Generalized diffusion: A microscopic approach

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The Fokker-Planck equation for the probability $f(r,t)$ to find a random walker at position r at time t is derived for the case that the probability to make jumps depends nonlinearly on $f(r,t)$. The result is a generalized form of the classical Fokker-Planck equation where the effects of drift, due to a violation of detailed balance, and of external fields are also considered. It is shown that in the absence of drift and external fields a scaling solution, describing anomalous diffusion, is possible only if the nonlinearity in the jump probability is of the power law type $[\sim f^{\eta}(r,t)]$, in which case the generalized Fokker-Planck equation reduces to the porous media equation. Monte Carlo simulations are shown to confirm the theoretical results.

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I. INTRODUCTION

Random walks are typically characterized by the probability to find a walker at some position r at some time t, $f(r,t)$. This could equally well be the concentration of walkers at a given space-time location in the event that there is an ensemble of independent walkers. In the classical case of an unbiased random walk, it was first shown by Einstein that at length and time scales large compared to the typical step size and the time between steps, respectively, the distribution satisfies the classical diffusion equation

$$\frac{\partial}{\partial t}f(r,t)=D\frac{\partial^2}{\partial r^2}f(r,t), \qquad (1)$$

with a diffusion constant D and that the diffusion constant can be expressed in terms of the microscopic dynamics of the problem, namely, the probability for the walker to take a step of given length and the time between steps [1]. It is obvious by inspection that the diffusion equation admits of normalized scaling solutions of the form $f(r,t)=t^{-1/2}\phi((r-r_0)^2/t)$, which immediately implies typical diffusive scaling of the second moment, $\langle[r(t)-r_0]^2\rangle=2Dt$, which is the Einstein relation. However, there are many systems observed in nature where it seems natural to use the language of diffusion, but for which the mean-squared displacement scales as something other than linearly with time. In order to describe such systems, the functional form of Eq. (1) is often generalized so as to allow for other types of scalings. Two popular methods are (i) the introduction of fractional time and/or space derivatives giving the fractional Fokker Planck equation (FFPE) [2–6] and (ii) replacement of $f(r,t)$ on the right by $f^{\alpha}(r,t)$, giving the porous media equation (PME) [7–9]. The FFPE can be understood as the equation of motion of the probability density of the continuum limit of a continuous time random walk in which the waiting times and jumps obey generalizations of the usual Poisson and Gaussian processes: for example, fractional time derivatives arise when the jump probabilities are sampled from the Mittag-Leffler distribution [3,4,10,11] (a generalization of the Poisson distribution in which the probability for a jump decays algebraically with time for long times). Alternatively, it can also be understood within the context of the generalized Langevin equation as the result of a memory function that depends algebraically on time [12]. In either case, it is therefore possible to relate the mathematical formalism (the FFPE) to a microscopic description (power-law-distributed waiting times or algebraic memory function). The purpose of this paper is to describe a similar class of microscopic dynamics for which the PME arises naturally as the corresponding Fokker-Planck equation.

There have been several attempts to provide some dynamical context for the PME. Abe and Thurner [13] attempted to generalize the classical derivation of Einstein by introducing the concept of escort probabilities into the master equation for a random walk. Aside from the *ad hoc* nature of the generalization, the result is the PME plus an additional term which is not well behaved in the long-time limit. Several authors have described the relation of the PME to a continuous time random walk. In particular, Curado and Nobre [14] show that the PME arises from a continuous time random walk in which the transition rates, which are constants in the classical random walk, depend on some power of the distribution. Borland [15] and Anteneodo and Tsallis [16] discuss the fact that the PME corresponds to a Langevin equation with multiplicative noise but, given the equivalence of the Fokker-Planck and Langevin descriptions, this is just another way of writing the same result. Lutsko and Boon [17] show that an assumption of nonlinear response in an ordinary fluid leads to the PME, but with no indication of the origin of the nonlinear response. Another approach based on generalizing the cumulant expansion of the intermediate scattering function leads to a somewhat different generalization of classical diffusion [18].

Consider a discrete time random walk on a one-dimensional lattice under the condition that the probability that the walker makes a jump from one lattice site to another depends on the concentration of walkers everywhere on the lattice. In this way, we generalize and extend previous models in several ways. First, we allow for jumps of arbitrary length and with asymmetric probabilities so that detailed balance is violated and an intrinsic drift is generated. Second, we start with a discrete time model rather than the continuous time random walk which, combined with the drift, leads to additional terms in the Fokker-Planck equation. The con-

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tinuous time random walk is a special limit of our formulation. Third, we do not assume *a priori* power law nonlinearities as has commonly been the case. We allow for a quite general form of nonlinear dependence of the jump probabilities on the local distributions and we show that the resulting Fokker-Planck equation admits self-similar, i.e., scaling, solutions only if the nonlinearities take the form of power laws. Thus we derive the existence of power law nonlinearities rather than impose them. Finally, we also consider the effect of an external field. A preliminary discussion of these results has recently appeared [19].

In the next section, we start from the master equation and use a multiscale expansion to derive the Fokker-Planck equation. The modifications necessary to take into account the action of an external field are also discussed. In Sec. III, we explore the properties of the generalized diffusion equation. In particular, we show that self-similar solutions are possible only under conditions that reduce our equation to the PME. We also present numerical results which demonstrate the importance of the nonstandard terms occurring in the generalized diffusion equation and showing, in particular, the effect of breaking detailed balance. The last section gives our conclusions.

II. DERIVATION OF THE GENERALIZED FOKKER-PLANCK EQUATION

A. The master equation

Consider a walker on a lattice whose sites are labeled by a discrete index l. A classical random walk is characterized by a set of probabilities $\{p_j\}$ which give the likelihood for a jump of j lattice sites ($j>0$ corresponds to jumps to the right, $j<0$ to jumps to the left). An individual walker is characterized by the probability to be at site l at time step i, $\mathsf{f}_l(i)$. Equivalently, one could imagine a population of independent walkers which all start from the same site, in which case $\mathsf{f}_l(i)$ would be the concentration of walkers at site l at time step i. If the walk is symmetric, $p_{-j}=p_j$, the walker exhibits diffusive behavior whereas asymmetric probabilities give rise to diffusion superposed on a systematic drift.

In the present case, we generalize this picture by considering that the jump probability is a function of the occupation probability (or the concentration of particles) on the lattice. Consequently, the probability to make a jump of length j from site l will depend on the concentration at site l at time step i, $\mathsf{f}_l(i)$, and on the concentration at the end point of the jump, $\mathsf{f}_{l+j}(i)$. It is convenient to introduce the more general notation whereby the transition probability to jump from site l to site k at time t is $P(l\to k;t)$ so that the distribution obeys the master equation

$$\mathsf{f}_l(i+1)=\mathsf{f}_l(i)+\sum_{k=-\infty}^{\infty}[\mathsf{f}_k(i)P(k\to l;i)-\mathsf{f}_l(i)P(l\to k;i)], \tag{2}$$

where the first term on the right is the increase in population due to walkers jumping to site l from all other sites k, whereas the second term is the loss due to walkers leaving site l to go to site k. In the classical case, the jump probabilities take values drawn from a prescribed distribution, i.e., $P(k\to l;t)=p_{l-k}$, the simplest case being $p_{(k+1)-k}=p_{(k-1)-k}=\frac{1}{2}$. Here, we make the specific generalization that the probabilities have the form

$$P(k\to l;i)=p_{l-k}F(\mathsf{f}_k(i),\mathsf{f}_l(i)) \tag{3}$$

for some, as yet unspecified, function $F(x,y)$. Note that the probabilities must satisfy the obvious normalization

$$1=\sum_k P(l\to k;t). \tag{4}$$

This, together with the requirement that the probabilities be bounded, $0\le P(k\to l;t)\le 1$, places restrictions on the form of $F(x,y)$.

B. Smoothing

The goal is to examine the distribution on length and time scales that are large compared to the lattice spacing δr and time step δt. On these scales, it is expected that the distribution can be approximated by a continuous function. To formalize this, a smoothed version of the distribution is defined by the probability density

$$f(r,t)=\sum_{l,i}G(r-l\delta r,t-i\delta t)\mathsf{f}_l(i) \tag{5}$$

where the sum extends over all values of the indices and the function $G(r,t)$ is assumed to be localized near the point $r=0,t=0$. For example, the smoothing function could be a product of Gaussians,

$$G(r,t)=\frac{1}{2\pi\sqrt{\sigma_r\sigma_t}}\exp\left(-\frac{r^2}{2\sigma_r}\right)\exp\left(-\frac{t^2}{2\sigma_t}\right). \tag{6}$$

In general, the length and time scales associated with the smoothing can be as small as those of the random walk model. In the following, it makes no difference as long as both are small compared to the scale of typical variations in the distribution function. In general, we assume that, as in this example, there are scales such as σ_r and σ_t that characterize the range of the smoothing and henceforth that these scales are similar to the lattice spacing and time step,

$$1\lesssim \delta r/\sqrt{\sigma_r},\quad \delta t/\sqrt{\sigma_t}. \tag{7}$$

It will be necessary to also define the inverse transformation. To that end, notice that

$$f(k\delta r,j\delta t)=\sum_{l,i}G(k\delta r-l\delta r,j\delta t-i\delta t)\mathsf{f}_l(i) \tag{8}$$

and assume that this relation is invertible so that

$$\mathsf{f}_l(i)=\sum_{k,j}G^{-1}(k\delta r-l\delta r,j\delta t-i\delta t)f(k\delta r,j\delta t). \tag{9}$$

