Aging in models of nonlinear diffusion

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We show that for a class of problems described by the nonlinear diffusion equation $\partial/\partial t\,\phi^{\mu}=D\partial^2/\partial x^2\phi^{\nu}$ an exact calculation of the two time autocorrelation function gives $C(t,t')=f(t-t')g(t')$ $(t>t')$ exhibiting normal and anomalous diffusions, as well as aging effects, depending on the values of μ and ν. We also discuss the form in which the fluctuation-dissipation theorem is violated in this type of systems. Finally, we argue that in this kind of model, aging may be a consequence of the nonconservation of the ''total mass.'' [S1063-651X(97)11802-5]

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In a wide variety of physical systems, where some kind of diffusion takes place, it can be observed that the mean-squared displacement scales with time as $\langle x^2(t)\rangle\propto t^{\alpha}$ with α depending on the physical problem in question. $\alpha=1$ corresponds to the so-called *normal diffusion* (the simple random walk), of which a complete statistical description can be obtained, for example, from the solution of the well known *diffusion equation* $\partial/\partial t\,\phi(x,t)=D\partial^2/\partial x^2\phi(x,t)$, where $\phi(x,t)$ is the probability that the diffusing particle be at position x at time t provided it was at the origin $x=0$ at $t=0$ and D is the diffusion constant. If $\alpha\neq 1$ the diffusion is called *anomalous* with $\alpha<1$ corresponding to *subdiffusion* and $\alpha>1$ to *superdiffusion* [1]. Anomalous diffusion can be a consequence, for example, of some kind of disorder in the system [1,2], or more generically, of long-range correlations in space-time. The computation of the propagator $\phi(x,t)$, which contains all the spatiotemporal information of the system, is in general a difficult task. Without knowing the exact propagator for all times, its long-time form can be calculated in some cases using techniques like renormalization group and scaling arguments [3].

Recently Tsallis and Bukman [4] have obtained the *exact* solution of the nonlinear Fokker-Planck equation

$$\frac{\partial}{\partial t}\phi(x,t)^{\mu}=-\frac{\partial}{\partial x}\{F(x)[\phi(x,t)]^{\mu}\}+D\frac{\partial^2}{\partial x^2}[\phi(x,t)]^{\nu}, \tag{1}$$

where $(\mu,\nu)\in\mathbb{R}^2$, $D>0$ is a diffusion constant, $F(x)=-dV(x)/dx$ is an external force associated with the potential $V(x)$, and (x,t) is 1+1 space-time. They have found the solution for a drift of the form $F(x)=k_1-k_2x$ with k_1 and k_2 constants. This equation recovers the standard diffusion or Fokker-Planck equation when $\mu=\nu=1$. Other values of (μ,ν) represent interesting physical systems as well: in the case with $F(x)=0$ (a purely diffusive problem), for $\mu=1$ and arbitrary ν, Eq. (1) is known as the *porous medium equation* and models many nonequilibrium systems in fluid dynamics [5], particle diffusion in magnetic fields [6], and gas dynamics [7], depending on the value of ν. The information-theoretic aspects of this case have been studied by Plastino and Plastino [8] and recently the interplay between dynamic and thermodynamic aspects have been studied in [10] for the general case of diffusion in N dimensions. The case $\mu=1$ and $\nu=3$ has been studied by Spohn [9] and describes a solid-on-solid model of surface growth.

Restricting the situation to the one without drift (for the general case see Ref. [4]), the solution for the propagator $\phi_q(x,t)$ can be written as

$$\phi_q(x,t)=\frac{\{1-\beta(t)(1-q)[x-x_M(t)]^2\}^{1/(1-q)}}{Z_q(t)}, \tag{2}$$

with $q=1+\mu-\nu$ and $x_M(t)=x_M(0)$ is the mean position, which for a situation without drift is constant and equal to the initial position. This solution is closed by the relations satisfied by $\beta(t)$ and $Z_q(t)$, namely,

$$\frac{\beta(t)}{\beta(0)}=\left[\frac{Z_q(0)}{Z_q(t)}\right]^{2\mu} \tag{3}$$

and

$$Z_q(t)=\left\{[Z_q(0)]^{\mu+\nu}+\frac{2\nu(\nu+\mu)D\beta(0)[Z_q(0)]^{2\mu}}{\mu}t\right\}^{1/\mu+\nu}. \tag{4}$$

