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Effect of memory kernels on the speed of reaction-diffusion fronts

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Abstract – We study the role of a memory kernel, in the constitutive equation for the particle flux, on the speed of propagating fronts in reaction-diffusion systems. We prove for general memory kernels the existence of propagating fronts with a speed bounded by the characteristics of the transport process, even in the fast-reaction limit. This upper bound depends only on the zero-delay value of the memory kernel. To illustrate our results, we consider examples of some functional forms for the memory kernel.

Introduction. – Since the pioneering works by Fisher and Kolmogorov *et al.* in 1937 [1,2], propagating fronts have been studied in many areas of science such as physics, biology, ecology and chemistry [3]. The basic phenomena of front propagation have typically been described by parabolic reaction-diffusion (RD) equations. More recently, time-delays have been incorporated in the evolution equations to model biological invasions [4–7]. The time delay accounts for memory effects in the transport that arise from waiting times or correlations between successive jumps in the underlying random walk. The resulting RD equations are of hyperbolic type if the time-delay is small compared with the characteristic time scale of the front evolution. The physical interest of these hyperbolic reaction-diffusion equations lies in the fact that they avoid the well-known pathologies of the standard diffusion equation, such as the infinitely fast propagation of local disturbances [7,8].

The foundation of any macroscopic description of reacting and diffusing systems is the continuity equation for the particle density $n(x,t)$ together with the constitutive equation for the particle flux $J(x,t)$. To account for memory effects in the transport we replace the standard Fick's first law form of the constitutive equation by a nonlocal relation between the flux and the density gradient,

$$J(x,t) = -\int_0^t \varphi\,(t-s)\,\partial_x n(x,s)\mathrm{d}s, \qquad (1)$$

where $\varphi(t)$ is a memory kernel [9]. This form of the constitutive equation captures the physical fact that the particle flux does not instantaneously adjust to the particle density gradient. If $\varphi(t) = D\delta(t)$, then we have a Fick's law, while the exponential kernel $\varphi(t) = \frac{D}{\tau}\exp\left(-\frac{t}{\tau}\right)$ gives us the Cattaneo equation for the flux $J : J + \tau\partial_t J = D\partial_x n(x,s)$.

Combining the constitutive equation for the flux (1) with the continuity equation for the particle density, $\partial_t n + \partial_x J = f(n)$, we obtain the nonlocal RD equation

$$\partial_t n = \int_0^t \varphi\,(t-s)\,\partial_{xx} n(x,s)\mathrm{d}s + f(n), \qquad (2)$$

which is the focus of this work. We assume that the reaction term $f(n)$ is of the Kolmogorov-Petrovskii-Piskunov type [2], *i.e.*, fulfils the condition $\max_{n\in(0,1)} f(n)/n = U$, $f(0) = 0$, and $f(1) = 0$, where U is the constant growth rate.

The connection between the memory kernel (macroscopic) and the waiting-time distribution (mesoscopic) between successive jumps was initially obtained by Kenkre and collaborators [10–12]. Below, we present a different but brief and direct derivation. However, the main objective of this work is to find the front propagation speed for RD equation of the form given in (2). The present work generalizes results about hyperbolic RD equations, viz., the hyperbolic Fisher equation with a nonlinear damping term [7,8]. The latter is a special case of (2) and is obtained for an exponential memory kernel. We consider

general memory kernels and derive a relation between the front speed and the Laplace transform of the memory kernel. We find that fronts travel at finite speed in the fast reaction limit only if the zero-delay value of the memory kernel is positive definite. Our general results are applied to some specific memory kernels. In particular, we deal with forms not previously studied, such as Lévy and long-tailed memory kernels.

