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Persistent random walk with exclusion

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Abstract. Modelling the propagation of a pulse in a dense *milieu* poses fundamental challenges at the theoretical and applied levels. To this aim, in this paper we generalize the telegraph equation to non-ideal conditions by extending the concept of persistent random walk to account for spatial exclusion effects. This is achieved by introducing an explicit constraint in the hopping rates, that weights the occupancy of the target sites. We derive the mean-field equations, which display nonlinear terms that are important at high density. We compute the evolution of the mean square displacement (MSD) for pulses belonging to a specific class of spatially symmetric initial conditions. The MSD still displays a transition from ballistic to diffusive behaviour. We derive an analytical formula for the effective velocity of the ballistic stage, which is shown to depend in a nontrivial fashion upon both the *density* (area) and the *shape* of the initial pulse. After a density-dependent crossover time, nonlinear terms become negligible and normal diffusive behaviour is recovered at long times.

1 Introduction

Random walks (RW) are widely studied stochastic processes with a wealth of different applications in many fields [1,2]. The persistent random walk (PRW) identifies a special class of RWs, where agents also have a bias to keep hopping in the same direction as they did in the past (with finite memory). While the continuum limit of standard RWs is the diffusion equation, yielding infinite propagation velocity, the continuum limit of the PRW is the so-called telegraph equation, which displays a transition from ballistic to diffusive transport at a characteristic time. The telegraph equation is also obtained from the so-called dichotomous (or sometimes also called *telegraph*) noise (random switches between two states) when the distribution of switching times is exponential and the process is drift-less [3].

The telegraph equation was first studied by Lord Kelvin, who was interested in the distortion and dissipation of electromagnetic waves in telegraph lines, motivated by the design of the first transatlantic cable [4], while PRW and its connection with the telegraph equation were first studied by Goldstein in 1951 [5]. The telegraph equation is notoriously used in many contexts, from transport of relativistic particles [6,7] in different *milieux*, such as in multiply scattering media [8], to second sound in liquid helium II and inertial effects in heat transport [9,10]. An interesting discussion of many applications of the telegraph equation can be found in a recent review by Weiss [11].

Macroscopic transport equations can be derived in a straightforward manner from *microscopic* stochastic processes, the diffusion equation being the classical text-book example. In one dimension, for example, if $P_i(n)$ denotes the probability that an agent is at site i on some discrete manifold at time $n\Delta t$, a simple unbiased RW corresponds to the update rule

$$P_i(n) = \frac{1}{2}[P_{i-1}(n-1) + P_{i+1}(n-1)] \qquad (1)$$

as it is assumed that at each time step the walker can either jump to its right or to its left with equal probability. Letting the lattice spacing a and the time step Δt go to zero, such that $\lim_{a,\Delta t\to 0}(a^2/\Delta t) = D$, one obtains the diffusion equation $\partial P(x,t)/\partial t = D\,\partial^2 P(x,t)/\partial x^2$. Of course, in performing the continuum limit one is tacitly assuming that many walkers are performing as many uncorrelated random walks and that a probability of being at x at time t can be defined by averaging over such uncorrelated trajectories. This requires the walkers to be transparent to each other. It is then interesting to ask the following question. If some exclusion rule is enforced, such that a walker can only jump on an *empty* site, how will the macroscopic equations be modified? And what kind of process will they describe? The macroscopic counterpart of this problem implies transport in a non-ideal *milieu*,

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e.g., a dense fluid or a complex scattering medium. Examples from optics include pulse diffusion in whole blood and in a dense distribution of particulate matter in the atmosphere and the ocean. Indeed it has been shown that the telegraph equation can be derived as an approximation to a physically more realistic transport equation [12].

Microscopic jump processes that implement exclusion rules go under the name of simple exclusion processes (SEP). In general, SEPs are space-discrete, agent-based stochastic processes modeling some kind of transport according to specific rules and bound to the constraint that no two agents can ever occupy the same site. SEPs play a central role in non-equilibrium statistical physics [13,14]. While the first theoretical ideas underlying such processes can be traced back to Boltzmann's works [15], SEPs were introduced and widely studied in the 70s as simplified models of one-dimensional transport for phenomena like hopping conductivity [16] and kinetics of biopolymerization [5]. Along the same lines, the asymmetric exclusion process (ASEP), originally introduced by Spitzer [17], and the associated macroscopic mean-field equations [18] have become a paradigm in non-equilibrium statistical physics [19–21] and have now found many applications, e.g. to the study of molecular motors [22], transport through nano-channels [23] and dynamics of microtubule depolymerization [24].

