Collective transport of particles in a ''flashing'' periodic potential

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We consider the collective motion of finite size Brownian particles induced by a one-dimensional, spatially asymmetric, periodic potential which is turned ''on'' and ''off'' dichotomously. The particles interact through simple hard-core repulsion. We show analytically that this simple system exhibits an interesting collective behavior: (i) the direction of motion can change many times as the density of particles is increased; (ii) close to the maximal density, the average velocity depends on the size of the particles in a very complex way, both in sign and magnitude. [S1063-651X(96)50407-1]

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Recent theoretical and experimental works have shown that dissipative processes in structures possessing vectorial symmetry can induce macroscopic average motion, even in the absence of any macroscopic driving force or field gradient [1–9]. On the one hand, these studies may provide an appropriate framework to analyze the operation of the motor proteins in charge of, e.g., cellular transport or muscle contraction [10]. On the other hand, they can also lead to novel separation techniques. Indeed, a man-made device that creates a spatially asymmetric periodic potential switched on and off periodically in time was predicted to generate a net current which is highly sensitive to the diffusion coefficient of the particles [1], a claim experimentally confirmed with electrode devices [11,12] and optical tweezers [13].

Recently, special attention has been paid to collective effects which are clearly important: in many biological situations numerous motors operate together, and in artificial structures the effect of interactions is crucial for separation. Two models have been recently studied: (i) finite size particles (interacting through hard-core repulsion) in an asymmetric potential tilted back and forth [14]; (ii) a collection of motors, rigidly attached to each other, that independently adsorb and desorb (i.e., switch from on to off) from a periodic structure [15]. In both cases, collective effects lead to new features.

In this paper we focus on a situation closer in spirit to what would arise in one-dimensional (1D) artificial structures: we consider particles with hard-core repulsion, in an asymmetric potential that is switched on and off *at the same time for all the particles* and that is *at every instant flat on large scales*. This natural extension to many particles of the on-off model of Ref. [1] also leads to a rich phenomenology. In particular, for long enough duration of the ''off'' intervals, we prove analytically that the average velocity can change sign a few times as particle density is increased from 0 to 1, and that its sign and amplitude at high density is extremely sensitive to the particles size. The outline of the paper is as follows: we first introduce our model and the considered regime. After recalling the low-density limit we examine the high-density one. We then calculate how the average velocity evolves between these two limits before confirming our picture through simulations.

To set notations, we consider N overdamped Brownian particles of size b moving on a segment of length L. They are submitted to a ''sawtooth'' periodic potential $V(x,t)$, which is periodically turned ''on'' $[V=V_{\rm on}(x)]$ for a time $\tau_{\rm on}$ and then ''off'' for a time $\tau_{\rm off}$ $[V=V_{\rm off}=0]$ (see Fig. 1). Units are chosen so that the potential spatial period λ is 1, as well as the friction coefficient of the particles. The asymmetry of the potential is characterized by the length a of its steepest slope.

If x_j denotes the position of the (center of) particle j, the evolution of the system is then described by the Langevin equations:

$$\dot{x}_j = -\partial_x V(x_j,t) + \xi_j(t), \quad j=1,\ldots,N \tag{1}$$

which are coupled by the constraint that neighbor particles are not allowed to overlap: $(x_j - x_{j-1}) > b$. $\xi_j(t)$ is a Gaussian white noise of autocorrelation function $\langle \xi_j(t)\xi_i(t')\rangle$

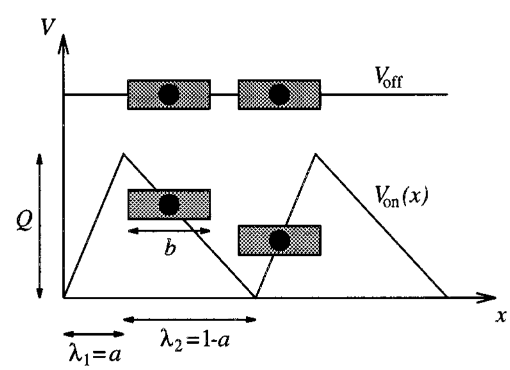

FIG. 1. Schematic picture of the system showing two particles of size b submitted periodically to the sawtooth periodic potential $V_{\rm on}(x)$ for a time $\tau_{\rm on}$, and then to the flat potential $V_{\rm off}$ for a time $\tau_{\rm off}$. The sawtooth potential has a period $\lambda=1$, sum of a short size $\lambda_1=a$ and a long one $\lambda_2=1-a$. The corresponding energy barrier is Q.

