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Non-Markovian random walks and nonlinear reactions: Subdiffusion and propagating fronts

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The main aim of the paper is to incorporate the nonlinear kinetic term into non-Markovian transport equations described by a continuous time random walk (CTRW) with nonexponential waiting time distributions. We consider three different CTRW models with reactions. We derive nonlinear Master equations for the mesoscopic density of reacting particles corresponding to CTRW with arbitrary jump and waiting time distributions. We apply these equations to the problem of front propagation in the reaction-transport systems with Kolmogorov-Petrovskii-Piskunov kinetics and anomalous diffusion. We have found an explicit expression for the speed of a propagating front in the case of subdiffusive transport.

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I. INTRODUCTION

This paper addresses the problem of the mesoscopic description of reaction-transport system of particles performing a continuous time random walk (CTRW) [1]. One of the main challenges is an implementation of the description of chemical reactions in non-Markovian transport processes governed by CTRW with nonexponential waiting time distributions. There exist several approaches and techniques to deal with this problem [2–11]. In particular, there are many efforts to incorporate the chemical reactions into subdiffusive transport. Different models lead to various fractional reaction-diffusion equations corresponding to kinetic regimes [12–20] and subdiffusion-limited reactions [21].

Our main objective here is to discuss how to incorporate the *nonlinear* kinetic term into *non-Markovian* transport equations which is still an open problem. We consider a one-component reaction-transport system consisting of independent particles X that follow CTRW. Let $\rho(x,t)$ represent the density of these particles at point x and time t. The main purpose is to derive the nonlinear Master equation for the density $\rho(x,t)$ in the following form:

$$\frac{\partial \rho}{\partial t} = L\rho, \tag{1}$$

where the nonlinear evolution operator L has to be determined. The challenge is to derive the Master equation for an arbitrary CTRW model coupled with nonlinear reaction. We assume that the chemical reaction follows the mass action law and the reaction term is of the form $r(\rho)\rho$. The density of other species participating in the reactions are held constant. It has been shown recently that for non-Markovian transport we cannot just add the term $r(\rho)\rho$ to the right-hand side of evolution Eq. (1) [12–16]. It is convenient to represent the nonlinear reaction rate $r(\rho)$ as the difference between the birth rate $r^{+}(\rho)$ and the death rate $r^{-}(\rho)$,

$$r(\rho) = r^{+}(\rho) - r^{-}(\rho). \tag{2}$$

As an illustration, let us consider the classical Schlögl first model [22],

$$A + X \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A + 2X, \quad X \overset{k_3}{\rightarrow} B, \tag{3}$$

where k_1, k_2, and k_3 are the reaction-rate constants. If we denote the densities of particles X and A by ρ and ρ_A respectively, then the birth and death rates are

$$r^{+}(\rho) = k_1\rho_A, \quad r^{-}(\rho) = k_3 + k_2\rho. \tag{4}$$

In what follows the density ρ_A of the catalyst A is assumed to be constant.

In what follows we consider three different non-Markovian models for reaction and transport processes. We apply these models to the problem of propagating fronts in reaction-transport systems with nonstandard diffusion [23,24] (see also a recent review [25]). The theory of subdiffusive propagation of a front is presented in [3,11,26–30], the superdiffusive propagation is studied in [31].

II. MODEL A

Non-Markovian behavior of particles performing CTRW occurs when diffusive particles get trapped for random times with nonexponential distribution. Let $\phi(t)$ and $w(z)$ denote the waiting time probability density function and the dispersal kernel respectively. For simplicity we consider the uncoupled case when jumps and waiting times are independent. If the distribution of waiting times is exponential: $\phi(t) = \lambda \exp(-\lambda t)$, the transport model is Markovian, and the difficulty of implementation of a nonlinear reaction term does not arise. In this case the Master Eq. (1) takes the form of the Kolmogorov-Feller equation with reaction

$$\frac{\partial \rho}{\partial t} = \lambda \int_{\mathbb{R}} \rho(x-z,t)w(z)dz - \lambda\rho + r(\rho)\rho \tag{5}$$

