Front Propagation in Reaction-Superdiffusion Dynamics: Taming Lévy Flights with Fluctuations

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We investigate front propagation in a reacting particle system in which particles perform scale-free random walks known as Lévy flights. The system is described by a fractional generalization of a reaction-diffusion equation. We focus on the effects of fluctuations caused by a finite number of particles per volume. We show that, in spite of superdiffusive particle dispersion and contrary to mean-field theoretical predictions, wave fronts propagate at constant velocities, even for very large particle numbers. We show that the asymptotic velocity scales with the particle number and obtain the scaling exponent.

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One of the fundamental processes involved in nonequilibrium pattern formation is the spatial propagation of interfaces or fronts. Front propagation usually emerges when a local reaction dynamics interplays with diffusion in space of the reacting agents and has been observed in a wide range of physical, chemical, and biological systems [1–6]. One of the most prominent models which displays propagating fronts is the Fisher-Kolmogorov-Petrovsky-Piscounov (FKPP) equation for the spatial concentration $u(x, t)$ of a reacting agent,

$$\partial_t u = \gamma u(1 - u) + D\Delta u. \tag{1}$$

In epidemiological contexts the field $u(x, t)$ may quantify the concentration of infected individuals relative to the endemic value [7]. In Eq. (1) diffusive motion of the reacting agents is assumed and quantified by the diffusion coefficient D in units of m^2/s. However, this assumption cannot be justified for a number of systems. In fact, superdiffusive dispersion in space has been observed in a wide range of biological and population dynamical systems [8–11].

One of the most successful theoretical concepts devised for the understanding of superdiffusion is a class of random walks known as Lévy flights [12]. A Lévy flight consists of random single steps Δx which are drawn from an inverse power-law probability density function (PDF) $p(\Delta x) \sim |\Delta x|^{-(1+\mu)}$ characterized by a Lévy exponent $0 < \mu < 2$. Because of the heavy tail, the variance in step size is divergent, the process lacks a spatial scale, and the position $X(t)$ of a Lévy flight scales heuristically with time t as $X(t) \sim t^{1/\mu}$. The associated diffusion equations contain fractional generalizations of ordinary derivatives [13,14]. These fractional Fokker-Planck equations can exhibit behaviors strikingly different from ordinary ones [15] and have found wide application in physics, e.g., protein motion on folded heteropolymers [16] and the dynamics of modern epidemics [17].

In two recent studies wave front dynamics was shown to be drastically different from ordinary reaction-diffusion dynamics when the reacting agents move superdiffusively [18,19]. The authors considered fractional generalizations of Eq. (1) and showed that the spatiotemporal shape $u(x, t)$ of the leading edge of a propagating front has a power-law tail along the spatial coordinate and accelerates exponentially in time as opposed to the constant velocity and exponential decay in space exhibited by ordinarily diffusive systems. The predictions made by mean-field theory thus indicate that scale-free, superdiffusive dispersion of the reacting agents excludes constant velocity wave fronts and induces an entirely different spatiotemporal behavior.

However, as has been shown in a number of recent studies, the effect of fluctuations can be rather profound in these systems [20]. A finite albeit large number N of particles or reacting agents leads to significant corrections to the mean-field approximation even for very large values of N. Brunet and Derrida [21,22] extended mean-field dynamics by an effective cutoff parameter ε for the concentration of particles below which no reaction and hence no exponential growth of the leading edge of a front is possible. Despite the fact that a rigorous equivalence with multiplicative noise is still lacking, the effective cutoff approach is very intuitive and in remarkable agreement with simulations of the full probabilistic dynamics.

Here, we focus on the effect of fluctuations on reaction-superdiffusion kinetics. We show that for arbitrarily small fluctuations (i.e., arbitrarily large particle numbers N), wave fronts propagate asymptotically at constant velocities. Furthermore, we show that as soon as fluctuations enter the description the algebraic tail along the spatial coordinate of the leading edge disappears and is replaced by an exponential decay. Thus, despite the fact that reacting agents move superdiffusively in space, the wave front patterns are qualitatively the same as in the ordinary diffusion case. We show that a front speed v is selected after a transient time and that v scales with particle number as $v \sim N^{1/\mu}$ for Lévy exponents $\mu < 2$. The results reported here are rather counterintuitive, deviate strongly from the predictions cast by mean-field theory, and indicate that fluctuations affect reactions-superdiffusion systems severely and must not be neglected.

