Wave-front dynamics in systems with directional anomalous diffusion

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(Received 23 December 2005; revised manuscript received 29 March 2006; published 27 October 2006)

In this paper we study the solutions of a generalized reaction-diffusion system with a bistable reaction term, and considering directional anomalous diffusion. We use the well-known properties of fractional derivatives to model asymmetric anomalous diffusion, and obtain traveling wave solutions that propagate in a direction that depends on the metastability of the front, the fractional exponent and the asymmetry of the diffusion.

DOI: 10.1103/PhysRevE.74.046116 PACS number(s): 82.20.−w, 05.20.−y, 82.56.Lz

I. INTRODUCTION

Anomalous diffusion has attracted considerable attention in the last decade, this is partly due to the development of new experimental results [1] and to the realization that random walks with Lévy flights diffuse anomalously.

Anomalous diffusion is generally defined by a mean square displacement which grows with time as

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

with $\alpha \neq 1$. Superdiffusion corresponds to $\alpha > 1$ and subdiffusion to $\alpha < 1$. Some authors have used fractional derivatives to model anomalous diffusion. In some cases fractional derivatives affect the time evolution [2], while in others it is involved in the space operator [3]. Metzler and Klafter [4] report a general overview of fractional transport processes and, among other things, they mix fractional derivatives both in time and in space.

Spatial fractional derivatives are used to model superdiffusion, associated with Lévy flights [3,5], while the time fractional derivatives are used to model subdiffusion [2]. Of course, one may describe a diffusion problem with a master equation, but in this case there is not a straightforward way to incorporate force fields and boundary value problems.

Lévy flights produce a step length distribution whose second moments diverges [6]. However, if one restricts the occurrence of flights in space and time, the time dependence of the second moment behaves anomalously, as we shall demonstrate in this paper. This is the reason why Lévy flights are widely used to model problems with anomalous diffusion.

Fractional derivatives are asymmetric operators and one can define right and left versions of them. The sum of right and left fractional derivatives is symmetric and has been used by Zumofen *et al.* [7] to study the problem of segregation in a simple reaction under Lévy mixing. This approach is specially useful in reaction diffusion systems and permits the study of the effects that anomalous diffusion has on those systems [8]. Evidence of systems with anomalous diffusion is found in many fields as diffusion in porous media [9], plasmas [10], biological tissues [11], and many other physical systems [12].

There is the need for a general study of the properties of nonlinear systems under different conditions of anomalous diffusion. For example, previous works in Turing systems with space [8] and time [2] fractional operators show that the range of diffusion coefficient ratios of the two morphogens, in which the instability appears, widens up due to the dependence of the Turing bifurcation conditions on the fractional exponents. A Turing bifurcation is present even in the case when this ratio is one. Furthermore, the resulting spatial Turing patterns may acquire a velocity.

The main purpose of this paper is to study a reaction-diffusion system with superdiffusion and kinetics that gives the possibility of bistability. Our motivation is that these systems produce shape preserving smooth fronts that move with constant velocity in normal diffusion conditions. We concentrate on the propagation of wave fronts when diffusion is asymmetric. There are previous works dealing with the symmetric case using a parabolic double well potential [13] and some studies on asymmetric anomalous diffusion in a Fisher-Kolmogorov reaction-diffusion equation [3].

This paper is organized as follows, in Sec. II we present the model used by Zanette [13] and extend it to the case of asymmetric diffusion. We choose this model for its simplicity and clarity. In Sec. III the results of asymmetric diffusion are discussed. In Sec. IV some calculations are done by using another model with a more general and analytical bistable potential, and we discuss the similarities with the previous case and the model-independent results. Finally, in the last section we draw some conclusions.

II. THE MODEL

We start with a one-dimensional model proposed by Zanette [13] for the evolution of the density of diffusing particles $\phi(x,t)$ written in Fourier space,

$$\partial_t\tilde{\phi} = -D_{\gamma}^{0}|k|^{\gamma}\tilde{\phi} + \omega\tilde{f}, \tag{2}$$

where a tilde over a quantity stands for the Fourier transform, $\tilde{\phi}=\int \exp(ikx)\phi(x,t)dx/\sqrt{2\pi}$, D_{γ}^{0} is the generalized diffusion coefficient, in units of length$^{\gamma}$/time, ω is the strength of the reaction term, $f(\phi)=-\phi+\phi_h\Theta(\phi-\phi_c)$. The Heaviside function Θ sets ϕ_c as the critical value, where the function has the discontinuity. We generalize this model to the case in which anomalous diffusion is asymmetric. Here we may use the Lévy Khintchine theorem [1] which defines β-stable Lévy distributions with arbitrary skewness. Therefore, we may write