with a clear separation of the transport and reactive terms on the RHS [23]. In the non-Markovian case these terms are not additive [12,15–17]. The key question is how the chemical reaction influences the transport process. For model A, we assume that transport processes associated with CTRW and chemical reactions are independent. This case has been considered in the series of papers [12,13,15]. The main assumption here is that when particles are trapped, the waiting time is the same for all particles including newborn particles. One can think of biological applications when cells or bacteria are trapped in some confined region, say, at time $\tau < t$, they proliferate over the trapping (waiting) time $t-\tau$, and then they are released at time t. In particular, for the problem of virus infection and its propagation, the random waiting time occurs due to virus reproduction inside infected cells [32].

A. Conservation laws for particles

The first step in the derivation of non-Markovian Master Eq. (1) is to formulate the integral balance equations for the density $\rho(x,t)$ and the auxiliary density $j(x,t)$. The latter describes the number of particles arriving at point x *exactly* at time t (see, for example [10,12],). The balance equations for $\rho(x,t)$ and $j(x,t)$ can be written in the following form:

$$\rho(x,t) = \rho_0(x) e^{\int_0^t r(\rho(x,u))du} \Psi(t) + \int_0^t j(x,\tau) e^{\int_\tau^t r(\rho(x,u))du} \Psi(t-\tau) d\tau, \qquad (6)$$

$$j(x,t) = \int_{\mathbb{R}} \rho_0(x-z) e^{\int_0^t r(\rho(x,u))du} w(z)\phi(t)dz + \int_0^t \int_{\mathbb{R}} j(x-z,\tau) e^{\int_\tau^t r(\rho(x-z,u))du} w(z)\phi(t-\tau)dz d\tau. \qquad (7)$$

These equations represent the balance of particles due to nonlinear chemical reaction and transport process described by CTRW [1]. Equation (6) is the conservation law for particles' density $\rho(x,t)$ at point x at time t. The first term on the RHS of Eq. (6) represents the particles that stay at their initial position up to time t. Their density grows with the rate $r(\rho(x,t))$ during time interval $(0,t)$. The first term involves also the survival function $\Psi(t) = \int_t^\infty \phi(t)dt$ which is the probability that particles stay at their initial location up to time t. The second term gives the number of particles that arrive at point x at previous time $\tau < t$ and grow with rate $r(\rho)$ during time interval (τ,t) so that no jumps take place during this time interval. Note that the initial distribution of particles $\rho_0(x)$ is set up in such a way that a random walk for all particles starts at $t=0$ (no aging effects) [33]. Equation (6) is the conservation law for the particles that arrive at point x *exactly* at time t. The first term on the RHS of Eq. (7) represents the particles that are at the point $x-z$ at time $t=0$. Their density increases with the rate $r(\rho)$ during time interval $(0,t)$ and they jump to the point x at time t. The second term describes the particles that arrive at the point $x-z$ at some time $\tau < t$ and react up to time t at which the particles jump to position x. It should be noted that Eqs. (6) and (7) are mesoscopic mean-field equations. We neglect the internal fluctuations due to the finite number of particles. In general random fluctuations could modify the macroscopic behavior of the reaction-transport systems (see, for example, [34,35]).

B. Nonlinear Master equation

Let us now derive the evolution equation for the density $\rho(x,t)$. Since balance Eqs. (6) and (7) are nonlinear, we cannot apply directly the standard technique of Fourier-Laplace transforms. Instead, we differentiate the density $\rho(x,t)$ given by Eq. (6) with respect to time

$$\frac{\partial \rho}{\partial t} = j(x,t) + r(\rho)\rho - \rho_0(x) e^{\int_0^t r(\rho(x,u))du} \phi(t) - \int_0^t j(x,\tau) e^{\int_\tau^t r(\rho(x,u))du} \phi(t-\tau) d\tau. \qquad (8)$$