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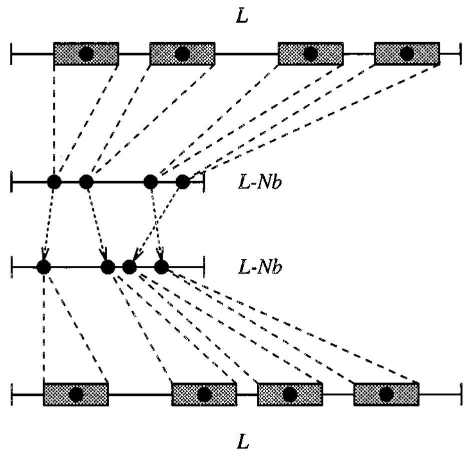

FIG. 2. During the motion of the particles in the flat potential $V_{\rm off}$, the real system can be reduced to a system of size $L-Nb$ with N noninteracting pointlike particles. The intervals between the particles are kept constant when switching from one system to the other.

$=2kT\delta_{j,i}\delta(t-t')$. We consider $0\le b<1$ as a system of particles of size $k+b$ (k integer) can readily be mapped back to the case $k=0$ (with the change $L\to L-Nk$).

Before going further let us briefly comment on a simple way to describe the diffusive ''off'' stage in a general case (see Fig. 2). The system can be ''compressed'' to a set of N *pointlike* particles in a system of size $L-Nb$, keeping the intervals between particles unchanged. Since these point particles are identical, whether or not they are allowed to cross does not affect the evolution of the system: when two pointlike particles meet we can either let them cross and swap (rename) them afterwards, or forbid crossing, the choice does not affect their final position. This means that the particles can be handled as *noninteracting* ones as long as they are reordered at the end of the ''off'' stage [16]. Inverting the ''compression'' procedure leads back to the original system.

Let us now investigate how the average velocity v of the particles depend on their size b and density $\varrho=bN/L$, in the limit of large systems (N and L go to infinity while ϱ remains finite). To get *analytical* solutions we focus on specific regimes, as was done for the simpler, one particle limit ($\varrho\to 0$) [1]. First the pinning potential $V_{\rm on}$ is taken strong enough so that during the time $\tau_{\rm on}$ the particles drift quickly to the positions corresponding to the nearest local energy minimum of the system, where they get trapped. This deep potential valley limit ($Q\gg kT$) furthermore suits fast separation purposes. Second, most of our results will be obtained in the limit where $\tau_{\rm off}$ is long enough for the particles to forget (modulo the period) their initial position on the sawtooth during an ''off'' period. The average displacement over a cycle is then that of initially randomly distributed particles during a single ''on'' phase.

In the low-density limit, a particle with random initial position in the $[-\lambda_2,\lambda_1]$ period [average $x=\frac{1}{2}(\lambda_2-\lambda_1)$] ends at $x=0$ after an ''off'' phase. The average progression per cycle is thus $\langle d\rangle=\frac{1}{2}(\lambda_2-\lambda_1)=1/2-a$ [1]. Let us now turn to the other extreme: an almost packed system $\varrho\approx 1$. As in previous studies of collective effects [14,15], the *commensuration* of the particle system to the potential period will play a crucial role.

To see this, consider the limit case $\varrho=1$ ($L/N=b$), where the system is equivalent to a single particle of size L, the position of which is measured by x_1 for example. Take now the limit of a very large system: $N\to\infty$. In the incommensurate case (b irrational), the particles are then uniformly distributed in the periods whatever the value of x_1, so that the whole system feels a flat potential whether the sawtooth potential is ''on'' or ''off'': the average velocity of the particles is zero. This is to be contrasted to the case of Ref. [15] where, as particles switched between ''on'' and ''off'' independently, motion could be obtained in the incommensurate situation. We now turn to the much richer commensurate case: $b=n/m$ in irreducible form. Simple algebra shows that the effective potential seen by the equivalent L-size particle during ''on'' periods is a sawtooth potential of period $\lambda'=1/m$ with two linear pieces of lengths $\lambda_1'=\{ma\}/m$ and $\lambda_2'=\{m(1-a)\}/m$ [14] (the notation $\{\ \}$ means the fractional part). The barrier height is NQ', where

