Transport of elastically coupled particles in an asymmetric periodic potential

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We study the motion of a chain of elastically coupled particles in an asymmetric potential. The particles are also subject to thermal fluctuations and a stochastic driving force of zero temporal average. The main motivation for investigating such systems originates from their partial analogy with a number of important models, including stochastic ratchets, the Frenkel-Kontorova model, and the various approaches to the microscopic description of friction and stick-slip motion having attracted great interest recently. We find that the collective behavior of the elastically coupled particles under certain conditions leads to an average velocity v which is larger than that of a single particle. The dependence of v on the coupling constant shows interesting anomalies discussed in the paper. [S1063-651X(97)05905-9]

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I. INTRODUCTION

In contrast to the macroscopic experience that transport phenomena are driven by a field gradient, recent studies have proposed a basically different transport mechanism. The key ingredients of this new transport process are broken spatial symmetry and nonequilibrium fluctuations. The latter is essential to avoid the consequences of the second law of thermodynamics, while the broken spatial symmetry selects the direction of the transport. There is no need for macroscopic driving forces to produce nonzero flux under these circumstances. A particle moving under such conditions is called a *ratchet*, referring to Feynman's example [1], demonstrating that it is impossible to extract work from a single heat source.

Assuming an underlying ratchetlike motion one can easily explain the—at first sight paradoxical—phenomenon of mass transport in living cells, frequently being sustained against a concentration gradient (e.g., in ion channels). This concept gave rise to the term *molecular motors* referring to the transport occurring by conformational changes of proteins on microscopical scale. The basic idea of ratchets may also be applied in technology as a tool for separating mixtures of granular materials [2].

The temporally correlated noise originates from interaction with an environment that is out of equilibrium. From a theoretical point of view this interaction can be represented either as a fluctuating force [3,5] or as a fluctuating potential [2,4]. In this paper we have restricted ourselves to the case of fluctuating force, also called the *correlation ratchet*.

Although most of the studies of ratchets have concentrated on the motion of a single particle, motivated by the experimental relevance of many interacting particles possible effects of collectivity have also been discussed in various contexts. Derényi and Vicsek [6] investigated the motion of an array of correlation ratchets interacting via hard-core repulsion. They found strong and complex dependence of the average velocity on the density and size of particles. Jülicher and Prost [7] showed the existence of dynamical phase transition for a rigid assembly of ratchets independently attaching and detaching to an asymmetric potential, while Derényi and Ajdari [8] studied the motion of finite size walkers in a fluctuating potential. These studies revealed that the collective motion of particles introduces a range of new and complex effects compared to the behavior of a single particle.

Our goal is to investigate the motion of particles coupled via springs with variable strength in an asymmetric periodic potential. This allows us to study the crossover from single to collective ratchet motion. We consider both the case when a different driving force, i.e., correlated noise, acts on each particle (asynchronous driving) and when the driving is uniform (synchronous driving).

This study may be useful not only in understanding collective behavior in ratchets, but also in models of friction and stick-slip motion, because there are many common features between the two problems. The starting point in many of the studies of friction is the equation of motion for a set of N elastically coupled oscillators that are subjected to a periodic potential due to the substrate. A special case is the Frenkel-Kontrova model [9], which has been used to study commensurate-incommensurate phase transitions. Similar models are also used in the study of energy transfer in long one-dimensional (1D) chains adsorbed on a periodic substrate [10].

The outline of the paper is as follows. In Sec. II we introduce the model and discuss the type of potential and the driving force that we use. The algorithm for solving the equations is discussed in Sec. III. The numerical results are presented in Sec. IV.