The last two terms can be interpreted as the density of particles that leave the point x exactly at time t,

$$i(x,t) = \rho_0(x) e^{\int_0^t r(\rho(x,u))du} \phi(t) + \int_0^t j(x,\tau) e^{\int_\tau^t r(\rho(x,u))du} \phi(t-\tau) d\tau. \qquad (9)$$

It follows from Eqs. (7) and (9) that

$$j(x,t) = \int_{\mathbb{R}} i(x-z,t) w(z) dz. \qquad (10)$$

Then Eq. (8) can be rewritten as

$$\frac{\partial \rho}{\partial t} = \int_{\mathbb{R}} i(x-z,t) w(z) dz - i(x,t) + r(\rho)\rho. \qquad (11)$$

This equation has a very simple meaning of a balance of particles at point x. The first term on the RHS gives the number of particles coming to x from different positions $x-z$, where the jump size z has the distribution $w(z)$. The second term gives the rate at which the particles leave the position x. The last term describes the growth of particles due to chemical reactions. In the linear case, a similar equation has been used [12,13]. The advantage of having this equation is that we do not need the Fourier transform to get the closed equation for the density $\rho(x,t)$. We can now find an expression for the density $i(x,t)$ in terms of $\rho(x,t)$. We divide Eqs. (6) and (9) by the factor $\exp(\int_0^t r(\rho(x,u))du)$ and take the Laplace transform of both equations

$$\mathcal{L}\{\rho(x,t) e^{-\int_0^t r(\rho(x,u))du}\} = [\rho_0(x) + \mathcal{L}\{j(x,t) e^{-\int_0^t r(\rho(x,u))du}\}] \tilde{\Psi}(s),$$

$$\mathcal{L}\{i(x,t) e^{-\int_0^t r(\rho(x,u))du}\} = [\rho_0(x) + \mathcal{L}\{j(x,t) e^{-\int_0^t r(\rho(x,u))du}\}] \tilde{\phi}(s),$$

where $\tilde{\Psi}(s) = \mathcal{L}\{\Psi(t)\}$ and $\tilde{\phi}(s) = \mathcal{L}\{\phi(t)\}$. From these equations, we obtain

$$\mathcal{L}\{i(x,t) e^{-\int_0^t r(\rho(x,u))du}\} = \frac{\tilde{\phi}(s)}{\tilde{\Psi}(s)} \mathcal{L}\{\rho(x,t) e^{-\int_0^t r(\rho(x,u))du}\}.$$

Inverse Laplace transform gives

$$i(x,t) = \int_0^t K(t-\tau) \rho(x,\tau) e^{\int_\tau^t r(\rho(x,u))du} d\tau, \qquad (12)$$

where $K(t)$ is the standard memory kernel defined by its Laplace transform

$$\tilde{K}(s) = \frac{\tilde{\phi}(s)}{\tilde{\Psi}(s)} = \frac{s\tilde{\phi}(s)}{1-\tilde{\phi}(s)}. \tag{13}$$

Substitution of Eq. (12) into Eq. (11) gives us the nonlinear Master equation

$$\frac{\partial \rho}{\partial t} = \int_0^t K(t-\tau)\left[\int_{\mathbb{R}} \rho(x-z,\tau)e^{\int_\tau^t r(\rho(x-z,u))du}w(z)dz - \rho(x,\tau)e^{\int_\tau^t r(\rho(x,u))du}\right]d\tau + r(\rho)\rho. \tag{14}$$

This nonlinear equation is the main result of this paper. For some particular cases, it can be reduced to known equations in the literature. For example, when the reaction rate $r(\rho) = r = \text{constant}$, Eq. (14) takes the form

$$\frac{\partial \rho}{\partial t} = \int_0^t K(t-\tau)e^{r(t-\tau)}\left[\int_{\mathbb{R}} \rho(x-z,\tau)w(z)dz - \rho(x,\tau)\right]d\tau + r\rho, \tag{15}$$

and this model with constant rate r has been formulated in [15]. Since the effective memory kernel $K(t-\tau)e^{r(t-\tau)}$ depends on the reaction rate, it is tempting to conclude that this equation describes the coupling of chemical reaction and transport. We believe that this conclusion is misleading. In fact this equation describes the complete decoupling of transport with memory effects and linear reaction. To show this, let us make a substitution