We begin with a simple two particle type (A, B) reaction scheme,

$$A_x + B_x \xrightarrow{k_1} 2A_x, \qquad A_x + B_x \xrightarrow{k_2} 2B_x, \tag{2}$$

$$A_x, B_x \xrightarrow{f(|x-y|)} A_y, B_y. \tag{3}$$

Particles of type A and B either react to produce two particles of type A or two particles of type B at rate k_1 and k_2, respectively. The units of rates $k_{1/2}$ and f are m^d/s and s^{-1}, respectively, where d is the Euclidean dimension. Furthermore, particles of both types may jump from position x to position y with a probability density rate $f(|x-y|)$ which we assume to be a decreasing function of distance $|x-y|$. The dynamic stochastic variables are the particle numbers $n_A(x,t)$ and $n_B(x,t)$ of particles in a volume of size Ω (in units m^d) around x of type A and B, respectively. The volume Ω is assumed to be large enough to contain a large number of particles but small compared to the spatial extend of the system. The total number of particles in Ω around x is given by $N(x,t) = n_A(x,t) + n_B(x,t)$.

In the limit of an infinite particle number per unit volume, fluctuations can be neglected and one obtains $\partial_t u = \gamma u(1-u)$ for the relative abundance of A particle $u = n_A/\Omega$ where $\gamma = k_1 - k_2$ (in units m^d/s). In a spatially extended system with dispersal governed by Eq. (3) we have $u = u(x,t)$ and the mean-field dynamics is augmented by a dispersal operator $\mathcal{L}$, i.e., $\partial_t u = \gamma u(1-u) + \mathcal{L}u$. When particles perform ordinary random walks the operator $\mathcal{L}$ can be approximated by the ordinary Laplacian Δ. However, this description is no longer valid if $f(x) \sim |x|^{-(1+\mu)}$ with $0 < \mu < 2$. In this case individual jumps lack a scale, particles perform Lévy flights, and $\mathcal{L}$ is proportional to a nonlocal singular integral operator,

$$\Delta^{\mu/2} u(x,t) = C_\mu \int dy \frac{[u(y,t) - u(x,t)]}{|x-y|^{1+\mu}}, \tag{4}$$

where C_μ is a dimensionless constant [23]. In Fourier space the operator $\Delta^{\mu/2}$ is equivalent to a multiplication by $-|k|^\mu$, generalizing the well-known $-k^2$ factor corresponding to the ordinary Laplacian which is why $\Delta^{\mu/2}$ is frequently referred to as a fractional Laplacian. In this case one obtains

$$\partial_t u = \gamma u(1-u) + D_\mu \Delta^{\mu/2} u, \tag{5}$$

which is the Fisher equation (1) for $\mu = 2$ and its superdiffusive mean-field generalization for $\mu < 2$. The generalized diffusion coefficient D_μ has units $\mathrm{m}^\mu/\mathrm{s}$. For $\mu = 2$ Eq. (5) is solved by exponential fronts traveling at a constant speed v [24], i.e., $u(x,t) \sim u_0 \exp[-\lambda(x - vt)]$, whereas when $\mu < 2$ fronts possess an algebraic tail along the spatial coordinate and are accelerating exponentially fast [18,19].

For large but finite N one may account for fluctuations by expanding a master equation associated with Eq. (2) for the local dynamics in terms of short time moments and obtain a Fokker-Planck equation [25]. This introduces a multiplicative noise term to Eq. (5), i.e., the system is governed by the Ito-stochastic partial differential equation

$$du = \gamma u(1-u)dt + D_\mu \Delta^{\mu/2} u dt + \frac{\sigma}{\sqrt{N}} \times \sqrt{u(1-u)} dW(t), \tag{6}$$

where $\sigma^2 = k_1 + k_2$ and $W(t) = W(x,t)$ is a spatially uncorrelated family of Wiener processes. Note that the noise amplitude decreases with particle number as $N^{-1/2}$ and the mean-field description is recovered in the thermodynamic limit. In the following we address the question of how and in what magnitude these fluctuations impact the front propagation of the system.

