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Different microscopic interpretations of the reaction-telegrapher equation

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Abstract

In this paper we provide some new insights into the microscopic interpretation of the telegrapher's and the reaction-telegrapher equations. We use the framework of continuous-time random walks to derive the telegrapher's equation from two different perspectives reported before: the kinetic derivation (KD) and the delayed random-walk derivation (DRWD). We analyze the similarities and the differences between both derivations, paying special attention to the case when a reaction process is also present in the system. As a result, we are able to show that the equivalence between the KD and the DRWD can break down when transport and reaction are coupled processes. Also, this analysis allows us to elaborate on the specific role of relaxation effects in reaction–diffusion processes.

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1. Introduction

The telegrapher's equation (TE) owes its name to the original works by Lord Kelvin on the propagation of an electric signal through a long cable [1]. He and some contemporaries found that the evolution of the electric current $I(x, t)$ through the cable was described by the equation

$$\frac{\partial^2 I}{\partial t^2} + a_1 \frac{\partial I}{\partial t} + a_2 I = a_3 \frac{\partial^2 I}{\partial x^2}, \tag{1}$$

where a_i are constants which depend on the characteristic parameters of the corresponding electric circuit. Since then, similar equations have arisen as a useful description for many other physical and mathematical situations, specially in transport theory. If one denotes the probability density $\rho(x, t)$ that a particle is at position x at time t, then most authors in modern literature refer to the form

$$\frac{\partial^2 \rho}{\partial t^2} + \frac{1}{\tau} \frac{\partial \rho}{\partial t} = c^2 \frac{\partial^2 \rho}{\partial x^2} \tag{2}$$

as the TE, with a a positive constant. This expression can be obtained straightforward from (1) after an exponential transformation of the type $\rho(x,t) \sim I(a,t)\exp(\xi t)$ and proper choice of ξ as a function of the parameters τ and c. The fact that (2) behaves as a wave equation in the limit $t \to 0$ and as a diffusion equation for $t \to \infty$, makes it a very convenient expression in order to solve the problem of the infinite propagation speed of signals that one finds for the classical diffusion equation [2, 3]. This idea has been deeply discussed and fruitfully exploited, for example, in the framework of extended irreversible thermodynamics (EIT) [4, 5]. Also, equation (2) has been proved of interest as an approximate solution for the general transport equation [6], with additional potential applications in the field of relativistic quantum mechanics [7], single-file flows [8], etc. A more comprehensive review on the applications and the properties of the TE can be found in [2, 3, 9] and the references therein.

In many areas, with special focus on thermal conduction and thermodynamics, the TE is usually related to the Maxwell–Cattaneo equation

$$J + \tau \frac{\partial J}{\partial t} = -D\frac{\partial \rho}{\partial x}, \tag{3}$$

where $J(x,t)$ is defined as the flux of particles passing through x at time t, τ is the characteristic relaxation time of the system and D is the diffusion coefficient. It is straightforward to see that (2) arises naturally from (3) together with the continuity equation

$$\frac{\partial \rho}{\partial t} = -\frac{\partial J}{\partial x} \tag{4}$$

and the identity $D = c^2/\tau$. So, the Maxwell–Cattaneo equation represents a generalization of Fick's law to the case where relaxation effects (characterized by the parameter τ) are considered, and so from this point of view the TE can also be interpreted as a generalized diffusion equation. These ideas, however, have been questioned by some authors [10, 11]. The Maxwell–Cattaneo equation has been criticized because it is not frame invariant and so it cannot be a valid conduction equation. This problem, however, has been seemingly resolved in a recent paper by Christov and Jordan [12]. The extension of the TE to two or more dimensions involves some formal problems too, as the solutions $\rho(x,t)$ can become negative in that case (due to this behavior, the TE has been said to be of the *dangerous* class as defined in [13]). Some thermodynamical arguments can be used to show that negative values of $\rho(x,t)$ are prevented for the case of thermal conduction [14]. However, there is no direct generalization of the 1D TE in higher dimensions [6, 15].

In the present paper, we will focus specially on the microscopic interpretations of the 1D equation (2) and the behavior of the reaction-telegrapher equation which results from considering both reaction kinetics and transport effects. We will explore and compare two different mathematical derivations that have been proposed before for the TE, the kinetic derivation (KD) and the delayed random walk derivation (DRWD). The differences at the microscopic level between these two derivations, as we shall see, become negligible at the macroscopic level. However, the interplay between transport and an extra process (a reaction process, in our case) can make these microscopic differences become apparent. If it happens, the macroscopic analogy between the KD and the DRWD will break down. Here, we illustrate these ideas for three different implementations of a reaction process and show that, for the breakdown of the analogy between KD and DRWD, a necessary (but not sufficient) condition is that the reaction and transport processes are coupled. The differences at the macroscopic level between both derivations are shown by analyzing the traveling front solutions for each case. As an interesting consequence, we find that for the three implementations of the reaction process considered, the fronts exhibit different qualitative behaviors with respect to the parameter τ. This allows us to review the discussion about the role of the relaxation time in the context of the reaction-telegrapher equation (see, for example, [16]).

