Directed particle diffusion under ''burnt bridges'' conditions

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We study random walks on a one-dimensional lattice that contains weak connections, so-called ''bridges.'' Each time the walker crosses the bridge from the left or attempts to cross it from the right, the bridge may be destroyed with probability p; this restricts the particle's motion and directs it. Our model, which incorporates asymmetric aspects in an otherwise symmetric hopping mechanism, is very akin to ''Brownian ratchets'' and to front propagation in autocatalytic $A+B\rightarrow 2A$ reactions. The analysis of the model and Monte Carlo simulations show that for large p the velocity of the directed motion is extremely sensitive to the distribution of bridges, whereas for small p the velocity can be understood based on a mean-field analysis. The single-particle model advanced by us here allows an almost quantitative understanding of the front's position in the $A+B\rightarrow 2A$ many-particle reaction.

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Models based on particle's diffusion in one-dimensional systems that lack mirror symmetry have attracted much attention in the last years. Such essentially one-particle models include ''Brownian ratchets'' [1–3], ''thermal ratchets'' (an extensive literature on this subject is partly reviewed in Ref. [4]), and several other models with strongly asymmetric transition rates [5,6]; they are relevant for the description of many biological and chemical processes and are also of interest in general thermodynamical contexts (see, e.g., [7]). On the other hand, much attention was paid to the front-propagation problem, say as in the simple $A+B\rightarrow 2A$ autocatalytic reaction, see Refs. [9–11]. Such reactions show (especially in $d=1$) many peculiarities connected with the discrete nature of the system [12–27]. As we will show, some aspects of such many-particle problems can also be reproduced by the one-particle model that we proceed to discuss.

Here we put forward a one-dimensional model of directed propagation based on random walks over a one-dimensional semi-infinite chain extending to the right of the origin. In each realization of the process we have a single walker that performs at regular time intervals steps to nearest-neighbor positions along the chain. Some of the links connecting nearest neighbors are, however, prone to be destroyed by the walker. We will call such links ''bridges'' and a destroyed link a ''burnt bridge.'' The bridge is burnt with probability p if the random walker crosses it from left to right, or if it attempts to cross it from right to left. In any case, if the bridge is burnt the walker stays right of it and cannot cross it back anymore; by this the walker gets to be separated from the left part of the chain. Initially we have a concentration c of intact bridges. At $t=0$ the walker starts at the origin and moves in random walk fashion. In Fig. 1 we sketch our model, in which the random walker is shown as an open circle, the dots represent the chain's sites, and the bridges are indicated by thin lines; a burnt bridge carries a vertical bar. In this figure, two bridges are burnt out. Such bridges hinder leftward motion creating an overall drift to the right; we denote the drift velocity by v, and study its dependence on c and on p.

Special cases of our burnt-bridges model (BBM) appear in several recent contexts that treat rectifying Brownian motion. The case $p=1$ reproduces the Brownian ratchet model of Refs. [1–3], which depicts closely several kinds of intracellular processes. In Refs. [2,3] a small particle (so-called Brownian motor) moves diffusively along a one-dimensional (1D) track on which barriers are located. The barriers act asymmetrically: they are totally transparent for rightward steps and totally reflecting (impenetrable) for leftward steps. The motor performs, thus, a random walk in a system containing a number of sites with asymmetric transition rates. A similar situation is also encountered in hopping lattice models with asymmetric transitions [5,6] and in resistor-diode networks (cf. Ref. [8]). Furthermore, our BBM for general p resembles to a large extent situations found in networks containing imperfect rectifiers [2] and is related to asymmetric hopping models in which backward rates are small but nonzero. The new aspect introduced by our BBM is that through the burning of bridges the system acquires a memory, which renders the overall process non-Markovian. A realization of such a situation is encountered in biological systems of gated channels, see e.g., [28], where a channel (like the bridges here) can be irreversibly blocked after the passage of an ion.

