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Continuous-time random walks and traveling fronts

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We present a geometric approach to the problem of propagating fronts into an unstable state, valid for an *arbitrary* continuous-time random walk with a Fisher–Kolmogorov-Petrovski-Piskunov growth/reaction rate. We derive an integral Hamilton-Jacobi type equation for the action functional determining the position of reaction front and its speed. Our method does not rely on the explicit derivation of a differential equation for the density of particles. In particular, we obtain an *explicit* formula for the propagation speed for the case of anomalous transport involving non-Markovian random processes.

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Recently there has been considerable effort to find the rate at which traveling waves propagate into a linearly unstable state [1–6]. The main reason for this is that a variety of physical, chemical, and biological phenomena can be explained in terms of the propagation of local perturbations into generically unstable states. Examples include the spread of epidemics [7], population dispersion [8,9], combustion waves [10], magnetic fronts [11], etc. However, most of the work has focused on finding the traveling wave solution for a given partial differential, integrodifferential, or difference equation [12]. A comprehensive review of up-to-date methods can be found in Ref. [5].

It has been found recently [13] that the *macroscopic* dynamics of propagating fronts are dependent on the choice of the underlying random walk model for the *mesoscopic* transport process. Since the dynamics of fronts are not universal and depend on statistical characteristics of underlying *mesoscopic* random processes, it is an important problem to find the *universal* rules relating both levels of description. The aim of this paper is to address this problem.

Most studies involving explicit *mesoscopic* descriptions of particle transport, so far, have concerned systems with additional simplifying features regarding the random walk, for example, a Markovian character of random processes, and other assumptions (see, for example, the review [4]). Recently, a simple non-Markovian model has been considered [14]. Here we are interested in exploring the physical properties of those systems of particles which react and disperse according to a general continuous-time random walk (CTRW) [15,16]. During the last two decades CTRW theory has been used as a general and physically based approach to quantify transport. It has been applied to semiconductors [17], turbulent diffusion [18], geological materials [19], econophysics [20], and many others (see the review [21]). However, it is well known that when dispersal and growth/reaction are coupled processes there may exist traveling wave front solutions. Recent studies have addressed the Turing conditions for pattern formation in CTRW with growth/reaction [22]. In this paper we present a geometric approach to the problem of propagating waves, derived from *mesoscopic* principles and valid for *arbitrary* random walk models.

Let us introduce the *mesoscopic* concentration $n(t,x)$ of particles performing a continuous random walk. The complete description of *mesoscopic* transport processes is given by the joint probability density $\Phi(s,z)$ of making a jump of length z in the time interval s to $s+ds$ [15]. We assume that the local growth rate of these particles Fisher–Kolmogorov-Petrovski-Piskunov (Fisher-KPP) type [1,23,24], that is,

$$U(\varepsilon x)nf(n), \qquad \max_{0\leqslant n\leqslant 1} f(n)=f(0), \qquad f(1)=0, \tag{1}$$

where the growth rate parameter $U(\varepsilon x)$ is a slowly varying function of the space coordinate x with ε being a small parameter.

The governing equation for $n(t,x)$ can be written in the form [15,16]

$$\begin{aligned} n(t,x)=\Psi(t)n(0,x)+\int_0^t\int_{-\infty}^{\infty}\Phi(s,z)n(t-s,x-z)dzds \\ +U(\varepsilon x)\int_0^t\Psi(s)n(t-s,x)f(n(t-s,x))ds, \end{aligned} \tag{2}$$

where $\Psi(t)$ is the survival probability that can be written as follows [15]:

$$\Psi(t)=1-\int_0^t\psi(s)ds, \qquad \psi(s)=\int_{-\infty}^{\infty}\Phi(s,z)dz. \tag{3}$$