Memory kernel and waiting time distribution. – In this section, we propose an alternative way to link the phenomenological description (1) of the transport with a mesoscopic description in terms of a continuous time random walk (CTRW) [13]. To this end, we express the flux $J(x,t)$ and the particle density $n(x,t)$ in terms of two probabilistic quantities, namely the joint probability density function $\Phi(z,s)$ of making a jump of length z in the time interval $(s, s+\mathrm{d}s)$ and the density of particles $j(x,s)$ that arrive at x at time s. Then the particle density $n(x,t)$ can be written as follows:

$$n(x,t) = \int_0^t j(x,s)\Psi(t-s)\mathrm{d}s. \tag{3}$$

Here $\Psi(t)$ is the survival probability which is related to the waiting time probability density function ψ,

$$\begin{aligned}\Psi(t) &= 1 - \int_0^t \psi(s)\mathrm{d}s,\\ \psi(s) &= \int_{-\infty}^{\infty} \Phi(z,s)\mathrm{d}z.\end{aligned} \tag{4}$$

Defining the flux as the balance between particles arriving at x at time t from the left and particles arriving at x at time t from the right, we have [14]

$$\begin{aligned}J(x,t) \;=\; & \ell \int_0^t \mathrm{d}s \int_{-\infty}^{x} j(z,t-s)\Phi(x-z,s)\mathrm{d}z\\ & -\ell \int_0^t \mathrm{d}s \int_{x}^{\infty} j(z,t-s)\Phi(x-z,s)\mathrm{d}z,\end{aligned} \tag{5}$$

where ℓ is a characteristic (mesoscopic) length scale of the CTRW. If the jump length distribution, $\rho(z)$, and the waiting time distribution, $\psi(s)$, are independent, $\Phi(z,s) = \rho(z)\psi(s)$, one has

$$\hat{\varphi}(H) = \frac{2\ell \langle z\rangle H}{(\hat{\psi}(H)^{-1} - 1)}. \tag{6}$$

This establishes a link between the phenomenological and the mesoscopic descriptions, namely a relation between the memory kernel (macroscopic) $\hat{\varphi}(H)$ and the waiting time pdf (mesoscopic) $\hat{\psi}(H)$. Equation (6) has the same form as eq. (9a) in [10], except for the factor $2\ell\langle z\rangle$. It is also equivalent to eqs. (35) and (42) in [11].

Consider now the situation when the mean waiting time $\langle t\rangle_\psi \equiv -\hat{\psi}'(0)$ is finite and small; then $\hat{\psi}(H)^{-1} \simeq 1 + \langle t\rangle_\psi H$ up to first order. Inserting this expression into (5), we obtain Fick's first law after applying the inverse Fourier-Laplace transform. Inserting the expression into (6), we obtain $\hat{\varphi}(H) = D$ or $\varphi(t) = D\delta(t)$, where the diffusion coefficient D is given by

$$D \equiv \frac{2\ell\langle z\rangle}{\langle t\rangle_\psi}. \tag{7}$$

Up to second order we have $\hat{\psi}(H)^{-1} \simeq 1 + \langle t\rangle_\psi H + \left(\langle t\rangle_\psi^2 - \frac{1}{2}\langle t^2\rangle_\psi\right) H^2$. Inserting this expression into (5), we obtain the Maxwell-Cattaneo form of the constitutive equation after applying the inverse Fourier-Laplace transform. Inserting the expression into (6), we obtain

$$\begin{aligned}\hat{\varphi}(H) = \frac{D\langle t\rangle_\psi H}{\hat{\psi}(H)^{-1} - 1} = \frac{D}{1 + \left[\langle t\rangle_\psi - \frac{1}{2}\frac{\langle t^2\rangle_\psi}{\langle t\rangle_\psi}\right] H} \simeq\\ D - D\left[\langle t\rangle_\psi - \frac{1}{2}\frac{\langle t^2\rangle_\psi}{\langle t\rangle_\psi}\right] H + \ldots.\end{aligned} \tag{8}$$

On the other hand $\hat{\varphi}(H) \simeq \hat{\varphi}(0) + \hat{\varphi}'(0)H + \ldots = \hat{\varphi}(0)(1 - \langle t\rangle_\varphi H + \ldots)$. Comparing this expression with (8), we obtain

$$\langle t\rangle_\varphi = \langle t\rangle_\psi - \frac{1}{2}\frac{\langle t^2\rangle_\psi}{\langle t\rangle_\psi}. \tag{9}$$

This is a relation between the mean memory or relaxation time (macroscopic) $\langle t\rangle_\varphi = -\hat{\varphi}'(0)/\hat{\varphi}(0)$ and the mean waiting time (mesoscopic) $\langle t\rangle_\psi \equiv -\hat{\psi}'(0)$.