A particularly close connection exists between BBM and front propagation in autocatalytic reactions, exemplified, say, by $A+B\rightarrow 2A$. In a mean-field picture front propagation is described by a quadratic Fisher equation [9,10] that is, however, as shown both analytically and by Monte Carlo simulations [12–27] quite deficient in low dimensions ($d=1$ and $d=2$), the reason being that in low dimensions the reactions are very sensitive to particle correlations and fluctuations [29,30]. As discussed in Refs. [16,23,26] the velocity at which A-cluster expands is determined by the form of the front, ''leading edge.'' We show now that BBM can repro-

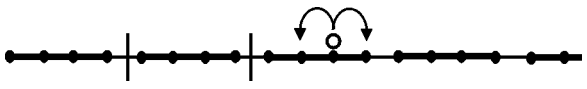

FIG. 1. The 1D propagation scheme. The open circle represents the random walker, the dots are the lattice sites. The bridges are depicted by thin links, the burnt bridges are marked by vertical bars.

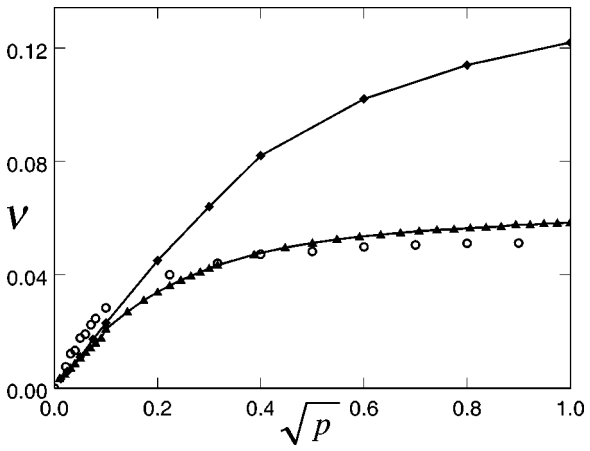

FIG. 2. The propagation velocity v is shown as a function of $\sqrt{p}$, where p is the probability of burning a bridge. The triangles are the results of our simulations for randomly distributed bridges, the diamonds those for regularly distributed (equidistant) bridges. The circles display the results of Monte Carlo simulations of the $A+B \rightarrow 2A$ reaction. See text for details.

duce the dynamics of the front's position in $1D$ quite closely; this is a theoretically very important finding, since it shows that autocatalytic reactions display features very akin to the rectification of Brownian motion.

We recall now that in modeling the $A+B \rightarrow 2A$ reaction one lets particles A and B react with probability q when they meet on the same site. In standard fashion one starts the reaction by placing one A particle at the origin of a semi-infinite chain, on which otherwise only B's are found. The position of the front is given by that of the rightmost A particle (which plays the role of a marker). Since the marker is always the rightmost A, the other A's are a left boundary for it. Thus, the motion of the marker to the right is free (it may be modulated by reaction acts), whereas its motion to the left is restricted by mobile obstacles (the other A's). The front's velocity is given by $v=\overline{x}/\overline{t}$ (see Ref. [16]), where $\overline{x}$ is a typical distance from the site at which the last reaction has taken place and $\overline{t}$ is the typical elapsed time between such reactions. The BBM presented above is a simplified version of this picture; in it all particles with the exception of the marker (the walker) are frozen, fact that reverts the many-body problem to a one-walker scheme.

We now address the study of our BBM and highlight its behavior through Monte Carlo simulations. We use a 1D lattice of length $L=30\,000$ (which is sufficient for 200 000 time steps, i.e., walker's moves) and impose a reflecting boundary condition at the origin. For the positioning of the bridges we consider two alternatives: (i) random distribution and (ii) regular, equidistant positions. The obtained propagation velocities are shown in Fig. 2 for $c=0.1$ as a function of $\sqrt{p}$. Case (i) is represented by triangles and case (ii) by diamonds. One sees that for small p, $p \ll 1$, both models behave similarly and that v depends almost linearly on $\sqrt{p}$, which is the mean-field result, see Eq. (15) below. For larger p deviations from the mean-field case are evident, and the models start to behave differently, indicating that the fluctuations in the interbridge distances become important. In Fig. 2 we also present (through thick open circles) the results of Monte Carlo simulations for the $A+B \rightarrow 2A$ reaction, Ref. [16]. Note that in the whole p -range investigated, case (i) (BBM with randomly distributed bridges) reproduces the $A+B \rightarrow 2A$ reaction results closely.

