

Cooperative Transport of Brownian Particles

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We consider the collective motion of finite-sized, overdamped Brownian particles (e.g., motor proteins) in a periodic potential. Simulations of our model have revealed a number of novel cooperative transport phenomena, including (i) the reversal of direction of the net current as the particle density is increased and (ii) a very strong and complex dependence of the average velocity on both the size and the average distance of the particles.

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The most common and best known transport phenomena occur in systems in which there exist macroscopic driving forces or gradients of potentials of various origin (typically due to external fields or concentration gradients). However, recent interesting theoretical and experimental studies have shown that nonequilibrium dissipative processes in structures possessing vectorial symmetry can induce macroscopic motion on the basis of purely microscopic effects [1–10].

This newly suggested mechanism is expected to be essential for biological transport processes such as the operation of molecular combustion motors or the contraction of muscle tissues. In these cases Brownian particles (myosin, kinesin, and dyenin) convert the energy of ATP molecules into mechanical work while moving along periodic structures (myosin along actin filaments, kinesin and dyenin along microtubules) [11–13]. A transport mechanism of this kind has also been experimentally demonstrated in simple physical systems [14,15].

So far the models for the transport of Brownian particles in periodic structures have been based on the description of the motion of one single particle, but in real systems one can rarely find this situation. Experimental evidence shows that several motor proteins can carry one larger molecule, and a large number of free motors can move along the same microtubule [11]. Furthermore, in separation processes a large number of particles are moving in the same medium [14].

Therefore we propose a simple one-dimensional model via many interacting Brownian particles moving with overdamped dynamics in a periodic potential. According to our computer simulations the model displays a number of novel cooperative phenomena. (i) First we show that for a range of frequencies of a periodic external driving force the average velocity v of the particles changes its direction as the number density of the particles is increased. (ii) In addition, v has a sensitive dependence on the size of the migrating particles. This effect is demonstrated for two kinds (periodic and constant) of driving forces. In the last part of the paper we present analytical results indicating that in the case of constant driving force and nearly zero distance between the particles the

dependence of the velocity on the particle size becomes extremely complex (nondifferentiable).

The motion of a single particle (in the absence of other particles) is described by the Langevin equation

$$\dot{x}_j = f(x_j) + \xi_j(t) + F_j(t), \quad j = 1, \dots, N, \quad (1)$$

where N is the number of particles, x_j denotes the position of the center of mass of the j th particle, $f(x) \equiv -\partial_x V(x)$ is a force field due to the sawtooth shaped periodic potential $V(x)$, $\xi_j(t)$ is Gaussian white noise with the autocorrelation function $\langle \xi_j(t) \xi_i(t') \rangle = 2kT \delta_{j,i} \delta(t - t')$, and $F_j(t)$ is a “driving force” with zero time average, which may be stochastic. Since in most of the experimental situations we can suppose that the interaction between two particles can be well approximated with a hard core repulsion, we assumed that the particles are hard rods (see Fig. 1). The hard core interaction means that during the motion the particles are not allowed to overlap (a particle does not continue to move in its original direction if it touches another one). This rule complements Eq. (1). All particles have the same size b , while the period of the potential is $p = 1$. The size of the system or in other words the number of the periods is L . We have applied periodic boundary conditions. The positions of the particles were updated sequentially (one after another, from left to right) using the finite difference version of (1). We have checked other types of updating (random, from right to

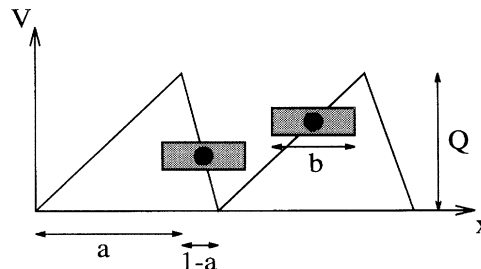


FIG. 1. Schematic picture of the system we consider showing two particles with size b subject to the sawtooth shaped periodic potential $V(x)$. The period of the potential is $p = 1$, where the lengths of the slopes are $\lambda_1 = a$ and $\lambda_2 = 1 - a$. The potential difference between the top and the bottom is Q .

left), with no change in the results. N and L go to infinity, while L/N remains finite, but usually $N \approx 20$ is large enough. During the integration of (1) δt was typically equal to 0.0001. Most of the runs required several days on a fast IBM RISC 6000/375 workstation.