II. THE MODEL

We consider a linear chain of particles connected by springs and subject to an asymmetric potential $V(x)$ of period l (Fig. 1). It is assumed that the particles are put in a thermal bath represented by a white noise $\xi_i(t)$ and, in addition, they are subject to an external temporally correlated noise $y_i(t)$. We neglect inertia effects, thus the equation of motion of the particle i reads

$$\gamma\dot{x}_i = k(x_{i-1} - 2x_i + x_{i+1}) - \frac{\partial V(x_i)}{\partial x_i} + y_i(t) + \sqrt{2D}\,\xi_i(t), \tag{1}$$

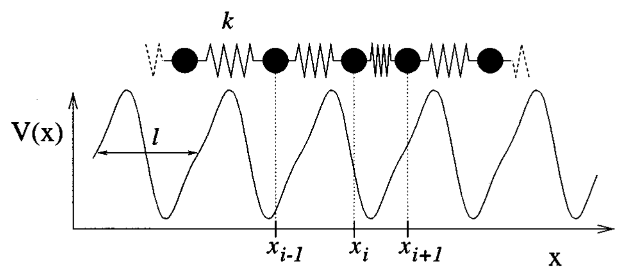

FIG. 1. Schematic representation of our system.

where k is the spring constant and D is the temperature. The initial length of the springs a does not enter Eq. (1), but it sets the density of particles: on average $\varrho = a/l$ particles fall into a period of the potential. We set the physical scales of the problem by putting $\gamma = 1$ and $V_{\max} - V_{\min} = O(1)$. The quantity of our major concern is the average velocity defined as the temporal average of the system's mean velocity

$$v = \lim_{T\to\infty} \frac{1}{TN} \sum_{t=1}^{T} \sum_{i=1}^{N} \dot{x}_i(t),$$

where N is the number of particles in a system of length L. The average velocity is a macroscopic quantity which can be measured in a real experiment in contrast to the position and velocity of individual particles.

As a ratchet potential we have used a differentiable potential of period $l = 1$

$$V(x) = -\tfrac{1}{2}\sin(2\pi x) - \tfrac{1}{8}\sin(4\pi x). \tag{2}$$

The span of this potential is about 1.1 and its asymmetry parameter (the ratio of the downhill region to the uphill region) is around 1/4. Motion in the potential Eq. (2) has been studied by several authors [11,12] and it has an advantage over the sawtooth potential: it is easier to treat numerically the movement in a differentiable potential than in a potential with discontinuous derivatives.

For synchronous driving we used a simple harmonic driving force

$$y_i(t) = A\cos\omega t \tag{3}$$

and for nonsynchronous driving we choose independent Ornstein-Uhlenbeck (OU) processes for each particle

$$\dot{y}_i = \frac{1}{\tau}(\sqrt{2Q}\,\eta_i(t) - y_i). \tag{4}$$

The noises ξ and η are uncorrelated both in space and in time, $\langle \xi_i(t)\xi_j(t')\rangle = \langle \eta_i(t)\eta_j(t')\rangle = \delta_{ij}\delta(t-t')$, yielding a temporally correlated but spatially uncorrelated fluctuating force $y_i(t)$: $\langle y_i(t) y_j(t')\rangle = \delta_{ij}(Q/\tau)e^{-|t-t'|/\tau}$. It is important to note that both of these driving forces have zero average. The finite velocity of the particles will develop due to the asymmetry in the potential $V(x)$.

Let us review the two limiting cases for the values of the spring constant k. If $k=0$, the particles are decoupled, the behavior of the system reduces to the much studied behavior of a single correlation ratchet (i.e., single particle) [3,5], and it is independent of the particle density.

In the limit when $k\to\infty$ the particles are strongly coupled, every particle ''feels'' the forces exerted on any other particle. As a consequence, the motion of the particles is uniform and given by the motion of a single particle in an effective potential

$$V_{\text{eff}}(x) = \frac{1}{N}\sum_{i=1}^{N} V(x+ia)$$

at effective noise strengths. This effective potential depends on the ratio of the period of the chain and the period of the ratchet potential. If ϱ is rational the system is commensurate, otherwise it is incommensurate. Commensurability, together with the synchronous or asynchronous nature of the driving, determines the behavior of the strongly coupled system by cancellation of various terms in Eq. (1).