Speed of fronts. – We choose "natural" initial conditions, *i.e.*, initial conditions that are localized or that decay faster than exponentially, *e.g.*, Heaviside initial conditions, $n(x,0) = 1$ for $x \leqslant 0$ and $n(x,0) = 0$ for $x > 0$. We assume that the solution of the nonlocal RD equation approaches a front propagating with constant speed in the long-time limit. Our choice of initial conditions ensures that the propagation speed of such a front is minimal [15]. We use the Hamilton-Jacobi approach [16] to determine this minimal speed v. The starting point is to consider the hyperbolic scaling $x \to x/\varepsilon$, $t \to t/\varepsilon$ and to represent the rescaled particle density $n^\varepsilon(x,t) = n(x/\varepsilon, t/\varepsilon)$ in terms of the action functional G^ε as $n^\varepsilon(x,t) = \exp[-G^\varepsilon(x,t)/\varepsilon]$ with $G^\varepsilon(x,t) \geqslant 0$. Applying these considerations to (2), we obtain the equation for the action functional G^ε:

$$\begin{aligned}&-\partial_t G^\varepsilon =\\ &\int_0^{t/\varepsilon} \varphi(s)\left\{e^{-\frac{G^\varepsilon(x,t-\varepsilon s) - G^\varepsilon(x,t)}{\varepsilon}}\left[\partial_x G^\varepsilon(x,t-\varepsilon s)\right]^2 + O(\varepsilon)\right\}\mathrm{d}s\\ &+ e^{G^\varepsilon/\varepsilon} f\left(e^{-G^\varepsilon/\varepsilon}\right).\end{aligned} \tag{10}$$

As long as the function $G(x,t) = \lim_{\varepsilon\to 0} G^\varepsilon(x,t)$ is positive, the rescaled particle density $n^\varepsilon(x,t) \to 0$ as $\varepsilon \to 0$. Therefore, the boundary of the set $G(x,t) > 0$ can be regarded as the location of the reaction-diffusion front, and the front position $x(t)$ can be determined by the equation

$G(x(t),t)=0$. We take the limit $\varepsilon\to 0$ of (10) and find that $G(x,t)$ obeys the nonlinear integral equation

$$\partial_t G+(\partial_x G)^2\int_0^\infty \varphi(s)e^{s\partial_t G}\mathrm{d}s+U=0. \tag{11}$$

This is the Hamilton-Jacobi equation for the action functional $G(x,t)$. When the memory kernel $\varphi(s)$ is the delta-function $D\delta(s)$, (11) can be written in the classical form $\partial_t G+D\left(\partial_x G\right)^2+U=0$.

We introduce the Hamiltonian $H=-\partial_t G$ and the generalized momentum $p=\partial_x G$. Then eq. (11) becomes

$$H=\hat{\varphi}(H)p^2+U, \tag{12}$$

where $\hat{\varphi}(H)=\int_0^\infty \varphi(t)e^{-Ht}\mathrm{d}t$ is the Laplace transform of the memory kernel $\varphi(t)$. The solution of eq. (11) is given by

$$G(x,t)=\int_0^t L[x(s),s]\mathrm{d}s \tag{13}$$

under the conditions $x(0)=0$ and $x(t)=x$. Here $L=p\mathrm{d}x/\mathrm{d}s-H$ is the Lagrangian. From Hamilton's equations we obtain $\mathrm{d}x/\mathrm{d}s=\partial_p H$ and p constant, which upon integration yields $x(s)=s\partial_p H$ with $x=t\partial_p H$, *i.e.* $v=\mathrm{d}x/\mathrm{d}t=\partial_p H$. On the other hand, $G(x,t)=0$ implies $p\partial_p H=H$, and the front speed is given by the set of equations $v=\partial_p H$, $p\partial_p H=H$, or equivalently

$$v=\frac{H}{p(H)},\quad \frac{\partial p}{\partial H}=\frac{p}{H}. \tag{14}$$

Making use of (12) and (14) we find

$$v(H)=H\sqrt{\frac{\hat{\varphi}(H)}{H-U}},\quad \frac{\partial p}{\partial H}=\frac{p}{H}. \tag{15}$$