2. Kinetic derivation versus delayed random walk derivation

Kinetic derivation. For this case, the dynamics of individual particles is assumed to follow a Markov process in the velocity, which takes randomly only two possible values $+v$ and $-v$. It means that each particle moves with velocity $+v$ during a certain sojourn time, then it switches instantaneously to velocity $-v$, switches again to $+v$ after a new sojourn time, and so on. The corresponding distribution of random sojourn times is of the form $\psi(t) = \lambda\, \mathrm{e}^{-\lambda t}$. This microscopic dynamics was first described by Goldstein [17] and Kac [18] from the point of view of a two-state model. Also, ideas from kinetic theory and the Maxwell equation have been used to derive the TE [5].

Delayed Random Walk Derivation. Consider now that the particles jump from one place to another on the 1D chain. If the random waiting times between consecutive jumps for each particle are distributed according to an Erlang distribution of the type $\psi(t) = t\lambda^2\, \mathrm{e}^{-\lambda t}$, then in the limit of small jumps (diffusive approximation) the TE is also recovered. This idea has recently been reviewed by one of us in the context of virus dynamics [19]. It is clear that the two processes described above (for the KD and the DRWD) are different at a microscopic level. However, the density of particles $\rho(x, t)$ follows in both cases a TE. This is a consequence of the similarities in the temporal statistics of the two processes, as we shall show below.

2.1. Continuous-time random walks: a unifying approach

The CTRW approach [20] brings the mathematical concept of semi-Markov process (developed by Pyke in 1961 [21]) into the context of physical transport. Unlike classical random walks, which are restricted to the Markov assumption, CTRWs can account for walks with memory effects by a joint probability distribution function (PDF) $\psi(x, t)$ for jump lengths and waiting times between jumps. Let $q(x, t)$ be the density of particles arriving at position x at time t; then we can write from the CTRW theory

$$q(x,t) = \int_0^t \int_{-\infty}^{\infty} q(x - x', t - t')\psi(x', t')\, \mathrm{d}x'\, \mathrm{d}t' + \int_{-\infty}^{\infty} \rho(x - x', 0)\psi(x', t)\, \mathrm{d}x'. \tag{5}$$

The first term in the rhs represents the contribution from all particles jumping from position $x - x'$ to position x after a waiting time t', while the second term gives the contribution from the initial density of particles. In order to find the form for the density of particles $\rho(x, t)$, one needs to consider the expression

$$\rho(x,t) = \int_0^t q(x, t - t')\Psi(t')\, \mathrm{d}t' + \rho(x, 0)\Psi(t), \tag{6}$$

where the function $\Psi(t)$ is the probability that a particle waits at least for a time t before jumping to a new position. So, the following identity between ψ and Ψ holds:

$$\Psi(t) = \int_t^{\infty} \int_{-\infty}^{\infty} \psi(x', t')\, \mathrm{d}x'\, \mathrm{d}t'. \tag{7}$$

The set of equations (5)–(7) constitutes the *jump* version of the CTRW. In contrast with that, it is also possible to derive a *velocity* version (this nomenclature is due to Zumofen and Klafter [22]) in which the particles do not jump from one place to another but travel always with a constant velocity whose value alternates between $+v$ and $-v$. The equivalent to (5)–(7) in the context of the *velocity* version reads

$$q_v(x,t) = \int_0^t \int_{-\infty}^{\infty} q_v(x - x', t - t')\psi_v(x', t')\, \mathrm{d}x'\, \mathrm{d}t' + \rho_v(x, 0) \tag{8}$$

$$\rho_v(x,t) = \int_0^t \int_{-\infty}^{\infty} q_v(x-x',t-t')\Psi_v(x',t')\,\mathrm{d}x'\,\mathrm{d}t' \tag{9}$$

$$\Psi_v(x,t) = \delta(x-vt)\int_t^{\infty}\int_x^{\infty} \psi_v(x',t')\,\mathrm{d}x'\,\mathrm{d}t', \tag{10}$$

where we have introduced the subindex v for *velocity* and $\delta(\cdot)$ represents the Dirac delta function. The meaning of $\rho_v(x,t)$ remains the same, i.e., it is density of particles' present (i.e., passing through) position x at time t, but now $q_v(x,t)$ represents the density of particles that arrive at position x at time t and change their direction exactly at that moment. $\psi_v(x,t)$ is the PDF of sojourn times and distances between two consecutive changes in the direction of the particles. Finally, $\Psi_v(x,t)$ is the probability that the particle travels a distance x in the same direction at least for a time t without changing direction. We will skip the details about the specific meaning of (8)–(10), as these expressions have accurately been discussed in [22]. The solutions for the two versions of the model were also found there: closed equations for the density of particles can be written in the Fourier–Laplace coordinates (k,s)

$$\widehat{\rho}(k,s) = \frac{\widetilde{\Psi}(s)}{1-\widehat{\psi}(k,s)}\widehat{\rho}(k,0) \tag{11}$$

$$\widehat{\rho_v}(k,s) = \frac{\widehat{\Psi_v}(k,s)}{1-\widehat{\psi_v}(k,s)}\widehat{\rho_v}(k,0), \tag{12}$$

where $\widetilde{\ }$ and $\widehat{\ }$ denote the Laplace and the Fourier–Laplace transforms, respectively.