Figure 1 illustrates the results obtained for the full stochastic model as defined by Eqs. (2) and (3), parameter values are provided in the figure caption. Figure 1(a) depicts the time evolution of the front velocity defined by the total mass $I(t)$ of particles of type A, where the total mass is given by the number of type A particles. After an initial nonlinear growth of $I(t)$ the front speed is asymptotically constant, in contrast to the behavior of the mean-field dynamics which exhibits exponential growth [18,19]. Note that this behavior is not a consequence of an effective cutoff in the power law of the dispersal due to a finite number of particles per site. In fact, the inset depicts the time evolution of the distance from its origin travelled by one reacting particle which scales with time according to

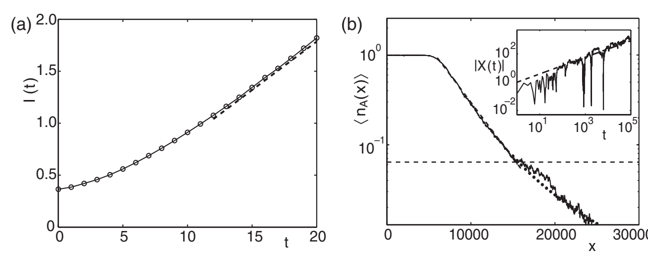

FIG. 1. Asymptotic front velocity in the full stochastic model. (a) The solid line depicts the total mass $I(t)$ of type A particles as a function of time. The system size is $L = 10^4$, the total number of A and B particles in the system is 200×10^4. Other parameters are $\gamma = 1$ and $\mu = 1.8$. A constant front velocity (constant $dI(t)/dt$) is attained asymptotically (dashed line). (b) Average shape of the wave front of type A particles in the linear regime [$t = 20$ in (a)] calculated from over 4000 realizations. The horizontal dashed line separates the exponential (dashed line) from the algebraic (dotted line) region. Note the log scale on the ordinate; below the dashed line the number of A particles is of the order of unity. The inset shows the distance from the starting point $|X(t)|$ of a Lévy flight with $\mu = 1.8$. The dashed line indicates the scaling $|X(t)| \sim t^{1/\mu}$.

$|X_t| \sim t^{1/\mu}$. This scaling only depends on the Lévy exponent μ and for $\mu < 1$ every particle travels superlinearly and thus "faster" than the wave front. The finite speed of the wave front is a consequence of the fact that even though particles of type A may jump far into the unstable region (where $n_B = 0$) the probability of absorption in that region is high enough to outweigh the local exponential growth of the number of A particles in that region unlike the mean-field dynamics which exhibits local exponential growth for arbitrarily small concentrations of type A particles.

Figure 1(b) depicts the shape of the moving front. In the moving coordinate frame $z = x - vt$ the expectation value of the number of A particles $\langle n_A(z)\rangle$ is shown on a semilogarithmic scale. Unlike the mean-field dynamics which exhibits an algebraic tail, the wave front decreases exponentially in the range where reaction kinetics play a role, i.e., $1 < n_A < N$. For values of z for which the concentration of A particles is too low and only dispersal plays a role it decreases algebraically.

The transition between exponential and algebraic decay in the shape of the asymptotic wave front indicates that effectively the dynamics near the tip of the wave front is governed by a threshold above which the reaction plays a dominant role and below which it does not.

