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Combining geometrical and dynamical disorder to enhance transport

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We look for the optimal way to distribute rectifiers in order to maximize their effect on the transport properties of Brownian particles. These rectifiers are introduced in the form of flashing asymmetric potentials distributed on a one dimensional lattice. We study the effects that different distributions of these rectifiers have on the generated current and on the energy cost of transport. Based on both analytical and numerical results, we observe an unexpected increase in the efficiency of the rectifiers and the magnitude of the current for the case in which geometrical and dynamical disorder are combined. We show that this effect is a direct consequence of the "hitchhiker" or "waiting time" paradox.

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I. INTRODUCTION

The subject of rectification of fluctuations has been extensively studied in the recent past, mainly due to its potential applications in biology and nanotechnology [1,2]. Pumps and motors within the cell seem to work not only in spite of the thermal fluctuations affecting proteins and organelles, but also profiting from these fluctuations by means of rectifiers [3]. A large family of models of Brownian ratchets has been introduced to obtain some insight into the basic mechanisms of noise rectification [1]. In addition, several models for collective rectifiers or Brownian motors have been proposed recently, most of them built from single Brownian ratchets coupled mechanically, via elastic or rigid interactions [4,5]. The reason is that *ensembles* of rectifiers working collectively need to be considered for the description of certain biological systems, such as muscle tissue, and for possible designs of some nanodevices.

We consider another aspect of ensembles of rectifiers in this article; namely, the purpose of this paper is to study the influence of the spatial distribution of rectifiers on their ability to transport Brownian particles. In particular, suppose we have at our disposal a given number of rectifiers and we are asked to distribute them along a line in order to transport particles in the most efficient way. We show that paradoxically, under certain conditions, the best performing scenario corresponds to the case when we combine dynamical and geometrical disorder.

This paper is organized as follows. Section II describes the model we propose to study rectification of fluctuations. Section III describes the mathematical details of our calculations and compares those results to our Monte Carlo simulations. Section IV summarizes our findings.

II. MODEL

Our system consists of particles describing a random walk on a one dimensional lattice, where rectifiers have been scattered with a concentration $c \in (0,1)$. Our rectifiers are *flashing* asymmetric potentials, each one consisting of an infinite well next to an infinite barrier. Figure 1 shows the potentials and the hopping probabilities used in our system. It is important to mention that nonflashing asymmetric potentials have been extensively used in the theory of surface growth in stepped surfaces and are called Ehrlich-Schwoebel (ES) potentials [6–9]. The ES potentials have also been introduced in the context of *cellular media*. These media consist of consecutive finite cells separated by permeable walls [10] and have been identified with multiple materials, ranging from biological tissues to the aforementioned stepped surfaces. Nonflashing finite ES potentials have also been used to study rectification in the presence of an external bias [9].

If the rectifiers in our system were permanently in place, a particle could move only within one cell. To achieve rectification, we have to *flash* our ES potentials. With this in mind, our ES potentials stay in place for $\tau-1$ units of time; then they all disappear for one unit of time. The process of having the potentials in place for $\tau-1$ units of time immediately followed by their disappearance for one unit of time is repeated continuously according to the following four different scenarios.

(1) *Periodic distribution:* the ES potentials are equally distributed and they reappear in the same places.

(2) *Spatial disorder:* the ES potentials are randomly dis-

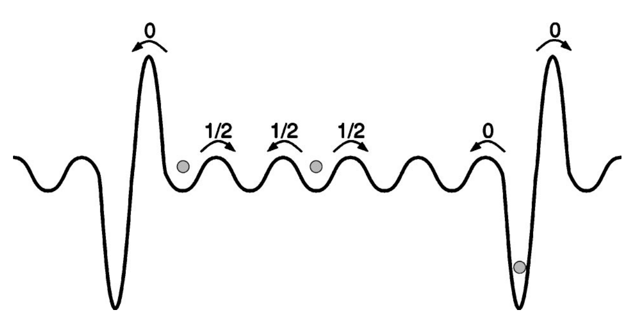

FIG. 1. Two Ehrlich-Schwoebel potentials confining Brownian particles within a cell. The hopping probabilities are indicated over the arrows.