In all our discussion above, we have tried to make it clear that the *jump* and the *velocity* version of the CTRW fit very well with the microscopic underlying process that was described in the DRWD and the KD, respectively. So that, the CTRW provides a unifying approach for both derivations. The DRWD can be described by the *jump* version by choosing an appropriate form of $\psi(x,t)$, and the KD can be described by the *velocity* version just by finding $\psi_v(x,t)$. For the case of DRWD, we have already mentioned above that waiting times were distributed according to $\psi(t) = t\lambda^2\,\mathrm{e}^{-\lambda t}$, and the diffusive approximation for transport (i.e., short-distance dispersal: $\sigma k \ll 1$, with σ being the characteristic jump length) was considered. Then, if waiting time and jump length distributions are assumed to be independent we find in the Fourier–Laplace space

$$\text{DRWD:}\quad \widehat{\psi}(k,s) \simeq \frac{\lambda^2}{(s+\lambda)^2}(1-\sigma^2k^2). \tag{13}$$

Note that this approximation is only valid for small values of σk so that the distribution $\widehat{\psi}(k,s)$ is prevented from becoming negative; this has been discussed to be a reason for the TE to be of the *dangerous* class [13].

For the KD, we need to consider the contribution from particles moving with velocity $+v$ and those moving with velocity $-v$. The PDF for the total distance covered and the total sojourn time during this cycle are given by the convolution product

$$\psi_v(x,t) = [\delta(x-vt)\lambda\,\mathrm{e}^{-\lambda t}] * [\delta(x+vt)\lambda\,\mathrm{e}^{-\lambda t}], \tag{14}$$

where the first term corresponds to the joint PDF for the particle moving from the left to the right, and the second one is for the backward movement. In the Fourier–Laplace space, (14) simplifies to

$$\text{KD:}\quad \widehat{\psi}_v(k,s) = \frac{\lambda^2}{(s+\lambda)^2+v^2k^2}. \tag{15}$$

If we introduce expressions (13) and (15) into (11) and (12), respectively, the models can easily be solved. By transforming back to the real coordinates (x, t), we obtain

$$\text{DRWD:} \quad \frac{1}{2\lambda}\frac{\partial^2\rho}{\partial t^2} + \frac{\partial\rho}{\partial t} = \frac{\sigma^2\lambda}{2}\frac{\partial^2\rho}{\partial x^2} \tag{16}$$

$$\text{KD:} \quad \frac{1}{2\lambda}\frac{\partial^2\rho}{\partial t^2} + \frac{\partial\rho}{\partial t} = \frac{v^2}{2\lambda}\frac{\partial^2\rho}{\partial x^2}. \tag{17}$$

These results confirm the equivalence at the macroscopic level between the KD and the DRWD, as in both cases we obtain a TE with the same form. The only difference appears in the definition of the diffusion coefficient ($D_j = \sigma^2\lambda/2$ and $D_v = v^2/2\lambda$) because of the different parameterization used in each case.

If we integrate those PDFs over the whole spatial domain (which is equivalent to evaluating the function at $k = 0$) we find that the distribution of waiting times is exactly the same in both cases, so both processes follow the same temporal statistics. This is not surprising, as the convolution of two exponential distributions $\lambda\,\mathrm{e}^{-\lambda t}$ as that considered in (14), is an Erlang distribution $t\lambda^2\,\mathrm{e}^{-\lambda t}$ as that used for the DRWD. Then, we conclude that the microscopic differences between the KD and the DRWD are only on the spatial statistics of jumps.

2.2. *Connection to the Maxwell–Cattaneo equation*

The Maxwell–Cattaneo equation can directly be obtained from the CTRW theory in the two cases considered above. To show this, note that we can use the continuity equation (4) as a definition for the fluxes $J(x, t)$ or $J_v(x, t)$. In the Fourier–Laplace space, that equation turns into $s\widehat{\rho}(k, s) - \rho(k, 0) = -\mathrm{i}k\widehat{J}(k, s)$. Then, it is easy to find from this expression together with (11) and (12) that

$$\widehat{J}(k, s) = \frac{\mathrm{i}}{k}\left(s - \frac{1 - \widehat{\psi}(k, s)}{\widetilde{\Psi}(s)}\right)\widehat{\rho}(k, s) \tag{18}$$

$$\widehat{J}_v(k, s) = \frac{\mathrm{i}}{k}\left(s - \frac{1 - \widehat{\psi}_v(k, s)}{\widehat{\Psi}_v(k, s)}\right)\widehat{\rho}_v(k, s). \tag{19}$$

Note that this definition for J coincides with the formal definition for the flux of particles in a CTRW that was first given by Compte and Metzler [23].