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

The effective temperature is also modified: $T'=T/N$ (diffusion is slower), so that $NQ'\gg kT'$. Applying the single particle limit to the equivalent particle, we get its average displacement per cycle (which is that of every real particle):

$$\langle d\rangle=\frac{1}{2}(\lambda_2'-\lambda_1')=\frac{1}{2m}(1-2\{ma\}). \tag{3}$$

A formal problem with the above analysis is that the diffusion coefficient of the equivalent particle is kT/N so that randomization in the ''off'' phase cannot be achieved in a finite time $\tau_{\rm off}$ (in the limit $N\to\infty$, $\varrho=1$). Consider instead the commensurate case with a density $\varrho=1-\varepsilon$, $0<\varepsilon\ll 1$, and take first the limit $N\to\infty$. What are the differences with the $\varrho=1$ case? At the end of an ''on'' pinning stage, there are now a few very distant empty spaces at the top of some potential barriers, the sizes of which are usually not greater than b, that separate groups of $\simeq 1/\varepsilon$ ''touching'' particles. This gives the initial conditions for the following diffusing stage: in the ''compressed'' picture (Fig. 2), each group consists of many pointlike particles located at the same position, separated by distances of order b. So if the ''off'' time allows a free particle to diffuse on distances of order b, the particles will be randomly distributed (typical separation $\simeq\varepsilon b$). Upon switching the sawtooth potential ''on,'' to zeroth order in ε the average displacement is $\langle d\rangle$ as given by Eq. (3). Thus, the average velocity tends towards $\simeq\langle d\rangle/(\tau_{\rm on}+\tau_{\rm off})$ as ε goes to zero, $\tau_{\rm off}$ being kept constant but large enough to allow free diffusion over distances larger than b: $\tau_{\rm off}>b^2/(kT)$ in our units. A crucial point of this argument is that N should be larger than $1/\varepsilon$, indicating that $N\to\infty$, $\varrho\to 1$ is a singular limit [16].

This leads to a quite strange behavior for the high-density ($N\to\infty$, $\varrho=1-\varepsilon$) drift as a function of the particles size as illustrated by Fig. 3 (similarly as in Ref. [14]). The limit average displacement per on-off cycle $\langle d\rangle$ is an erratic, discontinuous function with sharp peaks [given by Eq. (3)] for

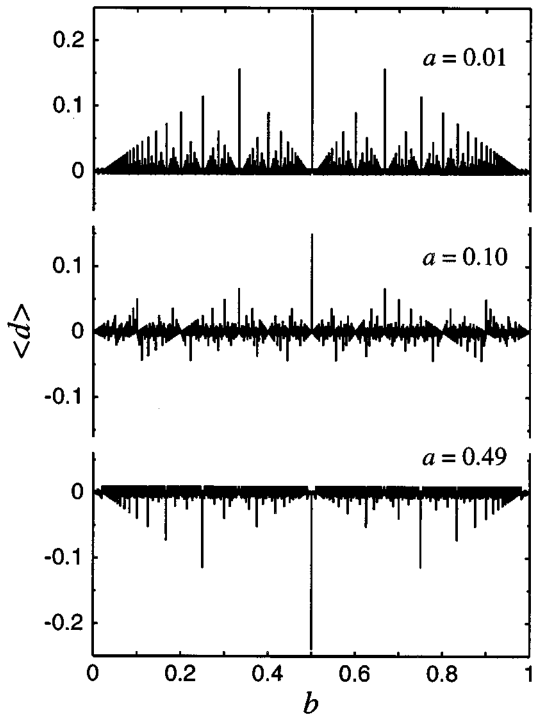

FIG. 3. High-density limit for the average particle displacement per on-off cycle $\langle d \rangle$ as a function of the particles size b, for different values of the asymmetry parameter a.

rational values of b, and zero otherwise. Both positive and negative peaks are present, in a pattern that depends on the value of the asymmetry parameter a.