$$\partial_t\tilde{\phi} = D_{\gamma}[s(ik)^{\gamma} + (1-s)(-ik)^{\gamma}]\tilde{\phi} + \omega\tilde{f}, \tag{3}$$

where $s=(\beta+1)/2$, $0\leq s\leq 1$ and $1\leq\gamma<2$. Observe that Eq. (2) corresponds to $s=1/2$, which is the symmetric case with a normalized diffusion coefficient $D_\gamma = D_\gamma^0/\cos(\pi\gamma/2)$. The term $(ik)^\gamma\tilde{\phi}$ is the Fourier transform of the right-hand fractional derivative ${}_{-\infty}D_x^\gamma\phi$ [3] and the term $(-ik)^\gamma\tilde{\phi}$ is its equivalent for the left-hand fractional derivative. Thus, for $s<1/2$ Lévy flights towards the left predominate over those to the right, so that s might be called the asymmetry parameter.

The physical motivation for using fractional derivatives to study Lévy flights is summarized in Ref. [3]. When $\tilde{f}=0$ our model describes a generalized diffusion equation with a spatial asymmetry controlled by s. The solution of the space fractional diffusion equation, subject to the initial condition $\phi(x,0)=\delta(x)$ in an infinite domain, is

$$\phi(x,t) = \frac{2}{\psi(D_\gamma t)^{1/\gamma}}\int_0^\infty e^{\xi\cos\psi}\cos[-\xi^{1/\gamma}\eta + \xi(2s-1)\sin\psi]\xi^{(1-\gamma)/\gamma}d\xi, \tag{4}$$

where $\xi = D_\gamma t k^\gamma$, $\eta = x/(D_\gamma t^{1/\gamma})$, and $\psi=\pi\gamma/2$. The derivation of this equation is in the appendix, and the form of ϕ for $D_\gamma=1$ and $t=1$ is shown in Fig. 1.

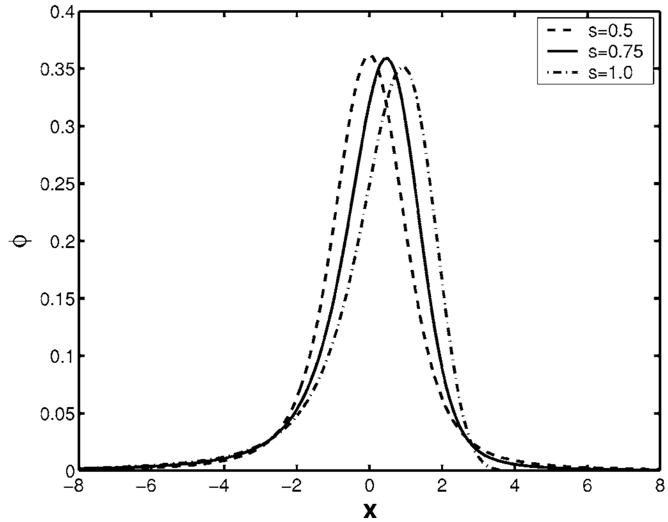

FIG. 1. Density profiles at fixed $\gamma=1.5$ and fixed time ($D_\gamma=1$ and $t=1$) for three values of the asymmetry parameter s. Notice that the three curves have power law tails on the left-hand side and only the totally asymmetric case ($s=1$) presents an exponential tail on the right-hand side. The skewness is inverted for $s<1/2$.