$$\rho(x,t) = n(x,t)e^{rt}. \tag{16}$$

Then we obtain the Master equation for $n(x,t)$,

$$\frac{\partial n}{\partial t} = \int_0^t K(t-\tau)\left[\int_{\mathbb{R}} n(x-z,\tau)w(z)dz - n(x,\tau)\right]d\tau \tag{17}$$

which is independent of the reaction and describes the transport of passive particles. So we have a complete decoupling in which the density $\rho(x,t)$ is the product of the density of passive particles $n(x,t)$ and the exponential factor e^{rt} due to the chemical reaction.

C. Subdiffusive transport

Now consider slow anomalous diffusion for which the waiting time probability density function (pdf) $\phi(t)$ has a power-law tail: $\phi(t) \sim (\tau_0/t)^{1+\gamma}$ with $0<\gamma<1$ as $t\to\infty$. Clearly, the first moment $\int_0^\infty t\phi(t)dt$ is divergent for $0<\gamma<1$. As a result, the mean-square displacement $\langle x^2\rangle$ depends on time t as t^γ [1]. Here we use the following expression for the survival probability:

$$\Psi(t) = E_\gamma\left[-\left(\frac{t}{\tau_0}\right)^\gamma\right], \quad 0<\gamma<1, \tag{18}$$

where $E_\gamma[x] = \Sigma_0^\infty x^n/\Gamma(\gamma n+1)$ is the Mittag-Leffler function. The waiting time pdf $\phi(t) = -\frac{d}{dt}E_\gamma[-(\frac{t}{\tau_0})^\gamma]$ has singular behavior $t^{\gamma-1}$ as $t\to 0$. The Laplace transforms of $\Psi(t)$ and $\phi(t)$ are

$$\tilde{\Psi}(s) = \frac{\tau_0(s\tau_0)^{\gamma-1}}{1+(s\tau_0)^\gamma}, \quad \tilde{\phi}(s) = \frac{1}{1+(s\tau_0)^\gamma}. \tag{19}$$

The advantage of using the Mittag-Leffler function is that we can find the fractional reaction-transport equation without passing to the long-time large-distance limit. We find from Eq. (13) that the Laplace transform of the memory kernel is

$$\tilde{K}(s) = \frac{s^{1-\gamma}}{\tau_0^\gamma}. \tag{20}$$

Equation (14) takes the form of a nonlinear fractional equation

$$\frac{\partial \rho}{\partial t} = \frac{e^{\int_0^t r(\rho(x-z,u))du}}{\tau_0^\gamma}D_t^{1-\gamma}\left(\int_{\mathbb{R}} \rho(x-z,t)e^{-\int_0^t r(\rho(x-z,u))du}w(z)dz\right) - \frac{e^{\int_0^t r(\rho(x,u))du}}{\tau_0^\gamma}D_t^{1-\gamma}\left(\rho(x,t)e^{-\int_0^t r(\rho(x,u))du}\right) + r(\rho)\rho, \tag{21}$$

where $D_t^{1-\gamma}$ is the Riemann-Liouville fractional derivative defined as

$$D_t^{1-\gamma}\rho(x,t) = \frac{1}{\Gamma(1-\gamma)}\frac{\partial}{\partial t}\int_0^t \frac{\rho(x,\tau)d\tau}{(t-\tau)^\gamma}.$$

Now assume that the dispersal kernel $w(z)$ is an even and rapidly decaying function for large z. We expand the expression in the brackets [Eq. (14)] for small z and truncate the Taylor series at the second moment. We obtain

$$\frac{\partial \rho}{\partial t} = \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2}\int_0^t K(t-\tau)\rho(x,\tau)e^{\int_\tau^t r(\rho(x,u))du}d\tau + r(\rho)\rho, \tag{22}$$

where $\sigma^2 = \int_{\mathbb{R}} z^2 w(z)dz$. Note that a similar nonlinear equation has been derived in [16,18].

