Wave fronts in bistable reactions with anomalous Lévy-flight diffusion

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Shape-preserving traveling solutions of an equation describing the interplay of bistable reaction processes and Lévy-flight anomalous diffusion are obtained and analyzed. The velocity of these wave fronts is determined as a function of the reaction parameters and the anomalous-diffusion exponent, and their shape is characterized in terms of simple quantities. [S1063-651X(97)09701-8]

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Anomalous diffusion is the underlying transport mechanism in a variety of physical systems of both theoretical and applied interest. It is characterized by a mean square displacement which depends on time as [1]

$$\langle r^2(t)\rangle \propto t^{\nu}, \tag{1}$$

with $\nu\neq 1$. More generally, this power-law dependence can be replaced by a generic function of time [2], but such a possibility has been scarcely studied. Power-law anomalous hyperdiffusion ($\nu>1$) occurs, for example, in developed turbulence [3] and phase-space dynamics of chaotic systems [4], whereas the subdiffusive case ($\nu<1$) is found in motion through highly heterogeneous media, such as disordered surfaces, porous materials, and gels [1].

A convenient model for anomalous diffusion is provided by random walks in which the jump probability $p(x)$ depends on the jump length x as a decreasing power law; for instance, in one dimension and for large $|x|$,

$$p(x)\propto |x|^{-1-\gamma}, \tag{2}$$

with $0<\gamma<2$. Lévy flights [5], defined through the Fourier transform of $p(x)$ as

$$p(k)=\exp(-|k/k_0|^{\gamma}) \quad (k_0=\text{const}), \tag{3}$$

are a paradigm of such random walks. For $\gamma\geqslant 2$, the one-step mean square displacement of a Lévy flight is finite and ordinary diffusion is recovered. For $\gamma<2$, instead, $\langle x^2\rangle$ is infinite, and Lévy flights produce hyperdiffusion. Although in this case the exponent ν in Eq. (1) is not defined, it has been shown that a confinement of the random walk gives place to a transitory regime in which one can identify $\nu=2/\gamma$ [6]. The combination of Lévy flights with power-law waiting time distributions makes it possible to consider a wider range of values of ν, including both hyperdiffusive and subdiffusive regimes [3,4].

It has been argued [6] that the one-dimensional ordinary-diffusion equation can be generalized to the case of Lévy-flight diffusion by writing, in the Fourier representation,

$$\partial_t \tilde{\phi}(k,t) = -D_{\gamma}|k|^{\gamma}\tilde{\phi}(k,t), \tag{4}$$

where

$$\tilde{\phi}(k,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\exp(ikx)\,\phi(x,t)\,dx \tag{5}$$

is the Fourier transform of the density of diffusing particles $\phi(x,t)$. The anomalous diffusion coefficient is given by $D_{\gamma}\propto\tau^{-1}|k_0|^{-\gamma}$, where τ is the (mean) waiting time of the random walk. The solution to Eq. (4) can be immediately written as

$$\tilde{\phi}(k,t)=\tilde{\phi}(k,0)\exp(-D_{\gamma}t|k|^{\gamma}), \tag{6}$$

but the antitransformed density $\phi(x,t)$ does not have a generic analytical expression.

This Brief Report is devoted to the study of some solutions of Eq. (4) when it is extended to consider reaction processes in the same spirit of ordinary reaction-diffusion equations. The interplay of anomalous diffusion and reaction processes has been recently addressed in connection with the anomalous kinetics of bimolecular reactions such as $A+A\rightarrow A$, $A+A\rightarrow 0$, and $A+B\rightarrow 0$ [7,8]. The study of such interplay in the frame of a formulation such as a generalized reaction-diffusion equation should provide insight into the effect of anomalous diffusion on self-organization phenomena, which are the main manifestation of complex behavior in reacting and diffusing systems [9,10]. One can then propose, in the Fourier representation, the reaction-anomalous diffusion equation

$$\partial_t\tilde{\phi}=-D_{\gamma}|k|^{\gamma}\tilde{\phi}+\omega\tilde{f}, \tag{7}$$

where $\tilde{f}$ is the Fourier transform of the reaction term $f(\phi)$, and ω is a constant that measures the strength of reactions. Note that, in general, $f(\phi)$ is a nonlinear function and, therefore, $\tilde{f}$ does not have an explicit form as a function of $\tilde{\phi}$.