In the commensurate case the effective potential is also a ratchet potential, but with a smaller amplitude. In this case a finite current is possible in a finite system, but in the thermodynamic limit ($N\to\infty, N/L=\varrho$) the current vanishes, since the amplitudes of the effective thermal noise and driving scale as N^{-1}. For synchronous driving, i.e., when the same external force acts on every particle, the driving does not cancel out, so the system becomes equivalent to a $D=0$ correlation ratchet in an effective potential. Nonzero current is possible provided the driving noise is strong enough.

If the period of the chain and of the potential are incommensurate then in the thermodynamic limit the potential cancels out ($V_{\text{eff}}=$ const), so that the current is zero, even for synchronous driving.

In the case of intermediate spring constants the behavior is governed by the interaction of the effective parameters which leads to nontrivial cooperative motion. We are going to investigate the behavior of the system in this regime by numerically integrating Eq. (1). In particular, we are interested in medium temperature and driving strength regimes since for large values of D or of the driving strength diffusion dominates and in the opposite limit the particles are not capable of hopping to the neighboring potential well. This region has been of major interest in previous studies since potential applications to biology require the fluctuations to be in the intermediate range.

Since the two models under consideration have ten parameters each the numerical exploration of the whole parameter space would have needed a prohibitively large amount of computer time. Three of the parameters fix the physical scales (mass, length, and time) but the rest can have any value. Many of the parameter sets correspond to trivial or previously studied behavior of the system, which is not interesting from our point of view. The considerations we have presented earlier in this section allow us to reduce the size of the parameter region to be scanned and thus make our goal achievable.

III. THE ALGORITHM

Equations (1) and (4) [or (3)] are of the form of $\dot{\mathbf{u}} = \mathbf{A}\mathbf{u} + \boldsymbol{\eta}$. If $\mathbf{A}$ was a constant then by diagonalizing $\mathbf{A}$ the model would simply reduce to an OU process. In our case **A** does depend on **u** and the equation can be only locally mapped into an OU process. For a small number of vector components in **u** it is worth diagonalizing matrix **A** each time step, perform an infinitesimal OU step, and then transform the result back into real space [13]. Since the linear chain in our model may consist of many particles this algorithm would be very time consuming. Instead we exploit the fact that half of **A** (the equations for y's) are already in diagonal form and thus they can be solved exactly

$$y(t+\Delta t)=y(t)e^{-\Delta t/\tau}+P\left(\left[\frac{Q}{\tau}(1-e^{-2\Delta t/\tau})\right]^{1/2}\right),$$

where $P(\sigma)$ denotes a random number drawn from a Gaussian distribution with zero average and variance σ. In the case of synchronous driving $y_i(t)$ is given by Eq. (3) so only the equations for x need to be integrated.

The equation of motion (1) was solved using an $\mathcal{O}(t^3)$ method, which is a variant of the numeric scheme used by Schneider and Stoll [14] for integrating stochastic partial differential equations. The method for the case of asynchronous driving reads

$$\Delta x_i^{(0)} \leftarrow \Delta t\left(k(x_{i-1}-2x_i+x_{i+1})-\partial_i V+\frac{\tau}{\Delta t}(1-e^{-\Delta t/\tau})y_i\right)$$

$$\Delta x_i^{(1)} \leftarrow \Delta x_i^{(0)}+\frac{\Delta t}{2}[k(\Delta x_{i-1}^{(0)}+\Delta x_{i+1}^{(0)})-(2k+\partial_i^2 V)\Delta x_i^{(0)}]$$
$$+P[\sqrt{Q\tau(2\Delta t/\tau-e^{-2\Delta t/\tau}+4e^{-\Delta t/\tau}-3)}]$$
$$+P(\sqrt{2D\Delta t})$$
$$x_i(t+\Delta t) \leftarrow x_i(t)+\Delta x_i^{(1)}. \qquad (5)$$

The first assignment is a simple Euler integration step, then the next order corrections are added to improve the method. The first stochastic part of $\Delta x_i^{(1)}$ is due to the randomness in the driving while the second part originates from the white thermal noise.