Note that when attention is restricted to the value of the smoothed function at lattice points, the relation between the original values and the smoothed values is just a discrete convolution which can be inverted using discrete Fourier transforms so long as the Fourier transform of the data and the smoothing functions exist and that of the smoothing function is nonzero [20]. This establishes the invertibility of the smoothing for a large class of functions. However, here, this expression will be developed in a Taylor expansion. Assuming that the smoothing function and its inverse are even functions of their arguments, as is natural, then

$$\mathsf{f}_l(i) = f(l\delta r, i\delta t)\sum_{k,j} G^{-1}(k\delta r - l\delta r, j\delta t - i\delta t) + \frac{1}{2}(\delta r)^2 \times \frac{\partial^2 f(l\delta r, i\delta t)}{\partial r^2}\sum_{k,j}(k-l)^2 G^{-1}(k\delta r - l\delta r, j\delta t - i\delta t) + \frac{1}{2}(\delta t)^2\frac{\partial^2 f(l\delta r, i\delta t)}{\partial t^2}\sum_{k,j}(j-i)^2 G^{-1}(k\delta r - l\delta r, j\delta t - i\delta t) + \cdots. \tag{10}$$

It is easy to see that if $G(k\delta r - l\delta r, j\delta t - i\delta t)$ is normalized, then so is the inverse function. The sums then characterize the width in space and time, respectively, of the inverse smoothing functions, which will be of the same order of magnitude as that of the actual smoothing functions. So we have that

$$\mathsf{f}_l(i) = f(l\delta r, i\delta t) + \gamma_r\sigma_r\frac{\partial^2 f(l\delta r, i\delta t)}{\partial r^2} + \gamma_t\sigma_t\frac{\partial^2 f(l\delta r, i\delta t)}{\partial t^2} + \cdots \tag{11}$$

for some dimensionless constants γ_r, γ_t which are of order unity. Note that this expansion makes sense, as does the whole smoothing procedure, provided the gradients of the distribution are small over the scales $\sqrt{\sigma_r}, \sqrt{\sigma_t}$.

C. Expansion of the master equation

In the limit of classical diffusion, when the transition probabilities take values from a given distribution, one could simply multiply the master equation by $G(r-l\delta r, t-i\delta t)$ and sum to get the exact master equation for the smoothed distribution,

$$f(r,t+\delta t) = f(r,t) + \sum_{m=-\infty}^{\infty}[f(r-k\delta r,t)p_m - f(r,t)p_{-m}]. \tag{12}$$

However, the nonlinearities of the generalized model do not permit this. Instead, Eq. (11) is used to get

$$f(r,t+\delta t) + \gamma_r\sigma_r\frac{\partial^2 f(r,t+\delta t)}{\partial r^2} + \gamma_t\sigma_t\frac{\partial^2 f(r,t+\delta t)}{\partial t^2} + \cdots = f(r,t) + \gamma_r\sigma_r\frac{\partial^2 f(r,t)}{\partial r^2} + \gamma_t\sigma_t\frac{\partial^2 f(r,t)}{\partial t^2} + \cdots + \sum_{m=-\infty}^{\infty}[f(r-m\delta r,t)F(f(r-m\delta r,t),f(r,t))p_m - f(r,t) \times F(f(r,t),f(r-m\delta r,t))p_{-m}] + \gamma_r\sigma_r\sum_{m=-\infty}^{\infty}\left(\frac{\partial^2 f(r-m\delta r,t)}{\partial r^2}F(f(r-m\delta r,t),f(r,t))p_m - \frac{\partial^2 f(r,t)}{\partial r^2}F(f(r,t),f(r-m\delta r,t))p_{-m}\right) + \cdots \tag{13}$$

where we have explicitly written only one of several terms in the sum proportional to σ_r (and none of the terms proportional to σ_t). The reason is that we will now further expand the distribution so as to give a superficially local expression. Then, it is found that the terms proportional to σ_r and σ_t contribute only to third order in the gradients, so that we have

$$\delta t\frac{\partial f(r,t)}{\partial t} + \frac{1}{2}(\delta t)^2\frac{\partial^2 f(r,t)}{\partial t^2} = -\delta r\frac{\partial f(r,t)}{\partial r}\sum_{m=-\infty}^{\infty} m p_m\left[\frac{\partial xF(x,y)}{\partial x} + \frac{\partial xF(x,y)}{\partial y}\right]_f + \frac{1}{2}(\delta r)^2\frac{\partial^2 f(r,t)}{\partial r^2}\sum_{m=-\infty}^{\infty} m^2 p_m\left[\frac{\partial xF(x,y)}{\partial x} - \frac{\partial xF(x,y)}{\partial y}\right]_f + \frac{1}{2}(\delta r)^2\left(\frac{\partial f(r,t)}{\partial r}\right)^2\sum_{m=-\infty}^{\infty} m^2 p_m\left[\frac{\partial^2 xF(x,y)}{\partial x^2} - \frac{\partial^2 xF(x,y)}{\partial y^2}\right]_f + O\left(\sigma_r^{3/2}\frac{\partial^3 f}{\partial r^3},\ldots\right), \tag{14}$$

where we have used the assumption that $\delta r < \sqrt{\sigma_r}$ to replace δr by σ_r in the error estimate. A compact notation has also been introduced whereby

$$\left[\frac{\partial xF(x,y)}{\partial x}\right]_f = \left[\frac{\partial xF(x,y)}{\partial x}\right]_{x=f(r,t),y=f(r,t)}. \tag{15}$$

D. Multiple time scales

We could simply truncate the expansion obtained so far on the grounds that the gradients are small over the scale of the smoothing (i.e., small over the scale of a few lattice spacings) but this is unsatisfactory on both physical and mathematical grounds. Physically, the resulting equation does not reduce to the diffusion equation in the appropriate limit of $F(x,y)=1$. Mathematically, this results in a second-order equation in time, whereas the exact master equation is clearly first order in time: knowledge of the distribution at time step i is sufficient to calculate it at all future time steps. These problems are not unrelated: both are due to the fact that changes in the distribution in time are driven by spatial gradients so that in some sense derivatives in time and in space are interchangeable. Ideally, we would like to say that the first-order spatial gradients drive the first-order time derivative, the second-order gradients second-order time derivatives, etc. However, we cannot simply equate these different terms separately as there is only one distribution and it can satisfy only one equation. The solution is to generalize the distribution to have many different, but related, time dependencies that can be satisfied at different length scales.

This leads to the method of multiple time scales.

To separate the different length and time scales in the problem, first define a length scale ℓ over which the relative variation of the distribution is of order 1,

$$\frac{1}{f}\frac{\partial f}{\partial r/\ell} \sim 1 \quad \text{or} \quad \ell \frac{\partial \ln f}{\partial r} \sim 1. \tag{16}$$

Then, a small parameter $\epsilon = \delta r/\ell$ is defined which quantifies the notion that the derivative of the distribution is small over the length scale of the smoothing function (which we assume is a few lattice spacings so that $\delta r \sim \sqrt{\sigma_r}$). A parameter τ is introduced by defining $\delta t = \epsilon\tau$, and dimensionless variables $z = r/\ell$ and $s = t/\tau$ are used to write the master equation as

$$\begin{aligned}\epsilon\frac{\partial f(z,s)}{\partial s} + \frac{1}{2}\epsilon^2\frac{\partial^2 f(z,s)}{\partial s^2}\\ = -\epsilon\frac{\partial f(z,s)}{\partial z}J_1\left[\frac{\partial xF(x,y)}{\partial x} + \frac{\partial xF(x,y)}{\partial y}\right]_f\\ + \frac{1}{2}\epsilon^2\frac{\partial^2 f(z,s)}{\partial z^2}J_2\left[\frac{\partial xF(x,y)}{\partial x} - \frac{\partial xF(x,y)}{\partial y}\right]_f\\ + \frac{1}{2}\epsilon^2\left(\frac{\partial f(z,s)}{\partial z}\right)^2 J_2\left[\frac{\partial^2 xF(x,y)}{\partial x^2} - \frac{\partial^2 xF(x,y)}{\partial y^2}\right]_f + O(\epsilon^3),\end{aligned} \tag{17}$$

where $J_n = \Sigma_m m^n p_m$. Additional time scales are now introduced by generalizing the distribution to a function of many time variables $f(z,s) \to f(z,s_0,s_1,\ldots)$ where the connection between this generalized function and the actual distribution is that $f(z,s) = f(z,s,\epsilon s,\epsilon^2 s,\ldots)$. Thus, the time derivatives must be replaced by

$$\frac{\partial}{\partial s} = \frac{\partial s_0}{\partial s}\frac{\partial}{\partial s_0} + \frac{\partial s_1}{\partial s}\frac{\partial}{\partial s_1} + \cdots = \frac{\partial}{\partial s_0} + \epsilon\frac{\partial}{\partial s_1} + \cdots. \tag{18}$$