For bistable reaction models—where $f(\phi)$ has two roots which correspond to homogenenous stable states—it is well known that the interplay of ordinary diffusion and reactions determines, as generic behavior, the development of smooth wave fronts in the density profile [10]. These shape-preserving fronts connect regions in which the density equals one of the two stable states, and have a well defined constant velocity, given by the parameters of the reaction function.

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Depending on those parameters, one of the two stable states dominates over the other, and the fronts move in such a way that the dominant state is eventually reached at any point in the system. A convenient form of a bistable reaction term is

$$f(\phi)=-\phi+\phi_h\theta(\phi-\phi_c), \tag{8}$$

with $0<\phi_c<\phi_h$, and where $\theta(\phi)$ is the Heaviside step function. The corresponding homogeneous stable states are $\phi=0$ and $\phi=\phi_h$. This piecewise-linear reaction function preserves the nonlinear character of more complex models, but makes possible an analytical treatment of the problem. It has been extensively used in the literature [11], along with other piecewise linearized models. In the following, this reaction model is considered in connection with Eq. (7), and wave-front solutions in bistable systems under the effect of anomalous diffusion are consequently obtained.

Shape-preserving wave fronts correspond to similarity solutions of the form $\phi(x,t)\equiv\phi(x-vt)$, where v is the front velocity. In the Fourier representation, one has $\tilde{\phi}(k,t)\equiv\exp(ikvt)\tilde{\phi}(k)$. For these special solutions and for the reaction term given in Eq. (8), the reaction-anomalous diffusion equation reads

$$ivk\tilde{\phi}=-D_\gamma|k|^\gamma\tilde{\phi}-\omega\tilde{\phi}-\frac{1}{ik}\frac{\omega\phi_h}{\sqrt{2\pi}}\exp(ik\xi_c). \tag{9}$$

Here ξ_c is the point at which $\phi(\xi=x-vt)$ reaches the critical value ϕ_c: $\phi(\xi_c)=\phi_c$. Since the problem is invariant under spatial shifts, it is possible to fix $\xi_c=0$. With this choice, the solution to Eq. (9) is

$$\tilde{\phi}(k)=-\frac{1}{ik}\frac{\omega\phi_h}{\sqrt{2\pi}}[D_\gamma|k|^\gamma+ivk+\omega]^{-1}. \tag{10}$$

This solution has to be antitransformed to obtain the density profile $\phi(\xi)$. To proceed with this antitransformation, it is first necessary to fix the asymptotic values of $\phi(\xi)$ for $\xi\to\pm\infty$. Taking $\phi(-\infty)\to0$ and $\phi(+\infty)\to\phi_h$, the density profile can be expressed as

$$\phi(\xi)=\frac{\phi_h}{2\pi}\lim_{\epsilon\to0^+}\int_{-\infty}^{+\infty}\frac{dk}{-ik+\epsilon}\frac{\exp(-iky)}{|k|^\gamma+iuk+1}, \tag{11}$$

where $y=\xi/(D_\gamma/\omega)^{1/\gamma}$ and $u=v/\omega^{1-1/\gamma}D_\gamma^{1/\gamma}$ are adimensionalized coordinate and front velocity, respectively. A more explicit, real form for the complex integral in Eq. (11) makes it possible to write

$$\phi(\xi)=\frac{\phi_h}{2\pi}\left[\pi+2\int_0^\infty dk\frac{k^{-1}(k^\gamma+1)\sin ky+u\cos ky}{(k^\gamma+1)^2+u^2k^2}\right]. \tag{12}$$