A static form of Eq. (2) with $\beta(t)=1/T$ (inverse temperature) and $Z_q(t)=Z_q(T)$ (partition function) has been obtained from a maximum entropy principle in the context of a generalized thermstatistics [11], and successfully applied for explaining, among many other problems, the thermodynamic foundations of Lévy anomalous diffusion [12,13]. We will see in the following that the above solution presents a very rich dynamical behavior characterized in general by anomalous diffusion and, for certain values of μ and ν, by aging phenomena, the long-term memory effects observed and nowadays extensively studied in amorphous polymers [14] and spin glasses [15]. Let us consider the two-time autocorrelation function

$$C(t,t')\equiv\langle y(t)x(t')\rangle \tag{5}$$

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$$= \int_{-\infty}^{\infty} dx\, dy\; x\, y\; \phi_q(x,0,t')\phi_q(y,x,t-t'), \tag{6}$$

in which $t'<t$ and where $\phi_q(u,v,z-z')$ is the probability that the particle was at position u at time z provided it was at position v at time z'. From Eq. (2) we obtain

$$C(t,t') = K_q\{Z_q(t-t')Z_q(t')[\beta(t-t')]^{1/2}[\beta(t')]^{3/2}\}^{-1}, \tag{7}$$

with K_q a constant that only depends on q. Now considering the regime in which $t-t'\to\infty$ and also $t,t'\to\infty$, from Eqs. (3), (4), and (7)

$$C(t,t') = A[B(t-t')]^{(\mu-1)/(\mu+\nu)}[Bt']^{(3\mu-1)/(\mu+\nu)}, \tag{8}$$

where

$$A = \frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{1}{q-1}-\frac{1}{2}\right)\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{1}{q-1}-\frac{3}{2}\right)}{\Gamma^2\left(\frac{1}{q-1}\right)(q-1)^2}\,\frac{1}{\beta^2(0)}\,\frac{1}{Z^{4\mu}(0)} \tag{9}$$

and

$$B = 2\,D\,\frac{\nu(\nu+\mu)}{\mu}\,\beta(0)Z^{2\mu}(0). \tag{10}$$

This result presents a variety of interesting characteristics. First we note that for $\mu=\nu=1$ we obtain the well known result for normal diffusion $C(t,t') = 2\,D\,\min(t,t')$. For the case of the porous medium equation, i.e., $\mu=1$, the asymptotic correlation simplifies to

$$C(t,t') = A[Bt']^{2/(1+\nu)}. \tag{11}$$

In this case the long-time behavior depends only on the minimum time (as in normal diffusion) but the diffusion is anomalous with exponent $2/(1+\nu)$. When $\nu>1$ the behavior is *subdiffusive* and for $\nu<1$ it is *superdiffusive*. This qualitative change can be conveniently observed in the shape of the propagator at a fixed time t^*, as shown in Fig. 1. In the subdiffusive regime, characteristic of the porous medium equation, the propagator presents a ''wave front'' that expands with time as

$$|x_{wf}| = \frac{1}{\sqrt{\beta(0)(\nu-1)}}\,\frac{Z_q(t)}{Z_q(0)}, \tag{12}$$

with $Z_q(t)$ given by Eq. (4). As $t\to\infty$ it flattens as $|x_{wf}| \propto t^{1/(1+\nu)}$. The wave front changes to the exponential decay of the normal Gaussian diffusion when $\nu=1$ and then to superdiffusion characterized by power law tails in the propagator that decays for $x\to\pm\infty$ and t fixed as

$$\phi(x) \propto |x|^{2/(\nu-1)}, \quad \nu<1. \tag{13}$$

Although the previous discussion considered $\mu=1$, it is valid in the general case in which the different regimes are more conveniently characterized by the parameter $q=1+\mu-\nu$ ($q<1$,1 and >1 corresponds to subdiffusive, normal and superdiffusive behaviors, respectively), and the relation defines the possible choices for μ and ν.