We can now demand that the terms cancel at each order in ϵ since this just defines the dependence of the distribution on the various time scales. The first two orders in ϵ give

$$\frac{\partial f}{\partial s_0} = -\frac{\partial f}{\partial z}J_1\left[\frac{\partial xF(x,y)}{\partial x} + \frac{\partial xF(x,y)}{\partial y}\right]_f,$$

$$\begin{aligned}\frac{\partial f}{\partial s_1} + \frac{1}{2}\frac{\partial^2 f}{\partial s_0^2} = \frac{1}{2}\frac{\partial^2 f}{\partial z^2}J_2\left[\frac{\partial xF(x,y)}{\partial x} - \frac{\partial xF(x,y)}{\partial y}\right]_f\\ + \frac{1}{2}\left(\frac{\partial f}{\partial z}\right)^2 J_2\left[\frac{\partial^2 xF(x,y)}{\partial x^2} - \frac{\partial^2 xF(x,y)}{\partial y^2}\right]_f.\end{aligned} \tag{19}$$

Now it is clear that the first equation can be used to rewrite the second derivative with respect to s_0 in terms of spatial gradients,

$$\begin{aligned}\frac{\partial^2 f}{\partial s_0^2} &= \frac{\partial}{\partial s_0}\left(-\frac{\partial f}{\partial z}J_1\left[\frac{\partial xF(x,y)}{\partial x} + \frac{\partial xF(x,y)}{\partial y}\right]_f\right)\\ &= J_1^2\frac{\partial}{\partial z}\left[\frac{\partial xF(x,x)}{\partial x}\right]_f^2\frac{\partial f}{\partial z},\end{aligned} \tag{20}$$

giving

$$\frac{\partial f}{\partial s_0} = -\frac{\partial f}{\partial z}J_1\left[\frac{\partial xF(x,y)}{\partial x} + \frac{\partial xF(x,y)}{\partial y}\right]_f,$$

$$\begin{aligned}\frac{\partial f}{\partial s_1} &= \frac{1}{2}\frac{\partial^2 f}{\partial z^2}J_2\left[\frac{\partial xF(x,y)}{\partial x} - \frac{\partial xF(x,y)}{\partial y}\right]_f\\ &+ \frac{1}{2}\left(\frac{\partial f}{\partial z}\right)^2 J_2\left[\frac{\partial^2 xF(x,y)}{\partial x^2} - \frac{\partial^2 xF(x,y)}{\partial y^2}\right]_f\\ &- \frac{1}{2}J_1^2\frac{\partial}{\partial z}\left[\frac{\partial xF(x,x)}{\partial x}\right]_f^2\frac{\partial f}{\partial z}.\end{aligned} \tag{21}$$

Summing gives the desired result,

$$\begin{aligned}\frac{\partial f}{\partial s} &= -\frac{\partial f}{\partial z}J_1\left[\frac{\partial xF(x,y)}{\partial x} + \frac{\partial xF(x,y)}{\partial y}\right]_f\\ &+ \frac{1}{2}\frac{\partial^2 f}{\partial z^2}J_2\left[\frac{\partial xF(x,y)}{\partial x} - \frac{\partial xF(x,y)}{\partial y}\right]_f\\ &+ \frac{1}{2}\left(\frac{\partial f}{\partial z}\right)^2 J_2\left[\frac{\partial^2 xF(x,y)}{\partial x^2} - \frac{\partial^2 xF(x,y)}{\partial y^2}\right]_f\\ &- \frac{1}{2}J_1^2\frac{\partial}{\partial z}\left(\frac{\partial xF(x,x)}{\partial x}\right)_f^2\frac{\partial f}{\partial z} + O(\epsilon^2).\end{aligned} \tag{22}$$

In terms of the original variables, this reads

$$\begin{aligned}\frac{\partial}{\partial t}f(r,t) + C\frac{\partial}{\partial r}[xF(x,x)]_f\\ = \bar{D}\frac{\partial}{\partial r}\left[\frac{\partial xF(x,y)}{\partial x} - \frac{\partial xF(x,y)}{\partial y}\right]_f\frac{\partial}{\partial r}f(r,t)\\ - \frac{1}{2}C^2\delta t\frac{\partial}{\partial r}\left[\frac{\partial xF(x,x)}{\partial x}\right]_f^2\frac{\partial}{\partial r}f(r,t) + O(\epsilon^3),\end{aligned} \tag{23}$$

where

$$C = \frac{\delta r}{\delta t}J_1,$$

$$\bar{D} = \frac{1}{2}\left(\frac{\delta r}{\delta t}\right)^2 J_2. \tag{24}$$

Alternatively, the diffusion coefficient can be written in terms of the second cumulant as

$$D = \frac{1}{2}\frac{(\delta r)^2}{\delta t}(J_2 - J_1^2), \tag{25}$$

and the equation rearranged to give

$$\frac{\partial f}{\partial t}+C\frac{\partial}{\partial r}[xF(x,x)]_f=D\frac{\partial}{\partial r}\left[\frac{\partial xF(x,y)}{\partial x}-\frac{\partial xF(x,y)}{\partial y}\right]_f\frac{\partial f}{\partial r}+\frac{1}{2}C^2\delta t\frac{\partial}{\partial r}\left[\frac{\partial xF(x,y)}{\partial x}-\frac{\partial xF(x,y)}{\partial y}-\left[\frac{\partial xF(x,x)}{\partial x}\right]^2\right]_f\frac{\partial f}{\partial r}. \quad (26)$$

Equations (23) and (26) give the generalized Fokker-Planck equation and are the main result of this section.

E. Effect of an external field

If the walkers are subject to an external field $V(r)$, the derivation given above must be further generalized. In stochastic algorithms, such as the standard Metropolis Monte Carlo algorithm, the goal is to generate the canonical distribution [21]. In fact, similar reasoning also lies behind the fluctuation-dissipation relation that is needed to specify the autocorrelations of the noise in Langevin models. Here, we can adopt the same approach and demand that the effect of the field be to modify the jump probabilities so as to generate some specified steady state distribution. Alternatively, one can adopt the position often used in modeling nonequilibrium processes and assume that the effect of the field is the same as in an equilibrium system—which would be equivalent to an assumption of local equilibrium. Both possibilities are explored here.

1. Detailed balance

The idea is that the stationary distribution is specified *a priori* as some function of the external field. If the stationary probability to find a walker at site k is π_k, then the master equation demands that

$$0=\sum_{k=-\infty}^{\infty}[\pi_k p_{l-k}F_{kl}(\pi_k,\pi_l)-\pi_l p_{k-l}F_{lk}(\pi_l,\pi_k)], \quad (27)$$

where the subscripts on the F functions indicate that these now depend on position via the field. The usual condition of detailed balance would be that forward and backward jumps must balance,

$$\pi_k p_{l-k}F_{kl}(\pi_k,\pi_l)=\pi_l p_{k-l}F_{lk}(\pi_l,\pi_k). \quad (28)$$

However, this assumption is problematic since the elementary probabilities p_{l-k} may make the forward and backward directions asymmetrical—in the extreme case, backward jumps might be forbidden altogether. This is simply a manifestation of the fact that asymmetric elementary probabilities give rise to drift, and in the case of drift it makes no sense to speak of the stationary distribution. So we can only attempt to enforce detailed balance when the elementary probabilities are symmetrical, in which case (28) reads

$$\pi_k F_{kl}(\pi_k,\pi_l)=\pi_l F_{lk}(\pi_l,\pi_k). \quad (29)$$

Then, making the usual separation of the jump probabilities into the probability to generate a particular jump, $F(\pi_{l-m},\pi_l)$, as before, and the probability to accept a jump, $G_{l-m,l}$, the balance condition becomes

$$\pi_k F(\pi_k,\pi_l)G_{kl}=\pi_l F(\pi_l,\pi_k)G_{lk}, \quad (30)$$

which is solved, e.g., by the Metropolis ansatz

$$G_{kl}=\min\left(1,\frac{\pi_l F(\pi_l,\pi_k)}{\pi_k F(\pi_k,\pi_l)}\right). \quad (31)$$

To proceed, we make the further assumption that the stationary distribution is a local function of the field, $\pi_l=\Phi(\beta V_l)=\Phi(\beta V(l\delta r))$. It is shown in the Appendix that in this case the generalized equation becomes

$$\frac{\partial f}{\partial t}+\frac{\partial}{\partial r}\left(C-D'(r)K(\beta V(r))\frac{\partial \beta V(r)}{\partial r}\right)[xF(x,y)]_f=\frac{\partial}{\partial r}\left(\bar{D}\left[\frac{\partial xF(x,y)}{\partial x}-\frac{\partial xF(x,y)}{\partial y}\right]_f-\frac{1}{2}C^2\delta t\left[\frac{\partial xF(x,x)}{\partial x}\right]_f^2\right)\frac{\partial f}{\partial r}, \quad (32)$$

where

$$K(V)=\left[\frac{\partial \ln xF(x,y)}{\partial y}-\frac{\partial \ln xF(x,y)}{\partial x}\right]_{\Phi(V)}\frac{d}{dV}\Phi(V) \quad (33)$$

and

$$D'(r)=\frac{(\delta r)^2}{\delta t}\sum_{m=-\infty}^{\infty}m^2 p_m\Theta\left(-mK(\beta V(r))\frac{\partial}{\partial r}\beta V(r)\right). \quad (34)$$

If the elementary probabilities are symmetric, then $D'(r)=D$. In this case, the advection-diffusion equation can be written explicitly as

$$\frac{\partial f}{\partial t}+D\frac{\partial}{\partial r}\left(\frac{[xF(x,y)]_f}{[xF(x,y)]_\Phi}\left[\frac{\partial xF(x,y)}{\partial x}-\frac{\partial xF(x,y)}{\partial y}\right]_\Phi\frac{\partial \Phi}{\partial r}\right)=D\frac{\partial}{\partial r}\left[\frac{\partial xF(x,y)}{\partial x}-\frac{\partial xF(x,y)}{\partial y}\right]_f\frac{\partial f}{\partial r}, \quad (35)$$

where the fact that $f=\Phi$ is a stationary solution is obvious.