Starting from this setting, we shall here generalize the concept of persistent random walk to cases of interest where exclusion effects are to be accounted for. More precisely, we will introduce a modified PRW featuring an explicit constraint in the hopping probabilities, that are now gauged by the occupancy of the target sites. We will proceed on to deriving the mean-field equations for the concentration. These will be shown to display nonlinear terms, that prove however negligible in the diluted limit. Working at high densities, excluded-volume corrections do matter, as we shall here substantiate both analytically and numerically.

The paper is organized as follows. In Section 2 we introduce the persistent simple exclusion process (PSEP) and derive the mean-field equations for the continuum densities. In Section 3 we characterize the evolution of the mean square displacement for a pulse belonging to a specific class of spatially symmetric initial conditions. Interestingly, as a result of the excluded-volume constraint, the ballistic-to-diffusive transition becomes dependent on the density. Moreover, the effective velocity that characterizes the ballistic stage becomes a function of the crowding level too, but also turns out to depend on the *shape* of the initial pulse. Finally, in Section 4 we summarize our results and sketch possible interesting directions along which to pursue this work.

2 The persistent simple exclusion process (PSEP)

Let us consider a bunch of N walkers on a one-dimensional lattice with spacing d and length L. According to the definition of persistent random walk [5], at regular intervals Δt a walker can jump in the same direction as it did at the previous step with probability p or invert its direction with probability q. We take $q = 1 - p$, which amounts to assuming that there is no leakage [5] in the system. Let us denote with $a_i(n)$ the probability that a walker is at site i at time $n\Delta t$ having been at site $i-1$ at time $(n-1)\Delta t$ (right-bound flow) and with $b_i(n)$ the probability that a walker is at site i at time $n\Delta t$ having been at site $i+1$ at time $(n-1)\Delta t$ (left-bound flow). If walkers are invisible to each other, the following relations hold:

$$a_i(n) = p\, a_{i-1}(n-1) + q\, b_{i-1}(n-1) \tag{2}$$
$$b_i(n) = p\, b_{i+1}(n-1) + q\, a_{i+1}(n-1). \tag{3}$$

The above equations describe a discrete stochastic process. The continuum limit can be obtained by introducing the continuous probability density $P(x,t) = \langle P_i(n)\rangle \equiv \langle a_i(n) + b_i(n)\rangle$, where $\langle \dots \rangle$ denotes an average over the trajectories of many agents, by letting $d \to 0$, $\Delta t \to 0$, $q \to 0$. By doing this, it is known that one gets the telegraph equation [11]

$$\frac{\partial^2 P}{\partial t^2} + 2r\frac{\partial P}{\partial t} = v^2 \frac{\partial P}{\partial x} \tag{4}$$

with

$$\lim_{d,\Delta t\to 0} \frac{p}{\Delta t} = v \qquad \lim_{q,\Delta t\to 0} \frac{q}{\Delta t} = r. \tag{5}$$

In this paper we wish to study how the persistent random walk is modified if we introduce the constraint that no two walkers can occupy the same site at the same time. That is, the probability to jump to a given site is gauged by the current occupancy of that site. Along the same line of reasoning of SEPs and ASEPs, we modify equations (2) and (3) in the following way:

$$\begin{aligned} a_i(n) - a_i(n-1) = {} & [p\, a_{i-1}(n-1) + q\, b_{i-1}(n-1)] \\ & \times [1 - P_i(n)] - a_i(n-1) \\ & \times \Big\{ p[1 - P_{i+1}(n-1)] \\ & + q[1 - P_{i-1}(n-1)](TM) \Big\} \end{aligned} \tag{6}$$

$$\begin{aligned} b_i(n) - b_i(n-1) = {} & [p\, b_{i+1}(n-1) + q\, a_{i+1}(n-1)] \\ & \times [1 - P_i(n)] - b_i(n-1) \\ & \times \Big\{ p[1 - P_{i-1}(n-1)] \\ & + q[1 - P_{i+1}(n-1)] \Big\} \end{aligned} \tag{7}$$

where $P_i(n) = a_i(n) + b_i(n)$. Again, the idea is to gauge jump probabilities by the occupancy of the target sites. For example, the first term in the r.h.s of equation (6) states that a net increase of the probability at site i associated with the right-bound flow is only possible with a transition rate proportional to the amount of *free room* at site i, i.e., $1 - P_i$. If all walkers happen to be at site i at the same time, then $P_i = 1$ and no further increase of a_i nor of b_i is possible.