We now discuss the asymptotic behavior of the BBM in the case of very high ($p \simeq 1$) and very low ($p \ll 1$), reaction probabilities. For $p \simeq 1$, a bridge burns practically at every crossing event. As a consequence one has a renewal situation: the walker takes the newly burnt bridge as its new origin. In the segment comprised between a left, burnt bridge and a right, intact one, the random walk motion corresponds to diffusion with a reflecting boundary condition at the left and an absorbing boundary condition at the right.

Let us first concentrate on the case when the bridges are equidistant, and separated by a distance $l=c^{-1}$. In this case one has evidently $\overline{x}=l$, so that our only task will be to evaluate $\overline{t}$. In our case $\overline{t}$ is the first-passage time through l and can be evaluated through the probability that the walker remains in the interval, $\psi(t)=\int_0^l \Psi(x,t)dx$, where the joint probability density $\Psi(x,t)$ to find a walker at point x at time t is given by the solution of the diffusion equation

$$\frac{\partial \Psi}{\partial t}=D\frac{d^2\Psi}{\partial x^2}, \tag{1}$$

under the boundary conditions $\Psi'(x,t)=0$ at $x=0$ and $\Psi(x,t)=0$ at $x=l$, where the initial condition is $\Psi(x,0)=\delta(+0)$. The mean sojourn time of a walker in this interval is well known, namely, $\overline{t}=l^2/2D$, so that the front's velocity, $\overline{v}=l/\overline{t}$, is [2]

$$\overline{v}_{reg}=2D/l=2cD. \tag{2}$$

On the other hand, in the case of randomly distributed bridges we must average $\overline{t}$ over the distribution of distances l between the bridges; taking the distribution to be Hertzian we have $p(l)=c\exp(-cl)$, from which $\overline{t}=l^2/D$ and

$$\overline{v}_{rand}=D/l=cD \tag{3}$$

follow. One may note the difference of a factor of 2 between Eqs. (2) and (3); this shows that the walker's velocity is strongly influenced by fluctuations in the interbridge distances, a fact that has its conterpart in the front propagation problem, both in discrete [27] and also in continuous systems [11]. In connection with the Brownian rectifier this means that a disordered distribution of barriers leads to a considerably lower drift velocity when compared to that found when the same number of barriers is equidistantly distributed. Note that Eqs. (2) and (3) neglect the existence of an underlying lattice and are exact only in the limit $c \rightarrow 0$. Using $p=1$ and $c=0.1$ in Fig. 2 we are still distant from a quantitative agreement. On the other hand, for even smaller c values the results of the simulations tend towards the values given by Eqs. (2) and (3); namely we find numerically for $c=0.1$, 0.05, and 0.025 that $v/cD=1.17$, 1.07, and 1.04 in case (i) and $v/2cD=1.22$, 1.15, and 1.05 in case (ii).

We now turn to the case $p \ll 1$. Again, the mean-drift velocity is given by the mean distance between two consecutively burnt bridges and by the mean time between these events. After burning a bridge, the overall process is renewed; the walker restarts its motion at the leftmost point of an interval, with a reflecting boundary condition there. On the other hand, for small p, bridges have a small probability to burn when crossed, and thus the mean walker's displacement between two renewals is much larger than c^{-1}, the mean distance between bridges. To approximate the situation we use here a separation of scales: a burning event will be pictured as a *reaction* of the walker with the bridge; the walker will disappear, burning the bridge: Then a new walker will be created just to the right of the burnt bridge. Given that p is small we can now assume the bridges to be a part of a continuous *reacting* medium.

The probability $\Phi(x,t)$ to find the nonreacted walker at point x at time t is now governed by the continuous reaction-diffusion equation

$$\frac{\partial \Phi}{\partial t} = D\frac{d^2\Phi}{\partial x^2} - k\Phi. \tag{4}$$

The boundary conditions are $\Phi'(0,t)=0$ and $\Phi(\infty,t)\to 0$, and the initial condition is $\Phi(x,0)=\delta(+0)$. The solution of Eq. (4) is a decaying ''half Gaussian,''

$$\Phi(x,t) = \frac{1}{\sqrt{\pi D t}}\exp\left(-\frac{x^2}{4Dt}\right)\exp(-kt). \tag{5}$$

