



A LETTERS JOURNAL EXPLORING
THE FRONTIERS OF PHYSICS

OFFPRINT

**Nonlinear diffusion from Einstein's master
equation**

J. P. BOON and J. F. LUTSKO

EPL, **80** (2007) 60006

Please visit the new website
www.epljournal.org

TAKE A LOOK AT THE NEW EPL

Europhysics Letters (EPL) has a new online home at
www.epljournal.org



Take a look for the latest journal news and information on:

- reading the latest articles, free!
- receiving free e-mail alerts
- submitting your work to EPL

www.epljournal.org

Nonlinear diffusion from Einstein's master equation

J. P. BOON^(a) and J. F. LUTSKO^(b)

Physics Department, Université Libre de Bruxelles - CP 231 B-1050 Bruxelles, Belgium

received 8 September 2007; accepted in final form 19 October 2007
published online 13 November 2007

PACS 05.40.Fb – Random walks and Levy flights

PACS 05.60.-k – Transport processes

PACS 05.10.Gg – Stochastic analysis methods (Fokker-Planck, Langevin, etc.)

Abstract – We generalize Einstein's master equation for random-walk processes by considering that the probability for a particle at position r to make a jump of length j lattice sites, $P_j(r)$, is a functional of the particle distribution function $f(r, t)$. By multiscale expansion, we obtain a generalized advection-diffusion equation. We show that the power law $P_j(r) \propto f(r)^{\alpha-1}$ (with $\alpha > 1$) follows from the requirement that the generalized equation admits scaling solutions ($f(r; t) = t^{-\gamma} \phi(r/t^\gamma)$). The solutions have a q -exponential form and are found to be in agreement with the results of Monte Carlo simulations, so providing a microscopic basis validating the nonlinear diffusion equation. Although its hydrodynamic limit is equivalent to the phenomenological porous media equation, there are extra terms which, in general, cannot be neglected as evidenced by the Monte Carlo computations.

Copyright © EPLA, 2007

Introduction. – A standard procedure to describe the microscopic mechanism of a diffusion process is to consider a test particle executing a random walk on some substrate. The idea goes back to 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 long-time limit, $f(r, t)$ is Gaussian in space [2]. This result had been known since Fick's law was established for diffusion; what was new in Einstein's work was the microscopic content, in particular the expression of the diffusion coefficient in terms of the particle velocity autocorrelation function, a form that was further generalized to the general class of transport coefficients known since the 1960s as the Green-Kubo coefficients [3].

The classical diffusion equation has been extensively used and successfully applied to 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 does not hold in more complicated situations such as when there is an interactive process between the particle and the substrate, or in heterogeneous media. In the 1930s, a nonlinear diffusion equation was proposed on a purely phenomenological basis devised in particular to describe diffusive transport in porous media, hence the name *porous media equation* [4]:

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

where D is the diffusion coefficient. This equation, when generalized with an advective term, has a q -Gaussian solution [5] and exhibits the interesting feature that the scaling $\langle r^2 \rangle \propto t^\gamma$ can be non-classical ($\gamma \neq 1$)¹. It was not until the 1990s that a more fundamental basis was proposed for the (generalized) porous media equation using various statistical mechanical approaches. The reason for the various approaches can be found in the variety of problems where non-classical (non-Gaussian) distributions are observed: transport in porous media, viscous fingering, information diffusion in social networks or in the internet, financial market distributions,...

^(a)E-mail: jdboon@ulb.ac.be

^(b)E-mail: jlutsko@ulb.ac.be

¹When $\alpha=1$, 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: $\langle r^n \rangle \propto t^{n\gamma/2}$.

The proposed approaches use formulations such as the generalized entropy [6], the Langevin equation [7,8], the master equation [9], the nonlinear response [10], the escort distribution [11], or the generalized generating function [12]; for a review, see [13].

Generalized master equation. – Here we use the microscopic approach by going back to Einstein’s original derivation 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

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

where the Boolean variable $n(r; t) = \{0, 1\}$ denotes the occupation at time t of the site located at position r and ξ_{\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]:

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

where $P_j(\ell)$ denotes the probability that the walker at site ℓ make a jump of j sites². 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:

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

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

As discussed in the introductory section, in more complex situations, when the linear response hypothesis is no longer valid, one observes non-Gaussian behavior, *i.e.* the long-time dynamics is different from that described by the classical Fokker-Planck equation (or the usual advection-diffusion equation). 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. 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 displacements³, we

²In Einstein’s formulation the particle jumps are restricted to symmetrical displacements, *i.e.* $P_{+j} = P_{-j}$.