It is interesting to observe here a rather surprising fact. From the above discussion, one may think that a modified diffusion equation including finite-density effects could be derived through occupancy-gauged hopping rules such as those appearing in equations (6) and (7) from a standard random walk without drift (Eq. (1)). However, as first noticed by Richards in 1977 [16], nonlinear terms cancel exactly in doing this, and one is left with the standard diffusion equation in the continuum limit.

In order to take the continuum limit, we first divide equations (6) and (7) by Δt and substitute $q = 1 - p$. Then, recalling the definitions (5), we get

$$\begin{aligned} \frac{\partial a}{\partial t} + v\frac{\partial}{\partial x}[a(1-P)] &= -rJ(1-P) \\ \frac{\partial b}{\partial t} - v\frac{\partial}{\partial x}[b(1-P)] &= rJ(1-P) \end{aligned} \quad (8)$$

where $P(x,t) = a(x,t) + b(x,t)$ and $J(x,t) = a(x,t) - b(x,t)$.

For the sake of the argument, let us consider the propagation of pulses in a fluid, i.e. travelling density fluctuations. Equations (8) contain the single-particle probability field P, which is a number between zero and one. The value $P = 1$ should then correspond to the maximum density allowed in the system. Thus, more *physical* equations can be obtained by introducing the agent densities

$$\rho(x,t) \equiv \rho_{\scriptscriptstyle M} P(x,t) \quad (9)$$
$$\mathcal{J}(x,t) \equiv \rho_{\scriptscriptstyle M} J(x,t) \quad (10)$$
$$\rho_+(x,t) = \rho_{\scriptscriptstyle M} a(x,t) \quad (11)$$
$$\rho_-(x,t) = \rho_{\scriptscriptstyle M} b(x,t) \quad (12)$$

where $\rho_{\scriptscriptstyle M}$ is the maximum allowed density, which in principle could be regarded as a parameter of the model. If we imagine that the agents have a finite size σ, i.e. we regard them as hard rods[1], one simply have $\rho_{\scriptscriptstyle M} = 1/\sigma$. Introducing the density $\rho_{\scriptscriptstyle M}$, equations (8) become

$$\begin{aligned} \frac{\partial \rho_+}{\partial t} + v\frac{\partial}{\partial x}\left[\rho_+\left(1-\frac{\rho}{\rho_{\scriptscriptstyle M}}\right)\right] &= -r\mathcal{J}\left(1-\frac{\rho}{\rho_{\scriptscriptstyle M}}\right) \\ \frac{\partial \rho_-}{\partial t} - v\frac{\partial}{\partial x}\left[\rho_-\left(1-\frac{\rho}{\rho_{\scriptscriptstyle M}}\right)\right] &= r\mathcal{J}\left(1-\frac{\rho}{\rho_{\scriptscriptstyle M}}\right). \end{aligned} \quad (13)$$

A system of equations for the densities $\rho(x,t)$ and $\mathcal{J}(x,t)$ can be obtained by adding and subtracting the two equations (13):

$$\begin{aligned} \frac{\partial \rho}{\partial t} + v\frac{\partial}{\partial x}\left[\mathcal{J}\left(1-\frac{\rho}{\rho_M}\right)\right] &= 0 \\ \frac{\partial \mathcal{J}}{\partial t} + v\frac{\partial}{\partial x}\left[\rho\left(1-\frac{\rho}{\rho_M}\right)\right] &= -2r\mathcal{J}\left(1-\frac{\rho}{\rho_M}\right). \end{aligned} \quad (14)$$

[1] It should be emphasized that it is in principle possible to write mean-field equations for an exclusion process that accounts for *extended* objects on a line from the beginning. In reference [25] the authors derive a modified diffusion-advection equation from a microscopic exclusion process (RW with drift) for hard rods. However, even if it would be intriguing to do so, it is rather unclear how to apply the same technique in the context of the PRW.

As a general remark, we see that the microscopic exclusion constraint results in the appearance of nonlinear terms. The standard evolution of the PRW leading to the telegraph equation is obtained in the *dilute* limit $\rho \ll \rho_M$. Conversely, we may consider the full system (14) as describing transport in a *crowded* medium. More precisely, the nonlinear equations (14) embody the microscopic excluded-volume constraint that emerges at high densities.