The front speed is given by $v(H^*)$, where H^* is the solution of

$$\frac{\mathrm{d}}{\mathrm{d}H}\left(\frac{H-U}{\hat{\varphi}(H)}\right)=\frac{2(H-U)}{H\hat{\varphi}(H)}. \tag{16}$$

Equation (15) shows that we only need the Laplace transform of the memory kernel $\hat{\varphi}(H)$ in order to determine the front speed v.

The existence of the front and the value of the minimal speed depend crucially on the behavior of $v(H)$ as $H\to\infty$. To see this, note that $v(H)\to\infty$ as $H\to U^+$. Therefore, if $v(H)$ is a monotonically decreasing function in the limit $H\to\infty$, then the minimum value is 0 and no propagating front exists. If, on the other hand, $v(H)$ is monotonically increasing with H, then a minimum speed exists. We assume that $\varphi(t)$ is a smooth function. The limit $H\to\infty$ is equivalent to the limit $t\to 0$. We write $\varphi(t)=\varphi(0)+\dot{\varphi}(0)t+\ddot{\varphi}(0)t^2/2+\ldots$, which has the Laplace transform $\hat{\varphi}(H)=\varphi(0)H^{-1}+\dot{\varphi}(0)H^{-2}+\ddot{\varphi}(0)H^{-3}+\ldots$, where the overdot means temporal derivative. Then, in the limit $H\to\infty$, $\hat{\varphi}(H)\simeq\varphi(0)H^{-1}$ and $v(H\to\infty)=\sqrt{\varphi(0)}$. This speed value can be selected by the front because it fulfils the condition $\partial_H p=p/H$, if $\varphi(0)>0$, as may be easily shown. We conclude that

$$v=\begin{cases} H^*\sqrt{\frac{\hat{\varphi}(H^*)}{H^*-U}}, & \varphi(0)=0,\\ \min\left[H^*\sqrt{\frac{\hat{\varphi}(H^*)}{H^*-U}},\sqrt{\varphi(0)}\right], & \varphi(0)>0,\end{cases} \tag{17}$$

where H^* is the solution of eq. (16). It is interesting to note that v is a monotonically increasing function of the reaction rate; $\partial_U v>0$ as may be checked. However, if $\varphi(0)>0$, this growth saturates at $\sqrt{\varphi(0)}$, a value that is not affected at all by the reaction process and depends only on the characteristics of the transport through the memory kernel. From eq. (6) it is clear that the memory kernel contains all the physical information we need to determine the propagation speed. Indeed, the upper bound for the front speed equals the speed of propagation of periodic disturbances in the high-frequency limit for the pure transport equation, *i.e.*, eq. (2) with $f=0$. Equation (17) demonstrates that for an infinitely differentiable memory kernel with $\varphi(0)>0$ the front speed is bounded from above by the transport process, even if the reaction process is very fast. The flux at time t is a weighted average of the particle density gradients at previous times, see eq. (1). The weight of the gradient at time t, $\partial_x n(x,t)$, is given by $\varphi(0)$. If $\varphi(0)=0$, the "instantaneous" particle gradient at time t does not contribute to the particle flux at time t and the front speed is unbounded.