Our model is one dimensional because the macromolecules serving as highways in biological transport can be assumed to be linear representing well-defined tracks. Thus, due to the hard core interaction, we also exclude the possibility of "passing." In higher dimensions (where the particles can get around each other) further effects are expected to take place. In addition to the case of periodic driving force, in the second part of the paper we shall also consider the case of constant driving force, because the latter case is (i) conceptually simpler, thus, it allows more direct interpretation of the simulational results and the analytic treatment of some limiting cases and (ii) a zero-mean signal can always be constructed as an alternating ($+F$ and $-F$) piecewise constant signal.

Normally, one single particle moves in the direction corresponding to the smaller uphill slope of the potential. However, there is a range of the parameters of the *periodic* driving force for which the particle migrates into the opposite direction [4–7]. In this regime we have found that *the gradual addition of particles* into the system *results in the change of their average velocity* back to the "normal" direction. We have tested this result for several different cases (including driving forces periodic in time [7] and distributed according to "kangaroo" statistics [4]), and we have found that this change of the current's direction is a universal property of the collective motion in our model. Figure 2 shows a simple example, where the driving forces are $F_j(t) = A \sin(\omega_j t)$ and the ω_j values are chosen randomly around a fixed value ω

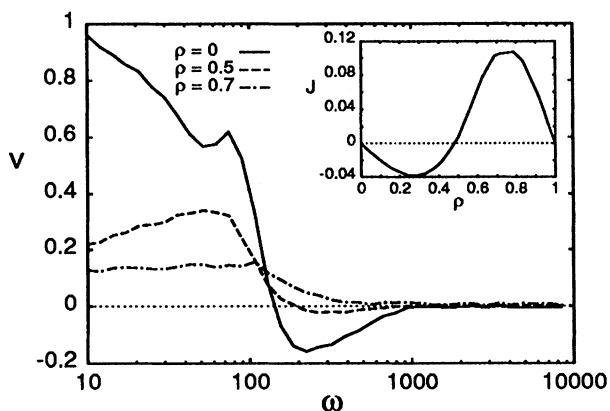


FIG. 2. The plot of the average velocity v as a function of the average frequency ω of the sinusoidal driving forces for three different values of the average covering $\rho \equiv bN/L$. The inset demonstrates the reversal of the particle current $J \equiv vN/L$ as a function of the average covering ρ , for $\omega = 175$. ($Q = 4$, $a = 0.8$, $b = 0.5$, $T = 1$, and the amplitude of the driving forces $A = 32$.)

with a dispersion of several percentage of ω (to avoid synchronization). The plot shows the average velocity as a function of ω , for various values of the average covering defined as $\rho \equiv bN/L$ ($0 < \rho < 1$). In the inset we have plotted the fundamental diagram: the particle current $J \equiv vN/L$ as a function of the average covering for $\omega = 175$.

Another interesting feature is observed if the average distance between two neighboring particles is fixed ($d \equiv L/N - b = \text{const}$) and we are changing the size of the particles.

Before describing our results we mention that it is easy to show that a system of length L consisting of N particles of size $k + b$ ($0 \leq b < 1$, $k = 1, 2, \dots$) is equivalent to a system of length $L - kN$ consisting of N particles of size b . Obviously, this kind of transformation has no effect on the motion of particles, therefore, it is enough to consider particles with sizes less than 1. In other words, any quantity is a periodic function of the size of the particles with period 1, i.e., with period equal to the period of the underlying potential.

Figure 3 shows the average velocity as a function of the size of the particles in the above mentioned case with sinusoidal driving forces for various values of ω . The velocity has very drastic changes. A large peak can be observed for b somewhat smaller than 1, and a smaller peak for b somewhat smaller than $1/2$. In most of the other cases we have studied, a large peak is observed just before b reaches 1 or for b a bit larger than 0 (or equivalently larger than 1), and a minimum (valley) on the opposite side of this integer value. This structure is repeated around $1/2$, but on a smaller scale. Sometimes this structure can be observed around $1/3$ and $2/3$.