³Any distribution for which the moments are finite, for instance, $p_j \sim e^{-j}$ or $p_j \sim t^{-\mu}$ with a cutoff.

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 equation. – Along the same lines as the classical diffusion equation is obtained from Einstein’s master equation, we perform a multi-scale expansion of the generalized master equation (5) using an expansion of the time and space derivatives of the form⁴

$$\frac{\partial}{\partial t} = \epsilon \frac{\partial^{(1)}}{\partial t} + \epsilon^2 \frac{\partial^{(2)}}{\partial t} + \dots, \quad (6)$$

$$\frac{\partial}{\partial r} = \epsilon \frac{\partial}{\partial r} + \epsilon^2 \frac{\partial^2}{\partial r^2} + \dots,$$

and a corresponding expansion of the distribution as

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

To first order, we have

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

and to second order

$$\begin{aligned} \mathcal{O}(\epsilon^2): \quad & \frac{\partial^{(1)}}{\partial t} f_1(r; t) + \frac{\partial^{(2)}}{\partial t} f_0(r; t) \\ & + \frac{1}{2} (\delta t) \frac{\partial^{(1)2}}{\partial t^2} f_0(r; t) = \\ & - \left(J_1 \frac{\delta r}{\delta t} \right) \frac{\partial^{(1)}}{\partial r} \left(\left. \frac{dgF(g)}{dg} \right|_{g=f_0(r; t)} f_1(r; t) \right) \\ & - \left(\frac{\delta r}{\delta t} J_1 \right) \frac{\partial^{(2)}}{\partial r} F(f_0(r; t)) f_0(r; t) \\ & + \frac{1}{2} \left(\frac{(\delta r)^2}{\delta t} J_2 \right) \frac{\partial^{(1)2}}{\partial r^2} F(f_0(r; t)) f_0(r; t), \quad (9) \end{aligned}$$

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:

$$\begin{aligned} & \frac{\partial}{\partial t} f(r; t) + C \frac{\partial}{\partial r} [F(f(r; t)) f(r; t)] = \\ & D \frac{\partial^2}{\partial r^2} [F(f(r; t)) f(r; t)] + \frac{1}{2} (C^2 \delta t) \frac{\partial}{\partial r} \mathbb{E}(r; t). \quad (10) \end{aligned}$$

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

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

⁴The smallness parameter is defined as the ratio of δr to the length scale over which the relative variation of the distribution is of order one and similarly for the time scale; see [14].

and

$$\begin{aligned} E(r; t) = & \frac{\partial}{\partial r} [F(f(r; t))f(r; t)] \\ & - \left(\left| \frac{dgF(g)}{dg} \right|_{g=f(r; t)} \frac{\partial}{\partial r} [F(f(r; t))f(r; t)] \right). \end{aligned} \quad (12)$$

When there is an external force acting on the particle, eq. (10) is further generalized as discussed elsewhere [14].

Scaling solution. – Under which conditions is there a scaling solution to the generalized equation? For simplicity, consider the diffusion equation with no drift, *i.e.* the jump probability is space symmetrical and consequently the first moment $J_1 = 0$ and $C = 0$, and (10) reduces to

$$\frac{\partial}{\partial t} f(r; t) = D \frac{\partial^2}{\partial r^2} [F(f(r; t))f(r; t)]. \quad (13)$$

Assuming that $f(r; t) = t^{-\gamma/2} \phi(r/t^{\gamma/2}) = t^{-\gamma/2} \phi(x)$, and expressing the time and space derivatives in terms of x , eq. (13) is rewritten as (see [14] for details)

$$-\gamma \frac{d}{dx} x \phi(x) = 2 D t^{1-\gamma} \frac{d^2}{dx^2} F(t^{-\gamma/2} \phi(x)) \phi(x). \quad (14)$$

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.*

$$\gamma = \frac{2}{2 + \eta}. \quad (15)$$

Thus, when $\eta \neq 0$, this describes anomalous diffusion: $\langle r^2 \rangle \sim t^{\frac{2}{2+\eta}}$ (and more generally $\langle r^n \rangle \sim t^{\frac{n}{2+\eta}}$). In this case, eq. (14) becomes

$$D \frac{d^2}{dx^2} \phi^{1+\eta}(x) + \frac{1}{2+\eta} \frac{d}{dx} x \phi(x) = 0, \quad (16)$$