In bistable models, like Eq. [3], there are always wavefront solutions [14] of the form $\phi(x,t)=\phi(x-vt)$, whose Fourier transform is $\tilde{\phi}(k,t)=\exp(ikvt)\tilde{\phi}(k,0)$. Substituting these expressions into Eq. [3] we obtain

$$ikv\tilde{\phi}(k,0) = D_\gamma[s(ik)^\gamma + (1-s)(-ik)^\gamma]\tilde{\phi}(k,0) - \omega\tilde{\phi}(k,0) - \frac{\omega\phi_h}{\sqrt{2\pi}}\frac{1}{ik}e^{ik\theta_c}, \tag{5}$$

where $\theta=x-vt$ and θ_c is the point where $\phi(\theta_c)=\phi_c$. In here we have set the boundary conditions $\phi(-\infty,t)=0$ and $\phi(\infty,t)=\phi_h$. Since the problem is translational invariant, we set $\theta_c=0$ and we solve for $\tilde{\phi}(k,0)$,

$$\tilde{\phi}(k,0) = -\frac{\omega\phi_h}{\sqrt{2\pi}}\frac{1}{ik}\{\omega + ivk - D_\gamma[s(ik)^\gamma + (1-s)(-ik)^\gamma]\}^{-1}. \tag{6}$$

This is only a function of k. Transforming back we obtain

$$\phi(\theta,0) = \frac{\phi_h}{2\pi}\lim_{\epsilon\to 0+}\int_{-\infty}^{\infty}\frac{\omega e^{-ik\theta}dk}{(-ik+\epsilon)\{ivk - D_\gamma[s(ik)^\gamma + (1-s)(-ik)^\gamma] + \omega\}}. \tag{7}$$

Simplifying the notation, using the variables

$$y = \left(\frac{\omega}{D_\gamma}\right)^{1/\gamma}\theta \quad \text{and} \quad u = \left(\frac{\omega}{D_\gamma}\right)^{1/\gamma}\frac{v}{\omega}$$

and writing $i=e^{i\pi/2}$, we can see that Eq. [7] is real and its form is

$$\phi(y) = \frac{\phi_h}{2}\left(1 + \frac{2}{\pi}\int_0^\infty dk\frac{k^{-1}\{\sin(ky)[1-k^\gamma\cos(\psi)] + \cos(ky)[uk - k^\gamma\sin(\psi)]\}}{[1-k^\gamma\cos(\psi)]^2 + [k^\gamma\sin(\psi)(1-2s)+uk]^2}\right). \tag{8}$$

At the discontinuity ($y=0$), this can be written as

$$\phi(0) = \phi_c = \frac{\phi_h}{2}\left(1 + \frac{2}{\pi}\int_0^\infty\frac{u - k^{\gamma-1}\sin(\psi)(2s-1)dk}{[1-k^\gamma\cos(\psi)]^2 + [k^\gamma\sin(\psi)(1-2s)+uk]^2}\right). \tag{9}$$