Examples. – In this section we illustrate our results for some typical memory kernels. Consider first the case $\varphi(t)=D\delta(t)$. In this case, (17) cannot be applied because $\delta(t)$ is not differentiable near $t=0$. However, the speed may be computed from (15) to yield $v=2\sqrt{UD}$ as expected. For the exponential kernel $\varphi(t)=D\tau^{-1}e^{-t/\tau}$ one recovers the hyperbolic RD equation. From (17), as $\varphi(0)=D/\tau>0$, we recover the known result

$$v=\min_{z>a}\left[\sqrt{D/\tau},\frac{z}{\sqrt{z+1}\sqrt{z-a}}\sqrt{D/\tau}\right]=\begin{cases}2\sqrt{D/\tau}\frac{\sqrt{a}}{1+a}, & a\leqslant 1,\\ \sqrt{D/\tau}, & a>1,\end{cases} \tag{18}$$

where $z\equiv H\tau$ and $a=U\tau$. Note that the front speed is bounded from above by the limiting speed of the transport process, $\sqrt{D/\tau}$. Both cases are depicted in fig. 1.

Lévy kernel: $\hat{\varphi}(H)=D\left[1+(H\tau)^\gamma\right]^{-1}$ with $0<\gamma\leqslant 1$. In this case $\varphi(0)$ is not defined and

$$v(H)=\sqrt{D/\tau}\frac{z}{\sqrt{z^\gamma+1}\sqrt{z-a}}, \tag{19}$$

where $z\equiv H\tau$ is a solution of $(z-2a)/(z-a)=\gamma z^\gamma/(1+z^\gamma)$. The front speed growths without bound with a as can be seen in fig. 2, where we plot the front speed *vs.* a for different values of the exponent γ. The figure also shows that as γ tends to 1 (the hyperbolic limit) the speed curves

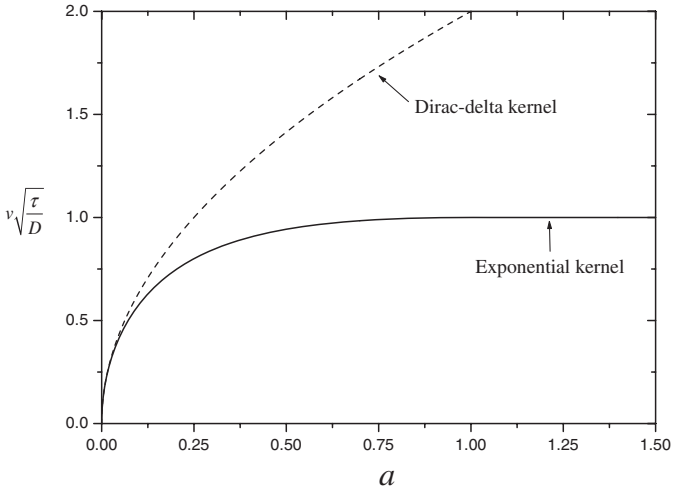

Fig. 1: Dimensionless front speed *vs.* a for the Dirac-delta (unbounded) and exponential kernels (bounded).

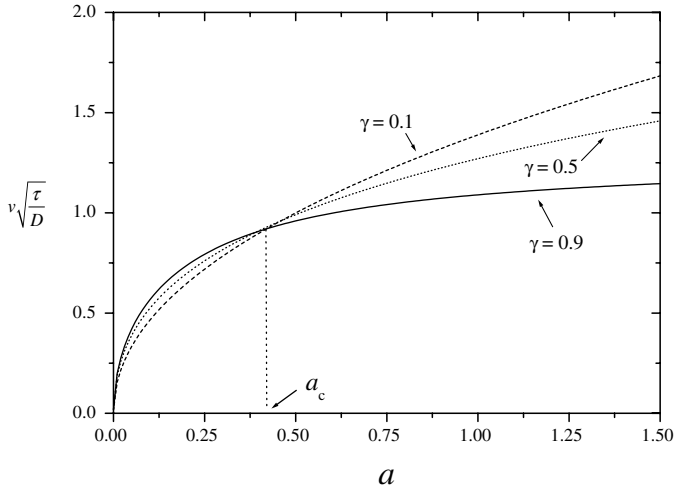

Fig. 2: Dimensionless front speed *vs.* a for the Lévy kernel. In this case the front speed is unbounded, and there exists a critical value a_c such that for $a > a_c$ slower transport produces faster fronts.