IV. NUMERICAL RESULTS

The numerical solution of Eq. (1) was performed for a system of size L incorporating N particles. We have applied periodic boundary conditions. The integration time step was $\Delta t=0.01$ which allowed us to integrate until reasonably large times ($t \simeq 10^5$). We have checked the stability of our numerical scheme by using smaller time steps, but they yielded no visible difference in the data. Most of our investigations were performed at $L=10$. The results were checked against finite size effects by reproducing them on a larger ($L=100$) system. In this case the actual data changed only by a small amount, but the overall qualitative behavior remained the same. We have concentrated on investigating the stationary velocity v as a function of various parameters of the model. The values of the parameters were chosen to represent the regions where we expect the most interesting phenomena to be present. First we study the effect of varying the driving amplitude and the coupling constant k, then we analyze the dependence on the density and some dynamical aspects of the motion. In all cases described below we used $D=0.1$ to ensure that thermal fluctuations are large enough, but are not too strong, which would result in an unbounded diffusion of the particles.

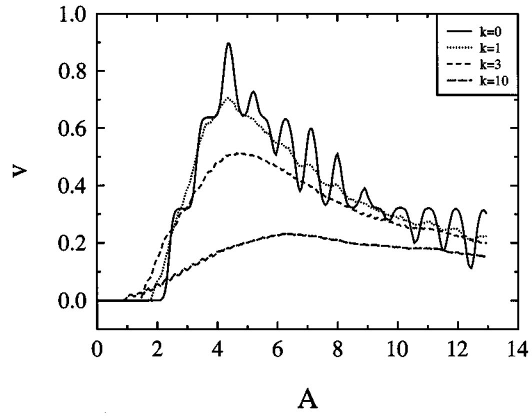

FIG. 2. The current vs the synchronous driving amplitude for various couplings.

For synchronous driving [Eqs. (1) and (3), $\omega=1$] with no coupling ($k=0$, solid line in Fig. 2) we obtained a typical velocity-driving curve of a thermally activated, periodically driven single ratchet [15]. Using larger coupling the curve flattens out, mostly velocity decrease can be observed. Nevertheless, at low driving strengths (below $A\simeq 2$) there is a region where the velocity *increases*, as is shown in Fig. 3. At this particular set of parameters the maximal velocity is reached at $k\simeq 3$. In the uncoupled ($k=0$) case the velocity was extremely small, so, in this case, it is appropriate to speak about coupling activated motion in analogy with thermal noise activated motion for a single stochastically driven ratchet [3].

In the case of asynchronous driving ($\tau=1$), to obtain a global picture of the behavior, we measured v in an incommensurate system (Fig. 4). Increasing the driving amplitude the velocity at small coupling strengths (i.e., nearly independent particles) increased as has been seen in previous studies of the single particle motion [3,11]. Introducing stronger coupling between the particles the velocity decreased as ex-

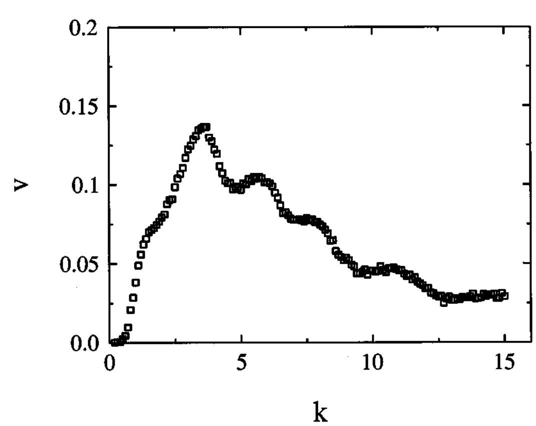

FIG. 3. The current v as a function of spring constant k for $A=1.9$.