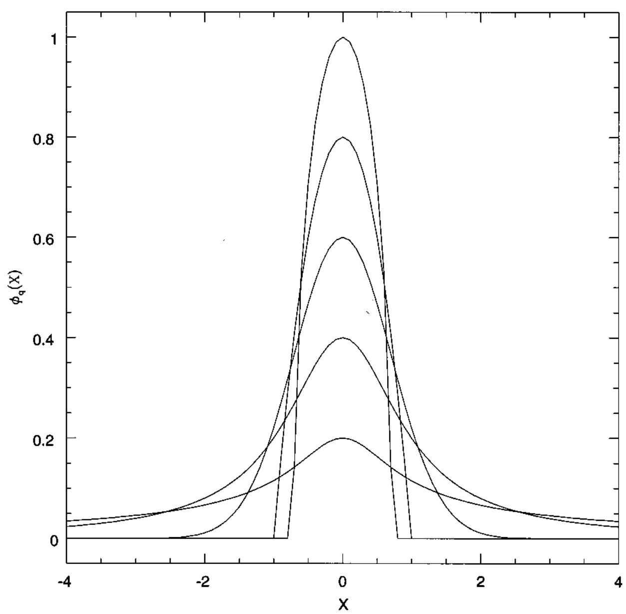

FIG. 1. Qualitative shape of the propagator $\phi_q(x,t)$ for fixed t. From top to bottom $q=-1,0,1,2,3$.

For $\mu\neq 1$ the autocorrelation function depends explicitly on both times, on all time scales, a feature characteristic of systems with long term memory. These effects of *aging* are common in disordered systems (e.g., spin glasses) where the time correlations present particular scaling forms (see [15] and references therein). Aging effects have also been studied in models without an explicit disorder as scalar fields, the XY model, and spinodal decomposition [16], and also in random walks in disordered media [17,18]. In order to compare the present scalings with those found in spin glasses it is convenient to normalize the correlation function in order to have $C(t,t)=1$. This normalization is natural in magnetic systems but it is not so for an arbitrary random walk. In our problem a suitable definition may be

$$C_n(t,t') = \frac{C(t,t')}{\sqrt{C(t,t)C(t',t')}}. \tag{14}$$

With this definition we obtain

$$C_n(t,t') \propto (t-t')^{(\mu-1)/(\mu+\nu)}\left(\frac{t'}{t}\right)^{(3\mu-1)/[2(\mu+\nu)]}, \tag{15}$$

when $t,t'\to\infty$ and $t-t'\to\infty$. This normalized correlation presents the commonly seen scaling with t'/t. The breaking of time translation invariance can be clearly seen in the so-called displacement function

$$B(t,t') \equiv \langle [y(t)-x(t')]^2\rangle \tag{16}$$

$$= C(t,t)+C(t',t')-2C(t,t'). \tag{17}$$

By definition $B(t,t)=0$. Writing $\tau=t-t'$

$$B(t'+\tau,t') \propto t'^{(3\mu-1)/(\mu+\nu)} + (t'+\tau)^{(3\mu-1)/(\mu+\nu)} - 2\tau^{(\mu-1)/(\mu+\nu)}t'^{(3\mu-1)/(\mu+\nu)}. \tag{18}$$

We see that in general $B(t'+\tau,t')$ depends on both t' and τ and consequently time translation invariance is broken. When $\mu=1$ and $\tau \gg t'$

$$B(t'+\tau,t') \approx \tau^{2/(1+\nu)}. \qquad (19)$$

The displacement depends only on the time difference τ and time translation invariance is recovered.