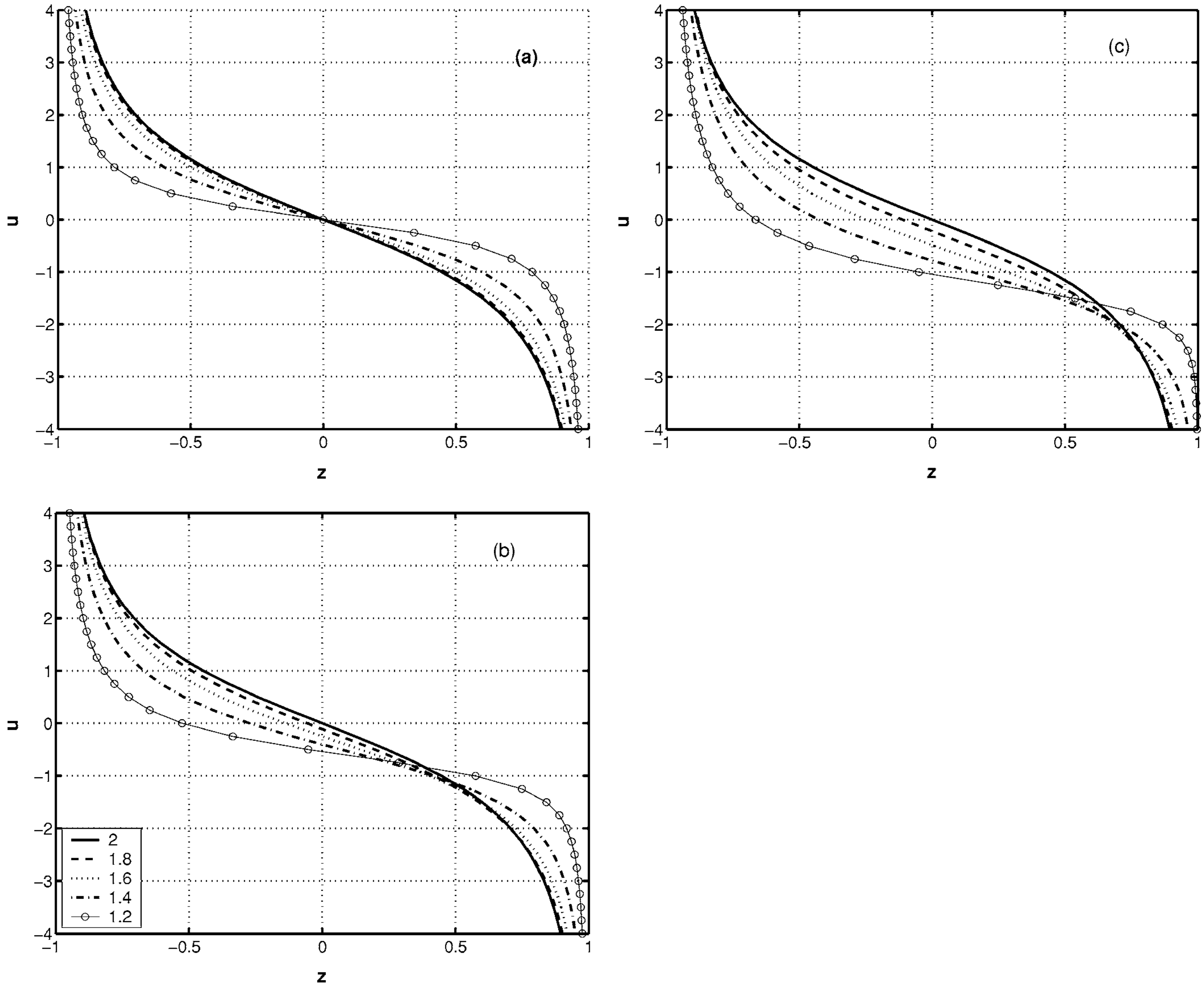

FIG. 2. Adimensional velocity u, as a function of the reaction parameter z for the piecewise linearized bistable model for different values of the Lévy flight exponents. In (a) the flights are symmetric ($s=0.5$), in (b) $s=0.25$ and the flights are partially asymmetric, and in (c) $s=0$ and the flights are completely asymmetric towards the left.

This equation reduces to Eq. (14) of Ref. [13] when $s=1/2$, except for the normalizing diffusion factor $\cos(\psi)$. The case of normal diffusion is recovered by substituting $\gamma=2$. We define the variable $z=1-2\phi_c/\phi_h$, which runs from -1 to 1 and that tells us about the relative prevalence of the two stable states in the bistable model. It is clear that z is just the negative of the integral indicated in Eq. [9]. In the case of $\gamma=2$ the dependence of the adimensional velocity with z is

$$u=-\frac{2z}{\sqrt{1-z^2}}. \tag{10}$$

In the general case of anomalous diffusion, the function $u(z)$ can be found numerically.

III. RESULTS

In Fig. 2 we show numerical results for the adimensional front velocity as a function of z. These data were constructed using Eq. (9). It is important to notice that in the symmetric case shown in Fig. 2(a) the velocities are always negative for $z>0$ and positive for $z<0$, meaning that the front always moves in such a way that the stable state gains over the metastable state. It is interesting to notice that in the symmetric case the dynamics are derivable from a grand potential $\Omega(\phi)$,

$$\partial_t\phi=-\frac{\delta\Omega(\phi)}{\delta\phi}, \tag{11}$$

with

$$\Omega=\int_{-\infty}^{\infty}F(\phi(x))dx-\frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}V(x-y)\phi(x)\phi(y)dxdy. \tag{12}$$