3 Mean square displacement

We turn now to analyzing how the excluded-volume constraint affects the propagation in an infinite medium of an initially localized pulse. It is well known that the PRW displays a transition from ballistic to diffusive transport, as exemplified by the mean square displacement (MSD),

$$\mu_2(t) \equiv \frac{1}{\mathcal{N}}\left[\left\langle x^2(t)\right\rangle_\rho - \left\langle x(t)\right\rangle_\rho^2\right] \quad (15)$$

with $\langle x^m(t)\rangle_\rho = \int x^m \rho(x,t)\,dx$ and $\mathcal{N} = \int \rho(x,t)\,dx$. As it is customarily done, we shall here restrict to a class of symmetric initial pulses, namely such that $\rho(x,t=0) = \rho(-x,t=0)$, $\mathcal{J}(x,t=0) = 0$, meaning that the initial distribution of the right-headed agents is equal to that of the left-headed ones. In this case, it is straightforward to show that $\langle x(t)\rangle \equiv 0\ \forall t$.

For the PRW one has

$$\begin{aligned} \mu_2(t) - \mu_2(0) &= \frac{v^2}{2r^2}(2rt - 1 + e^{-2rt}) \\ &\simeq \begin{cases} v^2t^2 & \text{for} \quad t \ll 1/2r \\ \left(\frac{v^2}{r}\right)t & \text{for} \quad t \gg 1/2r. \end{cases} \end{aligned} \quad (16)$$

When excluded-volume effects are important, it appears impossible to obtain a closed expression for $\mu_2(t)$. However, one can still capture the asymptotic regime at short times for a certain class of symmetric initial conditions in an infinite medium (see Ref. [4] for a critical discussion of reflecting and absorbing boundary conditions for the telegraph equation in a bounded domain). Let us consider the Taylor expansion of $\mu_2(t)$

$$\mu_2(t) = \mu_2(0) + \mu_2'(0)\,t + \frac{1}{2}\mu_2''(0)\,t^2 + O\left(t^3\right). \quad (17)$$

In order to evaluate the coefficients of the expansion, let us multiply the first equation of equation (14) by x^2 and the second one by x and integrate. Integrating by parts and assuming that boundary terms vanish, we obtain:

$$\begin{aligned} &\frac{d}{dt}\langle x^2\rangle_\rho - 2v\langle x\rangle_{\mathcal{J}} + \frac{2v}{\rho_M}\langle x\rangle_{\mathcal{J}\rho} = 0 \\ &\frac{d}{dt}\langle x\rangle_{\mathcal{J}} - v\int \rho\left(1-\frac{\rho}{\rho_M}\right)dx \\ &\qquad + 2r\langle x\rangle_{\mathcal{J}} - \frac{2r}{\rho_M}\langle x\rangle_{\mathcal{J}\rho} = 0 \end{aligned} \quad (18)$$

where $\langle \ldots \rangle_{\mathcal{J}}$ and $\langle \ldots \rangle_{\mathcal{J}\rho}$ denote averages with respect to the corresponding (products of) densities.

Since the initial condition is symmetric, the first equation of (18) shows that $\mu_2'(0) = 0$. Differentiating the same equation with respect to time, recalling equations (14) and integrating by parts eventually leads to:

$$\begin{aligned}\frac{d^2}{dt^2}\langle x^2\rangle_\rho &= 2v\frac{d}{dt}\langle x\rangle_{\mathcal{J}} - \frac{2v}{\rho_M}\frac{d}{dt}\langle x\rangle_{\mathcal{J}\rho}\\ &= 2v\left(v\int \rho\left(1-\frac{\rho}{\rho_M}\right)dx\right.\\ &\quad\left. - 2r\langle x\rangle_{\mathcal{J}} + \frac{2r}{\rho_M}\langle x\rangle_{\mathcal{J}\rho}\right)\\ &\quad - \frac{2v}{\rho_M}\left(v\int \rho^2\left(1-\frac{\rho}{\rho_M}\right)dx\right.\\ &\quad\left. + v\int x\rho\left(1-\frac{\rho}{\rho_M}\right)\frac{\partial\rho}{\partial x}dx\right). \qquad (19)\end{aligned}$$