Now, we can introduce (18) and (19) into the Maxwell–Cattaneo equation (3), with $\tau = 1/2\lambda$. If we do that, we obtain that the necessary conditions for the PDF's ψ and ψ_v, in order that the Maxwell–Cattaneo equation is satisfied, read

$$\widehat{\psi}(k, s) = \widehat{\psi}(0, s) - \frac{\widetilde{\Psi}(s)D_j}{s + 2\lambda}k^2 \tag{20}$$

$$\widehat{\psi}_v(k, s) = \widehat{\psi}_v(0, s) - \frac{\widehat{\Psi}_v(k, s)D_v}{s + 2\lambda}k^2. \tag{21}$$

It is an easy mathematical exercise to prove that (13) and (15) satisfy these conditions, respectively. So, it formally proves that the KD and the DRWD are compatible with the existence of a Maxwell–Cattaneo equation for J.

All this discussion is of importance because the Maxwell–Cattaneo equation (3) has been often interpreted as a first-order Taylor expansion (see for example [24]) of the phenomenological constitutive equation

$$J(x, t + \tau) = -D\frac{\partial\rho(x, t)}{\partial x}$$

that takes into account relaxation (delay) effects in the response of the system to local variations in the density of particles ρ. According to that, it could be thought that the Maxwell–Cattaneo equation can only be valid in the limit when τ is small. However, we have derived above the Maxwell–Cattaneo equation in the framework of the CTRWs without imposing any constriction on the relaxation parameter λ. It proves that the Maxwell–Cattaneo equation can represent an exact formula (not just an approximation) for the relaxation response of a system in some specific situations.

3. The effects of a reaction process

After introducing the CTRW framework for the analysis of the TE equation, we can now explore the main idea of this paper, which is to find out if the equivalence between the KD and the DRWD breaks down in the presence of a reaction process. Usually, one introduces mathematically reaction processes by using the ideas from classical kinetics and the mass action law (see case 1 below). However, different alternatives have been explored recently [25–27]. In the present paper we will explore these cases:

Case 1. The reaction process is independent of transport. This corresponds to the standard situation used in chemical kinetics.

Case 2. The reaction process takes place exactly when the particle lands in a new position after a jump or, alternatively, when it changes direction in the velocity version. This case has been studied in the framework of anomalous diffusion with reaction for CTRWs [25]. The idea is that the reaction process is coupled to transport, so that every transport event (i.e., a jump or a change in direction) yields a reaction event.

Case 3. The reaction process takes place after a distributed waiting time, provided that a jump or a change in direction does not occur first. Similarly to the case of jumps, we can consider that consecutive reaction events for a particle are separated by distributed waiting times. Then we need to introduce two internal waiting times for each particle, one for motion and the other for reaction. However, we have recently explored [26] the simplified case where those waiting times are mutually exclusive, it is, if there is a jump (reaction event) then the waiting time for reaction (jumps) starts from zero again. This may serve, for example, to explain situations where it is necessary a direct contact with a fixed substrate in order that the particle becomes activated and can react.

3.1. Traveling front solutions

In the following subsections, we will show that any of the three cases mentioned above leads in the asymptotic regime $t \to \infty$ to a hyperbolic reaction-telegrapher equation with the general form

$$\frac{\partial^2 \rho}{\partial t^2} + b_1 \frac{\partial \rho}{\partial t} = b_2 \frac{\partial^2 \rho}{\partial x^2} + b_3 \rho - F(\rho) - \frac{\partial F(\rho)}{\partial t}, \tag{22}$$

where $F(\rho)$ represents a nonlinear death term that is responsible for saturation effects in the system (for example, for the case of a logistic growth $F(p) \sim p^2$). The properties of the traveling solutions of (22) are widely known since many years ago (see, for example [28, 29]) and have been employed for modeling of forest fires [30], biological invasions [31], bistable systems [32] and many other [16].

We summarize how to compute the front velocity for the hyperbolic reaction–diffusion equation (22) by using the Hamilton–Jacobi method [33]. As we want to compute the velocity

reached by the traveling front in the long-time and large-distance limit when it evolves from the initial condition $\rho(x,0)=\theta(-x)$ ($\theta(\cdot)$ is the Heaviside function) it is convenient to introduce the hyperbolic scaling $x \to x/\varepsilon$ and $t \to t/\varepsilon$ where $\rho^\varepsilon(x,t) = \rho(x/\varepsilon, t/\varepsilon)$. Defining the auxiliary field $G^\varepsilon(x,t) = -\varepsilon \ln \rho^\varepsilon(x,t)$ one obtains

$$\left(\frac{\partial G^\varepsilon}{\partial t}\right)^2 - \varepsilon\frac{\partial^2 G^\varepsilon}{\partial t^2} - b_1\frac{\partial G^\varepsilon}{\partial t} = b_2\left(\frac{\partial G^\varepsilon}{\partial x}\right)^2 - b_2\varepsilon\frac{\partial^2 G^\varepsilon}{\partial x^2} + b_3 - \mathrm{e}^{G^\varepsilon/\varepsilon}F(\mathrm{e}^{-G^\varepsilon/\varepsilon}) - \mathrm{e}^{G^\varepsilon/\varepsilon}\frac{\partial F(\mathrm{e}^{-G^\varepsilon/\varepsilon})}{\partial t}. \tag{23}$$

