A briefing of applications was given in Ref. [49].

The most common definition, the Riemann-Liouville definition, goes back to Cauchy's multiple integral

$$\begin{aligned} {}_{t_0}D_t^{-n} f(t) &= \int_{t_0}^{t} dt_{n-1} \int_{t_0}^{t_{n-1}} dt_{n-2} \cdots \int_{t_0}^{t_1} dt_0 f(t_0) \\ &= \frac{1}{(n-1)!} \int_{t_0}^{t} dt' (t-t')^{n-1} f(t'), \end{aligned} \tag{A1}$$

replacing the factorial by a gamma function

$$ {}_{t_0}D_t^{-p} f(t) = \frac{1}{\Gamma(p)} \int_{t_0}^{t} d\tau \frac{f(\tau)}{(t-\tau)^{1-p}} \tag{A2}$$

for arbitrary complex p with $\mathrm{Re}(p)>0$, and with $t_0=0$,

$$ {}_{0}D_t^{-p} f(t) = \frac{1}{\Gamma(p)} \int_{0}^{t} d\tau \frac{f(\tau)}{(t-\tau)^{1-p}}. \tag{A3}$$

A derivative of order q, $q>0$, is consequently established via the definition

$$\frac{d^q}{dt^q} f(t) \equiv {}_0D_t^q f(t) = \frac{d^n}{dt^n}\, {}_0D_t^{q-n} f(t), \tag{A4}$$

where $n \geqslant q$ is a natural number. Here, also, we introduce the short-hand notation d^q/dt^q used in the text which we use for both $q<0$ and $q>0$, in the above spirit.

The Laplace transform of a fractional integral expression is very convenient,

$$\int_0^\infty dt\, e^{-ut} \frac{d^{-q}}{dt^{-q}} f(t) = u^{-q} f(u), \tag{A5}$$

where $f(u)$ is the Laplace transform of $f(t)$ [27]. Note that we deal with initial value problems, according to the generalization of the differentiation theorem of the Laplace transformation.

APPENDIX B: APPROXIMATION OF A SUM

In Eq. (90) we introduced the constant $d>0$ Here we show, that it is indeed positive. To this end, we have to evaluate the sum (note that due to the Gamma function in the denominator only even terms remain)

$$s = \sum_2^\infty \frac{1}{n\Gamma([1-n]/2)} = \underbrace{\frac{1}{2\Gamma(-1/2)}}_{\approx -0.141} + \underbrace{\sum_4^\infty \frac{1}{n\Gamma([1-n]/2)}}_{\equiv r}. \tag{B1}$$

We know, on the other hand, that

$$s' = \sum_{0}^{\infty} \frac{1}{\Gamma([1-n]/2)} = e[1-\mathrm{erf}(1)] \approx 0.428 \tag{B2}$$

and

$$r' = \sum_{4}^{\infty} \frac{1}{\Gamma([1-n]/2)} = e[1-\mathrm{erf}(1)] - \frac{1}{\Gamma(1/2)} - \frac{1}{\Gamma(-1/2)} \approx 0.145. \tag{B3}$$

Now we see that

$$|r| = \left| \sum_{4}^{\infty} \frac{1}{n\Gamma([1-n]/2)} \right| < \frac{1}{4} |r'| \approx 0.036. \tag{B4}$$

This proves that $|r| < |[2\Gamma(-1/2)]^{-1}|$, so that $s < 0$. This again proves the result given in Eq. (90), i.e. the approaching of the constant value from below. Note that s cannot be evaluated numerically in an easy way, due to the huge summation terms occurring. It is therefore much easier to prove above inequalities.

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