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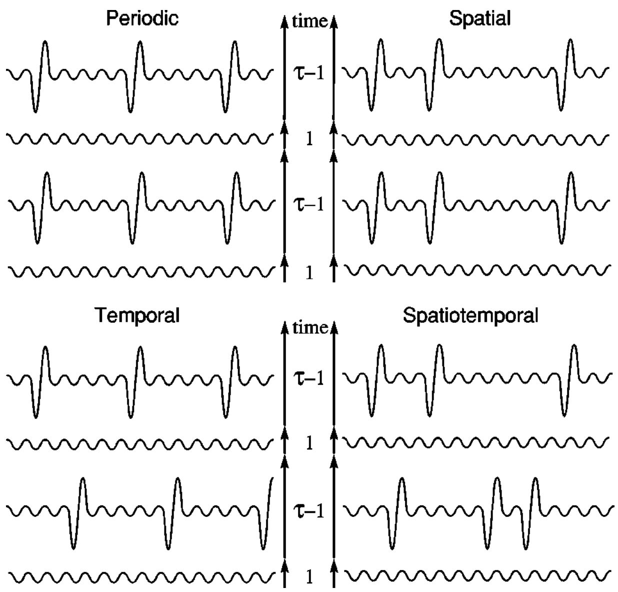

FIG. 2. Schematic representation of the time evolution for the different scenarios used in this paper. "Normal" symmetric potentials replace the ES potentials for one unit of time after every $\tau-1$ units of time. In this figure, the concentration of rectifiers is $c=0.2$ for the periodic and temporal scenarios, yielding a spatial period $l=5$.

tributed and they reappear in the same places.

(3) *Temporal disorder:* the ES potentials are equally distributed and they reappear in different places.

(4) *Spatiotemporal disorder:* the ES potentials are randomly distributed and they reappear in random places.

We refer to scenario 1 as having no disorder, scenario 2 as having geometrical disorder only, scenario 3 as having dynamical disorder only, and scenario 4 as having both geometrical and dynamical disorder. A schematic representation of the different scenarios is shown in Fig. 2.

We create the spatial and spatiotemporal distributions by assigning ES potentials on the lattice with a probability c per site. $\overline{l}=1/c$ is the average distance between two ES wells and $\overline{l}-1$ the average length of a cell. In the periodic and temporal scenarios, $l=1/c$ (which must be an integer number) is the distance between two consecutive ES wells, whereas the length of a cell is $l-1$.

III. ANALYTICAL RESULTS AND SIMULATIONS

Our main goal is to study the current of Brownian particles in our four different scenarios. The quantity of central interest to us is the average particle current

$$J=\lim_{t\to\infty}\frac{\langle x(t)\rangle}{t}. \tag{1}$$

We have performed Monte Carlo simulations for these four scenarios to measure the current J as a function of the period τ. The simulations consist of particles moving under the rules described above. Each trajectory consists of 3×10^4 units of time. A total of 10^5 trajectories for a selection of c and τ is explored. Periodic boundary conditions are used to simulate an infinite lattice. Notice that when $\tau=1$ the system effectively has no ES potentials for any value of c. The results of the simulations with $c=0.2$ are shown in Fig. 3.

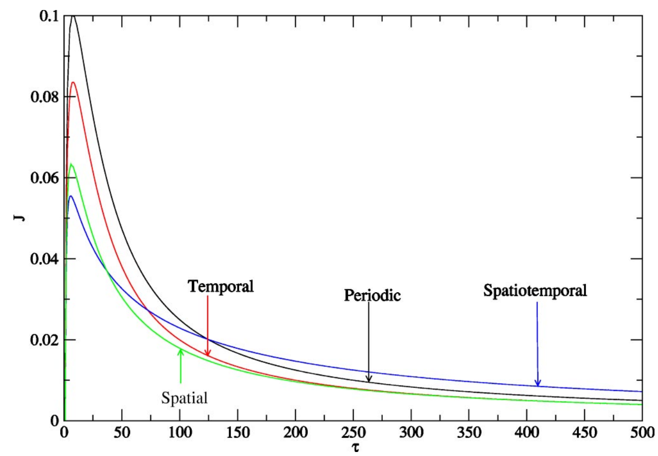

FIG. 3. Results from Monte Carlo simulations for the different scenarios. We have plotted the average particle current (J) vs the period (τ) for a concentration of ES potentials $c=0.2$.