Investigating the origin of this strange behavior of the particle size dependence on the average velocity we

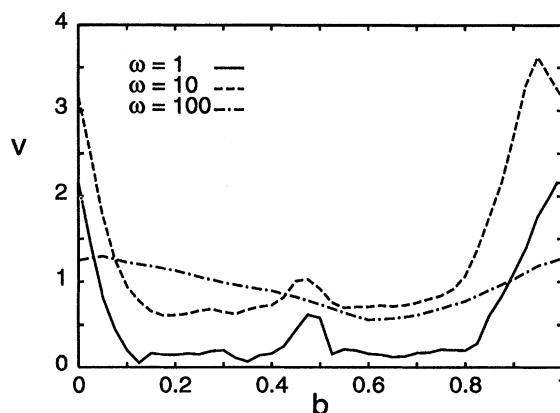


FIG. 3. The plot of the average velocity v as a function of the size of the particles b for three different values of the frequency ω of the sinusoidal driving forces. The average distance between two neighboring particles is $d = 0.5$. ($Q = 4$, $a = 0.8$, $T = 1$, and $A = 32$.)

examine the simplest case when the driving force is stationary: $F_j(t) = F$ and smaller than the uphill gradient of the potential.

Let us consider the case when the size of the particles is somewhat less than 1 and there are two particles in the neighboring valleys of the potential. Then the second particle is not able to jump further ahead until the first one jumps away. So the first one hinders the second one. Thus the average velocity is smaller than the velocity of a single particle. Figure 4(a) shows this situation for 15 particles. A *vacancy type* current can be observed, as a consequence of the traffic jams arising from the hindering of particles. This phenomenon is also related to jams common in one-dimensional driven diffusive systems and traffic models [16]. If the size of the particles is a bit larger than 1 and there are also two particles in the neighboring valleys, both of them cannot be in the minimum in the same time, therefore, the first one has a larger chance to jump further. In this case the second one indirectly “pushes” the first one. (But the first one also hinders the second one.) Thus, in spite of the hindering effects, the average velocity can be larger than

the velocity of a single particle. This situation can be seen in Fig. 4(b) for 12 particles. There are no jams and the density waves show that the particles help each other to jump through to the next valley. In case of slowly alternating external forces these effects (hindering and pushing) are expected to influence the net transport.

Figure 5(a) shows the average velocity as a function of the size of the particles in this stationary case, for various values of the average distance $d \equiv L/N - b$ between two neighboring particles. When d is infinity, the velocity is independent of the size of the particles, and identical to the velocity of a single particle. Decreasing d a velocity peak starts to develop for d just larger than $b = 0$, and a valley appears for b close to, but smaller than $b = 1$. This was explained in the previous paragraphs. As d is further decreased, another peak appears beyond $b = 1/2$ and also a valley before $b = 1/2$. This can also be explained in the above mentioned manner, taking into consideration that two particles can sit in the same potential valley if $b \approx 1/2$, and we can handle them as one particle with size $b \approx 1$. Decreasing the average

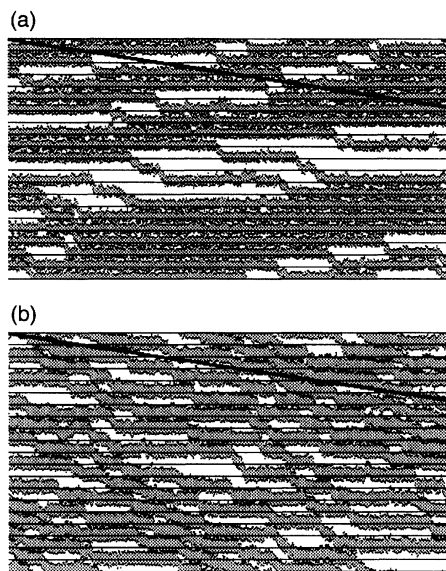


FIG. 4. Motion of the particles in the space-time domain. The time increases from left to right and the particles are moving downwards under the influence of the stationary driving force F . Horizontal lines represent the bottom of the potential valleys, and the wide slanted line represents the average motion of a single noninteracting particle. (a) 15 particles with size $b = 0.833$. A vacancy type current can be observed, as a consequence of the hindering effect of particles. The average velocity v is smaller than the average velocity of one single particle. (b) 12 particles with size $b = 1.166$. There are no jams, and the density waves show that the particles assist each other in jumping over to the next valley. v is larger than the velocity of a single particle. The average distance between particles is $d = 0.5$ in both cases.