Here $\psi(s)$ is the waiting time probability density functioin (PDF) that plays a very important role in what follows. Recall that $\int_0^t\psi(s)ds$ is the probability that at least one jump is made in the interval $(0,t)$. Equation (2) describes the balance of particles at the position x at time t. The first term on the right-hand side of Eq. (2) represents the number of particles remaining at their initial position x up to time t. The second term gives the number of particles arriving at x up to time t from position z and time s and the last term is a production term due to growth (1). To ensure an evolution with the minimal propagation speed we specify the frontlike initial condition

$$n(0,x)=\begin{cases}1, & x\leqslant 0\\ 0, & x>0.\end{cases} \tag{4}$$

We assume that after a long enough time there exists a traveling wave solution to the integral equation (2) with the initial condition (4). The main problem is to find the rate u at which this wave propagates. In this paper we develop a Hamilton-Jacobi approach to this problem valid for a general CTRW with a Fisher-KPP growth rate (1). The starting point for the geometric description of wave propagation is the hyperbolic scaling procedure $t\rightarrow t/\varepsilon$, $x\rightarrow x/\varepsilon$ and the representation of the rescaled concentration $n^{\varepsilon}(t,x)=n(t/\varepsilon,x/\varepsilon)$ in the WKB form

$$n^{\varepsilon}(t,x)=\exp\left(-\frac{G^{\varepsilon}(t,x)}{\varepsilon}\right),\quad G^{\varepsilon}(t,x)\geqslant 0, \tag{5}$$

where the action functional G^{ε}, describing the logarithmic asymptotic form of the concentration field, has to be found. It follows from Eq. (5) that, as long as the function $G(t,x)=\lim_{\varepsilon\rightarrow 0}G^{\varepsilon}(t,x)$ is positive, the rescaled field $n^{\varepsilon}(t,x)\rightarrow 0$ as $\varepsilon\rightarrow 0$. The boundary of the set where $G(t,x)>0$ can be regarded as a reaction front. Therefore, we may argue that the reaction front position $x(t)$ can be determined from the equation $G(t,x(t))=0$. The justification of this procedure for relatively simple reaction-diffusion systems can be found in Refs. [23,24].

Now we are in a position to derive the equation for the function $G(t,x)$. Substitution of Eq. (5) into the rescaled equation for $n^{\varepsilon}(t,x)$ gives the equation for $G^{\varepsilon}(t,x)$,

$$\begin{aligned}1-&\int_0^{t/\varepsilon}\int_{-\infty}^{\infty}\Phi(s,z)\exp\left[\frac{-G^{\varepsilon}(t-\varepsilon s,x-\varepsilon z)+G^{\varepsilon}(t,x)}{\varepsilon}\right]\\ &\times dz ds-U(x)\int_0^{t/\varepsilon}\Psi(s)\exp\left[\frac{-G^{\varepsilon}(t-\varepsilon s,x)+G^{\varepsilon}(t,x)}{\varepsilon}\right]\\ &\times f(e^{-G^{\varepsilon}/\varepsilon})ds=0.\end{aligned} \tag{6}$$

Here we have used the condition that the action functional $G^{\varepsilon}(t,x)\rightarrow\infty$ as $t\rightarrow 0$ for $x>0$. Now let us derive the equation for $G(t,x)=\lim_{\varepsilon\rightarrow 0}G^{\varepsilon}(t,x)$ by considering the limit $\varepsilon\rightarrow 0$. Since $\lim_{\varepsilon\rightarrow 0}f(\exp(-G^{\varepsilon}/\varepsilon))=1$ provided $G^{\varepsilon}(t,x)>0$ it follows from Eq. (6) that the limiting function

$$G(t,x)=-\lim_{\varepsilon\rightarrow 0}\varepsilon\ln n^{\varepsilon}(t,x) \tag{7}$$

obeys the nonlinear integral equation

$$\begin{aligned}1-&\int_0^{\infty}\int_{-\infty}^{\infty}\Phi(s,z)e^{-(\partial G/\partial t)s}e^{(\partial G/\partial x)z}dz ds-U(x)\\ &\times\int_0^{\infty}\left[1-\int_0^{s}\psi(z)dz\right]e^{-(\partial G/\partial t)s}ds=0,\end{aligned} \tag{8}$$

provided $G(t,x)>0$. This equation is the main result of our paper. It can be regarded as the generalized Hamilton-Jacobi equation for the action functional $G(t,x)$ determining the position of a reaction front. Recall that the equation $G(t,x(t))=0$ gives the position of the front $x(t)$ and the propagation rate $u=dx/dt$. Until now, no approximations regarding the random walk have been used; this equation is *exact* in the limit $\varepsilon\rightarrow 0$ and valid for *arbitrary* CTRW with Fisher-KPP growth rates.