The integral in this solution can be explicitly calculated only for the case of ordinary diffusion ($\gamma=2$) and for $\gamma=1$, when the Lévy distribution corresponds, in the coordinate space, to a Cauchy distribution, $p(x)\propto(1+k_0^2x^2)^{-1}$. Although for $\gamma=0$ the integral can also be found, the limit $\gamma\to0$ is singular with respect to Lévy distributions. In fact, for $\gamma=0$ Eq. (3) implies $p(k)=\text{const}$ and, therefore, $p(x)\propto\delta(x)$, which describes immobile particles. For noninteger values of γ, the profile $\phi(\xi)$ has to be calculated numerically.

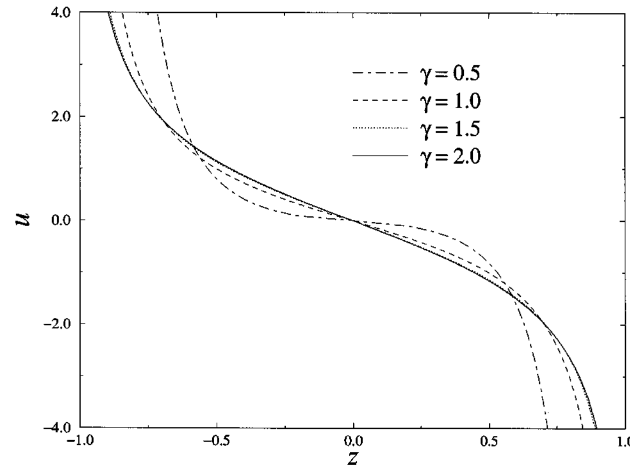

FIG. 1. Adimensionalized wave-front velocity u in a piecewise linearized bistable reaction model driven by Lévy-flight anomalous diffusion as a function of the reaction parameter z, for various values of the Lévy exponent γ.

The condition $\phi(0)=\phi_c$, given above by the choice of the critical point ξ_c, produces

$$\phi_c=\frac{\phi_h}{2\pi}\left[\pi+2\int_0^\infty dk\frac{u}{(k^\gamma+1)^2+u^2k^2}\right], \tag{13}$$

which can be rewritten as

$$z=-\frac{2u}{\pi}\int_0^\infty\frac{dk}{(k^\gamma+1)^2+u^2k^2}, \tag{14}$$

with $z=1-2\phi_c/\phi_h$. This implicit equation determines the value of the front velocity u as a function of the reaction parameters—combined in a single quantity z—and the anomalous-diffusion exponent γ. The parameter z ($-1<z<1$) is a direct measure of the relative prevalence of the two stable states in the reaction model. For $z>0$, $\phi=\phi_h$ dominates over $\phi=0$, and vice versa for $z<0$. In fact, Eq. (14) shows that the sign of z fixes the direction of motion of the wave front, irrespectively of the value of γ. For $z>0$ the front moves leftwards, and the density approaches the homogenenous state ϕ_h. For $z<0$ the front velocity is positive, and $\phi(x,t)$ vanishes asymptotically for all x.

In the case of ordinary diffusion, the adimensional front velocity is given by [11]

$$u(\gamma=2)=-\frac{2z}{\sqrt{1-z^2}}, \tag{15}$$

whereas for a Cauchy jump distribution one obtains

$$u(\gamma=1)=\cot\left[\frac{\pi}{2}z(1-|z|^{-1})\right]. \tag{16}$$

In Fig. 1, these two functions are plotted along with the numerical calculation of $u(z)$ for $\gamma=1.5$ and 0.5. The curves for $\gamma=2$ and 1.5 are practically indistinguishable. Appreciable differences appear only for $\gamma\approx1$, and for decreasing γ the dependence of the velocity on the parameter z is less smooth. The qualitative behavior of these curves is, however, independent on the anomalous diffusion exponent, and it can be proven from Eq. (14) that, for arbitrary γ, $u \to \mp\infty$ as $z \to \pm 1$.