2. Local equilibrium and superstatistics

If, on the other hand, we make the local equilibrium assumption that the acceptance probabilities are the same as in an equilibrium system,

$$G_{kl}=\min(1,\exp\{-\beta[V(l\delta r)-V(k\delta r)]\}), \quad (36)$$

then the results in the Appendix give the same form as Eq. (32), but with $K(V)=-1$.

The local equilibrium assumption can be relaxed by using the superstatistics approach [22], better suited for systems out of equilibrium where the Boltzmann distribution $\exp\{-\beta[V(r)]\}$ cannot be expected to hold. The acceptance probabilities are then written as

$$G_{kl}=\min(1,\exp\{-\tilde{\beta}[U(l\delta r)-U(k\delta r)]\}), \quad (37)$$

with

$$\exp[-\tilde{\beta}U(r)] = \int_0^\infty d\beta \frac{f(\beta)}{Z(\beta)} e^{-\beta V(r)}, \tag{38}$$

where $f(\beta)$ is a prescribed distribution of the intensive variable β with the normalization $Z(\beta)$. We then obtain the generalized advection-diffusion equation (see the Appendix)

$$\frac{\partial f}{\partial t} + \left[C\frac{\partial}{\partial r} - \tilde{D}(r)\frac{\partial}{\partial r}\left(\frac{d\tilde{\beta}U(r)}{dr}\right)\right][xF(x,y)]_f = \frac{\partial}{\partial r}\left(D\left[\frac{\partial xF(x,y)}{\partial x} - \frac{\partial xF(x,y)}{\partial y}\right]_f - \frac{1}{2}C^2\delta t\left[\frac{\partial xF(x,x)}{\partial x}\right]_f^2\right)\frac{\partial f}{\partial r}, \tag{39}$$

with

$$\tilde{D}(r) = \frac{(\delta r)^2}{\delta t}\sum_{m=-\infty}^{\infty} m^2 p_m \Theta\left(m\frac{d\tilde{\beta}U(r)}{dr}\right). \tag{40}$$

III. PROPERTIES OF THE GENERALIZED DIFFUSION EQUATION

A. The generalized equation as a conservation law

The generalized diffusion equation contains an explicit velocity C. However, since it multiplies a nonlinear function of the distribution, it is not a drift in the usual sense that it can be eliminated by a Galilean transformation. Although it arises from the same physical source as the drift in classical diffusion—namely, the asymmetry of the jump probabilities—it corresponds in the present case to a position-dependent velocity. Of course, one could always make a transformation to an arbitrary moving frame, say with velocity C', and this would introduce the usual term $C'\partial_r f$ into the equation.

The generalized Fokker-Planck equation can also be cast in the usual form of a conservation law,

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial r}J = 0, \tag{41}$$

with flux

$$J = \left(C - D'(r)K(\beta V(r))\frac{\partial \beta V(r)}{\partial r}\right)[xF(x,y)]_f - \left(\bar{D}\left[\frac{\partial xF(x,y)}{\partial x} - \frac{\partial xF(x,y)}{\partial y}\right]_f - \frac{1}{2}C^2\delta t\left[\frac{\partial xF(x,x)}{\partial x}\right]_f^2\right)\frac{\partial f}{\partial r}. \tag{42}$$

Indeed, one interpretation of the result is that it describes ordinary diffusion with drift velocity C and diffusion constant D that are functions of the distribution, i.e.,

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial r}\left(\mathsf{C}(r) - D'(r)F(f,f)K(\beta V(r))\frac{\partial \beta V(r)}{\partial r}\right) f = \frac{\partial}{\partial r}\mathsf{D}(r)\frac{\partial f}{\partial r}, \tag{43}$$

where

$$\mathsf{C} = CF(x,y),$$

$$\mathsf{D} = \bar{D}\left[\frac{\partial xF(x,y)}{\partial x} - \frac{\partial xF(x,y)}{\partial y}\right]_f - \frac{1}{2}C^2\delta t\left[\frac{\partial xF(x,x)}{\partial x}\right]_f^2. \tag{44}$$

This makes clear that in the special case $F(x,y)=1$, classical diffusion is recovered.

B. Scaling solutions

We now specialize to the case that there is no drift, $C=0$, and no external field, and ask under what circumstances a scaling solution of the form $f(r,t)=t^{-\gamma/2}\phi(r/t^{\gamma/2})$ is possible; in other words, when does the general formulation describe diffusion? Without drift and without external force, the generalized diffusion equation reduces to

$$\frac{\partial f}{\partial t} = \bar{D}\frac{\partial}{\partial r}\left(M(f)\frac{\partial f}{\partial r}\right) \tag{45}$$

where we have introduced $M(f)=[\frac{\partial xF(x,y)}{\partial x} - \frac{\partial xF(x,y)}{\partial y}]_f$. Defining $\zeta = r/t^{\gamma/2}$ and introducing the scaling ansatz gives

$$-\frac{\gamma}{2}\left(\phi(\zeta) + \zeta\frac{d}{d\zeta}\phi(\zeta)\right) = \bar{D}t^{1-\gamma}\frac{d}{d\zeta}\left(M(t^{-\gamma/2}\phi(\zeta))\frac{d}{d\zeta}\phi(\zeta)\right). \tag{46}$$

It is only possible to eliminate the factors of the time if $M(f)=m_0 f^\eta$, for some constant m_0, giving

$$-\frac{\gamma}{2}\frac{d}{d\zeta}\zeta\phi(\zeta) = m_0\bar{D}t^{1-\gamma-\eta\gamma/2}\frac{d}{d\zeta}\left(\phi^\eta(\zeta)\frac{d}{d\zeta}\phi(\zeta)\right). \tag{47}$$

So scaling works provided that

$$\gamma = \frac{2}{\eta+2}, \tag{48}$$

and the equation for the scaling function is

$$m_0\bar{D}\frac{d}{d\zeta}\left(\phi^\eta(\zeta)\frac{d}{d\zeta}\phi(\zeta)\right) + \frac{\gamma}{2}\frac{d}{d\zeta}\zeta\phi(\zeta) = 0, \tag{49}$$

or

$$m_0\bar{D}\phi^\eta(\zeta)\frac{d}{d\zeta}\phi(\zeta) + \frac{\gamma}{2}\zeta\phi(x) = A \tag{50}$$

for some constant A. In the case $A=0$, the particular solution is easily found from $\frac{d}{d\zeta}\phi^\eta(\zeta) = -\frac{\eta\gamma}{2m_0\bar{D}}\zeta$, and is given by

$$\phi(\zeta) = \left(B - \frac{\eta}{2(2+\eta)m_0\bar{D}}\zeta^2\right)^{1/\eta}\Theta\left(B - \frac{\eta}{2(2+\eta)m_0\bar{D}}\zeta^2\right). \quad (51)$$

The constant B is determined by normalization:

$$B = \left(\frac{\eta(\eta+2)}{8m_0\bar{D}}\right)^{\eta/\eta+2} B\left(\frac{1}{\eta},\frac{1}{2}\right)^{-2\eta/\eta+2}, \quad (52)$$

where $B(x,y)=\Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the Beta function. The distribution can also be written as a q Gaussian by defining $\eta=1-q$,

$$\phi(\zeta) = B^{1/1-q}\left(1 - \frac{1-q}{2Bm_0\bar{D}(3-q)}\zeta^2\right)^{1/1-q} \times\Theta\left(1 - \frac{1-q}{2Bm_0\bar{D}(3-q)}\zeta^2\right). \quad (53)$$

Note that the scaling hypothesis demands that

$$M(f) \equiv \left[\frac{\partial xF(x,y)}{\partial x} - \frac{\partial xF(x,y)}{\partial y}\right]_f = m_0 f^\eta, \quad (54)$$

and the fact that the function F is defined in terms of the jump probabilities means that it must be bounded. From its definition, we expect that

$$0 \le xF(x,y) \le 1 \quad \text{and} \quad 0 \le yF(x,y) \le 1, \quad (55)$$

for all $x,y\in[0,1]$. If, for example, $F(x,y)=F(x)$, then the scaling hypothesis is: $F(x)\sim x^\eta$, so that the bounds given above demand that

$$\eta \ge 0, \quad 0 \le \gamma \le 1, \quad \text{and} \quad q \le 1. \quad (56)$$

All of the preceding concerning the scaling behavior applies only to the case that the constant A is taken to be zero in Eq. (50). For values of $A\neq 0$, no general solution of this equation could be found. However, note that if $\phi(\zeta)$ is analytic at $\zeta=0$, then from Eq. (50)

$$\lim_{\zeta\to 0}\frac{d}{d\zeta}\phi(\zeta) = \frac{A}{m_0\bar{D}\phi^\eta(0)}, \quad (57)$$

so that any solution with $A\neq 0$ is not symmetric about $\zeta=0$. Thus, we can say that the scaling behavior discussed here applies to the general case of symmetric solutions.