As can be seen, all the plots in Fig. 3 show a maximum in the current for a specific value of τ. This can be understood by focusing on the two limits of τ. When τ is small, the cell's lifetime is too short for the particle to reach the ES well inside the cell. The particle is barely affected by the rectifiers, its motion is almost symmetrical, and the current vanishes. On the other hand, for large τ, a particle spends too much time trapped at the bottom of the ES wells, which also inhibits its motion in one direction. In other words, there is no rectification for $\tau=1$ or $\tau\to\infty$, but there is rectification for intermediate values of τ.

We can also see that for short values of τ (short cell lifetime), the highest current corresponds to the most ordered case (periodic). However, this behavior quickly changes and the scenario that combines geometrical and dynamical disorder (spatiotemporal) exhibits the largest current. We offer an analytical description for this unexpected behavior in the remainder of this paper.

The models we proposed can be solved analytically for large τ. In this limit, we can assume that by the end of each period τ particles reach the corresponding ES wells with probability 1 for all scenarios. Equation (1) becomes

$$J=\frac{\overline{d}}{\tau}, \tag{2}$$

where $\overline{d}$ is the average distance covered by a particle in one period.

We start by discussing the periodic scenario. In this case, a particle has two equal possibilities of motion as the barriers disappear. The first option is to jump left, thus remaining within the same cell once the barriers reappear and covering a zero net distance in the following period of time τ. The second possibility carries the particle to the right into the next cell so that the net distance covered by the particle is l.

Therefore, the average distance covered by the particle in one period is

$$\overline{d_{\mathrm{p}}} = \frac{l}{2} = \frac{1}{2c}. \tag{3}$$

In the spatial scenario, when the asymmetric potentials are randomly distributed and reappear in the same place, a particle also has two equal possibilities of motion as the barriers disappear. If a particle moves right it covers the length l of the next cell to the right. If the particle jumps left, it remains in the same cell and covers a net distance of zero in the following period of time. However, this is no longer true if the cell's size is equal to one lattice site. In this particular case, the particle moves back to the next cell to the left and the net motion is -1. This situation occurs with a probability p_1, which is difficult to assess. The probability of having a cell of size 1 is c, but the probability of *being* in a cell of size 1 is greater than c. This is because the concentration of particles is larger in zones of the lattice where there are several consecutive cells of size 1. We will neglect the effect that these zones have on reducing the net current by taking $p_1 \simeq c$. With this additional approximation, the particle covers an average distance $-c$ with probability 1/2 in the first option, while it covers an average distance l in the second option. Then,

$$\overline{d_{\mathrm{s}}} = \frac{l-c}{2} = \frac{1-c^2}{2c}. \tag{4}$$

For the temporal scenario, once the barriers reappear, the next ES well is located to the right of the particle and can be in any site at a distance ranging from zero to $l-1$, with equal probability $1/l$. Since the average displacement in the first move is zero, then

$$\overline{d_{\mathrm{t}}} = \sum_{k=0}^{l-1} \frac{k}{l} = \frac{1-c}{2c}. \tag{5}$$

Finally, for the spatiotemporal case, the average displacement when there are no barriers is also zero. After the barriers reappear a particle moves to the right until it finds the ES well. The probability to have an ES well at a site is c; therefore the average displacement is

$$\overline{d_{\mathrm{st}}} = \sum_{k=0}^{\infty} kc(1-c)^k = \frac{1-c}{c}. \tag{6}$$

Using Eqs. (3)–(6) and Eq. (2) we obtain the corresponding current for large τ in each scenario:

$$J_{\mathrm{p}} = \frac{1}{2\tau c}, \quad J_{\mathrm{s}} = \frac{1-c^2}{2\tau c},$$

$$J_{\mathrm{t}} = \frac{1-c}{2\tau c}, \quad J_{\mathrm{st}} = \frac{1-c}{\tau c}. \tag{7}$$

Notice the factor $1/2$ present in all the expressions except in the spatiotemporal disorder. This is the main result of this paper: for small c and large τ, the current obtained for the spatiotemporal disorder is *double* the current obtained for the other three distributions of rectifiers. The following is our explanation of this result.