By using Laplace transform (20) and Eq. (22), we obtain the nonlinear reaction-subdiffusion equation,

$$\frac{\partial \rho}{\partial t} = D(\gamma)e^{\int_0^t r(\rho(x,u))du}D_t^{1-\gamma}\frac{\partial^2}{\partial x^2}\rho(x,t)e^{-\int_0^t r(\rho(x,u))du} + r(\rho)\rho, \tag{23}$$

where $D(\gamma) = \sigma^2/2\tau_0^\gamma$ is the anomalous diffusivity.

III. MODEL B

Model B deals with the case when the transport process described by CTRW depends on the chemical reaction. This model was considered by Vlad and Ross [2]. They introduced the notion of the age of the particle as the transition time between two successive jumps. The particles have zero age when they just arrive at some point x from which they will jump later. The main assumption for model B is that the newborn particles produced with the rate $r^+(\rho)\rho$ have zero age. In other words, when a new particle is born, it is given a new waiting time for a jump (zero age). The density $j(x,t)$ for model B can be interpreted as a zero-age density of particles arriving at the point x exactly at time t. The particles arrive at the point x because of the jumps in space and a birth process with the rate $r^{+}(\rho)$. Since the nonlinear reaction rate $r(\rho)$ is the difference between the birth rate $r^{+}(\rho)$ and the death rate $r^{-}(\rho)$, the balance equations for the densities $j(x,t)$ and $\rho(x,t)$ can be written as

$$\rho(x,t)=\rho_0(x)e^{-\int_0^t r^{-}(\rho(x,u))du}\Psi(t) + \int_0^t j(x,\tau)e^{-\int_\tau^t r^{-}(\rho(x,u))du}\Psi(t-\tau)d\tau \tag{24}$$

and

$$j(x,t)=r^{+}(\rho)\rho+\int_{\mathbb{R}}\rho_0(x-z)e^{-\int_0^t r^{-}(\rho(x,u))du}w(z)\phi(t)dz + \int_0^t\int_{\mathbb{R}} j(x-z,\tau)e^{-\int_\tau^t r^{-}(\rho(x,u))du}w(z)\phi(t-\tau)dzd\tau. \tag{25}$$

This system of equations has been derived in [2,16]. The authors employed the Markov model with age-dependent density $\xi(x,t,\tau)$ such that $\rho(x,t)=\int_0^\infty \xi(x,t,\tau)d\tau$. Of course, Eqs. (24) and (25) can be formulated directly as the balance equations without introduction of $\xi(x,t,\tau)$. Equation (24) is the conservation law for the particles at point x at time t. Equation (25) describes the situation when the particles with zero age at point x are either produced with a rate $r^{+}(\rho)$ or arrive at point x from other positions. By using the method developed for model A, one can derive the nonlinear Master equation for the density $\rho(x,t)$

$$\frac{\partial\rho}{\partial t}=\int_0^t K(t-\tau)\left[\int_{\mathbb{R}}\rho(x-z,\tau)e^{-\int_\tau^t r^{-}(\rho(x-z,u))du}w(z)dz - \rho(x,\tau)e^{-\int_\tau^t r^{-}(\rho(x,u))du}\right]d\tau + r^{+}(\rho)\rho - r^{-}(\rho)\rho. \tag{26}$$

Note that Vlad and Ross stated that the balance Eqs. (24) and (25) could not be reduced to a nonlinear Master equation as Eq. (26) due to the nonlinear term $\exp(-\int_\tau^t r^{-}(\rho(x-z,u))du)$ [2]. However, Yadav and Horsthemke managed to overcome this difficulty by using the large-spatial scale and long-time limits [16]. They used the standard asymptotics for the Fourier transform of jump density $w(k)=1-\sigma^2k^2+o(k^2)$ and neglected the initial conditions in the long-time limit. If we expand $\rho(x-z,\tau)$ in Eq. (26) for small z, then we obtain the equation derived in [16]

$$\frac{\partial\rho}{\partial t}=\frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2}\int_0^t K(t-\tau)\rho(x,\tau)e^{-\int_\tau^t r^{-}(\rho(x,u))du}d\tau + r^{+}(\rho)\rho - r^{-}(\rho)\rho. \tag{27}$$

Thus, the Master Eq. (26) can be considered as the generalization of Eq. (27) derived in [16] for the arbitrary jump distribution $w(z)$.

