From Einstein to generalized diffusion

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Abstract. We show that from a generalization of Einstein's master equation for the random walk one obtains a generalized equation for diffusion processes. The master equation is generalized by making the particle jump probability $P_j(r)$ a functional of the particle distribution function $f(r,t)$. If one demands that the resulting generalized diffusion equation admits of scaling solutions: $f(r;t) = t^{-\gamma/2} \phi \left(r/t^{\gamma/2} \right)$, a power law $P_j(r) \propto f(r)^{\alpha-1}$ (with $\alpha > 1$) follows, and the solutions exhibit q-exponential forms which are found to be in agreement with the results of Monte-Carlo simulations, providing a microscopic basis validating the nonlinear diffusion equation. We also show that the phenomenological *porous media equation* is an approximation to the generalized advection-diffusion equation.

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INTRODUCTION

A canonical description of the microscopic mechanism of diffusion is that of a test particle executing a random walk as proposed by Einstein who, in one of his celebrated 1905 articles [1], showed how the diffusion equation follows from a mean-field description written in terms of the probabilities that the particle performs elementary displacements at each time step. The distribution function $f(r,t)$, that is the probability that, given the particle was initially at $r = 0$ at $t = 0$, it will be at position r at time t (for t large compared to the duration of an elementary displacement) is obtained as the solution to the Fokker-Planck equation for diffusion, and one finds that, in the the long-time limit, $f(r,t)$ is Gaussianly distributed in space [2]. The classical diffusion equation describes a large class of phenomena (ranging from particle dispersion in suspensions to diffusion of innovations in social networks) and is indeed applicable as long as the system responds linearly to a change in the quantity that is being transported. But the linear response hypothesis doesn't hold in more complicated situations such as when there is an interactive process between the particle and the substrate, or in heterogeneous media.

A nonlinear diffusion equation was proposed around 1935 on a phenomenological basis devised in particular to describe diffusive transport in porous media, hence the name *porous media equation* [3]

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

where D is the diffusion coefficient. This equation has a q-Gaussian solution [4] and exhibits the interesting feature that the scaling $\langle r^2 \rangle \propto t^\gamma$ can be non-classical (when

$\gamma \neq 1$) [1]. It was not until the 1990's that a more fundamental basis was proposed for the (generalized) porous media equation using various statistical mechanical approaches: the generalized entropy [5], the Langevin equation [6, 7], the master equation [8], the nonlinear response [9], the escort distribution [10], or the generalized generating function [11]; for a recent review, see [12].

MASTER EQUATION

Here we use Einstein's original microscopic approach based on the random walk. For simplicity consider a one-dimensional lattice where the particle hops to the nearest neighboring site (left or right) in one time step, a process described by the discrete equation

$$n(r;t+1) = \xi_- n(r+1;t) + \xi_+ n(r-1;t) , \qquad (2)$$

where the Boolean variable $n(r;t) = \{0,1\}$ denotes the occupation at time t of the site located at position r and $\xi_\pm$ is a Boolean random variable controlling the particle jump between neighboring sites ($\xi^+ + \xi^- = 1$). The mean field description follows by ensemble averaging Eq.(2). With $\langle n(r;t)\rangle = f(r;t)$ and $\langle \xi_j \rangle = P_j$ (using statistical independence of ξ and n), and extending the possible jump steps over the whole lattice, one obtains Einstein's master equation [1]

$$f(r;t+\delta t) = \sum_{j=-\infty}^{+\infty} P_j(r-j\delta r;t) f(r-j\delta r;t) , \qquad (3)$$

where $P_j(\ell)$ denotes the probability that the walker at site ℓ make a jump of j sites [2]. Using the normalization: $1 = P_0(\ell;t) + \sum_{j\neq 0} P_j(\ell;t)$, Eq.(3) takes the form of a Boltzmann like difference equation

$$f(r;t+\delta t) - f(r;t) = \sum_{j=0}^{\infty} [P_j(r-j\delta r;t) f(r-j\delta r;t) - P_j(r;t) f(r;t)] , \qquad (4)$$

which simply describes the rate of change of the particle distribution as the difference between the incoming and outgoing fluxes at location r.