IV. NUMERICAL TESTS

In order to test the validity of the generalized diffusion equation, we have performed numerical simulations of the underlying random walk model. Our simulations begin with a population of N independent random walkers at position $r=0$ at time $t=0$. At time step i, each walker makes a jump of m lattice sites from its present position, say site l, with a probability $p_m F(\mathsf{f}_l(i),\mathsf{f}_{l+m}(i))$ where the distribution $\mathsf{f}_k(i)$ is simply the fraction of walkers at site k at time step i. All of the simulations discussed below were performed using a population of size $N=10^5$.

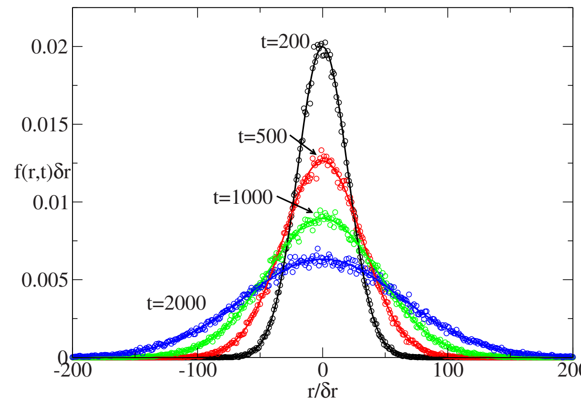

FIG. 1. (Color online) Evolution of an initial δ-function distribution for the case $q=0.999$ and equal elementary probabilities for jumps up to length 2. The symbols are from Monte Carlo simulation of the random walk and the solid lines are the analytic q Gaussian solution (58) to the generalized diffusion equation.

The first simulation is for the case of no drift, elementary probabilities $p_j=\frac{1}{5}$ with $j\in[-2,2]$, and $F(x,y)=x^{1-q}$, for which the theory gives

$$f(r,t) = t^{-1/3-q}\phi_q(r/t^{1/3-q}),$$

$$\phi_q(\zeta) = B_q^{1/1-q}\left(1 - \frac{1-q}{2B_q(2-q)(3-q)\bar{D}}\zeta^2\right)^{1/1-q} \times\Theta\left(1 - \frac{1-q}{2B_q(2-q)(3-q)\bar{D}}\zeta^2\right),$$

$$B_q = \left(\frac{(1-q)(3-q)}{8(2-q)\bar{D}}\right)^{1-q/3-q} B\left(\frac{1}{1-q},\frac{1}{2}\right)^{-2-2q/3-q}. \quad (58)$$

As stated above, only the range $q\le 1$ is permitted, and the value $q=1$ corresponds to classical diffusion. Since the initial condition and jump probabilities are symmetric, there is no drift and the scaling solution applies. Figures 1–3 show the analytic results, given by Eq. (58), and the results of the microscopic simulations for $q=0.999$ (essentially the classical case), 0.5, and 0.0. These correspond to anomalous dif-

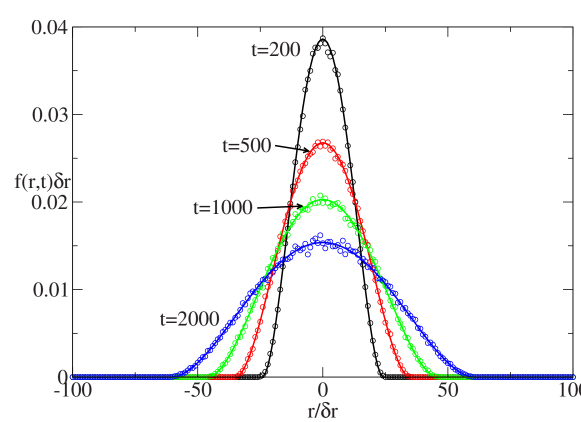

FIG. 2. (Color online) Same as Fig. 1, but for $q=0.5$.

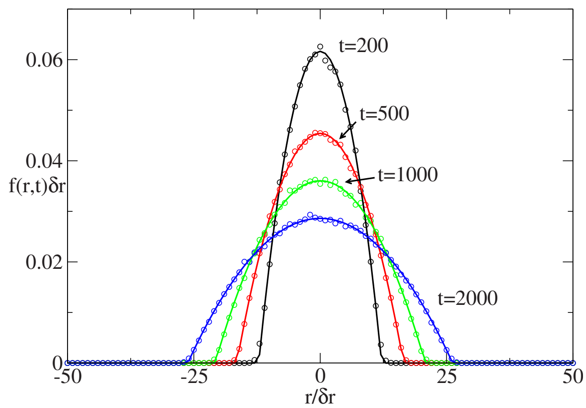

FIG. 3. (Color online) Same as Fig. 1, but for $q=0.0$.

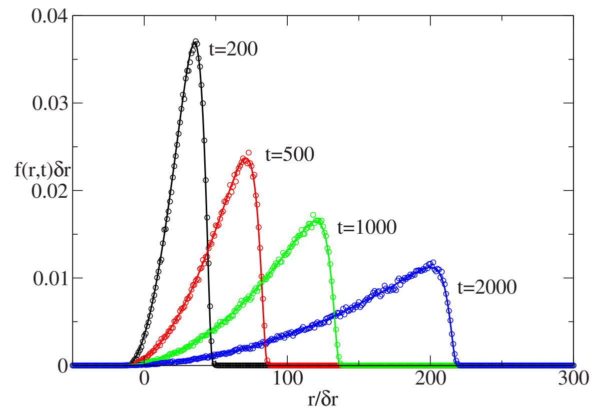

FIG. 5. (Color online) Same as Fig. 4, but for $q=0.5$.

fusion with scaling exponent $\gamma=0.9995$, $\frac{4}{5}$, and $\frac{2}{3}$, respectively. In all cases, the agreement between the simulations and the scaling solution is very good, even at the earliest times.

In the second set of simulations, particles are subjected to drift. In this case, the elementary probabilities are taken to be $p_j=\frac{j+3}{15}$ for $j\in[-2,2]$. Figures 4–6 show the evolution of the distributions for the same values of q as for the no-drift case. As mentioned above, it is then no longer possible to solve the generalized diffusion equation analytically. So comparison is made to a numerical solution of Eq. (26) with $F(x,y)=x^{1-q}$. The numerical solution was performed using centered finite differences in the spatial variable and a simple, first-order scheme in the time, with the lattice spacing fixed at δr and the time step equal to $0.001\delta t$. For $q=0.999$, the process is essentially that of the classical case of advection-diffusion. For the smaller values of q however, the distribution is very different, becoming increasingly asymmetrical as time progresses. As q becomes smaller, and the processes becomes more subdiffusive, the velocity of the peak of the distribution also decreases. Even with these significant qualitative changes for decreasing values of q, the generalized diffusion equation is again seen to give very good agreement with the Monte Carlo simulations.

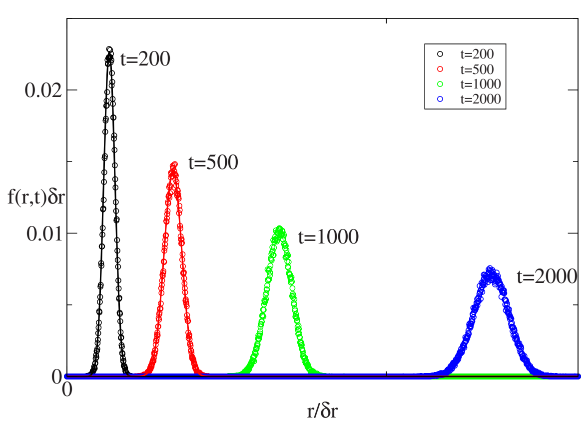

FIG. 4. (Color online) The evolution of an initial δ-function distribution for the case $q=0.999$ and $p_j=(j+3)/15$ for $j\in[-2,2]$. Since the probabilities violate detailed balance, there is a nonzero drift velocity $C=2\delta r/3\delta t$. The symbols are from Monte Carlo simulation of the random walk and the solid lines are the numeric solution of the generalized diffusion equation (26).