The essence of the model B and the main difference with model A is that it describes the situation when the newborn particles are given the new waiting time for a jump. One can think of a situation in which the trapping mechanism has been induced by chemical binding of newborn molecules. In this case we have to take into account the aging effects. Of course, we should make a clear distinction between the age of a jump event and the age of a particle from $t=0$. The latter effect is not considered in this paper.

IV. MODEL C

This model corresponds to the phenomenological generalization of the CTRW model for the case when the chemical reaction is taken into account. We can incorporate the local growth rate of diffusing particles by adding a term $\int_0^t r^{+}(\rho(x,t-\tau))\rho(x,t-\tau)\Psi(\tau)d\tau$ to the balance equation for the density of particles. We write

$$\rho(x,t)=\rho(x,0)\Psi(t)+\int_0^t\int_{\mathbb{R}}\rho(x-z,t-\tau)w(z)\phi(\tau)dzd\tau + \int_0^t r^{+}(\rho(x,t-\tau))\rho(x,t-\tau)\Psi(\tau)d\tau. \tag{28}$$

This equation has been used in [3,4] as a starting point. Henry *et al.* modified it in [15] and pointed out that the model C is not justified at the mesoscopic level and what is more its interpretation is not clear. The purpose of this section is to show that model C has a very natural physical interpretation.

Here we assume that the reaction is a pure birth process: $r^{+}(\rho)$, and $j(x,t)$ is a zero-age density of particles arriving at the point x exactly at time t. The balance equations are

$$\rho(x,t)=\rho_0(x)\Psi(t)+\int_0^t j(x,t-\tau)\Psi(\tau)d\tau \tag{29}$$

and

$$j(x,t)=r^{+}(\rho)\rho+\int_{\mathbb{R}}\rho_0(x-z)w(z)\phi(t)dz + \int_0^t\int_{\mathbb{R}} j(x-z,t-\tau)w(z)\phi(\tau)dzd\tau. \tag{30}$$

These equations do not involve nonlinear terms inside the integrals. Therefore, the standard technique of Fourier-Laplace transforms can be employed to reduce two balance Eqs. (29) and (30) to a single equation for $\rho(x,t)$. It turns out that this equation can be written as a phenomenological balance Eq. (28). So Eq. (28) corresponds to a mesoscopic situation when the newborn particles are given a new waiting time for a jump. Note that it has been found [15] that we cannot use balance Eq. (28) with negative reaction term, since it leads to the negative density for the subdiffusive transport. Of course, model C is just a particular case of model B when the death rate $r^{-}(\rho)=0$.

From Eq. (28) one can obtain the Master equation for the density $\rho(x,t)$ in the following form:

$$\frac{\partial\rho}{\partial t}=\int_0^t K(t-\tau)\left[\int_{\mathbb{R}}\rho(x-z,\tau)w(z)dz-\rho(x,\tau)\right]d\tau + r^{+}(\rho)\rho$$

in which the transport term does not directly depend on the chemical reaction as in models A and B.

V. SPEED OF TRAVELING WAVES

In this section we address the problem of wave-front propagation for model A. We assume that the reaction rate $r(\rho)$ is of the Kolmogorov-Petrovskii-Piskunov (KPP) type [10,36],

$$\max_{0\leq\rho\leq 1} r(\rho) = r(0) > 0, \quad r(1) = 0. \tag{31}$$

Note that the standard logistic growth corresponds to $r(\rho) = 1-\rho$ [37]. We start with the nonlinear Master equation for the density $\rho(x,t)$,

$$\frac{\partial\rho}{\partial t} = \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2}\int_0^t K(t-\tau)\rho(x,\tau)e^{\int_\tau^t r(\rho(x,u))du}d\tau + r(\rho)\rho \tag{32}$$

with an initial condition in the form of a step function

$$\rho(x,0) = \theta(x), \tag{33}$$

where $\theta(x)=1$ for $x\leq 0$ and $\theta(x)=0$ for $x>0$. This condition describes the initial segregation of an unstable state ($\rho=0$) for $x>0$ and a stable state ($\rho=1$) for $x\leq 0$.