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

$$\phi(x) = \left(\frac{1+2\eta}{1+\eta} B \right)^{\frac{1}{\eta}} \left[1 - \frac{\eta}{2(2+\eta)(1+2\eta)BD} x^2 \right]^{\frac{1}{\eta}}, \quad (17)$$

where B is an integration constant. With $\eta = 1 - q$, and returning to the original space and time variables, (17) takes the canonical q -exponential form

$$f(r; t) = B_q t^{-\frac{1}{3-q}} \left[1 - (1-q) M_q \frac{r^2}{D t^{\frac{2}{3-q}}} \right]^{\frac{1}{1-q}} \quad (18)$$

with

$$\begin{aligned} B_q &= \left[\left(1 + \frac{1-q}{2-q} \right) B \right]^{\frac{1}{1-q}}, \\ M_q^{-1} &= 2(3-q)(3-2q)B. \end{aligned} \quad (19)$$

So, with no drift and no external field, the generalized random-walk model describes anomalous diffusion with

q -distributions⁵. It also follows from (18) that the distribution of the values taken by $f(r; t)$ at any fixed value of time has the form of a power law [15]; defining $\tilde{f}(r; t) = B_q^{-1} t^{\frac{1}{3-q}} f(r; t)$, we have

$$\mathcal{P}(\tilde{f}) = \int_{-\infty}^{\infty} dr D^{-\frac{1}{2}} t^{-\frac{1}{3-q}} \delta(\tilde{f}(r; t) - \tilde{f}) \sim \frac{\tilde{f}^{-q}}{\sqrt{1 - \tilde{f}^{1-q}}}. \quad (20)$$

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.

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 $\eta = \alpha - 1$)

$$\begin{aligned} \frac{\partial}{\partial t} f(r; t) + C \frac{\partial}{\partial r} f^\alpha(r; t) = \\ D \frac{\partial^2}{\partial r^2} f^\alpha(r; t) + \frac{1}{2} (C^2 \delta t) \frac{\partial}{\partial r} E(r; t), \end{aligned} \quad (21)$$

with

$$E(r; t) = (1 - \alpha f^{\alpha-1}(r; t)) \frac{\partial}{\partial r} f^\alpha(r; t). \quad (22)$$

Comparison of eq. (21) and eq. (1) shows that the two equations are the same in the absence of drift ($C = 0$). With non-zero drift, this corresponds to a generalized porous media equation when the second term on the r.h.s. of (21) 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. (21) contains an additional term which, in general, cannot be neglected (see next section).

Microscopic simulations. – Monte Carlo simulations are performed with the generalized master equation (5) using the 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), and the results are compared with the numerical solution of the generalized diffusion equation (21). 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 (18); 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

⁵One verifies straightforwardly that for $q \rightarrow 1$, one retrieves the classical Gaussian distribution.

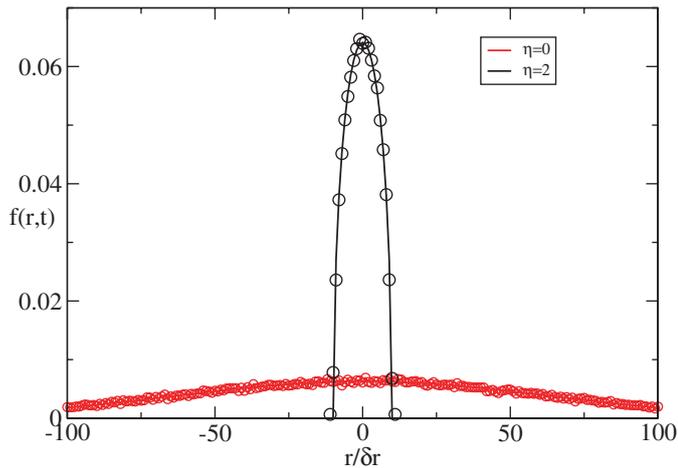


Fig. 1: (Color online) Generalized diffusion with no drift: the distribution function $f(r; t=2000$ time steps) obtained from Monte Carlo simulations (symbols) and the solution (18) of the generalized diffusion equation for $\alpha=3$ (upper curve) and $\alpha=1$ (10^5 walkers; initial condition: $f(r, t=0) = \delta(r)$).