Focusing attention now on the form of the density profile, it is first possible to show that the asymptotic tail of the solution given by Eq. (12), $\phi(\xi \to -\infty)$, depends in a rather strong way on the anomalous-diffusion coefficient γ. In fact, for $\gamma > 1$ and $u \neq 0$, one has

$$\phi(\xi \to -\infty) \propto \exp(-|y/u|), \tag{17}$$

i.e., an exponential decay which depends on the value of γ only through the velocity u. On the other hand, for $\gamma < 1$, the asymptotic tail decays as a power law,

$$\phi(\xi \to -\infty) \propto |y|^{-\gamma}, \tag{18}$$

which also holds for $\gamma > 1$ when $u = 0$. For $\gamma < 1$, therefore, the density profile decays relatively slowly and, in fact, its tail is not normalized: the total number of diffusing particles beyond a certain distance from the front is infinite. This contrasts with the case of $\gamma > 1$, where the exponential decay corresponds to a finite total particle number. This difference should be ascribed to the stronger effect of anomalous diffusion for lower values of γ. In the limit $\xi \to +\infty$, the density approaches its asymptotic value ϕ_h, with the same functional form as it vanishes for $\xi \to -\infty$.

Since the form of the solution given by Eq. (12) is relatively simple—it is a monotonic function with well defined, constant asymptotic values—the front profile can be qualitatively characterized by a single parameter, namely, its width Δ. A convenient definition for this quantity could be given in terms of the derivative of $\phi(\xi)$ at the origin: $\Delta^{-1} \propto d\phi/d\xi|_{\xi=0}$. However, it can be shown that, when $\gamma < 1$ and $u \neq 0$,

$$\frac{d\phi}{d\xi} = \frac{\phi_h}{\pi}\left(\frac{\omega}{D_\gamma}\right)^{1/\gamma} \int_0^\infty dk \frac{(k^\gamma+1)\cos ky - uk \sin ky}{(k^\gamma+1)^2 + u^2k^2} \tag{19}$$

has a finite discontinuity precisely at $\xi = 0$. Although the jump in this derivative is hard to obtain in an analytical way, Eq. (19) implies immediately that the average value of $d\phi/d\xi$ at the origin is given by

$$\frac{1}{2}\left[\frac{d\phi}{d\xi}(0^+) + \frac{d\phi}{d\xi}(0^-)\right] = \frac{\phi_h}{\pi}\left(\frac{\omega}{D_\gamma}\right)^{1/\gamma} \times \int_0^\infty dk \frac{k^\gamma+1}{(k^\gamma+1)^2 + u^2k^2}. \tag{20}$$

It is then convenient to define the adimensionalized width Δ according to

$$\Delta^{-1} = \frac{1}{2\phi_h}\left[\frac{d\phi}{dy}(0^+) + \frac{d\phi}{dy}(0^-)\right] = \frac{1}{\pi}\int_0^\infty dk \frac{k^\gamma+1}{(k^\gamma+1)^2 + u^2k^2}, \tag{21}$$

which is a function of z through its dependence on the adimensional velocity u.

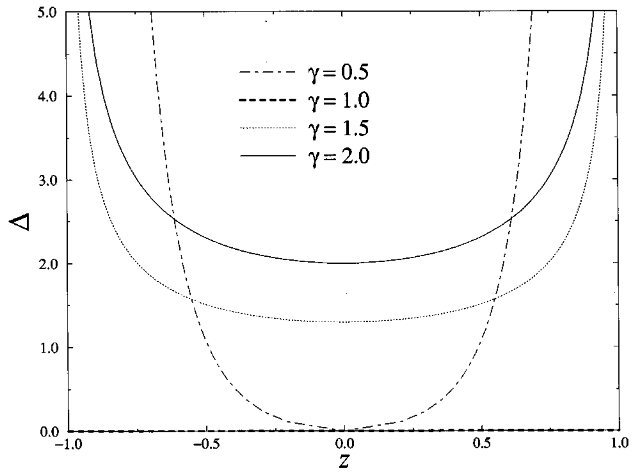

FIG. 2. Adimensionalized front width Δ as a function of the reaction parameter z, for various values of the Lévy exponent γ.