When the linear response hypothesis is no longer valid, one observes that the long-time dynamics is different from that described by the classical Fokker-Planck equation (i.e. non-Gaussian behavior). At the level of the mean field description, the breakdown of linear response means that the particle motion depends on the occupation probability in a non-trivial way. The jump probability then becomes a functional of the particle distribution function, and Einstein's equation describing the space-time evolution of the particle motion must be generalized in order to account for the functional dependence.

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[1] When $\alpha = 1$, Eq.(1) is the usual diffusion equation with a Gaussian solution [2] and classical scaling ($\gamma = 1$); note also that the scaling holds for all moments: $\langle r^n \rangle \propto t^{n\gamma/2}$.
[2] In Einstein's formulation the particle jumps are restricted to symmetrical displacements, i.e. $P_{+j} = P_{-j}$.

So introducing in (4) $P_j(\ell;t) = p_j F(f(\ell\delta r;t))$, with $j \neq 0$ and where p_j is a given distribution of displacements [3], we obtain the generalized master equation

$$f(r;t+\delta t) - f(r;t) = \sum_{j=0} p_j[F(f(r-j\delta r;t))f(r-j\delta r;t) - F(f(r;t))f(r;t)]. \quad (5)$$

GENERALIZED DIFFUSION

Proceeding as in classical diffusion theory from Einstein's master equation, we perform a multi-scale expansion of the generalized master equation (5). To characterize the fact that we are interested in the hydrodynamic regime, we introduce a small parameter ε so that an expansion of the time and space derivatives gives

$$
\begin{aligned}
\frac{\partial}{\partial t} &= \varepsilon\frac{\partial^{(1)}}{\partial t} + \varepsilon^2\frac{\partial^{(2)}}{\partial t} + \dots, \\
\frac{\partial}{\partial r} &= \varepsilon\frac{\partial^{(1)}}{\partial r} + \varepsilon^2\frac{\partial^{(2)}}{\partial r} + \dots;
\end{aligned} \quad (6)
$$

a corresponding expansion of the distribution yields

$$f(r;t) = f_0(r;t) + \varepsilon f_1(r;t) + \dots. \quad (7)$$

To first order, we obtain

$$\mathscr{O}(\varepsilon^1): \qquad \frac{\partial^{(1)}}{\partial t}f_0(r;t) = -\left(J_1\frac{\delta r}{\delta t}\right)\frac{\partial^{(1)}}{\partial r}F(f_0(r;t))f_0(r;t), \quad (8)$$

and to second order

$$\mathscr{O}(\varepsilon^2): \qquad \frac{\partial^{(1)}}{\partial t}f_1(r;t) + \frac{\partial^{(2)}}{\partial t}f_0(r;t) + \frac{1}{2}(\delta t)\frac{\partial^{(1)2}}{\partial t^2}f_0(r;t) =$$

$$-\left(J_1\frac{\delta r}{\delta t}\right)\frac{\partial^{(1)}}{\partial r}\left(\left.\frac{dgF(g)}{dg}\right|_{g=f(r;t)}f_1(r;t)\right) - \left(\frac{\delta r}{\delta t}J_1\right)\frac{\partial^{(2)}}{\partial r}F(f_0(r;t))f_0(r;t)$$

$$+\frac{1}{2}\left(\frac{(\delta r)^2}{\delta t}J_2\right)\frac{\partial^{(1)2}}{\partial r^2}F(f_0(r;t))f_0(r;t), \quad (9)$$

where J_n denotes the moments $J_n = \sum_{j\neq 0}j^n p_j$. Resummation of these results (see [14] for details) yields the hydrodynamic limit of the generalized master equation

$$\frac{\partial}{\partial t}f(r;t) + C\frac{\partial}{\partial r}[F(f(r;t))f(r;t)] =$$

$$D\frac{\partial^2}{\partial r^2}[F(f(r;t))f(r;t)] + \frac{1}{2}(C^2\delta t)\frac{\partial}{\partial r}\mathsf{E}(r;t). \quad (10)$$

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[3] For instance, $p_j \propto e^{-j}$, or $p_j \propto j^{-\mu}$.