Using this equation we find for the mean-traveled distance

$$\overline{x} = \int_0^\infty \int_0^\infty x\Phi(x,t)dxdt = D^{1/2}k^{-3/2} \tag{6}$$

and for the mean lifetime between events

$$\overline{t} = \int_0^\infty \int_0^\infty t\Phi(x,t)dxdt = k^{-1}. \tag{7}$$

According, now, to our coarse-grained model, the mean velocity of the walker is then $v=\overline{x}/\overline{t}=D^{1/2}k^{1/2}$. It remains to evaluate k. A simple consideration leads to the form

$$k \propto pc. \tag{8}$$

In the following we show that a more accurate approximation suggests that

$$k = 2pc. \tag{9}$$

We do this by supposing that the overall coarse-grained concentration Φ does not change considerably on the scale $l=c^{-1}$, the typical distance between bridges.

We now consider the evolution of the fine-grained survival probability $\Delta(x,t)$ of the walker between two traps situated at $\pm l/2$, from which $\Phi(x,t)$ follows by averaging over a spatial domain that is small compared to $\overline{x}$, but large compared to l. The change in $\Delta(x,t)$ is governed inside $[-l/2,l/2]$ by the diffusion equation

$$\frac{\partial \Delta}{\partial t} = D\frac{\partial^2 \Delta}{\partial x^2}, \tag{10}$$

to be solved with respect to the ''gray sphere'' (mixed) boundary condition at $x=\pm l/2$,

$$j = -D\frac{\partial \Delta}{\partial x} = p\Delta(l/2), \tag{11}$$

and a similar relation at $x=-l/2$ (one may note that the reaction probability p has the dimension of an inverse time, since it is the probability to react on contact *per time step*). Solving Eq. (10) through the variable separation $\Delta(x,t)=X(x)T(t)$ gives the solution in the form $\Delta(x,t)=\Sigma_n b_n \cos(a_n x)\exp(-\lambda_n t)$ with $\lambda_n = Da_n^2$. The boundary condition gives rise to an equation determining a_n: The a_n's are the (discrete) solutions of the transcendental equation

$$a = -\frac{p}{D}\cot\left(\frac{al}{2}\right). \tag{12}$$

The lowest mode, which determines the overall decay is given by the smallest nonzero solution of Eq. (12). For p small one can take $\cot(al/2)\simeq 2/al$ and obtains

$$a^2 = 2p/Dl, \tag{13}$$

from which

$$k = \lambda = 2p/l = 2pc \tag{14}$$

follows [as claimed above, Eq. (9)]. In this case

$$v = D^{1/2}k^{1/2} = \sqrt{2Dpc}. \tag{15}$$

Hence Eq. (8) and following lead to a linear dependence of v on $p^{1/2}$, behavior which is clearly supported by Fig. 2. Furthermore, for small p (as was to be theoretically expected) the results of the numerical simulations show that the walker's drift velocity is the same for regularly and for randomly distributed bridges.

We now compare the findings of the BBM to the $A+B\to 2A$ problem. For p large, the front velocity in the autocatalytic reaction behaves similarly to the walker's velocity in case (i), BBM with randomly distributed bridges, Eq. (3). The lowest order c dependence in these two models is the same, but the corrections of higher order in c differ. For small p, the velocity of the front in the $A+B\to 2A$ problem is slightly larger than the one in the BBM. This fact can be traced back to the fact that in the reaction problem the effective diffusion coefficient is larger than D [16].

Let us summarize our findings. We introduced a simple non-Markovian model, the BBM, in which a walker may destroy with probability p bridges that it crosses from left to right or attempts to cross from right to left. We monitored through Monte Carlo simulations the mean-drift velocity v of the walker as a function of p. For small values of p we

find that the mean-field result ($v \sim \sqrt{p}$) holds, and that this result does not depend on the spatial distribution (regular or random) of the bridges. At larger values of p deviations from the mean-field result appear. Moreover, at fixed c the value of v is twice larger for a regular than for a random bridge placement. Comparison of the BBM results to those of the $A+B \rightarrow 2A$ reaction shows that the BBM reproduces the $A+B \rightarrow 2A$ findings satisfactorily over the entire p range.

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