These results also reflect in the behavior of a suitable generalization of the fluctuation-dissipation theorem (FDT) for systems that may never attain equilibrium. This generalized form, firstly introduced for studying the off-equilibrium dynamics of spin glasses [19], states that

$$R(t,t') = \beta\theta(t-t')X(t,t')\frac{\partial C(t,t')}{\partial t'}. \qquad (20)$$

where $R(t,t')$ is the response at time t to an external force h applied at time t'

$$R(t,t') = \left.\frac{\delta\langle x(t)\rangle}{\delta h(t')}\right|_{h=0}, \qquad (21)$$

β is the inverse temperature and $\theta(z)$ is the step function. The function $X(t,t')$ measures the departure from FDT; if FDT is satisfied then $X(t,t')=1$. In general FDT will be violated by a system that never reaches equilibrium, as in the models we are considering here, but it is, nevertheless, instructive to analyze how the function X behaves. If we apply an external perturbation h at time t', the form of the propagator remains the same as in Eq. (2), but now $x_M(t)$ satisfies the differential equation

$$\frac{d}{dt}x_M(t) = h\,\delta(t-t'), \qquad (22)$$

whose solution is $x_M(t)=x_M(0)+h\,\theta(t-t')$. According to Eq. (21) the response function is $R(t,t')=\theta(t-t')$. Now, for the case of the usual random walk ($\mu=\nu=1$), an explicit calculation from Eq. (8) gives, for the correlation function, $C(t,t')=2Dt'$. Noting that in the standard Fokker-Planck equation $\beta \rightarrow 1/D$, we obtain from Eq. (20) that $X(t,t')=1/2$. Consequently, for the simple random walk, FDT is violated with a factor X that is a constant [16]. In the case of the porous medium equation ($\mu=1$, arbitrary ν), a similar analysis shows that $X(t,t')=f(t')$, i.e., the correction factor is a function of t' only. In the third case, for arbitrary μ and ν the function X depends explicitly on both times t and t'. From this analysis it is clear that, although all three cases violate FDT (as expected), the dynamics becomes more complex as we go from the simple random walk, to the porous medium equation and finally to arbitrary (μ,ν), and this is reflected in the structure of the function $X(t,t')$.

Finally and from another point of view, we argue that the absence (presence) of aging phenomena is a direct consequence of the ‘‘conservation of mass’’ (or not) in the system. For our model it can be verified that [4]

$$\int dx\ \phi_q(x,t) = \left[\frac{Z_q(t)}{Z_q(0)}\right]^{\mu-1}\int dx\ \phi_q(x,0), \qquad (23)$$

and consequently the norm of the distribution or ‘‘total mass’’ is independent of time only if $\mu=1$. As suggested by Goldendfeld for the case of the normal diffusion, the conservation of mass is directly connected with the fact that asymptotically the system loses memory of its history and becomes unable to distinguish between different initial conditions. The situation is completely different if the mass is not conserved, as, for example, in the modified porous medium equation [20] and in the problems we consider here when $\mu \neq 1$. Although we are not able to give a rigorous proof of this assertion, the different situations studied here are in agreement with it. Consequently, it would be a direct connection between conservation of the mass and aging in the class of systems considered: for our model equation, in the systems with $\mu=1$, the mass is conserved and the autocorrelation function does not present aging behavior. But if $\mu \neq 1$ there is no conservation of the mass and aging effects are seen.

Concluding, a number of interesting problems that can be modeled by nonlinear diffusion equations can be solved exactly and the diffusion presents very different characteristics depending on the degree of nonlinearity. An exact calculation of the two-time correlation functions shows that, besides the expected anomalous diffusion, some systems may exhibit aging effects as found in many other disordered systems. The aging satisfies particular scaling forms, depending on the problem considered, which in principle could be compared with experimental results. The different dynamical scenarios can be characterized also by studying the (violation of) the fluctuation-dissipation theorem. These aging effects, in systems modeled by partial differential equations, seem to be strongly related to the conservation of the ‘‘total mass.’’ It would be interesting to test the validity (or not) of this hypothesis in other models and also to study the extensions of these results for dimensions higher than one.

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