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This result is the generalized diffusion equation where C and D are the drift velocity and the diffusion coefficient respectively

$$C = \frac{\delta r}{\delta t} \sum_{j \neq 0} j p_j, \qquad D = \frac{(\delta r)^2}{2\delta t} \left(\sum_{j \neq 0} j^2 p_j - \left(\sum_{j \neq 0} j p_j \right)^2 \right), \qquad (11)$$

and

$$\mathsf{E}(r;t) = \frac{\partial}{\partial r} \left[F(f(r;t)) f(r;t) \right] - \left(\left| \frac{d g F(g)}{dg} \right|_{g=f(r;t)} \frac{\partial}{\partial r} \left[F(f(r;t)) f(r;t) \right] \right). \quad (12)$$

EXTERNAL FIELD

When there is an external field $V(r)$ acting on the particle, Eq.(10) is further generalized [14]. In stochastic algorithms, such as the standard Metropolis Monte Carlo algorithm, the goal is to generate the canonical distribution. The position often used in modeling nonequilibrium processes is to 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, i.e. that the acceptance probabilities are the same as in an equilibrium system. This assumption can be relaxed by using the *superstatistics* approach [15] to write the acceptance probabilities as

$$G_{k\ell} = \min \left(1, \exp \left(-\beta \left(U \left(\ell \delta r \right) - U \left(k \delta r \right) \right) \right) \right), \qquad (13)$$

with

$$\exp \left(-\tilde{\beta} U(r) \right) \propto \int_0^\infty d\beta \, e^{-\beta V(r)} f(\beta), \qquad (14)$$

where $f(\beta)$ is a prescribed distribution of the intensive variable β. We then obtain the generalized advection-diffusion equation [14]

$$
\begin{aligned}
\frac{\partial f}{\partial t} + C \frac{\partial}{\partial r} \left(x F(x,y) \right)_f &= D'(r) \frac{\partial}{\partial r} \left\{ \left(x F(x,y) \right)_f \left(\frac{d\beta U(r)}{dr} \right) \right\} \\
&+ \quad D \frac{\partial}{\partial r} \left(\frac{\partial x F(x,y)}{\partial x} - \frac{\partial x F(x,y)}{\partial y} \right)_f \frac{\partial f}{\partial r} \\
&- \quad C \delta t \frac{\partial}{\partial r} \left(\frac{\partial x F(x,x)}{\partial x} \right)_f^2 \frac{\partial f}{\partial r}, \qquad (15)
\end{aligned}
$$

with

$$D'(r) = \frac{(\delta r)^2}{\delta t} \sum_{m=-\infty}^{\infty} m^2 p_m \Theta \left(m \frac{d\beta U(r)}{dr} \right), \qquad (16)$$

and where the notation $\left(\frac{\partial x F(x,y)}{\partial x} + \frac{\partial x F(x,y)}{\partial y} \right)_f$ indicates that first the derivative should be evaluated with the variables being treated as independent and then both x and y replaced by $f(r,t)$.

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SCALING AND POWER LAW

Let us consider the generalized diffusion equation with no drift and ask under which conditions there is a scaling solution. When there is no drift, the jump probability is space symmetrical and consequently the first moment $J_1 = 0$ and $C = 0$, and (10) reduces to

$$\frac{\partial}{\partial t} f(r;t) = D \frac{\partial^2}{\partial r^2} [F(f(r;t)) f(r;t)].$$ (17)