Introducing the definitions for the Hamiltonian and momentum as $H = -\partial_t G$ and $p = \partial_x G$ respectively, equation (23) becomes in the limit $\varepsilon \to 0$

$$H^2 + b_1 H = b_2 p^2 + b_3,$$

which can be rewritten in the form of the relativistic Hamilton–Jacobi equation of a particle with mass M moving in the potential field V, that is, $H = \sqrt{M^2c^4 + c^2p^2} + V$ where c is the speed of light. By comparing both equations we find

$$c = \sqrt{b_2}, \qquad V = -b_1/2, \qquad M = \frac{\sqrt{b_3 + b_1^2/4}}{b_2}. \tag{24}$$

As in relativistic dynamics, c plays the role of an upper bound for the traveling front velocity. The general form of the front velocity is computed from [33]

$$v_f = \min_{p>0}\frac{H(p)}{p}.$$

In consequence,

$$v_f = \begin{cases} 2\sqrt{\dfrac{b_2 b_3}{b_1^2 + 4b_3}} & \text{if} \quad b_1 > 0 \\ \sqrt{b_2} & \text{if} \quad b_1 < 0, \end{cases} \tag{25}$$

where we can distinguish between two regimes: usually [16], $b_1 > 0$ corresponds to slow reaction (the characteristic reaction time is larger than the characteristic waiting time) and $b_1 < 0$ to fast reaction (the characteristic reaction time is smaller than the characteristic waiting time). It can be seen that the transition between both regimes at $b_1 = 0$ is always smooth, since $\mathrm{d}v_f/\mathrm{d}b_1\big|_{b_1=0} = 0$. Next, we will derive the reaction–diffusion equations for each case and will apply the analytical result (25) in order to compare the dynamics obtained.

3.1.1. Case 1. Equations (5) and (8) for the *jump* and the *velocity* version, respectively, turn now into

$$\text{DRWD}: \quad q(x,t) = \int_0^t\int_{-\infty}^{\infty} q(x-x',t-t')\psi(x',t')\,\mathrm{d}x'\,\mathrm{d}t' + \int_{-\infty}^{\infty}\rho(x-x',0)\psi(x',t)\,\mathrm{d}x' + \frac{r_1}{\lambda}\rho - F(\rho) \tag{26}$$

$$\text{KD}: \quad q_v(x,t) = \int_0^t\int_{-\infty}^{\infty} q_v(x-x',t-t')\psi_v(x',t')\,\mathrm{d}x'\,\mathrm{d}t' + \rho_v(x,0) + \frac{r_1}{\lambda}\rho_v - F(\rho_v), \tag{27}$$

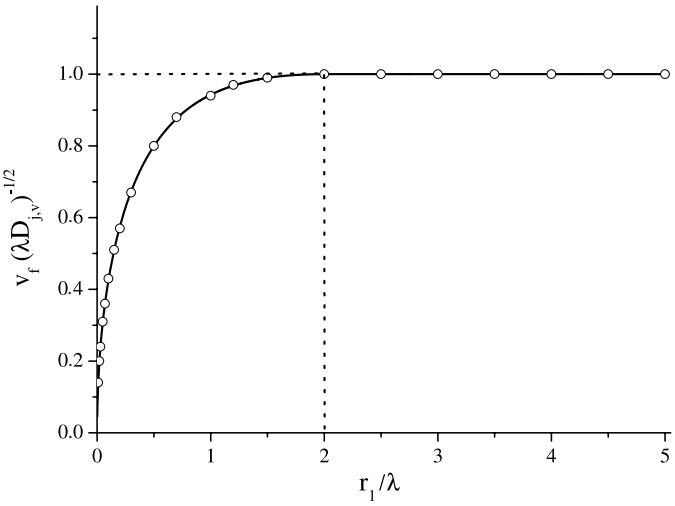

Figure 1. Comparison between the analytical expression for the velocity of traveling fronts in (30) (solid line) and the results from numerical integration of (28) and (29) (circles). Dotted lines indicate the transition point at $r_1 = 2\lambda$. The values of the parameters used in the plot are $D_{j,v} = 1, \lambda = 0.5$.