Physically, the front width is defined by the combined effect of reactions and transport. In fact, diffusion tends to widen the front steadily, and this effect should be enhanced for decreasing γ, when the transport mechanism becomes more efficient. On the other hand, reaction processes drive the density to locally approach one of the two stable states, making the fronts that connect such states sharper. In addition, the reaction rate is stronger when the difference between the actual value of the density and its stable state is larger. Therefore, diffusion can contribute—through the disbalance of chemical equilibrium caused by the transport of density—to the sharpening of the wave fronts by enhancing the effect of reactions. This complex interplay is well illustrated in Fig. 2, which shows the adimensionalized front width Δ as a function of z for various values of γ. For $\gamma > 1$, Δ has a finite minimum at $z = 0$, and increases as z approaches its limiting values. For fixed z, moreover, it decreases for increasing γ. In the case of Cauchy anomalous diffusion, $\gamma = 1$, the width vanished identically for all z, $\Delta \equiv 0$. This implies that, irrespectively of the reaction parameters, the front is infinitely steep at the origin. Finally, for

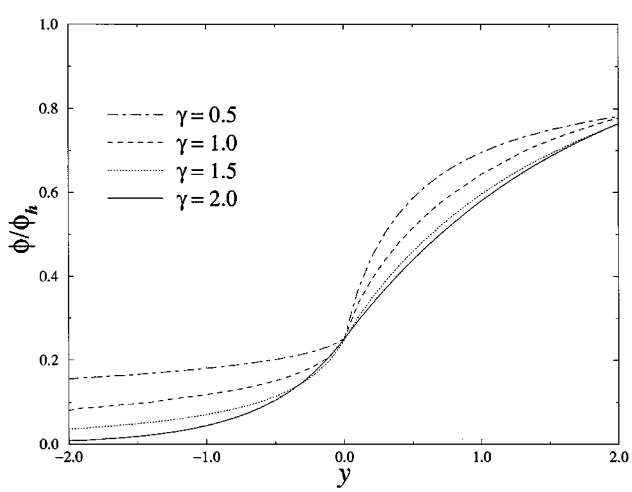

FIG. 3. Normalized density profile ϕ/ϕ_h as a function of the adimensionalized coordinate y, for various values of the Lévy exponent γ and $z = 0.5$.

$\gamma<1$ and $z\neq 0$, Δ is again finite, but vanishes for $z=0$. These generic properties can be analytically obtained from Eq. (21).

Figure 3 shows the (normalized) density profiles for various values of γ at a given value of z. Some of the main features discussed above are clearly displayed by these plots. Although these features have been here derived for a specific form of the reaction term, they are expected to be qualitatively reproduced for any bistable reaction model.

The shape-preserving wave fronts analyzed in this Brief Report are a generalization of well-known structures in bistable reaction-diffusion systems, to the case of anomalous diffusion. In ordinary-diffusion systems of arbitrary dimension, these essentially one-dimensional structures constitute a generic pattern, in the sense that (almost) any initial condition develops such fronts, whose further evolution governs the long-time behavior of the bistable system. The question about whether the wave fronts studied here play the same role of generic patterns in anomalous-diffusion systems arises then quite naturally. A more general question regards the validity of Eqs. (4) and (7) as a mathematical description of real anomalous diffusion and reaction-anomalous diffusion processes, respectively. Indeed, those equations are in principle valid for Lévy flights [6], whose connection with anomalous diffusion in the sense of Eq. (1) is only asymptotic. This question is also relevant to numerical simulations involving anomalous-diffusion transport. In fact, the Lévy distribution in coordinate space is extremely cumbersome, and such numerical simulations are generally performed using simpler jump distributions [8], which coincide with Lévy's only in their asymptotic behavior, Eq. (2). Answering these questions is the subject of work in progress.

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