Assuming that $f(r;t) = t^{-\gamma/2} \phi\left(r/t^{\gamma/2}\right) = t^{-\gamma/2} \phi(z)$, and expressing the time and space derivatives in terms of z, Eq.(17) is rewritten as (see [14] for details)

$$-\gamma \frac{d}{dz} z \phi(z) = 2 D t^{1-\gamma} \frac{d^2}{dz^2} F\left(t^{-\gamma/2} \phi(z)\right) \phi(z).$$ (18)

The time-dependence on the right can only be eliminated if $F(g) = g^\eta = t^{-\eta\gamma/2} \phi^\eta$ for some number η, and hence $1 = t^{1-\gamma} t^{-\eta\gamma/2}$, i.e.

$$\gamma = \frac{2}{2+\eta}.$$ (19)

Thus, when $\eta \neq 0$, this describes anomolous diffusion: $\langle r^2 \rangle \sim t^{\frac{2}{2+\eta}}$. In this case, Eq.(18) becomes

$$D \frac{d^2}{dz^2} \phi^{1+\eta}(z) + \frac{1}{2+\eta} \frac{d}{dz} z \phi(z) = 0,$$ (20)

and admits a q-exponential solution (see [14] for details)

$$\phi(z) = \left(\frac{1+2\eta}{1+\eta} B\right)^{\frac{1}{\eta}} \left[1 - \frac{\eta}{2(2+\eta)(1+2\eta) BD} z^2\right]^{\frac{1}{\eta}},$$ (21)

where B is an integration constant. With $\eta = 1 - q$, and returning to the original space and time variables, (21) takes the canonical q-exponential form

$$f(r;t) = B_q t^{-\frac{1}{3-q}} \left[1 - (1-q) M_q \frac{r^2}{D t^{\frac{2}{3-q}}}\right]^{\frac{1}{1-q}}$$ (22)

with

$$B_q = \left[\left(1 + \frac{1-q}{2-q}\right) B\right]^{\frac{1}{1-q}}, \qquad M_q^{-1} = 2(3-q)(3-2q) B.$$ (23)

So, with no drift and no external field, the generalized random walk model describes anomalous diffusion with q-distributions [4].

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[4] One verifies straightforwardly that for $q \to 1$, one retrieves the classical Gaussian distribution.
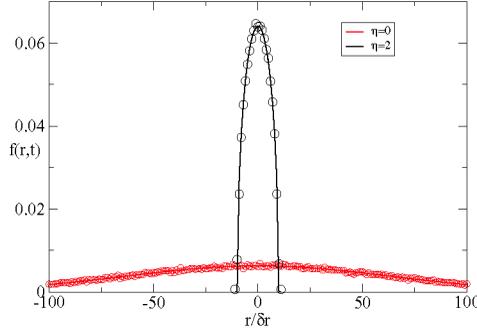
FIGURE 1. (Color online) Generalized diffusion with no drift: the distribution function $f(r;t = 2000$ time steps) obtained from Monte-Carlo simulations (symbols) and the solution (22) of the generalized diffusion equation (solid lines) for $\alpha = 3$ (upper curve) and $\alpha = 1$ (10^5 walkers; initial condition: $f(r,t = 0) = \delta(r)$).

An important result of the present analysis is that the power law dependence of the transition probability, $P_j = p_j F(f)$ with $F(f) = f^\eta$, is not introduced as an ansatz, but follows from the demand for a scaling (or self-similar) solution to the generalized diffusion equation.

NONLINEAR DIFFUSION EQUATION

Now introducing the power law dependence $F(f) = f^\eta$ (with $\eta \geq 0$ for normalization $\sum_j P_j = 1$) in the generalized equation (10), we obtain (with $\eta = \alpha - 1$)

$$\frac{\partial}{\partial t}f(r;t) + C\frac{\partial}{\partial r}f^\alpha(r;t) = D\frac{\partial^2}{\partial r^2}f^\alpha(r;t) + \frac{1}{2}\left(C^2\delta t\right)\frac{\partial}{\partial r}\mathsf{E}(r;t), \qquad (24)$$

with

$$\mathsf{E}(r;t) = \left(1 - \alpha f^{\alpha-1}(r;t)\right)\frac{\partial}{\partial r}f^\alpha(r;t). \qquad (25)$$