The reaction term ωf in Eq. (5) corresponds to $-\partial F/\partial\phi$, and

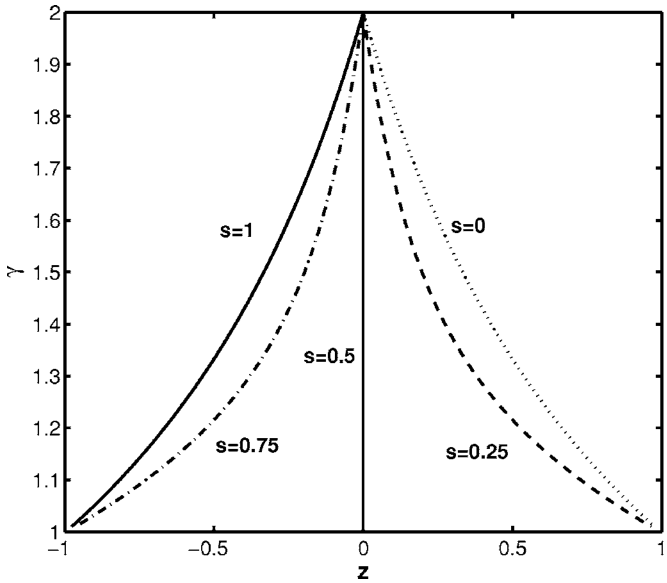

FIG. 3. Values of the Lévy exponent γ as a function of the reaction parameter z for different values of the asymmetry parameter s when the profile remains stationary, notice that $z=0$ for all γ only when $s=0.5$.

$$V(x-y)=\frac{1}{\Gamma(2-\gamma)}\partial_x^2\frac{1}{|x-y|^{(\gamma-1)}},\tag{13}$$

which comes from the definition of a fractional symmetric derivative (see the next section). So that $d\Omega/dt<0$ and the front always advances towards the metastable state region.

In Fig. 2(b) we show that in the case of asymmetric superdiffusion the velocities may be negative for $z<0$ which implies that the metastable state gains over the stable state. There is a competition between the metastability that moves the front towards the metastable state and the asymmetry of the Lévy flights, that in this case opposes this tendency. The region where the velocities are negative for $z<0$ increases as the anomalous exponent decreases. In Fig. 2(c) we show that in the extreme case $s=0$, when there is completely asymmetric diffusion, the behavior of u as a function of γ is the same as before but the region of negative velocity becomes larger.

In Fig. 3 we show that for any value of z there is a value of γ for which there is no wave propagation, except in the symmetric case where the only value of z consistent with $u=0$ is $z=0$. In this plot we see that all curves converge to the same point when $\gamma=2$ as expected for normal diffusion.

The shape preserving fronts can be integrated from Eq. (8). The form of the profiles $z(y)=1-2\phi(y)/\phi_h$ were calculated for $u=0$ and $z(0)=0.7$, and they are shown in Fig. 4(a). The profile form strongly depends on the asymmetry parameter, its width increases with asymmetry and it varies very rapidly near $y=0$, as it is made clear by its first derivative [see Fig. 4(b)]. This effect increases with decreasing s. Keeping the values of $u=0$ and $z(0)=0.7$ fixed, we calculated the values of γ by using Eq. (9). We find that $\gamma=1.176$ for $s=1$, $\gamma=1.128$ for $s=0.8$, and $\gamma=1.053$ for $s=0.6$.

IV. CONTINUOUS POTENTIAL

In this section we will show that the characteristics of the front velocity are independent of the piecewise linearized