Remember that at zero particle density, the average displacement per cycle is positive (if $a<0.5$), and independent of the size of the particles. Increasing the density from 0 to 1, it evolves to the discontinuous function of b shown in Fig. 3. The question is how this occurs. When the density is still less than one the function $\langle d(b) \rangle$ has to be continuous, due to the smoothing effect of the finite temperature. But we will now show that increasing the density from 0 to 1 while keeping the particle size b fixed, the velocity can vary nonmonotonically and can even change sign several times, along a route that will be sensitive to the actual value of b.

Let us start with a simple pedagogical example: $b=1/3$ and $a=0.5-b/4$. For very small particle densities, a particle is usually alone in some potential period or valley. Its average displacement per on-off cycle is about $b/4$, as it is the distance between its eventual position (the bottom of the valley) and its average starting position (the middle of the valley). At larger densities, when on average two particles fall into a valley, they will end in the configuration of minimal potential energy: the two particles touch each other, with the center of the right particle in the bottom of the valley. Thus, the center of mass of the two particles is $b/4$ far from the middle of the valley to the left. Therefore $\langle d \rangle$, the average drift during the ''on'' stage, is now about $-b/4$, a ''negative'' value. At even higher densities, with about three particles per valley, the average displacement will be about $b/4$ again.

Analytical calculations are actually possible for $b=1/m$ with $m=2,3,\ldots,$ as the valleys are then ''independent'':

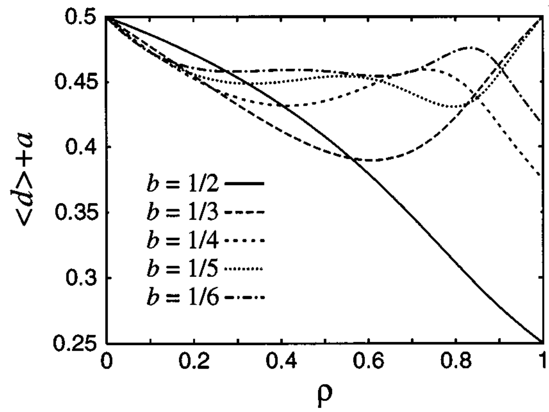

FIG. 4. The plot of $\langle d \rangle + a$ as a function of the density ϱ for five different values of b, valid if a lies in the appropriate interval, which is respectively [0,1/2], [1/3,1/2], [1/3,1/2], [2/5,1/2], and [2/5,1/2] in decreasing order of b.

when the potential is switched ''on,'' the particles remain in their starting valley, and the minimal energy configuration in each valley is independent of what happens in the neighboring ones. Always assuming that the particles are randomized before each ''on'' period, one can calculate the probabilities that $0,1,\ldots,m$ particles will start in the same valley (the

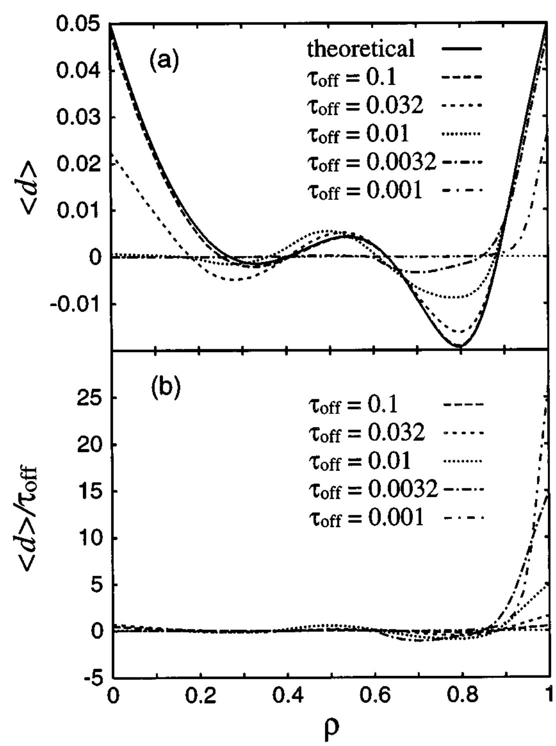

FIG. 5. The plots (a) and (b) show respectively $\langle d \rangle$ and $\langle d \rangle/\tau_{\mathrm{off}}$ as a function of the density ϱ in the case $b=1/5$, $a=0.5-b/4=0.45$, $kT=1$, for different values of τ_{off}. Supposing that Q is large τ_{on} can be chosen small enough ($\tau_{\mathrm{on}} \ll \tau_{\mathrm{off}}$) so that $\langle d \rangle/\tau_{\mathrm{off}}$ is a good approximation of the velocity $v=\langle d \rangle/(\tau_{\mathrm{on}}+\tau_{\mathrm{off}})$.