Evaluating the previous expression at $t = 0$ makes the terms that involve the function $\mathcal{J}$ disappear. Thus

$$\begin{aligned}\frac{d^2}{dt^2}\langle x^2\rangle_\rho\Big|_{t=0} &= 2v^2\int \rho\left(1-\frac{\rho}{\rho_M}\right)^2 dx\Big|_{t=0}\\ &\quad - \frac{2v^2}{\rho_M}\int x\rho\left(1-\frac{\rho}{\rho_M}\right)\frac{\partial\rho}{\partial x}dx\Big|_{t=0} \qquad (20)\end{aligned}$$

which leads to the approximation

$$\mu_2(t) \approx \mu_2(0) + v_e^2\, t^2 \qquad (21)$$

with

$$\begin{aligned}v_e = \frac{v}{\sqrt{\mathcal{N}}}\Bigg[\int \rho\left(1-\frac{\rho}{\rho_M}\right)^2 dx\Big|_{t=0}\\ -\frac{1}{\rho_M}\int x\rho\left(1-\frac{\rho}{\rho_M}\right)\frac{\partial\rho}{\partial x}\,dx\Big|_{t=0}\Bigg]^{1/2} \qquad (22)\end{aligned}$$

where we have used the fact the norm $\mathcal{N} = \int \rho(x,t)\,dx$ is constant if boundary terms can be neglected. This is the case of a broad choice of initial conditions, such as the propagation of pulses that are initially localized in a compact domain.

Figure 1 shows the time evolution of μ_2 obtained by integrating numerically the system (18) with a forward-difference approximation in time and replacing the spatial derivatives by centered Euler approximations. The initial conditions are generalized Gaussian pulses of the type

$$\rho(x, t=0) = \phi\, e^{-x^{2\beta}/2}. \qquad (23)$$

This allows us to investigate the propagation of a pulse whose shape varies continuously from Gaussian ($\beta = 1$) to a sharp, nearly piecewise constant step function ($\beta \gg 1$), while the parameter $\phi < 1$ gauges the level of crowding. It is not difficult to compute v_e analytically from equation (22) as a function of ϕ for a pulse of the kind (23). After straightforward calculations, one gets

$$v_e(\phi) = v\left[1 - \frac{3\,\phi}{2^\gamma} + \frac{2\,\phi^2}{3^\gamma}\right]^{1/2} \qquad (24)$$

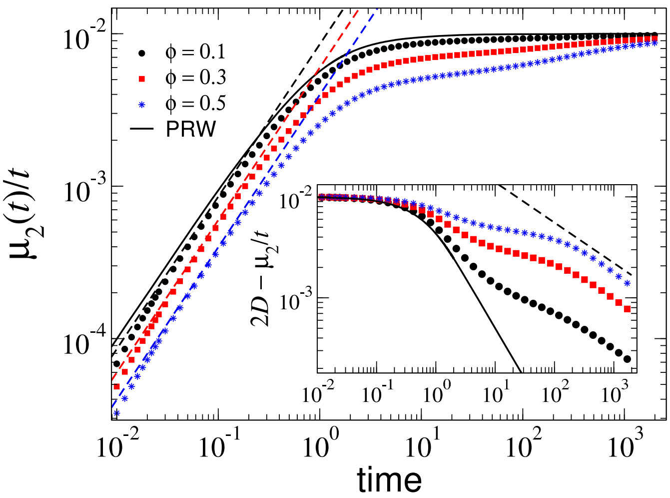

Fig. 1. Mean square displacement for a pulse of the kind (23) with $\beta = 10$ as a function of time for different choices of the crowding parameter ϕ. The dashed lines are straight lines of slope v_e as predicted by equation (24). Inset: approach to the diffusive regime. The parameter $D = v^2/2r$ is the theoretical diffusion coefficient. The solid line refers to the PRW and vanishes as t^{-1}. The dashed line is an inverse-power law with exponent 0.4, to be used as a guide for the eye.

where $\gamma = 1 + 1/2\beta$. It is clear from the figure that the approximation (24) captures to an excellent extent the initial ballistic stage. Furthermore, the numerical integration of equations (18) clearly shows that asymptotically the propagation becomes diffusive, with the same diffusion coefficient $v^2/2r$ as the PRW. This is to be expected as $\rho \to 0$ as $t \to \infty$ and therefore the excluded-volume constraints (that is, the nonlinear terms) become negligible. Nevertheless, the inset in Figure 1 clearly shows that the approach to the diffusive regime is considerably slowed down as a result of crowding – the more the greater the excluded-volume constraint.