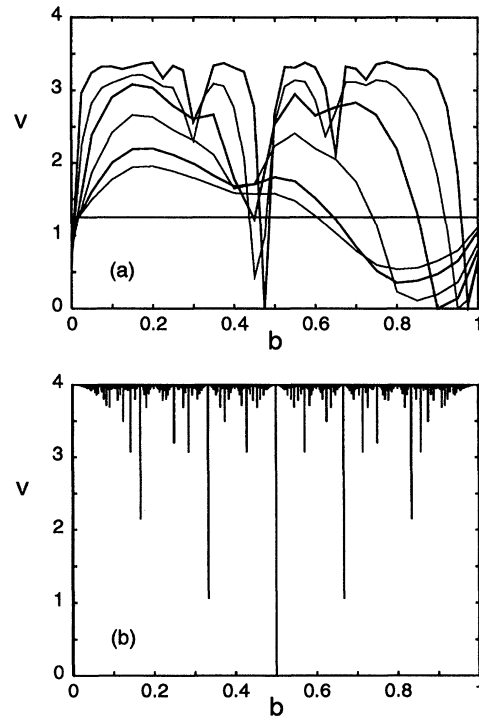


FIG. 5. The average velocity v as a function of the size of the particles b , when the driving force is stationary with $F = 4$. (a) The plot for different values of the average distance between two neighboring particles: $d = \infty$ (one single particle, the horizontal line) and $d = 0.6, 0.4, 0.2, 0.1, 0.05, 0.025$. (b) The plot in the limit when the average distance between two particles goes to zero. This discontinuous function has sharp minima for b rational and a value equal to F if b is irrational. ($Q = 4, a = 0.2$, and $T = 1$.)

distance further, valleys and peaks appear before and after $b = 1/3$ (three particles in one potential valley), $b = 2/3$ (three particles in two potential valleys), and so on at (almost) any rational value of b .

If the sum of the average distance and the size of the particles is a rational value, i.e., $b + d = n/m$, we can say that the structure is *commensurate*. For $d \ll 1$ the particles are distributed evenly and m particles can be found in n potential valleys. The minimum of the potential energy of the system is realized if every m th particle is sitting in the bottom of the potential valleys. Then, for $F = 0$, each particle has to jump a distance $1/m$ to reach the next minimum energy state of the system. Simple algebra shows that such a system (in which N particles are playing the role of a single particle) can also be described in terms of a modified sawtooth potential with a period $p' = 1/m$, where the lengths of the slopes are $\lambda'_1 = \{ma\}/m$ and $\lambda'_2 = \{m(1-a)\}/m$. The potential difference between the top and bottom states is NQ' , where

$$Q' = Q \frac{\{ma\}\{m(1-a)\}}{mam(1-a)}. \quad (2)$$

The notation $\{\dots\}$ means the fractional part of the value between the braces.

Thus, in the presence of the driving force F , we can calculate the average velocity as the velocity of a single particle using the formula derived by Magnasco [1] with parameters Q' , λ'_1 , λ'_2 , $F' = F$, and $T' = T/N$ ($T' \rightarrow 0$ for $N \rightarrow \infty$).

However, if the structure is incommensurate and the average distance is small, the corresponding modified potential of the whole system is almost flat and the system has a continuous translation symmetry. Therefore the particles can move with almost the maximum velocity $v_{\max} = F$.

The modified potential is also flat (or almost flat), if the structure is commensurate but ma is an integer number (or close to an integer number). This is the reason why we cannot see a valley before $1/5$, $2/5$, $3/5$, and $4/5$ on Fig. 5(a) as a consequence of $a = 0.2$.

Correspondingly, decreasing the average distance between the particles the minima of the valleys tend to the rational values. The values of the minima go to the values calculated from Magnasco's formula, and the width of the valleys goes to zero. For the other cases the velocity goes to $v_{\max} = F$. In the limit when the average distance is zero, we get a strange, discontinuous function with sharp minima for b rational and a value equal to F if b is irrational [Fig. 5(b)].

In conclusion, we have demonstrated that taking into account the interaction of Brownian particles migrating via overdamped dynamics along periodic structures re-

sults in a variety of novel cooperative effects. Among other possible applications, our results are expected to be pertinent from the point of biological transport involving finite density of protein molecules moving along substrates made of macromolecules. In particular, we have found a strong dependence of the average current on the particle size for sizes close to the period of the underlying potential. If thermal ratchet type models represent an adequate description of biological transport, our latter result is likely to be relevant in the understanding of the behavior of such molecular motors as kinesin or dyenin, since their size and the period of the corresponding microtubules are comparable (see, e.g., Ref. [12]). Effects caused by the finite size of the transported objects (e.g., other proteins, mitochondria, visualizing beads) represent potential subjects for further studies.

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