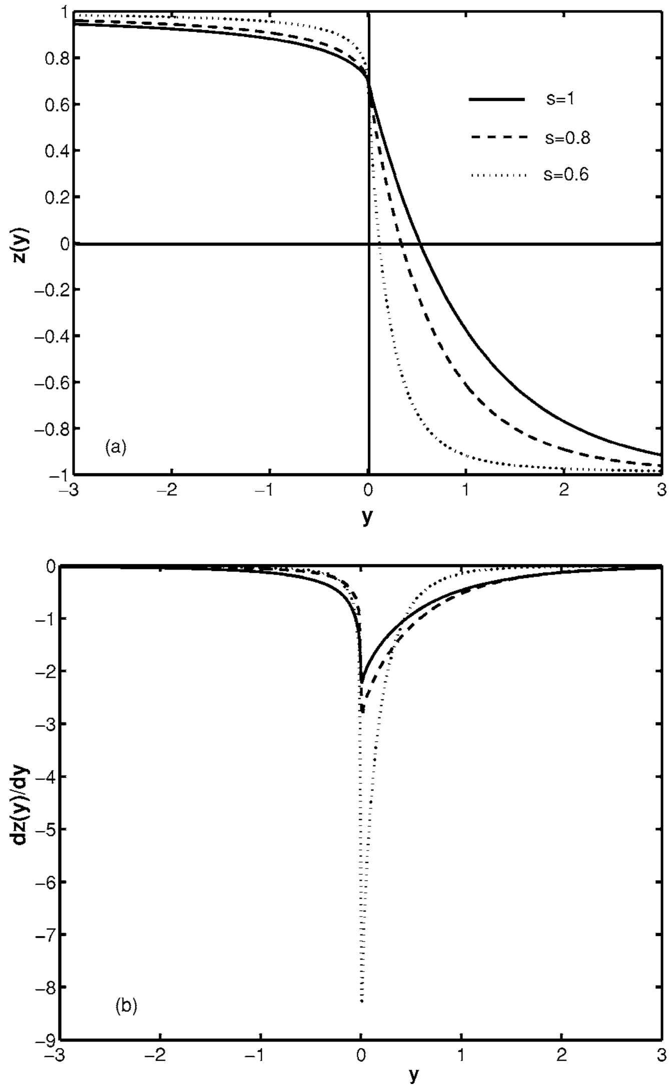

FIG. 4. In (a) we show the profiles $z(y)=1-2\phi(y)/\phi_h$ as a function of distance y for different values of the asymmetry parameter s. All the profile are stable ($u=0$) and the anomalous exponent was chosen so that $z(0)=0.7$ and increases with s. In (b) we show the first derivative $dz(y)/dy$ of the profiles as a function of y.

bistable reaction term used in Eq. (3). To show this we numerically analyze front-wave propagation produced by a continuous reaction term. The model is the following:

$$\partial_t\phi=\chi_\gamma({}_xD_\infty^\gamma\phi)-\frac{\partial F}{\partial\phi},\tag{14}$$

where

$${}_xD_\infty^\gamma\phi=\frac{1}{\Gamma(2-\gamma)}\partial_x^2\int_x^\infty\frac{\phi(y)}{(y-x)^{\gamma-1}}dy,\tag{15}$$

with $1\leqslant\mathrm{Re}(\gamma)<2$, and

$$F(\phi)=\tfrac{1}{4}(\phi^2-1)^2+\mu\phi.\tag{16}$$

This model corresponds to the case $s=0$, so that we have a process with completely asymmetric diffusion and then we shall use the left-hand fractional derivative. In this case the

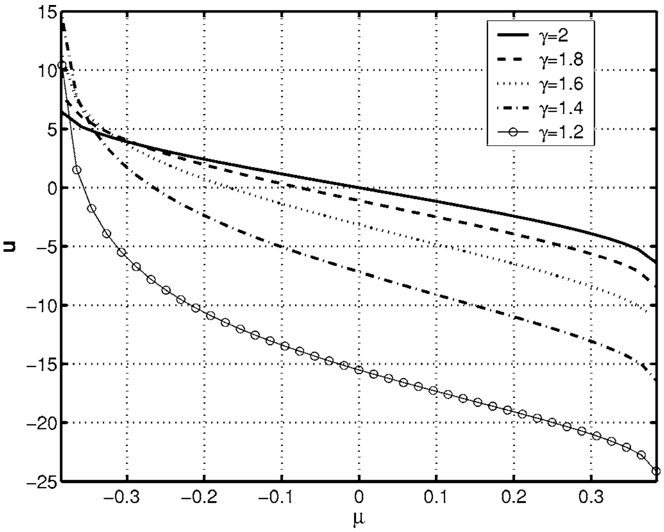

FIG. 5. Values of the front velocity u as a function of the reaction parameter μ for different values of the anomalous exponent γ.

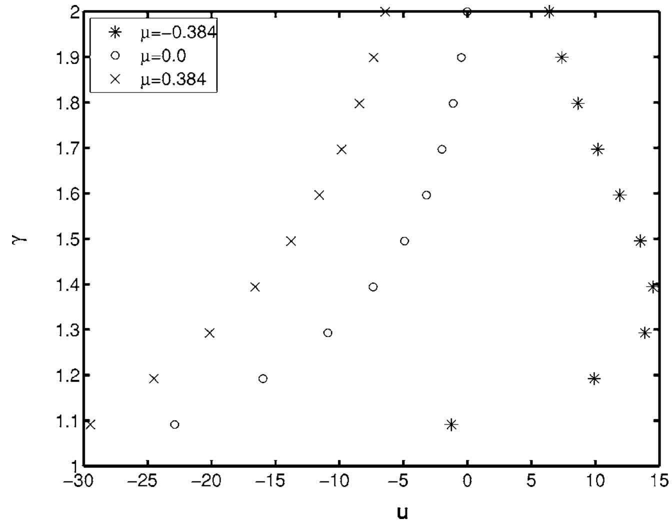

FIG. 6. Values of the front velocity u as a function of the anomalous exponent γ for different values of the reaction parameter μ.

parameter μ plays the same role as z in the preceding section, and it is the negative of a chemical potential. If $\mu \neq 0$ then the system has two homogeneous stable steady states, where one is metastable and the other is stable.