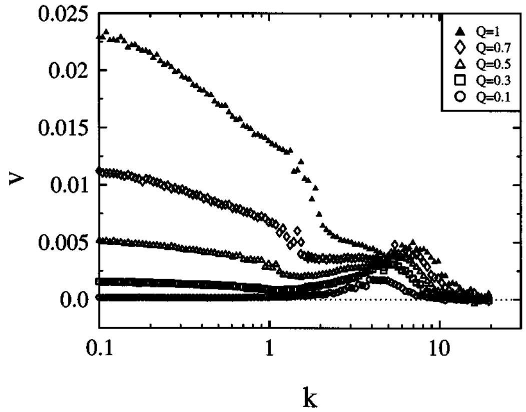

FIG. 4. The current vs the coupling for various asynchronous driving amplitudes.

pected from previous discussions. In the range $k \simeq 2-5$ one can observe a resonance in the velocity which comes from collective motion of the particles, as we show later. For large driving (large Q) this resonance is not able to compensate the decrease in the velocity. But for sufficiently small driving one can observe an *enhancement* of the velocity (Fig. 5, $Q=0.3$). The maximum velocity for this set of parameters is about twice the velocity produced by uncoupled particles. In Fig. 5 we have also plotted the data obtained for the same parameters except that $\varrho=1$ $(N=L)$, i.e., for a commensurate system. For that case the velocity goes to zero already for rather small values of k, whereas for the incommensurate system the velocity shows a resonant peak.

The observed resonance is a stochastic resonance [16] and its appearance is due to the interacting time scales of the correlation in the driving, the overdamped harmonic motion, and the motion in the potential. Consequently there must be a shift in the position of the resonance with the changing of the driving strength. This shift can be easily seen in Fig. 4. The peak current at the resonance becomes larger with increasing driving, but over some critical Q there is no enhancement compared to the uncoupled case. The resonance may occur only at medium coupling strengths and in incommensurate systems. The reason for this is that for a small coupling the particles are mostly confined to their own potential wells no matter what ϱ is, the coupling reduces the effective temperature but not the potential yielding a smaller average velocity. Also, for large coupling the current goes to zero even in the incommensurate case, so no resonance can develop.

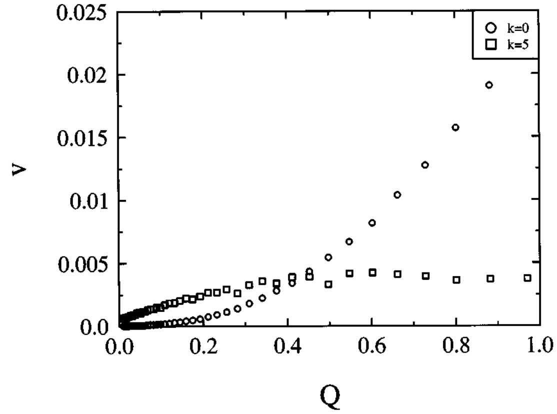

FIG. 6. The current as a function of driving amplitude for the uncoupled case ($k=0$, circles) and near resonant coupling ($k=5$, squares).

In Fig. 6 we show the current for two different couplings as a function of the driving amplitude in order to demonstrate the dependence of the enhancement on the driving. In agreement with Fig. 4 the velocity enhancement is seen for Q's smaller than 0.45 and no enhancement is observed for larger driving.

We have seen that the commensurability has an effect on the resonance. In order to study this effect we put a varying number of particles in our system and measured the stationary velocity. The size of the system is again $L=10$, so zero current is expected at multiples of 2 and 5. In fact, a vanishing current was observed mostly at multiples of 10 and at a smaller amount at 15, 25, and 35 (Fig. 7).

To characterize the dynamics of the resonant peak seen in Fig. 5 we studied the correlation function of the distance between neighboring particles. The distance function is defined as

$$\Delta_i(t) = x_{i+1}(t) - x_i(t),$$

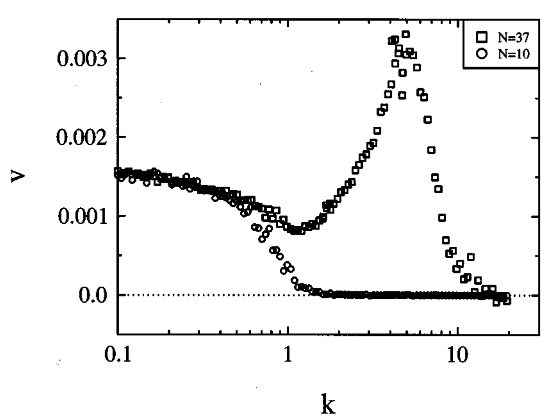

FIG. 5. The current v as a function of spring constant k for $Q=0.3$.