where r_1 is the characteristic reaction rate and $F(\rho)$ represents a nonlinear saturation term, as in (22). The final expressions we find for the density of particles, inverting back to the real space, are

$$\text{DRWD:} \quad \frac{\partial^2 \rho}{\partial t^2} + (2\lambda - r_1)\frac{\partial \rho}{\partial t} = \lambda D_j \frac{\partial^2 \rho}{\partial x^2} + 2\lambda r_1 \rho - F(\rho) - \frac{\partial F(\rho)}{\partial t} \tag{28}$$

$$\text{KD:} \quad \frac{\partial^2 \rho_v}{\partial t^2} + (2\lambda - r_1)\frac{\partial \rho_v}{\partial t} = \lambda D_v \frac{\partial^2 \rho_v}{\partial x^2} + 2\lambda r_1 \rho_v - F(\rho_v) - \frac{\partial F(\rho_v)}{\partial t}, \tag{29}$$

which have the same general form as (22). Note that the only difference between (28) and (29) is in the definition of the diffusion coefficients so we conclude that for case 1 the equivalence at the macroscopic level between the DRWD and the KD is still valid. Now, if we apply (25) to these equations we can find the form of the front velocity v_f

$$v_f = \begin{cases} 2\dfrac{\sqrt{2r_1 D_{j,v}}}{2 + r_1/\lambda} & \text{if} \quad r_1 < 2\lambda \\ \sqrt{\lambda D_{j,v}} & \text{if} \quad r_1 > 2\lambda. \end{cases} \tag{30}$$

We show the behavior of the dimensionless velocity $v_f/\sqrt{\lambda D_{j,v}}$ as a function of r_1/λ in figure 1. There, we have chosen the values of the parameters so that $D_j = D_v$ to make the results from the KD and the DRWD coincide. The results obtained have been compared in the plot with those obtained from the numerical integration of (28),(29) (circles), showing a perfect agreement. We observe that there is always a transition at $r_1 = 2\lambda$, so that for higher values of the reaction rate r_1 the front speed will not increase. This is due to the limitation imposed by the TE on the finite propagation of signals: traveling fronts in the reaction-telegrapher equation cannot propagate faster than the information signals in the TE. This important limitation has been discussed in detail in previous works [4, 16, 32, 34].

3.1.2. Case 2. Now, if the reaction can occur only at the moment of a jump in space (or change in velocity), it is obvious that we have to introduce the reaction directly in the transport term of the CTRW equations. So that, equations (5) and (8) become for this case

$$\text{DRWD:}\quad q(x,t) = (1+r_2)\int_0^t\int_{-\infty}^{\infty} q(x-x',t-t')\psi(x',t')\,\mathrm{d}x'\,\mathrm{d}t' + \int_{-\infty}^{\infty}\rho(x-x',0)\psi(x',t)\,\mathrm{d}x' - F(\rho) \tag{31}$$

$$\text{KD:}\quad q_v(x,t) = (1+r_2)\int_0^t\int_{-\infty}^{\infty} q_v(x-x',t-t')\psi_v(x',t')\,\mathrm{d}x'\,\mathrm{d}t' + \rho_v(x,0) - F(\rho_v), \tag{32}$$

where r_2 is now a (dimensionless) reaction parameter. We obtain the corresponding evolution equations for $\rho(x,t)$ and $\rho_v(x,t)$:

$$\text{DRWD:}\quad \frac{\partial^2\rho}{\partial t^2} + 2\lambda\frac{\partial\rho}{\partial t} = (1+r_2)\lambda D_j\frac{\partial^2\rho}{\partial x^2} + \lambda^2 r_2\rho - F(\rho) - \frac{\partial F(\rho)}{\partial t} \tag{33}$$

$$\text{KD:}\quad \frac{\partial^2\rho_v}{\partial t^2} + 2\lambda\frac{\partial\rho_v}{\partial t} = \lambda D_v\frac{\partial^2\rho_v}{\partial x^2} + \lambda^2 r_2\rho_v - F(\rho_v) - \frac{\partial F(\rho_v)}{\partial t}. \tag{34}$$

At the same time, if we apply (25) to (33) and (34), we find the values for v_f. Note that in this case the coefficient b_1 defined in (22) will always be positive, so we do not have any transition in v_f. The results obtained are

$$\text{DRWD:}\quad v_f = 2\sqrt{r_2\lambda D_j} \tag{35}$$

$$\text{KD:}\quad v_f = \sqrt{\lambda D_v\left(1 - \frac{r_2}{1+r_2}\right)}. \tag{36}$$

For case 2, equations (33) and (34) do not show the same dependence on the reaction parameter r_2. It implies that the equivalence between the KD and the DRWD breaks down in this case as a consequence of the coupling between transport and reaction. In figure 2 we show the different behavior of traveling fronts exhibited by the DRWD and the KD for this case. It is specially interesting to observe the behavior for the DRWD: as the coefficient b_2 in equation (33) is proportional to the reaction parameter r_2, then v_f is unbounded for $r_2 \to \infty$. This undesirable behavior contradicts the idea mentioned above that traveling fronts cannot be faster than the information signals for the TE. In consequence, we can conclude that the DRWD for case 2 does not represent apparently a convenient implementation of a reaction process; this point will be addressed in detail in the Conclusions section.