Our analysis shows that the initial behaviour of the mean square displacement is qualitatively the same as in the PRW, i.e., the propagation is ballistic. The effect of crowding is to decrease the velocity that characterizes the initial stage of the evolution. In Figure 2 the effective velocity v_e, normalized to the diluted limit v, is plotted as function of the level of crowding and for different choices of the parameter β. Remarkably, v_e also depends on the *shape* of the initially localized density pulse. The ballistic spreading of a super-Gaussian pulse, nearly a sharp step, proceeds with a considerably lower speed as compared to the spreading of a pure Gaussian pulse (see again Eq. (22)).

4 Conclusions and perspectives

The persistent random walk yields the so-called telegraph equation in the continuum limit, which displays a well known transition from ballistic to diffusive transport. In the classical microscopic formulation of the PRW, individual walkers are assumed to jump toward neighboring sites

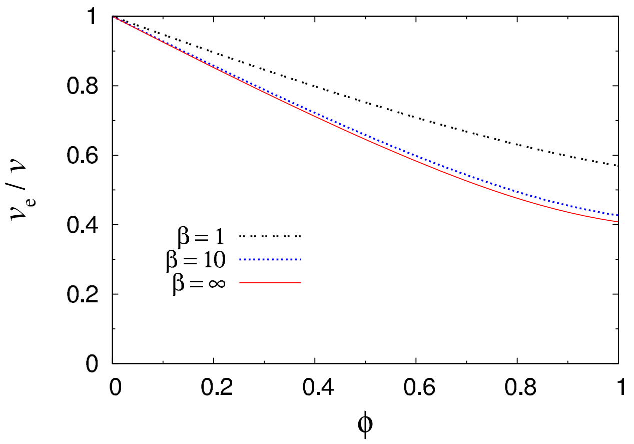

Fig. 2. Effective velocity (24) as a function of the level of crowding for a Gaussian pulse, a generalized Gaussian with $\beta = 10$ and a step pulse ($\beta \to \infty$).

with constant probability. However, one can account for excluded volume effects by gauging the hopping probability to the occupancy of the target sites. By doing so, we obtained a set of two coupled nonlinear transport equations, that reflect the microscopic competition for the available space. Microscopic processes which implement exclusion rules are called simple exclusion processes (SEPs). For this reason, we refer to the generalized model introduced here as the persistent simple exclusion process (PSEP).

We go on to investigate the mean-field limit of the PSEP process for a specific class of initial conditions. These are generalized Gaussian pulses, whose shape varies continuously from Gaussian to sharp steps depending on a control parameter. The pulse amplitude ϕ in this setting measures the degree of imposed crowding, i.e., the density of the medium. Numerical integration of our modified transport equations shows that the PSEP still undergoes a transition from ballistic to diffusive behaviour of the MSD. However, the velocity of the initial ballistic stage is found to decrease with the density of the medium (ϕ). This might be relevant in many cases where the telegraph equation is used to model physical situations. Think for example to gel electrophoresis (GEP), first modeled as a two-state process yielding the telegraph equation in the 50s [26]. As a molecule moves along a channel in response to an applied electric field, it may become entangled in the gel matrix at random times and after some time detach from the gel fibers because of thermal fluctuations. Here $a(x,t)$ and $b(x,t)$ represent the concentration of bound and free molecules. Of course, the available theory does not describe the migration of molecules in crowded solutions, which may be however interesting to analyze through GEP.

Remarkably, as a consequence of the excluded-volume constraint, the velocity of the ballistic stage also depends on the *shape* of the initial pulse. In particular, at equal values of crowding ϕ, our calculations show that pulses with sharper edges display smaller velocities and hence cross over later to diffusive spreading. At long times, the propagation becomes diffusive, with the same diffusion coefficient as for the long-time limit of the telegraph equation. This is because, as the pulse spreads, the density decreases and nonlinear terms become eventually irrelevant.

We envisage to extend this work along different lines. On the one side it would be interesting to account from the very beginning for the finite size of the agents along the lines of [25], beyond the point-like version of the crowding considered here (i.e., fully penetrable entities). Moreover, it would also be engaging to establish a link between our treatment and the dichotomous noise picture, in order to investigate the connection between excluded-volume constraints and modifications of the switching time statistics.

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