One interesting question is whether the new terms appearing in the generalized diffusion equation (23) and (26) play any role, or whether they could be neglected, giving a result closer to the porous media equation [7] which (with drift term) reads

$$\frac{\partial}{\partial t}f(r,t)+C\frac{\partial}{\partial t}f^{\alpha}(r,t)=D\frac{\partial^2}{\partial r^2}f^{\alpha}(r,t). \tag{59}$$

To investigate this, we repeated the solution of two modifications of the generalized diffusion equation. In the first case, the "extra" terms are simply omitted from Eq. (23) giving

$$\frac{\partial f}{\partial t}+C\frac{\partial}{\partial r}[xF(x,y)]_f=\bar{D}\frac{\partial}{\partial r}\left[\frac{\partial xF(x,y)}{\partial x}-\frac{\partial xF(x,y)}{\partial y}\right]_f\frac{\partial f}{\partial r}. \tag{60}$$

One objection to this approximation is that it does not reduce to the expected result in the limit of classical diffusion, since then the extra term would combine with the diffusive term to make the replacement $\bar{D}\to D$. This leads to the second modification considered here, namely, omitting the extra term from Eq. (26), which then reads

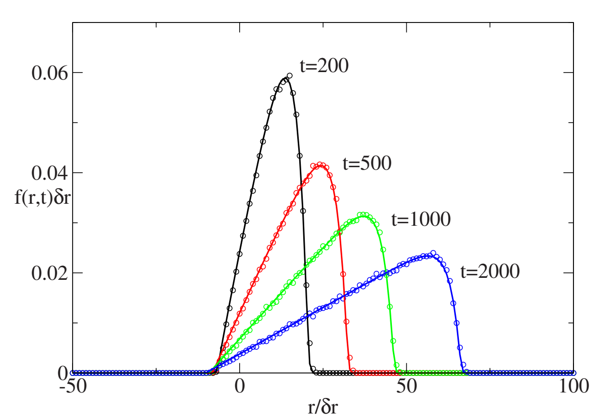

FIG. 6. (Color online) Same as Fig. 4, but for $q=0.0$.

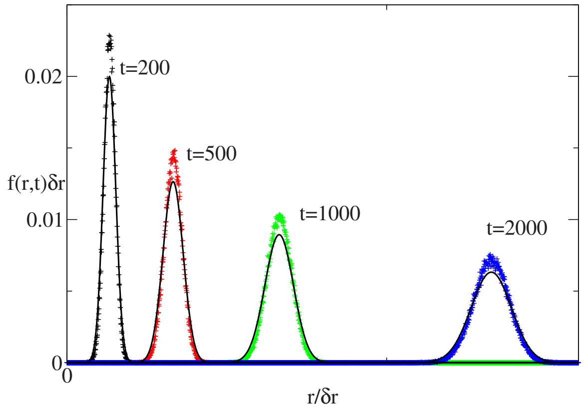

FIG. 7. (Color online) Simulation data for $q=0.999$ and the predictions of the Fokker-Planck equation with the type I modification. Type II is not shown as it gives virtually the same result as the full Fokker-Planck equation, as shown in Fig. 4, and is in almost perfect agreement with the data.

$$\frac{\partial f}{\partial t} + C\frac{\partial}{\partial r}[xF(x,y)]_f = D\frac{\partial}{\partial r}\left[\frac{\partial xF(x,y)}{\partial x} - \frac{\partial xF(x,y)}{\partial y}\right]_f \frac{\partial f}{\partial r}. \tag{61}$$

For want of better terms, these will be referred to as modifications I and II, respectively. Figures 7 and 8 show the numerical solution of these equations compared to the simulation data for the two cases $q=0.999$ and 0. For $q=0.999$, the type II modification is a much better approximation to the data than is the type I modification, as might be expected since type II becomes exact for $q=1$. However, the results for $q=0$ are exactly reversed: type I is a noticeably better approximation than is type II. The conclusion is that the full equation is necessary to provide a good description of the system for all values of q.

V. CONCLUSIONS

We have shown that a simple modification of the classical random walk gives rise to subdiffusive behavior. The required modification is that the probability to make a jump from one lattice site to another depends on the occupation probability of the walker on the lattice. Using a multiscale expansion of the exact master equation, we derived a generalized Fokker-Planck equation. In the limit of symmetric probabilities to jump left and right, this equation gives rise to diffusive behavior of the moments of the distribution, provided the dependence of the jump probabilities takes the form of a power law. In this case, our result reduces to the porous media equation. Unlike other approaches that begin with a continuous time random walk, we specifically consider a microscopic model in the *hydrodynamic* limit of large length and time scales. This is responsible for the appearance of a new term in the generalized diffusion equation which, as comparison to simulations of the microscopic model shows, is necessary to correctly describe the evolution of the distribution.

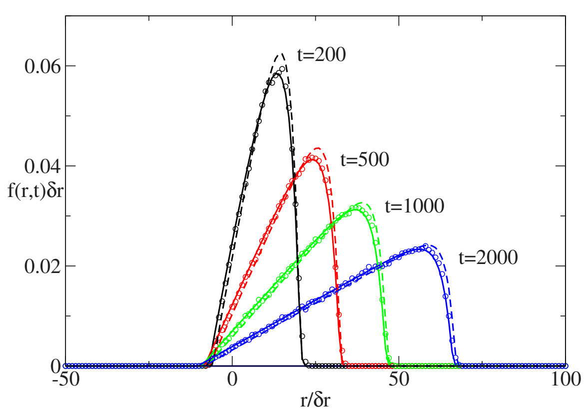

FIG. 8. (Color online) Simulation data for $q=0$ together with the predictions of the Fokker-Planck equation with the type I (full line) and type II (broken line) modifications.

Our generalized equation reduces to previous results in the appropriate limits. Most simply, if the function $F(x,y)=1$ the Fokker-Planck equation becomes the classical advective-diffusive equation. The continuous time random walk results from the scaling

$$\delta t \to \epsilon^2 \delta t, \quad \delta r \to \epsilon \delta r, \quad J_1 \to \epsilon J_1, \tag{62}$$

and the limit $\epsilon \to 0$. (Note that this limit is easily deduced directly from the smoothed master equation without need for the multiscale expansion.) With the further approximations of (i) no drift ($C=0$) and (ii) hops of only one lattice site, our result agrees with those of Curado and Nobre [14] and Nobre *et al.* [23].

We have shown that exact self-similar solutions of the generalized diffusion equation (without drift) are possible only if the jump probabilities scale as power laws. In this case, the distribution turns out to be the so-called q Gaussian often introduced in an *ad hoc* manner to describe anomalous diffusion. The model presented here therefore gives one answer to the question of what underlying dynamics could give rise to the observed q Gaussian distributions: a dependence of the jump probabilities on the local distribution (or, more likely, local concentration) of walkers is sufficient. Note that the dependence need not be an exact power law: it is enough that the long-time limit of the diffusion equation admits scaling, which in turn implies that the function $F(x,y)$ becomes algebraic in x in the limit of very small or very large x, depending on the various scaling exponents. One restriction of the exact scaling result, however, is that our model is well defined only if $F(x,y)=x^\eta$ for $\eta>0$, which in turn implies subdiffusive scaling of the moments. To describe superdiffusion there are only two possibilities. Either one could construct a function $F(x,y)$ that gives the proper normalization of the jump probabilities and that gives superdiffusion in the long-time limit or one could modify the basic description of the jump probabilities, Eq. (3), so as to introduce nonlinearity in some other way.

The generalized diffusion equation (GDE) is in some ways similar to the fractional Fokker-Planck equation: both describe subdiffusion and both require power law probabilities to give the subdiffusion (the GDE in the jump probabilities, the FFPE in the waiting times). It is natural to ask whether, given some experimental data which show subdiffusion, there is any way to choose between the two descriptions. On physical grounds, the idea of waiting times that are distributed as a power law might be more appropriate, in which case the FFPE should be preferred; if it makes more sense to think in terms of an interaction between the walkers, then the GDE might be more appropriate. Empirically, if the distribution of walkers is measured, it might be possible to choose a model based on the fact that the GDE predicts that the distribution of walkers in a system showing subdiffusion with no external forces should obey a q Gaussian distribution, whereas in the case of the FFPE there is also a scaling solution, but the distribution is a stretched Gaussian [2]. In fact, in two studies, one of subdiffusion induced by a random walk on a Sierpinski gasket [24] and the other of superdiffuson induced by a raondom walk on a tree structure [25], it was shown that the FFPE and GDE results were sufficiently different as to allow an empirical distinction to be made.

In the presence of either drift (i.e., nonsymmetric jump probabilities) or an external field, the GDE is more complex than the equivalent extension of the porous media equation. This is true even when a power law dependence of the jump probabilities is assumed since in this case the GDE becomes

$$\frac{\partial f}{\partial t}+\frac{\partial}{\partial r}\left(C+(1+\eta)D'(r)\frac{\partial \ln \Phi(\beta V(r))}{\partial r}\right)f^{1+\eta} = \frac{\partial}{\partial r}\left((1+\eta)\bar{D}f^{\eta}-\frac{1}{2}(1+\eta)^2C^2\delta t f^{2\eta}\right)\frac{\partial f}{\partial r}, \tag{63}$$

where

$$D'(r)=\frac{(\delta r)^2}{\delta t}\sum_{m=-\infty}^{\infty} m^2 p_m \Theta\left((1+\eta)m\frac{\partial \ln \Phi(\beta V(r))}{\partial r}\right), \tag{64}$$

or, with $1+\eta=\alpha$,

$$\frac{\partial f}{\partial t}+\frac{\partial}{\partial r}\left(C+\alpha D'(r)\frac{\partial \ln \Phi(\beta V(r))}{\partial r}\right)f^{\alpha} = \frac{\partial}{\partial r}\left(D+\frac{\delta t}{2}C^2(1-\alpha f^{\alpha-1})\right)\frac{\partial}{\partial r}f^{\alpha}, \tag{65}$$

to be compared with the PME (59). With no field, the drift does not generate a simple Galilean transformation of the equation without drift, as is usually assumed to be the case with the porous media equation, but instead generates new nonlinearities in the GDE. Because the drift term has the same number of powers of f but one fewer derivative, than the right-hand side, no simple scaling solution is evident. In the case of an external field but no drift, one has that $D'(r) \to \bar{D}$, so that the gradient terms on the left- and right-hand sides of the equation have the same numbers of powers of f and of spatial gradients. A scaling solution would then be possible, but only with a trivial external field. This superficial analysis suggests that exact scaling is possible in the GDE only in the case of no field and no drift. It leaves open the possibility of approximate scaling in the long-time limit, not to mention the possibility that more complex assumptions for the dependence of the jump probabilities might give completely different scaling properties. These questions are the subject of ongoing research.