In the periodic and spatial scenarios, the particle either stays in the same cell or moves to the beginning of the next cell. It covers either no distance or the average cell length, respectively. Hence, the average distance covered by a particle for small c and large τ is half of the cell length [see Eqs. (3) and (4)].

On the other hand, when dynamical disorder is introduced, the particle always finds itself in a new cell. Then the question is how much of that cell the particle will cover on the average. As it turns out, for the temporal scenario the particle covers, on the average, half of the cell length [Eq. (5)], whereas for the spatiotemporal scenario the particle covers, on the average, the entire cell length [Eq. (6)].

This unexpected result can be related to the "hitchhiker" or "waiting time" paradox [11] affecting a person trying to obtain a ride from cars traveling on a road. According to this paradox, if the interval of time between the cars traveling on that road corresponds to a Poisson process with an exponential distribution, then the average waiting time $\overline{d}$ for a person arriving at random is equal to the average time interval $\overline{s}$ between cars. This result is paradoxical, because we should expect the average waiting time $\overline{d}$ to be half of the mean interval $\overline{s}$ between cars. However, only when the cars pass by the hitchhiker separated by equal time intervals (periodically), i.e., s is constant, is the average waiting time $\overline{d}$ indeed half of the mean interval s, as intuitively expected. The effect is the same between our spatiotemporal and temporal scenarios if we interpret the arrival of cars as ES potentials (separating cells of length $s=l-1$) and the arrival of the hitchhiker as the position of the particle when the ES potentials reappear.

To ascertain the validity of our analysis, we compare the analytical results we obtained for the current [Eqs. (7)] against our Monte Carlo simulations for a concentration of ES potentials $c=0.2$. Figure 4 shows an excellent agreement between theory and simulations, which starts at $\tau \approx 50$ for the periodic and temporal cases and at $\tau \approx 1500$ for the spa-

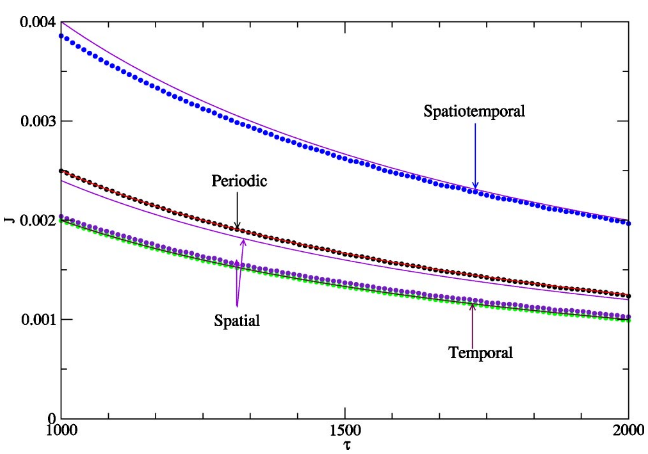

FIG. 4. Comparison between analytical results using Eqs. (7) (solid lines) and Monte Carlo simulations (dots). We have plotted the average current J vs τ for a concentration of ES potentials $c=0.2$.

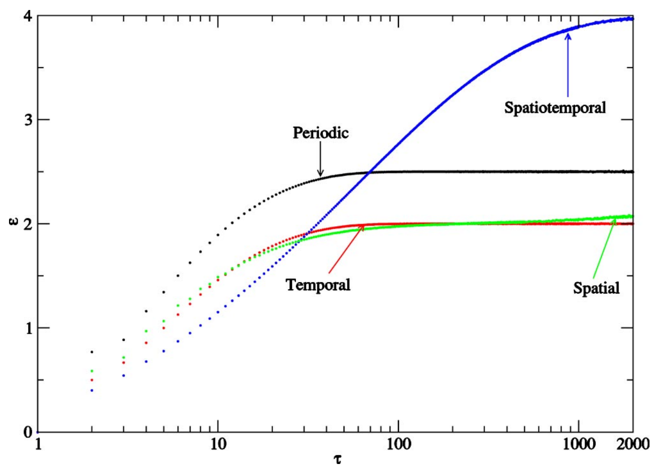

FIG. 5. The efficiency per load ε vs τ for a concentration of ES potentials $c=0.2$. Units of energy are such that the depth of the ES wells is $\Delta V=1$.

tiotemporal disorder. We observe only a slight discrepancy (approximately 5% for $\tau=2000$) for the scenario with spatial disorder. This discrepancy is due to the possible presence of several consecutive cells of length 1 as has already been discussed above.