In order to investigate this threshold mechanism we analyzed the dynamics within an approach originally introduced in Ref. [21] in which an effective cutoff $\varepsilon \sim 1/N$ is introduced directly by means of a step function in the nonlinear growth term of mean-field dynamics, i.e.,

$$\partial_t u = \gamma u(1-u)\Theta(u-\varepsilon) + D_\mu \Delta^{\mu/2} u, \tag{7}$$

in which Θ is the Heaviside function. For mathematically rigorous treatments of these type of fractional reaction-diffusion equations, see Ref. [26]. Qualitatively, this accounts for the fact that no growth on average can occur if the particle concentration u is less than a fixed small number of particles per unit volume. This approach has been applied successfully in the ordinary diffusion scenario [21]. In Eq. (7), mean-field theory implies $\varepsilon = 0$.

Figure 2 summarizes the front dynamics obtained from numerical integration of (7) for a concentration $u(x, t)$ initially peaked at the origin and which vanishes exponentially for small and large arguments. For various particle numbers N the velocity and shape of the front were computed. Figure 2(a) shows that even for very large particle numbers wave fronts move asymptotically at constant speeds, a remarkable difference from the mean-field limit (dashed line in the inset) which predicts exponentially accelerating front. Furthermore, the asymptotic speed is larger for larger particle number N per site. Figure 2(b) depicts snapshots of the wave fronts on a double-logarithmic scale. After a transient phase, the shape of the front approaches a steady state with a sharply decreasing boundary at intermediate values for the concentration and an algebraic tail for large x with concentrations $u(x, t)$ below the cutoff ε. The inset in 2(b) depicts the approach to the asymptotic front shape in the comoving frame. Therefore, the dynamical system (7) is in qualitative agreement with the dynamics of the full stochastic model.

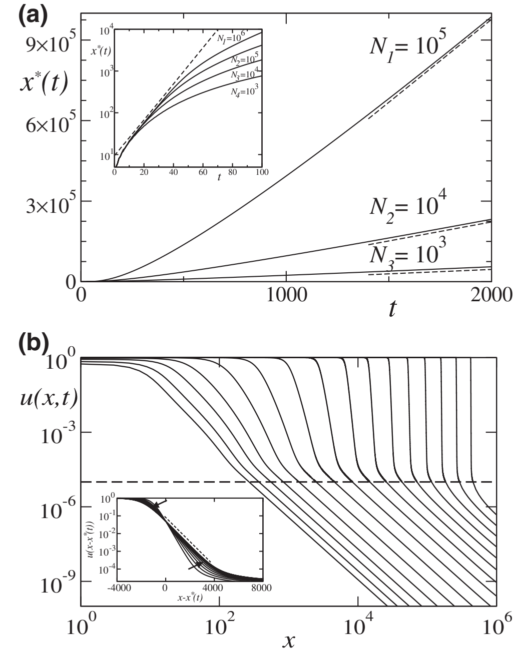

FIG. 2. Propagation of wave fronts in superdiffusive systems with effective cutoff. (a) Location of the wave front $x^*(t)$ as a function of time t for different particle numbers N (solid lines) for $\mu = 1.5$ and $\gamma = 0.1$ in Eq. (7). Following initial transients the velocity $v = dx^*(t)/dt$ is constant (dashed lines) and increases with N. The inset depicts a magnification of the initial phase. The wave front accelerates exponentially but deviates from the mean-field dynamics ($\varepsilon = 0$, dashed line) after the transient period. (b) Shape of the wave front at exponentially increasing time steps $t = 1.5^m$ with $m = 5, 6, \ldots, 20$ for $N = 10^4$. After a transient phase the shape remains unaltered, decays sharply for$1/N < u(x, t) < 1$, and follows a power law $u(x, t) \sim x^{-(1+\mu)}$ for large x. The dashed line indicates the effective cutoff $\varepsilon = 10^{-4}$. The spatial extent in the numerical integration was $L = 2^{23} \approx 8.38 \times 10^6$. Inset: Scaling behavior of the fronts' profiles in the reference frame of the front. Arrows indicate the temporal direction. The curves approach a steady state characterized by an exponential decay in space, $\exp - \lambda x$. The position of the front $x^*(t)$ is given implicitly by $u(x^*(t), t) = 0.05$.