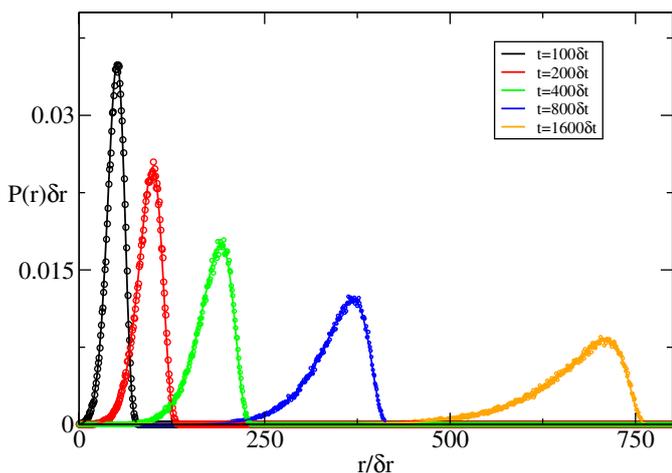


Fig. 2: (Color online) Generalized diffusion with drift: the distribution function $f(r; t=100$ to 1600 time steps) obtained from Monte Carlo simulations (symbols) and the numerical solution of the generalized diffusion equation (21) (solid lines) for $\alpha=1.1$, *i.e.* $q=0.9$ (10^5 walkers; initial condition: $f(r, t=0) = \delta(r)$).

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 $E(r; t)$ 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 (22) in the generalized equation (21) cannot be neglected. To the best of our knowledge the present results provide the first microscopically based demonstration of the nonlinear diffusion equation. Further results, including the case where the transition

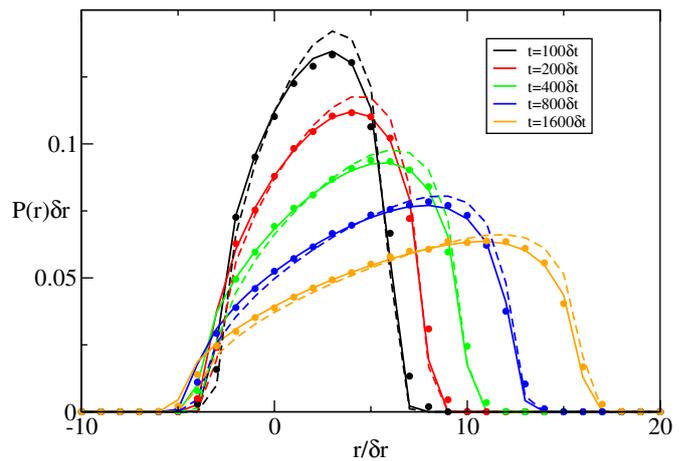


Fig. 3: (Color online) Same as fig. 2 for $\alpha=2$, *i.e.* $q=-1$. Dashed lines: see text.

probabilities have full spatial dependence (*i.e.* not only on the distribution at the originating location) and the generalization with an external force (*i.e.* the nonlinear advection-diffusion equation) are discussed in [14].

The work of JFL was supported in part by the European Space Agency under contract number ESA AO-2004-070.

REFERENCES

- [1] EINSTEIN A., *Ann. Phys. (Leipzig)*, **17** (1905) 549.
- [2] FELLER W., *An Introduction to Probability Theory*, Vol. 1, third edition (Wiley, New York) 1968, Sect. XIV.6.
- [3] BOON J. P. and YIP S., *Molecular Hydrodynamics* (Dover, New York) 1991, Chapt. 2.
- [4] MUSKAT M., *The Flow of Homogeneous Fluids Through Porous Media* (McGraw-Hill, New York) 1937.
- [5] PLASTINO A. R. and PLASTINO A., *Physica A*, **222** (1995) 347.
- [6] TSALLIS C. and BUKMAN D. J., *Phys. Rev. E*, **54** (1996) R2197.
- [7] BORLAND L., *Phys. Rev. E*, **57** (1998) 6634.
- [8] ANTENEODO C. and TSALLIS C., *J. Math. Phys.*, **44** (2003) 5194.
- [9] CURADO E. M. F. and NOBRE F. D., *Phys. Rev. E*, **67** (2003) 021107.
- [10] LUTSKO J. F. and BOON J. P., *Europhys. Lett.*, **71** (2005) 906.
- [11] ABE S. and THURNER S., *Physica A*, **356** (2005) 403.
- [12] BOON J. P. and LUTSKO J. F., *Physica A*, **368** (2006) 55.
- [13] CHAVANIS P. H., arXiv/cond-mat 0709.1829v1 (2007).
- [14] LUTSKO J. F. and BOON J. P., to be published in arXiv/cond-mat (2007).
- [15] GROSFILS P. and BOON J. P., *Europhys. Lett.*, **74** (2006) 609.