ACKNOWLEDGMENTS

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APPENDIX: ROLE OF THE EXTERNAL FIELD

The master equation is

$$\begin{aligned} f(r,t+\delta t) = f(r,t) + \sum_{m=-\infty}^{\infty} p_m [& f(r-m\delta r,t) \\ & \times F(f(r-m\delta r,t),f(r,t))G_{r-m,r} \\ & - f(r,t)F(f(r,t),f(r+m\delta r,t))G_{r,r+m}], \end{aligned} \tag{A1}$$

where

$$G_{l-m,l}=\frac{\Phi_l F(\Phi_l,\Phi_{l-m})}{\Phi_{l-m}F(\Phi_{l-m},\Phi_l)}\Theta\left(1-\frac{\Phi_l F(\Phi_l,\Phi_{l-m})}{\Phi_{l-m}F(\Phi_{l-m},\Phi_l)}\right) + \Theta\left(\frac{\Phi_l F(\Phi_l,\Phi_{l-m})}{\Phi_{l-m}F(\Phi_{l-m},\Phi_l)}-1\right) \tag{A2}$$

and

$$\Phi_l = \Phi(V(l\delta r)). \tag{A3}$$

This can also be written as

$$\begin{aligned} G_{l-m,l} &= 1+\left(\frac{\Phi_l F(\Phi_l,\Phi_{l-m})}{\Phi_{l-m}F(\Phi_{l-m},\Phi_l)}-1\right)\Theta\left(1-\frac{\Phi_l F(\Phi_l,\Phi_{l-m})}{\Phi_{l-m}F(\Phi_{l-m},\Phi_l)}\right) \\ &= 1+\left(\frac{\Phi_l F(\Phi_l,\Phi_{l-m})}{\Phi_{l-m}F(\Phi_{l-m},\Phi_l)}-1\right)\Theta(\Phi_{l-m}F(\Phi_{l-m},\Phi_l) \\ &\quad -\Phi_l F(\Phi_l,\Phi_{l-m})) = 1+H_{l-m,l} \end{aligned} \tag{A4}$$

where

$$H_{l-m,l}=\left(\frac{h[l\delta r,(l-m)\delta r]}{h[(l-m)\delta r,l\delta r]}-1\right)\Theta\left(1-\frac{h[l\delta r,(l-m)\delta r]}{h[(l-m)\delta r,l\delta r]}\right)$$

with

$$h(x,y)=\Phi(V(x))F(\Phi(V(x)),\Phi(V(y))). \tag{A5}$$

The goal is to develop the expansion of $H_{l-m,l}$ in terms of δr and to use this to derive the modified advection-diffusion equation. In the appendix, we use an abbreviated notation whereby $\partial_r = \frac{\partial}{\partial r}$, etc.

First, note that for present purposes we need the expansion of $H_{l-m,l}$ up to order $(\delta r)^2$ inclusive. For the step-function part, we have

$$\Theta\left(1-\frac{h(x,x-u)}{h(x-u,x)}\right)=\Theta(h(x-u,x)-h(x,x-u))$$
$$=\Theta\left(u(h_y-h_x)+\frac{1}{2}u^2(h_{xx}-h_{yy})+\cdots\right)$$
$$=\Theta\left(\frac{u}{|u|}(h_y-h_x)+\frac{1}{2}|u|(h_{xx}-h_{yy})+\cdots\right). \quad \text{(A6)}$$

Now, we assume that (h_y-h_x) is of order 1, so that in some formal sense we can expand to get

$$\Theta\left(1-\frac{h(x,x-u)}{h(x-u,x)}\right)=\Theta\left(\frac{u}{|u|}(h_y-h_x)\right)+\frac{1}{2}|u|(h_{xx}-h_{yy})\times\delta\left(\frac{u}{|u|}(h_y-h_x)\right)+\cdots. \quad \text{(A7)}$$

In general, the δ function (and higher-order terms) only contribute on a set of measure zero and can be neglected. [Furthermore, we will explicitly show that the δ function cannot contribute until at least order $(\delta r)^3$.] Expanding the coefficient of the step function gives

$$\left(\frac{h(x,x-u)}{h(x-u,x)}-1\right)=u\frac{h_x-h_y}{h}+\frac{1}{2}u^2\left(\frac{h_{yy}}{h}-2\frac{h_xh_y}{h^2}+2\frac{h_x^2}{h^2}-\frac{h_{xx}}{h}\right)+\cdots. \quad \text{(A8)}$$

Multiplying these two contributions, we see that the δ function first appears at order u^2, but in the form of $x\delta(x)$, which is always zero; so, as stated above, it cannot contribute until at least order u^3, if at all. The result is

$$\left(\frac{h(x,x-u)}{h(x-u,x)}-1\right)\Theta\left(1-\frac{h(x,x-u)}{h(x-u,x)}\right)=\left[u\left(\frac{h_x-h_y}{h}\right)+\frac{1}{2}u^2\left(\frac{h_{yy}}{h}-2\frac{h_xh_y}{h^2}+2\frac{h_x^2}{h^2}-\frac{h_{xx}}{h}\right)\right]\times\Theta(u(h_y-h_x))+O(u^3), \quad \text{(A9)}$$

and consequently

$$H_{l-m,l}=\left[(m\delta r)\left(\frac{h_x-h_y}{h}\right)+\frac{1}{2}(m\delta r)^2\left(\frac{h_{yy}}{h}-2\frac{h_xh_y}{h^2}+2\frac{h_x^2}{h^2}-\frac{h_{xx}}{h}\right)\right]\Theta(m(h_y-h_x)). \quad \text{(A10)}$$

Similarly

$$H_{l,l+m}=\left(\frac{\Phi_{l+m}F(\Phi_{l+m},\Phi_l)}{\Phi_lF(\Phi_l,\Phi_{l+m})}-1\right)\Theta(\Phi_lF(\Phi_l,\Phi_{l+m})-\Phi_{l+m}F(\Phi_{l+m},\Phi_l))$$
$$=\left(\frac{h[(l+m)\delta r,l\delta r]}{h[l\delta r,(l+m)\delta r]}-1\right)\Theta\left(1-\frac{h[(l+m)\delta r,l\delta r]}{h[l\delta r,(l+m)\delta r]}\right)$$
$$=\left[(m\delta r)\frac{h_x-h_y}{h}+\frac{1}{2}(m\delta r)^2\left(\frac{h_{xx}}{h}-\frac{2h_xh_y}{h^2}+\frac{2h_y^2}{h^2}-\frac{h_{yy}}{h}\right)\right]\Theta((m\delta r)(h_y-h_x))+O(m^3). \quad \text{(A11)}$$

Substituting back into the master equation gives

$$f(r,t+\delta t)=f(r,t)+\sum_{m=-\infty}^{\infty}p_m[f(r-m\delta r,t)F(f(r-m\delta r,t),f(r,t))-f(r,t)F(f(r,t),f(r+m\delta r,t))]+\sum_{m=-\infty}^{\infty}p_m[f(r-m\delta r,t)F(f(r-m\delta r,t),f(r,t))H_{r-m,r}-f(r,t)F(f(r,t),f(r+m\delta r,t))H_{r,r+m}. \quad \text{(A12)}$$