Comparison of Eq.(24) and Eq.(1) shows that the two equations are the same in the absence of drift ($C = 0$). With nonzero drift, this corresponds to a generalized porous media equation when the second term on the r.h.s. of (24) vanishes, i.e. for $\delta t \rightarrow 0$. So the phenomenological generalized porous media equation is an approximation which can be obtained in the hydrodynamic limit from the generalized master equation with a power law dependence for the transition probability (and in the absence of external force [14]). However Eq.(24) contains an additional term which, in general, cannot be neglected (see next section).
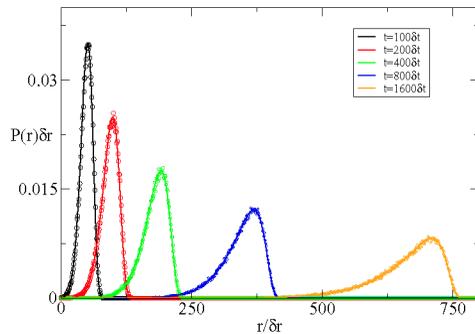
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FIGURE 2. (Color online) Generalized diffusion with drift: the distribution function $f(r;t = 100$ to 1600 time steps) obtained from Monte-Carlo simulations (symbols) and the numerical solution of the generalized diffusion equation (24) (solid lines) for $\alpha = 1.1$, i.e. $q = 0.9$ (10^5 walkers; initial condition: $f(r,t = 0) = \delta(r)$).

MICROSCOPIC SIMULATIONS

An important test of the theory will be given by confronting the solution of the generalized diffusion equation with the results of microscopic simulations. We therefore performed Monte-Carlo simulations with the generalized master equation (5) using power law dependent jump probabilities and prescribed p_j distributions: $p_j = \frac{1}{5}$ for $j = [-2, +2]$ (space symmetrical jumps and, so, C=0) and $p_j = \frac{j+3}{15}$ for $j = [-2, +2]$ (space asymmetrical jumps and so with non-zero drift velocity). The results are then compared with the numerical solution of the generalized diffusion equation (24). Figure 1 illustrates the case without drift for $\eta = 2$ ($\alpha = 3$ and $q = -1$) showing perfect agreement between the Monte-Carlo data and the q-exponential solution (22); for comparison the classical Gaussian result ($\eta = 0$, $q = 1$) is also shown.

Two examples with drift are given in Figs.2 and 3 for $\alpha = 1.1$ ($q = 0.9$) and $\alpha = 2$ ($q = -1$) respectively showing excellent agreement between the simulation data and the solution of the nonlinear equation. We also computed the solution of the generalized diffusion equation without the extra term $\mathsf{E}(r;t)$ for the value $\alpha = 2$; the results are given by the dashed lines in Fig.3. The systematic discrepancy with the simulation results gives clear evidence that the term given by (25) in the generalized equation (24) cannot be neglected. The present results provide the first microscopically based demonstration of the nonlinear diffusion equation. Further results, including the case where the transition probabilities have full spatial dependence (i.e. not only on the distribution at the originating location) are discussed in [14].
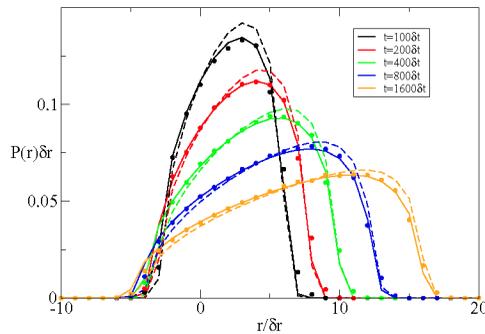
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FIGURE 3. (Color online) Same as Fig.2 for $\alpha = 2$, i.e. $q = -1$. Dashed lines: see text

ACKNOWLEDGMENTS

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