Equation (8) can be rewritten in a very useful form involving the moment generating function for a CTRW. Let us introduce some new notation, namely, the Hamiltonian function H and the generalized momentum p,

$$H=-\frac{\partial G}{\partial t},\quad p=\frac{\partial G}{\partial x}, \tag{9}$$

then by using the definitions of the moment generating functions

$$\hat{\Phi}(H,p)=\int_0^{\infty}\int_{-\infty}^{\infty}\Phi(s,z)e^{-Hs}e^{px}dz ds,$$

$$\hat{\psi}(H)=\int_0^{\infty}\psi(s)e^{-Hs}ds. \tag{10}$$

Equation (8) can be rewritten as an equation for the Hamiltonian function H,

$$1-\hat{\Phi}(H,p)-\frac{U(x)}{H}[1-\hat{\psi}(H)]=0. \tag{11}$$

By combining Eqs. (9) and (11) we arrive at the Hamilton-Jacobi type equation written in terms of the moment generating functions of the underlying CTRW,

$$\frac{\partial G}{\partial t}\left[1-\hat{\Phi}\left(-\frac{\partial G}{\partial t},\frac{\partial G}{\partial x}\right)\right]+U(x)\left[1-\hat{\psi}\left(-\frac{\partial G}{\partial t}\right)\right]=0. \tag{12}$$

The solution G has to be chosen in a such way that $H=-\partial G/\partial t$ is the root of Eq. (11) with the largest real part. It should be noted that since the parameters of Eq. (8) do not involve time explicitly, we can conclude that the corresponding Hamiltonian system is conservative, that is, $H(p,x)=E$.

If the jump length and waiting time are independent random variables we can write the moment generating function $\hat{\Phi}(H,p)$ in the decoupled form

$$\hat{\Phi}(H,p)=\hat{\psi}(H)\hat{\phi}(p), \tag{13}$$

where

$$\hat{\psi}(H)\equiv\textstyle\int_0^{\infty}\psi(s)\exp(-Hs)ds,$$

$$\hat{\phi}(p)\equiv\textstyle\int_{-\infty}^{\infty}\rho(z)\exp(pz)dz,$$

and $\rho(z)$ is the jump PDF.

We may consider several examples. First, let us look at the classical case when the waiting time pdf is of exponential form $\psi(t)=\tau^{-1}\exp(-t/\tau)$ and the jump PDF is Gaussian $\rho(z)=(\sigma\sqrt{2\pi})^{-1}\exp(-z^2/2\sigma^2)$. Then

$$\hat{\psi}(H)=\frac{1}{1+H\tau},\quad \hat{\phi}(p)\simeq 1+\sigma^2p^2/2, \tag{14}$$

and the Hamilton-Jacobi equation takes a classical form corresponding to the Fisher-KPP-equation [23,24]

$$\frac{\partial G}{\partial t}+\frac{\sigma^2}{\tau}\left(\frac{\partial G}{\partial x}\right)^2+U(x)=0, \tag{15}$$

while for a general $\rho(z)$ we have [13]

$$\frac{\partial G}{\partial t}+\frac{1}{\tau}\left[\int_{-\infty}^{\infty}e^{z(\partial G/\partial x)}\rho(z)dz-1\right]+U(x)=0. \tag{16}$$

Now let us consider a long-tailed (Levy) waiting time distribution $\psi(t)$ with the Laplace transform [16]

$$\hat{\psi}(H)=\frac{1}{1+(H\tau)^{\gamma}},\qquad 0<\gamma\leqslant 1. \tag{17}$$

In this case we have a class of CTRW that are non-Markovian and lead to slow anomalous diffusion. The density $\psi(t)$ behaves like $t^{-(\gamma+1)}$ for large t, and its expectation diverges when $0<\gamma\leqslant 1$. If the moment generating function for the jump PDF is $\hat{\phi}(p)\simeq 1+\sigma^2p^2/2$, then Eq. (12) takes the form of the anomalous Hamilton-Jacobi equation

$$\left(-\frac{\partial G}{\partial t}\tau\right)^{\gamma}-U(x)\tau\left(-\frac{\partial G}{\partial t}\tau\right)^{\gamma-1}-\frac{\sigma^2}{2}\left(\frac{\partial G}{\partial x}\right)^2=0. \tag{18}$$