The purpose is to find the traveling-wave solution $\rho(x,t) = f(x-vt)$ of the initial value problem [Eqs. (32) and (33)]. Here v is the speed at which the wave profile f invades the unstable state with $\rho=0$. When the memory kernel $K(t-\tau) = \tau_0^{-1}\delta(t-\tau)$, then Eq. (32) becomes the KPP equation (Fisher equation)

$$\frac{\partial\rho}{\partial t} = D\frac{\partial^2\rho}{\partial x^2} + r(\rho)\rho \tag{34}$$

with the diffusion coefficient $D=\sigma^2/2\tau_0$. This case corresponds to the exponential waiting time pdf $\phi(t) = \lambda\exp(-\lambda t)$ with $\lambda=\tau_0^{-1}$. It is well known [37] that the minimal propagation speed v for Eq. (34) is $2\sqrt{Dr(0)}$.

To find the propagation rate for the non-Markovian initial value problem [Eqs. (32) and (33)], we use the Hamilton-Jacobi approach [23,36]. The starting point is to apply hyperbolic scaling $x\to x/\varepsilon$, $t\to t/\varepsilon$ with $\varepsilon\to 0$ which corresponds to the long-time large-distance behavior of the traveling wave. When the scaling parameter $\varepsilon\to 0$, the rescaled density $\rho^\varepsilon(x,t)=\rho(x/\varepsilon,t/\varepsilon)$ can take only two values 0 and 1 everywhere except in the narrow front region where the transport and reaction terms are balanced. In another words, the wave profile $f((x-vt)/\varepsilon)$ tends to a unit step function $\theta(x-vt)$. The aim is to find the location of the front and rate at which it moves.

We introduce the action functional G^ε as

$$\rho^\varepsilon(x,t) = \exp\left[-\frac{G^\varepsilon(x,t)}{\varepsilon}\right]. \tag{35}$$

It follows from Eq. (35) that if the function $G(x,t) = \lim_{\varepsilon\to 0} G^\varepsilon(x,t)$ is positive, the rescaled density $\rho^\varepsilon(x,t)\to 0$ as $\varepsilon\to 0$. The boundary of the set $G(x,t)>0$ can be regarded as the reaction front [23,36]. Then, the front position $x(t)$ can be determined by the equation $G(x(t),t)=0$. Since we are interested in the leading edge of the traveling wave ($\rho^\varepsilon\approx 0$), we write the equation for the rescaled density in the linear form

$$\frac{\partial\rho^\varepsilon}{\partial t} = \frac{\varepsilon\sigma^2}{2}\frac{\partial^2}{\partial x^2}\int_0^{t/\varepsilon} K(\tau)e^{r(0)\tau}\rho^\varepsilon(x,t-\varepsilon\tau)d\tau + \frac{r(0)\rho^\varepsilon}{\varepsilon}. \tag{36}$$

Substituting Eq. (35) into Eq. (36) and taking the limit $\varepsilon\to 0$, we obtain

$$\frac{\partial G}{\partial t} + \frac{\sigma^2}{2}\left(\frac{\partial G}{\partial x}\right)^2\int_0^\infty K(\tau)e^{r(0)\tau}e^{\tau(\partial G/\partial t)}d\tau + r(0) = 0. \tag{37}$$

This is the Hamilton-Jacobi equation for the action functional $G(x,t)$ (see [3,23,28]). If we introduce the Hamiltonian $H=-\frac{\partial G}{\partial t}$ and the generalized momentum $p=\frac{\partial G}{\partial x}$, then Eq. (37) can be written as

$$H + \tilde{K}(H-r(0))\frac{\sigma^2p^2}{2} - r(0) = 0, \tag{38}$$

where $\tilde{K}(s)$ is the Laplace transform of the memory kernel $K(t)$. This equation is different from the analogous one in [3,28].