3.1.3. Case 3. Finally, we show how the CTRW theory can be used to introduce the ideas of a reaction process where the reaction events are separated by distributed waiting times. We will call $R(t)$ the PDF of waiting times for reaction, and $R^*(t)$ the corresponding survival probability (i.e., the probability that the particle has not reacted after a waiting time t). By introducing these ideas into the CTRW framework, equations (5) and (6) for the *jump* version

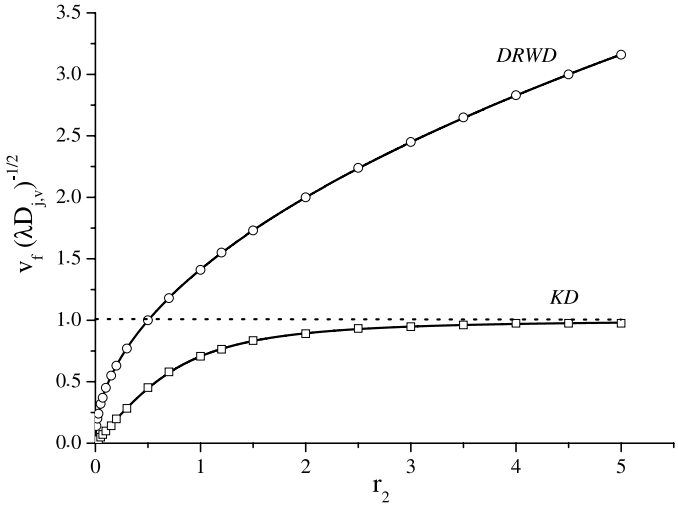

Figure 2. Comparison between the analytical expressions for the DRWD and the KD for the velocity of traveling fronts (equations (35) and (36), solid lines) and the results from numerical integration of (33) and (34) (symbols), respectively. The values of the parameters used in the plot are the same as in figure 1.

become (see [26] for further details)

$$\begin{aligned} q(x,t) = &\int_0^t \int_{-\infty}^{\infty} q(x-x',t-t')R^*(t')\psi(x',t')\,\mathrm{d}x'\,\mathrm{d}t' \\ &+ 1 + r_3 \int_0^t q(x,t-t')R(t')\Psi(t')\,\mathrm{d}t' \\ &+ \int_{-\infty}^{\infty} \rho(x-x',0)R^*(t')\psi(x',t)\,\mathrm{d}x' \\ &+ 1 + r_3\rho(x,0)R(t)\Psi(t) - F(\rho) \end{aligned} \tag{37}$$

$$\rho(x,t) = \int_0^t q(x,t-t')R^*(t')\Psi(t')\,\mathrm{d}t' + \rho(x,0)R^*(t)\Psi(t), \tag{38}$$

with r_3 being the reaction parameter. For the *velocity* version we have, equivalently,

$$\begin{aligned} q_v(x,t) = &\int_0^t \int_{-\infty}^{\infty} q_v(x-x',t-t')R^*(t')\psi(x',t')\,\mathrm{d}x'\,\mathrm{d}t' \\ &+ 1 + r_3 \int_0^t \int_{-\infty}^{\infty} q_v(x-x',t-t')R(t')\Psi(x',t')\,\mathrm{d}x'\,\mathrm{d}t' \\ &+ \int_{-\infty}^{\infty} \rho_v(x-x',0)R^*(t)\psi(x',t)\,\mathrm{d}x' \\ &+ 1 + r_3 \int_{-\infty}^{\infty} \rho_v(x-x',0)R(t)\Psi(x',t)\,\mathrm{d}x' - F(\rho_v) \end{aligned} \tag{39}$$

$$\rho_v(x,t) = \int_0^t \int_{-\infty}^{\infty} q_v(x-x',t-t')R^*(t')\Psi(x',t')\,\mathrm{d}x'\,\mathrm{d}t'. \tag{40}$$

Although the equations obtained are slightly more complex than those for the two previous cases, they can still be transformed to the Fourier–Laplace space in order to solve the problem.

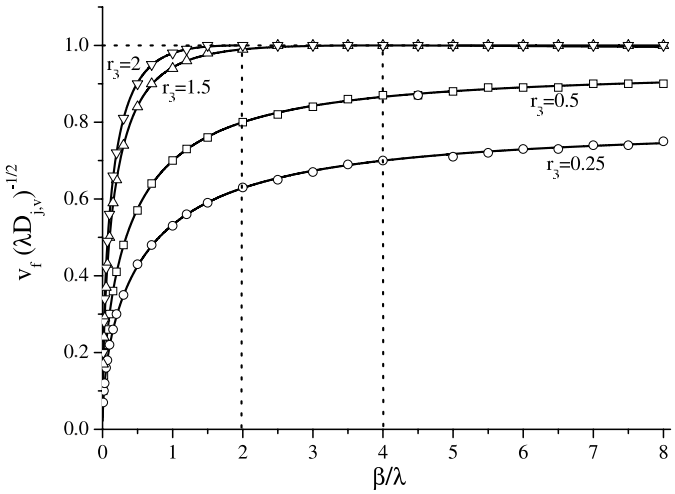

Figure 3. Comparison between the analytical expression for the velocity of traveling fronts in (43) (solid line) and the results from numerical integration of (41) and (42) (circles). Dotted lines indicate the transition points situated at $\beta/\lambda = 2/(r_3 - 1)$ for those cases where $r_3 > 1$. The values of the parameters used in the plot are the same as in figure 1 plus those indicated for r_3 in the legend.