The other quantity we study in this article is the efficiency of the system. To define the efficiency, we need to realize that our flashinglike ratchet works as a motor when there is a load force F opposite to the direction of the current $J(F)$. If the force is small enough, particles move against it, performing work equivalent to $FJ(F)$ [12]. On the other hand, energy is introduced into the system each time we switch off the ES potentials. A particle trapped in an ES well will then effectively increase its potential energy. For the dynamics of our model we have assumed that the ES wells are infinite. Now, to have a finite input energy we need to consider finite ES wells with depth $\Delta V \ll kT$. The efficiency of the system for a small load F is

$$\eta = \lim_{t\to\infty} \frac{F\langle x(t)\rangle_F}{\Delta V\langle w(t)\rangle_F} \simeq \lim_{t\to\infty} \frac{\langle x(t)\rangle_0}{\Delta V\langle w(t)\rangle_0}F, \tag{8}$$

where $\langle x(t)\rangle_F$ and $\langle w(t)\rangle_F$ are the average distance covered and the average number of ES wells visited by the particle in time t and for a load F, respectively. Based on Eq. (8), we will focus on the efficiency per load, $\varepsilon \equiv \eta/F$. $1/\varepsilon$ can be interpreted as the energy cost to transport a particle at zero load and per unit of length.

We have studied the efficiency ε under the different scenarios described in this paper. The results of our Monte Carlo simulations, for $c=0.2$ and $\Delta V=1$, are shown in Fig. 5.

For very large τ, the particle is assured of reaching an ES potential in every period τ. Therefore, the number of wells visited in $n\tau$ is precisely n, and $\varepsilon=\bar{d}$. We also obtain an excellent match between this approximation and our simulations for all scenarios when $\tau=2000$ (and as early as for $\tau \approx 100$ for the periodic and temporal scenarios). The efficiency for the spatiotemporal scenario is the smallest for short values of τ but it quickly becomes the largest as τ becomes larger. The efficiency for this scenario is exactly twice that for the temporal disorder. Also, from Eqs. (6), (3), and (5), we should expect the efficiency for the spatiotemporal disorder to be twice as large as the efficiency for all the other scenarios for small c and large τ.

IV. CONCLUSIONS

We have shown that for low values of τ (short cell lifetime), the highest current and efficiency correspond to what we consider to be the most ordered case (periodic). However, this behavior changes rapidly, and the scenario that combines both geometrical and dynamical disorder (spatiotemporal) exhibits the largest current and efficiency. Since the spatiotemporal scenario combines the two types of disorder studied in this paper, we consider this to be our most disordered case. We have shown that the current and the efficiency are the largest for the spatiotemporal scenario, starting at relatively low values of τ ($\tau \approx 100$ for $c=0.2$). The spatiotemporal disorder case contains the ingredients needed to yield the maximum current of the four scenarios considered in this article. We have seen that the absence of dynamical disorder reduces the effectiveness of the rectifiers because the particle has only a probability 1/2 to jump into the next cell. Also, we have observed that the absence of spatial disorder in the temporal scenario reduces the average distance covered by a particle ("waiting time" paradox). Since only in the spatiotemporal case does a particle cover the entire average cell length in a period τ, and since no other possible scenario would seem to achieve this more efficiently, we have arrived at the conjecture that our most disordered scenario should prove to be the most efficient way to distribute rectifiers in a one dimensional system. Finally, most of our results could apply for other types of rectifiers. We have used a precise design of ES barriers as a combination of a trap and a reflecting barrier to explain the behavior of the current and efficiency. However, our arguments are based on the average spacing among rectifiers and the hitchhiker paradox and could be extended, with some modifications, to different types of pumps and ratchets. Work in this direction is in progress.

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