The propagation rate v can be found from [23]

$$v = \frac{\partial H}{\partial p} = \frac{H}{p}. \tag{39}$$

Solving quadratic Eq. (38) for p, we obtain from Eq. (39) that

$$v = H^*\sigma\sqrt{\frac{\tilde{K}(H^*-r(0))}{2H^*-2r(0)}}, \tag{40}$$

where H^* is the solution of

$$\frac{\partial}{\partial H}\left(\frac{(H-r(0))}{\tilde{K}(H-r(0))}\right) = \frac{2(H-r(0))}{H\tilde{K}(H-r(0))}. \tag{41}$$

Front propagation rate for subdiffusive transport

Let us consider the reaction-subdiffusion case for which the Laplace transform of the waiting time pdf $\phi(t)$ is

$$\tilde{\phi}(s) = \frac{1}{1+(s\tau_0)^\gamma}, \quad 0<\gamma<1$$

and the Laplace transform of the memory kernel is given by Eq. (20). Then Eq. (41) has the solution $H^*=2r(0)/(2-\gamma)$. Substitution of this solution into Eq. (40) gives the propagation rate v corresponding to Master Eq. (32) with initial condition (33). We introduce the following notations for the propagation speeds: v_A for model A; v_B and v_C for model B and model C respectively. The minimal propagation speed v_A for model A with Eqs. (32) and (33) is

$$v_A = \sqrt{\frac{2r(0)^{2-\gamma}\sigma^2}{\tau_0^\gamma(2-\gamma)^{2-\gamma}\gamma^\gamma}}. \tag{42}$$

For simplicity, we consider the case when the death rate $r^-(\rho)$ obeys $r^-(0)=0$. For Schlögl first model (3), it means that $k_3=0$ [see Eq. (4)]. Then for model B and model C we have [3,28]

$$v_B=v_C=\sqrt{\frac{r(0)^{2-\gamma}\sigma^2(3-\gamma)^{3-\gamma}}{2\tau_0^{\gamma}(2-\gamma)^{2-\gamma}}}. \tag{43}$$

The case $k_3\neq 0$ was considered in [28].

For $\gamma=1$, we have the classical result $v=2\sqrt{Dr(0)}$ with $D=\sigma^2/2\tau_0$ that corresponds to the KPP equation (Fisher equation) [Eq. (34)]. For $0<\gamma<1$, the propagation speed v_B is greater than v_A. This is because the newborn particles in model B and model C are given new waiting times for the jump event. As a result the overall transport process and the propagation rate for model A are slower than those of model B and model C. It is also interesting to compare our results with those obtained in [29]. The authors considered the irreversible autocatalytic reaction $A+X\rightarrow 2X$ with subdiffusion. They found that the minimal propagation is zero. This finding seems to contradict with our result of finite speed propagation (42). In fact, model A and the subdiffusion-reaction model studied in [29] are different. In our model we keep the concentration of one of the component constant, while Froemberg *et al.* considered two-component system of equations for which both reactants A and X vary in space and time. For example, in our paper the density ρ_A of the catalyst A in Eq. (3) is assumed to be constant.

VI. CONCLUSIONS

In this paper we have given a mesoscopic description of a reaction-transport system of particles performing a continuous time random walk (CTRW) with nonexponential waiting time distributions. Our main objective has been to implement a *nonlinear* kinetic term into *non-Markovian* transport equations. We have considered three different CTRW models with reactions which have been discussed in the literature. We have derived nonlinear Master Eqs. (14) and (26) for the mesoscopic density of reacting particles corresponding to CTRW with arbitrary jump and waiting time distributions. We have applied the theory to the problem of front propagation in reaction-transport systems with KPP kinetics and non-Markovian diffusion. We have found an explicit expression for the speed of the propagating front in the case of subdiffusion transport.

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