In summary, the characteristic spatiotemporal wave front solution of Eq. (5) for large times is given by $u(x, t) \sim A\exp[-\lambda(x - vt)]$, for $1/N < u < 1$ followed by a power-law tail $u(x, t) \sim B(x - vt)^{-(1+\mu)}$ for $u < 1/N$ in which A and B are constants in units m^{-1} and $\mathrm{m}^{-\mu}$, respectively. The decay parameter λ (units m^{-1}) and the velocity v depend on the particle number N. Qualitatively, this dependence can be determined in the moving reference frame under the assumption that $u(x, t) = u(x - vt) = u(z)$. Figure 2(b) suggests that $u(z) = u_1(z) = A\exp - \lambda z$ for $z < z^\star$ and $\varepsilon < u \ll 1$ and $u(z) = u_2(z) = B/z^{1+\mu}$ for $z > z^\star$ $(u < \varepsilon)$ where $z^\star$ marks the crossover between exponential and algebraic decay. Heuristically a relation between the speed v of the wave front, the threshold ε, and

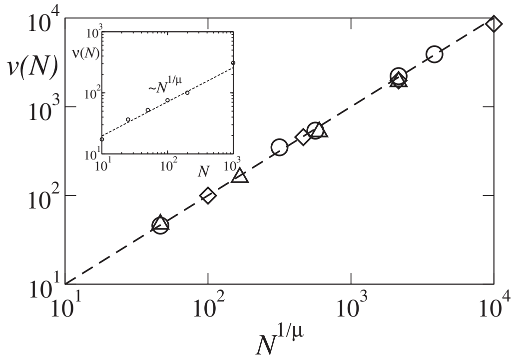

FIG. 3. Asymptotic front velocity $v(N)$ of the effective cutoff model as a function of the particle number N for different Lévy exponents $\mu = 1.2$, 1.5, and 1.8 (circles, diamonds, and triangles, respectively). The dashed line indicates the scaling $v(N) \sim N^{1/\mu}$. The inset shows the calculated asymptotic front velocity of the full stochastic model for $\mu = 1.8$.

the exponential decay parameter λ can be obtained by analyzing the short time dynamics. In the exponential regime for small u values $u(x, t + \Delta t) = A \exp - \lambda(x - vt - v\Delta t)$ for small Δt. Because of the exponential growth term $u(x, t + \Delta t) \approx (1 + \gamma\Delta t) \exp - \lambda(x - vt)$. Assuming the exponential shape is stable both expressions are the same, which implies

$$v \sim \gamma/\lambda, \tag{8}$$

in units m/s. On the right-hand side of the crossover, the reaction term is irrelevant and a nonzero $u(x, t + \Delta t)$ is given by the dispersal term only. In particular, if the wave front is stable $u(x + v\Delta t, t + \Delta t) \approx \varepsilon \approx \Delta t D_\mu \Delta^{\mu/2} u(x, t)$. The last term can be approximated by integration of the tail over range to the left of the crossover, i.e., $\varepsilon \approx u^\star \Delta t D_\mu \int_{v\Delta t}^{\infty} y^{1+\mu} dy$, where $u^\star \approx 1$ which yields the scaling relation $v \approx C\varepsilon^{-1/\mu}$ with $C = \Delta t^{\mu-1}/(D_\mu u^\star)$ in units $\mathrm{m}^{\mu-1}/\mathrm{s}^\mu$. This implies, in combination with Eq. (8), how the wave front parameter λ and the velocity v scale with particle number N:

$$\lambda \propto N^{-1/\mu}, \qquad v \propto N^{1/\mu}. \tag{9}$$

Figure 3 shows the front velocity v as a function of particle number N obtained by numerical integration of the dynamics [Eq. (7)]. The numerics agree well with the scaling law (9) over several orders of magnitude and several choices of the Lévy exponent μ.

We are convinced that our results are of major importance for the understanding of front propagation in pattern-forming systems in which the reactive agents defy the rules of ordinary diffusion. We have shown that even when reacting agents move superdiffusively constant velocity fronts are typical for pulled front dynamics, contrary to what is expected from mean-field approximations, and we believe that our results will contribute to the understanding of more complex pattern-forming systems such as the geographic spread of human epidemics [27].

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