In Fig. 5 we show the numerically calculated front velocity as a function of the parameter μ for different values of the anomalous exponent γ. All calculations were performed using a simple Euler method in a grid with 2000 points, with a time step of $\Delta t=0.005$, and using fixed boundary conditions at the values of the two equilibrium states $\phi_+>0$ and $\phi_-<0$. A centered step function of the form $\phi_+ + (\phi_+ - \phi_-)\Theta(x-1000)$ was used as initial condition, and the diffusion coefficient that determines the length scale was $\chi_\gamma = 30$. There we see that the behavior of the front velocity as a function of the reaction parameter for different values of the anomalous exponent γ is very similar to that of Fig. 2(c) of the preceding section.

From these results, it is possible to see that for $\mu=0$ we have a front velocity different from zero that is always negative. This means that when the two stable steady states are completely symmetric there is always wave-front propagation, a fact that never occurs in normal diffusion. It is important to emphasize that the physical process responsible for these phenomenon is the asymmetric superdiffusion, modeled with the asymmetric fractional derivative of Eq. (14).

Notice that the operator defined in Eq. (15), is the Riemann-Liouville definition of a fractional derivative, and it is ill defined when $\gamma=2$. In the numerical calculations we use the Grünewald-Letnikov discretization [15] for all cases except for $\gamma=2$. In Fig. 5 we have included a numerical calculation for normal diffusion.

In Fig. 6 we show the front velocity as a function of the anomalous exponent for three values of the reaction parameter μ. The values are $\mu=0$ (when the two steady stable states are symmetric), and $\mu=\pm 0.384 \approx \pm \mu_c$, where μ_c is the value of the reaction parameter when one of the two steady stable states disappears.

In Fig. 6 it is possible to see how the asymmetry of the superdiffusion affects the behavior of the wave-front velocity. One important consequence is that for $\mu=0.384$ the front velocity reaches a maximum and then decreases until it changes its sign. This means that for certain values of the parameter reaction μ is possible to change the direction of wave-front propagation only by manipulating the anomalous exponent γ. This is equivalent to say that there are some values for the parameters of the model for which the metastable state overcomes the stable state as a result of a competition between the chemical potential and the asymmetry of the diffusion, the same result as obtained in Sec. II.

In Fig. 7 we show the front profiles for the reaction parameter $\mu=0$ after 2000 iterations. For this value the function F has two minima at the same level, and in absence of anomalous diffusion we have two phases in equilibrium and the front should not move. However, in the presence of asymmetric anomalous diffusion, the front acquires a velocity. The front velocity was measured by following the posi-

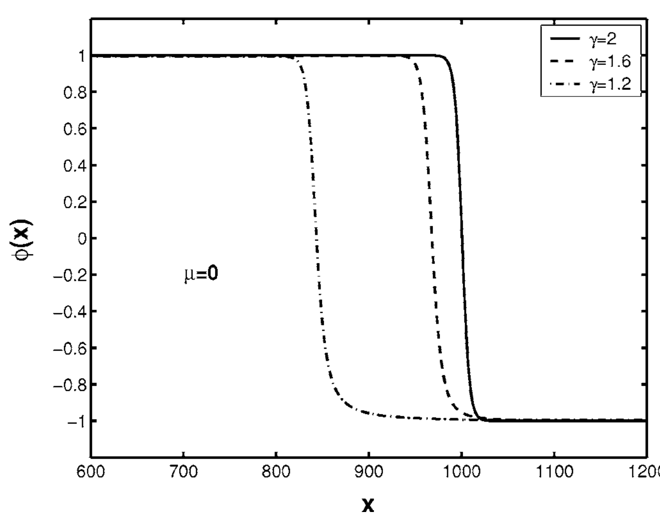

FIG. 7. Profile snapshots corresponding to $\mu=0$ for different values of γ.

tion where $\phi=0$. After 400 iterations the profile acquires a fixed form which then moves with constant velocity. We have also started with different, initial random conditions in a region near the center of the lattice and we find that after a number of iterations (depending on the initial conditions) the same front appears and moves with the same velocity. This answers the question posed by Zanette [13], concerning the behavior of ordinary bistable reaction-diffusion systems under general anomalous diffusion conditions. This behavior reveals that for almost any initial conditions the system develops shape preserving fronts, traveling with constant velocity.