tend to saturate at $\sqrt{D/\tau}$. Moreover, we observe an interesting behavior: There is a critical value for a, namely a_c, such that for $a < a_c$ the front speed is higher for $\gamma \to 1$ than for $\gamma \to 0$, in agreement with the subdiffusive transport. However, for $a > a_c$ this behavior is inverted and in clear disagreement with the subdiffusive transport. This fact has been already observed for hyperbolic fractional reaction-diffusion equations [17]. Let us note that reaction-transport problems involving spatial Lévy kernels with an infinite first moment were considered in [18].

Long-tailed kernel: We consider the power-law kernel $\varphi(t) = \frac{D(\gamma-1)}{\tau}\left(1+\frac{t}{\tau}\right)^{-\gamma}$ with $\gamma > 1$ and finite moments. As $\varphi(0) = \frac{D(\gamma-1)}{\tau} > 0$, eq. (17) implies that the front speed is bounded by $\sqrt{D(\gamma-1)/\tau}$. The Laplace transform of

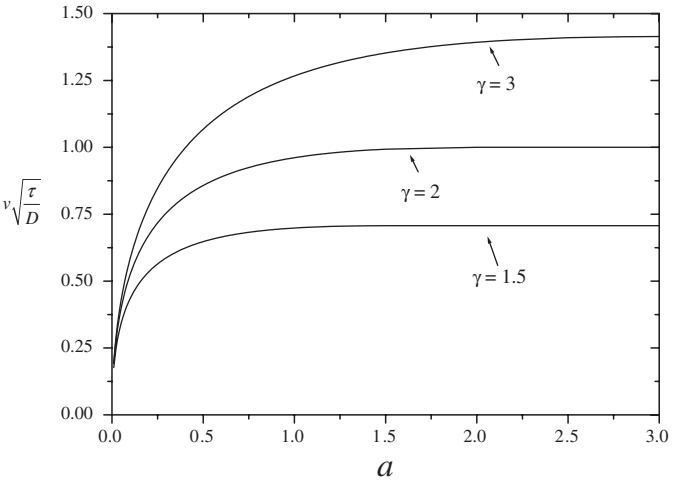

Fig. 3: Dimensionless front speed *vs.* a for the long-tailed kernel. In this case the dimensionless front speed is bounded by $\sqrt{\gamma-1}$. For higher values of the index γ the kernel tail decays faster than for low γ and this generates faster fronts.

the kernel is $\hat{\varphi}(H) = D(\gamma-1)\,(H\tau)^{\gamma-1}\,e^{H\tau}\Gamma\,(1-\gamma, H\tau)$ where $\Gamma(,)$ is the incomplete gamma-function. The front speed has to be calculated numerically from eqs. (16) and (17). In fig. 3 we plot the front speed *vs.* a for different values of γ. The saturation effect at $\sqrt{D(\gamma-1)/\tau}$ is observed. Note that when γ increases, the front speed also increases due to the faster decay of the memory kernel tail. It is noteworthy that for the family of gamma distributions $\varphi(t) = D(t/\tau)^m e^{-t/\tau}$ with $m \geqslant 1$ one has $\varphi(0) = 0$, and then no bounded front speed is obtained.

Conclusions. – We consider a reaction-diffusion equation with a memory kernel in the constitutive equation for the particle flux. The corresponding transport equation is not new and is widely known, however no attention has been paid to the investigation of traveling fronts when this equation is combined with a reaction term. The speed of traveling fronts emerging from initial conditions with compact support is obtained within the framework of the Hamilton-Jacobi theory, and a general result for any $\varphi(t)$ is derived. Our main result is the existence of an upper bound for the front speed in the fast reaction limit, if the memory kernel does not vanish at $t = 0$. This bound depends only on the characteristics of the transport process through the zero-delay value of the memory kernel. The Laplace transform of the memory kernel contains all the information necessary to specify the propagation speed. Our general results are applied to some typical memory kernels, in particular to Lévy and long-tailed kernels.

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