In a similar fashion one can write the time-fractional Hamilton-Jacobi equation for the case in which the waiting density $\psi(t)$ is stable with the index of stability γ. The corresponding Laplace transform is $\hat{\psi}(H)=\exp[-(H\tau)^{\gamma}]$ [15]. The solution of all the Hamilton-Jacobi equations (12), (15), (18) can be written as

$$G(t,x)=\min_{x(\cdot)}\left\{\int_0^t L(x'(s))ds : x(0)=x, x(t)=0\right\}, \tag{19}$$

where $L(q)=\max_p[pq-H(p)]$ is the Lagrangian associated with H.

When the growth rate U is independent of the coordinate x, $G(t,x)$ corresponds to the action of a free particle $-Et+px$. The propagation rate u can then be found [5,13] from three equations: Eq. (11) and

$$u=\frac{\partial H}{\partial p},\quad pu=H(p). \tag{20}$$

It turns out that for the long-tailed waiting time distribution (17) the propagation rate u can be found exactly. From Eq. (18) we obtain the momentum p in terms of the Hamiltonian $p=f(H)$, where $f(H)=[2\tau(H-U)(H\tau)^{\gamma-1}]^{1/2}\sigma^{-1}$. This, together with Eq. (20), gives the equation for H, namely, $1=Hd\ln f(H)/dH$, the solution of which is $H=U(3-\gamma)(2-\gamma)^{-1}$. From Eq. (20) we readily obtain an explicit expression for u,

$$u=\frac{\sigma}{\tau\sqrt{2}}(U\tau)^{1-(\gamma/2)}(3-\gamma)^{(3-\gamma)/2}(2-\gamma)^{-1+\gamma/2}. \tag{21}$$

For the case $\gamma=1$, Eq. (21) is in agreement with the corresponding classical expression $u=2(DU)^{1/2}$, where $D=\sigma^2/\tau$ is the diffusion coefficient. In the absence of reaction $(U=0)$, the mean squared displacement (MSD) of particles grows as t^{γ} so that the physical meaning of the exponent γ is clear; for a fixed time, the MSD grows monotonically with γ. It means that the intensity of transport increases with γ. One can think of γ as a measure of the tail length of the waiting time distribution $\psi(t)$ (17). When the waiting time PDF has a long tail it is expected that the mean rate of jumps is lower. That is, waiting time PDF with a long tail decrease the rate of the spread of the particles and therefore the speed of the front, because some particles have long rests before starting the following jump. As a result, the speed of the front, when reaction is present, should also be a monotonically increasing function of γ, that is, $du/d\gamma>0$. This physical condition, applied to Eq. (21), yields $U<U_{\max}=\tau^{-1}(2-\gamma)/(3-\gamma)$ and therefore the reaction rate cannot be arbitrarily large. The meaning of this condition on the reaction rate is the same that one can obtained for the hyperbolic reaction-diffusion equations (see, for example, Refs. [3–6]). Moreover,

$$u<u_{\max}=\sqrt{\frac{D}{\tau}}\sqrt{\frac{3-\gamma}{2}}.$$

It should be noted that, in general, the rate of the propagation u depends on the explicit behavior of the initial condition $n(0,x)$ as $x\to\infty$ [1]. In this paper we have considered only the frontlike initial condition (4) for which formulas (20) gives the lower boundary of possible propagation speeds. The Hamilton-Jacobi technique can be easily adopted to the nonzero initial conditions of the form $n^{\varepsilon}(0,x)=\exp[-G_0(x)/\varepsilon]$ $(x\geqslant 0)$ for which an infinite set of propagation speeds might exist.

In summary, a Hamilton-Jacobi type equation which describes the *macroscopic* dynamics of fronts for *arbitrary* CTRW with growth/reaction of Fisher-KPP type has been derived in terms of the *mesoscopic* properties of the motion of the particles. These properties are related to the probability density functions of jump length and waiting times. We have derived an *exact* expression for the speed of propagating fronts for anomalous transport involving non-Markovian random processes. We have shown, in this case, that there exists an upper bound for the *macroscopic* parameters, such as the reaction rate U and the speed of the front u, which depend on the *mesoscopic* parameter γ.

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