The last term on right-hand side is

$$f(r,t)F(f(r,t),f(r,t))\sum_{m=-\infty}^{\infty}p_m(H_{r-m,r}-H_{r,r+m})+\delta r(\partial_rf)\sum_{m=-\infty}^{\infty}mp_m\left(-\frac{dxF}{dx}H_{r-m,r}-\frac{dxF}{dy}H_{r,r+m}\right)+\cdots$$
$$=f(r,t)F(f(r,t),f(r,t))\sum_{m=-\infty}^{\infty}\frac{1}{2}(m\delta r)^2p_m\left[\left(\frac{h_{yy}}{h}-2\frac{h_xh_y}{h^2}+2\frac{h_x^2}{h^2}-\frac{h_{xx}}{h}\right)-\left(\frac{h_{xx}}{h}-\frac{2h_xh_y}{h^2}+\frac{2h_y^2}{h^2}-\frac{h_{yy}}{h}\right)\right]\Theta(m(h_y-h_x))$$
$$+(\delta r)^2(\partial_rf)\sum_{m=-\infty}^{\infty}m^2p_m\left[-\frac{dxF}{dx}\left(\frac{h_x-h_y}{h}\right)-\frac{dxF}{dy}\left(\frac{h_x-h_y}{h}\right)\right]\Theta(m(f_y-f_x))$$
$$=(\delta r)^2f(r,t)F(f(r,t),f(r,t))\left(\frac{h_{yy}}{h}-\frac{h_y^2}{h^2}+\frac{h_x^2}{h^2}-\frac{h_{xx}}{h}\right)\sum_{m=-\infty}^{\infty}m^2p_m\Theta(m(f_y-f_x))$$

$$+ (\delta r)^2(\partial_r f)\left(\frac{h_x - h_y}{h}\right)\left[-\frac{dxF}{dx} - \frac{dxF}{dy}\right]\sum_{m=-\infty}^{\infty} m^2 p_m \Theta(m(f_y - f_x))$$

$$= (\delta r)^2\left[f(r,t)F(f(r,t),f(r,t))\left(\frac{d^2 \ln h}{dy^2} - \frac{d^2 \ln h}{dx^2}\right) + (\partial_r f)\left(\frac{dxF}{dx} + \frac{dxF}{dy}\right)\left(\frac{d \ln h}{dy} - \frac{d \ln h}{dx}\right)\right]\sum_{m=-\infty}^{\infty} m^2 p_m \Theta(m(f_y - f_x))$$

$$= \frac{\partial}{\partial r}\left[f(r,t)F(f(r,t),f(r,t))\left(\frac{d \ln h}{dy} - \frac{d \ln h}{dx}\right)\right](\delta r)^2 \sum_{m=-\infty}^{\infty} m^2 p_m \Theta(m(f_y - f_x)).$$

Since this term only contributes to the master equation at order $(\delta r)^2$, it is easy to see that the complete Fokker-Planck equation now reads

$$\partial_t f + C\partial_r[yF(y)]_f = D'(r)\partial_r\left[f(r,t)F(f(r,t),f(r,t))\left(\frac{d \ln h}{dy} - \frac{d \ln h}{dx}\right)_{x=y=r}\right] + D\partial_r\left[F(y) - y\frac{\partial F(y)}{\partial y}\right]_f \partial_r f - \frac{1}{2}\delta t C^2 \partial_r\left[F(y) - y\frac{\partial F(y)}{\partial y} + \left(\frac{\partial yF(y)}{\partial y}\right)^2\right]_f \partial_r f, \tag{A13}$$

where

$$D'(r) = \frac{(\delta r)^2}{\delta t}\sum_{m=-\infty}^{\infty} m^2 p_m \Theta(m(h_y - h_x)). \tag{A14}$$

Note that in the case of symmetric elementary probabilities

$$\frac{(\delta r)^2}{\delta t}\sum_{m=-\infty}^{\infty} m^2 p_m \Theta(m(f_y - f_x)) = \frac{(\delta r)^2}{\delta t}\sum_{m>0}^{\infty} m^2[p_m \Theta(m(f_y - f_x)) + p_{-m}\Theta(-m(h_y - h_x))]$$

$$= \frac{(\delta r)^2}{\delta t}\sum_{m>0}^{\infty} m^2 p_m[\Theta(m(f_y - f_x)) + \Theta(-m(h_y - h_x))]$$

$$= \frac{(\delta r)^2}{\delta t}\sum_{m>0}^{\infty} m^2 p_m = \frac{1}{2}\frac{(\delta r)^2}{\delta t}\sum_{m=-\infty}^{\infty} m^2 p_m = \bar{D}. \tag{A15}$$

The final form of the advection-diffusion equation can be clarified. Writing it as

$$\partial_t f + C\partial_r(yF(y))_f = D'(r)\frac{\partial}{\partial r}\left[\frac{fF(f,f)}{h(r,r)}\left(\frac{\partial h}{\partial y} - \frac{\partial h}{\partial x}\right)_{x=y=r}\right] + D\partial_r\left[F(y) - y\frac{\partial F(y)}{\partial y}\right]_f \partial_r f - \frac{1}{2}\delta t C^2 \partial_r\left[F(y) - y\frac{\partial F(y)}{\partial y} + \left(\frac{\partial yF(y)}{\partial y}\right)^2\right]_f \partial_r f, \tag{A16}$$

and noting that

$$\frac{\partial}{\partial x}h(x,y) = \frac{\partial}{\partial x}\Phi(V(x))F(\Phi(V(x)),\Phi(V(y))) = \frac{\partial \Phi}{\partial x}\left[\frac{\partial xF(x,y)}{\partial x}\right]_\Phi, \tag{A17}$$

gives

$$\partial_t f + C\partial_r[yF(y)]_f = D'(r)\frac{\partial}{\partial r}\left(\frac{fF(f,f)}{\Phi F(\Phi,\Phi)}\left[\frac{\partial xF(x,y)}{\partial y} - \frac{\partial xF(x,y)}{\partial x}\right]_\Phi \partial_r \Phi\right) + \partial_r\left\{D\left[F(y) - y\frac{\partial F(y)}{\partial y}\right]_f - \frac{\delta t}{2}C^2\partial_r\left[F(y) - y\frac{\partial F(y)}{\partial y} + \left(\frac{\partial yF(y)}{\partial y}\right)^2\right]_f\right\}\partial_r f. \tag{A18}$$

The local equilibrium result can also be easily deduced. It corresponds to taking

$$h(x,y) = \exp[-\beta V(x)], \quad \text{i.e. } \frac{\partial}{\partial x}h(x,y) = -\beta\frac{\partial V(x)}{\partial x}\exp[-\beta V(x)]. \tag{A19}$$

Noting that the derivative of $D'(r)$ produces a term of the form $x\delta(x)$ that vanishes, $D'(r)$ can be taken under the derivative ∂_r in (A18), and in the local equilibrium case

$$D'(r)\frac{\partial}{\partial r}\left(\beta\frac{\partial V(r)}{\partial r}fF(f,f)\right)=\frac{\partial}{\partial r}\left(D'(r)\beta\frac{\partial V(r)}{\partial r}fF(f,f)\right). \tag{A20}$$

The resulting generalized Fokker-Planck equation reads

$$\partial_t f+\partial_r\left[C[yF(y)]_f-D'(r)\left(\beta\frac{\partial V(r)}{\partial r}fF(f,f)\right)\right]=+\partial_r\left(D\left[F(y)-y\frac{\partial F(y)}{\partial y}\right]_f-\frac{\delta t}{2}C^2\left[F(y)-y\frac{\partial F(y)}{\partial y}+\left(\frac{\partial yF(y)}{\partial y}\right)^2\right]_f\right)\partial_r f. \tag{A21}$$

[1] A. Einstein, Ann. Phys. **17**, 549 (1905).
[2] R. Metzler, E. Barkai, and J. Klafter, Phys. Rev. Lett. **82**, 3563 (1999).
[3] R. Metzler and J. Klafter, Phys. Rep. **339**, 1 (2000).
[4] I. M. Sokolov, J. Klafter, and A. Blumen, Phys. Today **55** (11), 48 (2002).
[5] R. Metzler, J. Klafter, and I. M. Sokolov, Phys. Rev. E **58**, 1621 (1998).
[6] D. Fulger, E. Scalas, and G. Germano, Phys. Rev. E **77**, 021122 (2008).
[7] M. Muskat, *The Flow of Homogeneous Fluids through Porous Media* (McGraw-Hill, New York, 1937).
[8] A. R. Plastino and A. P. A. Plastino, Physica A **222**, 347 (1995).
[9] C. Tsallis and D. J. Bukman, Phys. Rev. E **54**, R2197 (1996).
[10] I. Goychuk, E. Heinsalu, M. Patriarca, G. Schmid, and P. Hänggi, Phys. Rev. E **73**, 020101(R) (2006).
[11] R. Hilfer and L. Anton, Phys. Rev. E **51**, R848 (1995).
[12] I. Santamaria-Holek, J. Rubi, and A. Gadomski, J. Phys. Chem. B **111**, 2293 (2007).
[13] A. Abe and S. Thurner, Physica A **356**, 403 (2005).
[14] E. M. F. Curado and F. D. Nobre, Phys. Rev. E **67**, 021107 (2003).
[15] L. Borland, Phys. Rev. E **57**, 6634 (1998).
[16] C. Anteneodo and C. Tsallis, J. Math. Phys. **44**, 5194 (2003).
[17] J. F. Lutsko and J. P. Boon, Europhys. Lett. **71**, 906 (2005).
[18] J. P. Boon and J. F. Lutsko, Physica A **368**, 55 (2006).
[19] J. P. Boon and J. F. Lutsko, Europhys. Lett. **80**, 60006 (2007).
[20] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in C* (Clarendon Press, Oxford, 1993).
[21] D. Frenkel and B. Smit, *Understanding Molecular Simulation*, 2nd ed. (Academic Press, San Diego, CA, 2002).
[22] C. Beck and E. D. G. Cohen, Physica A **322**, 267 (2003).
[23] F. D. Nobre, E. M. F. Curado, and G. Rowlands, Physica A **334**, 109 (2004).
[24] C. Schulzky, C. Essex, M. Davison, A. Franz, and K. H. Hoffman, J. Phys. A **33**, 5501 (2000).
[25] A. Fischer, S. Seeger, K. H. Hoffman, C. Essex, and M. Davison, J. Phys. A **40**, 11441 (2007).