intervals between particles follow a Poisson distribution). By determining the corresponding minimal energy configurations at the end of the ''on'' stage, $\langle d\rangle$ can then be computed explicitly. This straightforward procedure becomes tedious for large m and leads to long formulas. Curves are plotted in Fig. 4, and we only give the simplest formula:

$$\langle d\rangle=\frac{1}{4}+\frac{1}{4}\left(\frac{1}{\varrho}-1\right)\left[1-\exp\left(-\frac{\varrho}{1-\varrho}\right)\right]-a \tag{4}$$

for $b=1/2$ and $0\leqslant a<0.5$. It is actually easy to see that for any rational value of b $(b=n/m)$, the quantity $\langle d(\varrho,a)\rangle+a$ does not depend on a within intervals where the minimal energy configurations are the same but for a shift of $-a$. Therefore, in Fig. 4, we have plotted $\langle d\rangle+a$ as a function of ϱ.

The figure shows that the average displacement (or velocity) of the particles is a nonmonotonous function of the density. For well chosen values of a (e.g., $a\approx 0.5-b/4$) the direction of motion can even change several times. The curves obtained are consistent with both the low-density result $\langle d\rangle+a=1/2$ and with our high-density ($\varrho\rightarrow 1$) estimate as quantified by Eq. (3).

Eventually, to investigate the range of validity of our analytical results, we performed numerical simulations using the compression picture, and present here (Fig. 5) the case $b=1/5$, $a=0.5-b/4=0.45$, $kT=1$, for different values of $\tau_{\rm off}$. For large values of $\tau_{\rm off}$ (e.g., $\tau_{\rm off}=0.3$), the simulation result is indistinguishable from our analytic predictions. Analysis also shows that the time for the randomization in the ''off'' state is larger at low density, in agreement with our estimate that it should scale as λ^2 at low density and rather as b^2 at high density [16]. More importantly, Fig. 5 shows that the features obtained in this paper survive the relaxation of the ''randomization'' hypothesis. It also proves that the high density velocities $v=\langle d\rangle/(\tau_{\rm on}+\tau_{\rm off})$ can be larger than the optimal low density ones: particles in the ''off'' state need not diffuse on a distance a but only on b, which allows us to reduce the cycle time.

In conclusion, we have analyzed the main features of the collective directed motion of finite size, overdamped Brownian particles in a one-dimensional, spatially asymmetric, ''flashing'' periodic potential. Through analytical arguments we have calculated the average particle velocity in certain limits, exhibiting a few striking points: its direction can alternate upon increase of the particle density, and its value is very sensitive to the particle size at high density. The one-dimensionality of the problem certainly favors the occurrence of such salient features. We, however, hope that this study will encourage the theoretical and experimental analysis of the influence of *collective effects* in real 1D, 2D, or 3D propelling devices [11–13]: a strong sensitivity to properties of particles and a highly nonlinear behavior are features that could be taken advantage of for separation purposes.

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[16] The ''compression'' picture of pointlike particles is valid in the continuous limit, when the underlying microscopic jump distance $\delta_{\rm mic}$ and time $t_{\rm mic}$ go to zero with the diffusion coefficient $\delta_{\rm mic}^2/t_{\rm mic}$ kept fixed. For very small but finite $\delta_{\rm mic}$ and $t_{\rm mic}$ this picture fails to describe the freezing of very large aggregates of ''touching'' particles. Our description thus holds up to a ''cap'' density (that tends towards 1 as $\delta_{\rm mic}$ and $t_{\rm mic}$ go to zero), beyond which the effective velocity will decrease to zero.