V. CONCLUSIONS

We have analyzed the traveling wave fronts that occur in reaction-diffusion bistable systems when superdiffusion is asymmetric. The main results are that the fronts may move even when the reaction term is symmetric for all values of the diffusion exponent $1 \leqslant \gamma < 2$, and for all $s \neq 1/2$. Likewise, the tendency of the front to move towards the metastable state region may be compensated by the asymmetry of the Lévy flights, when the fractional exponent is sufficiently small.

The importance of our work is that it completes the analysis of the behavior of reaction diffusion systems with anomalous diffusion with arbitrary asymmetry. This might turn out to be important in some applications to real systems, particularly when dealing with diffusion of chemicals in complex domains, such as tissues and composite media. Although our analysis is based on a particularly simple model, most of the conclusions drawn from it should be model independent. This was verified by using two different kinetics and finding no qualitatively different results. Of particular interest is the circumstance of having bistability in the kinetics, because anomalous diffusion has profound effects on the time evolution of the interfaces between chemicals allowing for transport. This is evidently of great importance in many practical applications.

APPENDIX: DIFFUSION WITH FRACTIONAL DIFFERENTIAL OPERATORS

In here we derive the solution of Eq. (3) when $\tilde{f}=0$, for arbitrary right-hand and left-hand fractional derivatives. If the initial condition is a δ-function centered at zero, one can write

$$\frac{\partial \tilde{\phi}}{\partial t} = D_\gamma[(ik)^\gamma s + (1-s)(-ik)^\gamma]\tilde{\phi}, \tag{A1}$$

where s is the asymmetry parameter and the factors $(ik)^\gamma$ come from the Fourier transform of the fractional derivative operators. This equation can be integrated immediately to obtain

$$\tilde{\phi}(k,t) = \frac{1}{\sqrt{2\pi}} e^{[(ik)^\gamma s + (1-s)(-ik)^\gamma]D_\gamma t},$$

since $\tilde{\phi}(k,0)=1$. Fourier transforming the equation above, one gets

$$\phi(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ikx + [(ik)^\gamma s + (1-s)(-ik)^\gamma]D_\gamma t} dk.$$

Separating the domain of integration in two parts around zero, one gets two integrals whose imaginary part vanishes when summing up. Therefore

$$\phi(x,t) = \frac{1}{\pi}\int_0^{\infty} e^{k^\gamma D_\gamma t \cos(\pi\gamma/2)} \cos[-kx + k^\gamma D_\gamma t(2s-1) \times \sin(\pi\gamma/2)]dk. \tag{A2}$$

Conveniently defining variables one gets Eq. (4) in the text.

This form exhibits the scaling behavior

$$\phi(x,t) = \frac{2}{\psi (D_\gamma t)^{1/\gamma}} G_\gamma\left(\frac{x}{(D_\gamma t)^{1/\gamma}}; s\right). \tag{A3}$$

Since $D_\gamma=1$ and $t=1$ in Fig. 1, one is plotting the universal function $2G_\gamma(x;s)/\psi$. This problem has been examined in detail before by Paradisi *et al.* [16] using discrete expressions for the fractional derivatives and calculating numerically the density distributions. Observe that the integral diverges for positive argument of the exponential, that is, it is only defined for $\cos(\psi)<0$, or $1<\gamma<3$. For subdiffusion $(2<\gamma<3)$ $\phi(x,t)$ is not well defined. However for $1<\gamma<2$, $\phi(x,t)$ represents a density distribution with superdiffusion. The second moment of the distribution can be written as

$$\langle x^2 \rangle = \frac{2(D_\gamma t)^{2/\gamma}}{\theta}\int_{-\infty}^{\infty} \eta^2 G_\gamma(\eta; s) d\eta = D_\gamma t^{2/\gamma} N_\gamma(s). \tag{A4}$$

This integral diverges, as it is well known, but for experimental applications one could set finite integration limits, since the physical system is confined in space, as it has been done in Ref. [17], and the mean square displacement grows with the same exponent $\alpha=2/\gamma$.

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