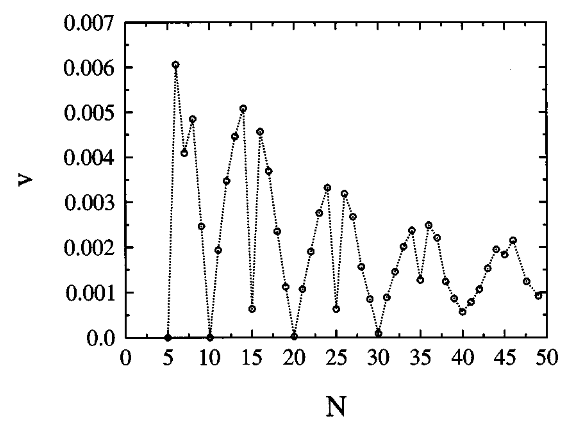

FIG. 7. The current for various numbers of particles in a system of size $L=10$.

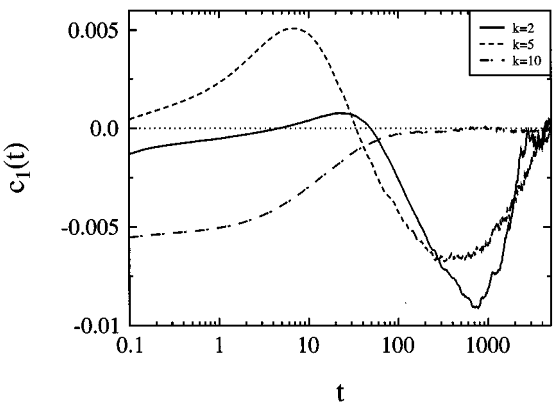

FIG. 8. The correlation function of two distances between three consecutive particles $[c_1(t)]$ for various couplings.

and it is straightforward to define a set of correlation functions as

$$c_i(t) = \langle \Delta_i(t)\Delta_0(t)\rangle - \langle \Delta_i(t)\rangle\langle \Delta_0(t)\rangle.$$

So, $c_0(t)$ gives the autocorrelation function of the distance between two particles and $c_1(r)$ gives the correlation function of the two distances between three consecutive particles. In Fig. 8 we show the correlation function $c_1(t)$ for some values of k using the same parameters as in Fig. 5 (asynchronous driving). For the resonant value of k $(k=5)$ positive temporal correlation develops, while in the other cases the correlation is negative, meaning that the motion of a particle is mostly localized oscillation. The positive correlation peak appears not at $t=0$ but at some positive time which corresponds to a traveling wavelike motion of the chain, as opposed to the biased random walks of the particles in the case of $k=0$. This shows that the observed stochastic resonance is a collective effect of the coupled particles. We have seen similar resonance not only by changing the coupling strength but also via changing the correlation time τ of the driving colored noise. In fact, the system can be tuned into its resonant state by many parameter combinations provided they result in characteristic time scales of the same order of magnitude.

Having explored the most relevant subset of the parameter space our results show that using a suitable coupling between individual particles in an asymmetric potential it is possible to enhance their average velocity. For the case of synchronous driving (harmonic external force) we show a regime where the motion in the system is activated by coupling the particles together, which is similar to the original noise activated ratchet motion. For the case of asynchronous driving (external colored noise), we also observe enhancement, but only for relatively small driving amplitudes. Although this effect is not as significant as the one in the synchronous case, it may be of larger importance for models of biological motion, where the driving is intrinsically stochastic.

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