For simplicity, we will consider that consecutive reaction events are uncorrelated, so we choose $R(t) = \beta\, \mathrm{e}^{-\beta t}$. It implies that we introduce a new characteristic rate β in the system.

For this specific case, the evolution equation for the density of particles in the real coordinates x, y can only be found if we obviate the effect of initial conditions. It means that we have to restrict ourselves to the asymptotic regime $t \to \infty$, where the effects of these initial conditions will be negligible. Using this approximation, we obtain from (37)–(38) and (39)–(40)

$$\frac{\partial^2 \rho}{\partial t^2} + [2\lambda + (1 - r_3)\,\beta]\,\frac{\partial \rho}{\partial t} = \lambda D_j \frac{\partial^2 \rho}{\partial x^2} + \beta r_3 (2\lambda + \beta)\rho - F(\rho) - \frac{\partial F(\rho)}{\partial t} \tag{41}$$

$$\frac{\partial^2 \rho_v}{\partial t^2} + [2\lambda + (1 - r_3)\,\beta]\,\frac{\partial \rho_v}{\partial t} = \lambda D_v \frac{\partial^2 \rho_v}{\partial x^2} + \beta r_3 (2\lambda + \beta)\rho_v - F(\rho_v) - \frac{\partial F(\rho_v)}{\partial t} \tag{42}$$

for DRWD and KD, respectively. By comparing (41) and (42), we observe that the equivalence between the DRWD and the KD holds as in case 1, albeit in this case we again have coupled effects between transport and reaction (because of the assumption of mutually exclusive waiting times). So that, we conclude that the existence of couplings between reaction and transport is a necessary (but not sufficient) condition for the breakdown of this equivalence.

Finally, we also show the result for the speed of traveling fronts, which reads in this case

$$v_f = \begin{cases} \sqrt{\lambda D_{j,v}} & \text{if} \quad \beta/\lambda < \frac{2}{r_3 - 1} \quad \text{and} \quad r_3 > 1 \\ 2\dfrac{\sqrt{r_3 \beta (2 + \beta/\lambda) D_{j,v}}}{2 + (1 + r_3)\beta/\lambda} & \text{otherwise.} \end{cases} \tag{43}$$

The plot of v_f as a function of the reaction parameter r_3 would be very similar to that shown in figure 1 for case 1. Instead, in order to stress the differences between the two cases we show in figure 3 the form of $v_f/\sqrt{\lambda D_{j,v}}$ as a function of the dimensionless parameter β/λ. There

it can be clearly seen that for $r_3 > 1$ there is a transition (at $\beta/\lambda = 2/(r_3 - 1)$, according to (43)) to the upper bound of the velocity, while for $r_3 < 1$ the velocity always increases asymptotically.

4. Conclusions

The works and discussions about the telegrapher's equation and the Maxwell–Cattaneo equation have extended for many years and they represent nowadays a classical topic in thermodynamics and transport theory. However, in this paper we have tried to show that there are still some aspects about these equations that are worth exploring. Specifically, we have tried to focus on the idea that different derivations of the telegrapher's equation correspond actually to different processes at a microscopic level. So that, we have tried to exploit these differences in order to see if the macroscopic equivalence between both cases breaks down in the presence of a growth (reaction) process. As a result of our analysis, some interesting conclusions can be mentioned.

(i) We have shown that in the context of the kinetic derivation and the delayed random walk derivation, the Maxwell–Cattaneo equation can be derived without imposing any constraints on the value of the characteristic relaxation time of the system, denoted by τ in (3). This is in contrast with previous works that seem to suggest that the Maxwell–Cattaneo equation is just an approximated result for small relaxation effects (i.e., τ small).

(ii) It is possible to derive a reaction-telegrapher equation where the equivalence between the kinetic derivation and the delayed random walk derivation breaks down. It can only occur in some situations (case 2 above) where transport and reaction are coupled, so that the microscopic differences in the transport dynamics are magnified by the effects of reaction.

(iii) The unbounded behavior of the front speed for the delayed random walk derivation (see figure 2) means that the finite propagation of signals imposed by the telegrapher's equation does not represent an upper bound for traveling fronts in that case. So, we have reported a case where the theoretical advantages of the telegrapher's equation, over the classical diffusion equation, are destroyed by the effect of an extra (reaction) process. Whether that situation reflects an unphysical behavior or not is still an open question.

(iv) We have also shown the different roles of the relaxation time on the reaction-telegrapher equations derived for cases 1–3. While the transition from a monotone front speed to a constant speed occur at a fixed value of the reaction parameter in case 1 (see equation (30)), the same transition does not exist in case 2 or only exists for a certain range of values in case 3. The fact that different microscopic implementations of the reaction process lead to a qualitatively different macroscopic behavior for traveling fronts makes evident the lack of universality in reaction–diffusion processes with relaxation effects. So, our work shows that the problem of how memory effects should be introduced in reaction–diffusion systems, which has been the focus of several recent works [26, 27], appears even in the case of the well-known telegrapher's equation.

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