Mirror symmetry breaking through an internal degree of freedom leading to directional motion

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We analyze here the minimal conditions for directional motion (net flow in phase space) of a molecular motor placed on a mirror-symmetric environment and driven by a center-symmetric and time-periodic force field. The complete characterization of the deterministic limit of the dissipative dynamics of several realizations of this minimal model reveals a complex structure in the phase diagram in parameter space, with intertwined regions of pinning (closed orbits) and directional motion. This demonstrates that the mirror symmetry breaking, which is needed for directional motion to occur, can operate through an internal degree of freedom coupled to the translational one.

The possibility of motion rectification at the Brownian scale from nonequilibrium fluctuations is an interesting question already posed by Smoluchowski [1] and Feynman [2]. It has been shown that directional motion (the appearance of net flow in phase space) of Brownian particles, without any macroscopic gradient or force, can be achieved provided that the potential exhibits spatial asymmetry and detailed balance is broken. This latter condition assures that the system is out of equilibrium. Systems with a periodic potential profile but spatial asymmetry, called *ratchets*, have been addressed as systems in which nonequilibrium fluctuations can induce directional motion [3]. They have attracted much attention on the basis that they can help to understand the physics of molecular motors [4], along with the possibilities they open for using these ideas in superconductors [5], Josephson junctions [6], quantum dots [7], and in the promising world of nanotechnology [8].

Hereon, we will focus on ''motor'' systems such that their internal degrees of freedom are essential for net directional motion to occur. The motivation for this problem came initially from the (bio)molecular motors field when it was found [9] that kinesin direction of motion along microtubules could be reversed by modifying the architecture of a small domain of the protein called ''neck region.'' These discoveries could suggest that the mirror-symmetry-breaking mechanism responsible for the directional motion performed by these proteins could lie in their own structure rather than in their environment. In this paper we will consider the type of systems with a mirror-symmetric environment for its translational degree of freedom (u^{tr}). The symmetry-breaking mechanism acts through an internal degree of freedom (u^{int}) coupled to it; that is, we will consider a dimer model (two degrees of freedom). We are interested in the minimal conditions for the operation of this system as a motor (being capable of moving against an applied field). Previous works have also analyzed directional motion in dimer models [10] but the potential for u^{tr} considered was ratchet *ab initio*. On the contrary, the dimer model we present in this paper is inmersed in a sym-

metric environment. This is also the case for the system recently studied by [11]. There, internal degrees of freedom (more than two) experience a flashing interaction potential, while ours is a rocked system. After a complete characterization of the deterministic limit of the dynamics, which reveals the basic nonlinear mechanics of directional motion, we will briefly discuss the gross features of the Langevin dynamics of this model and its utility as a help to design new technologies at microscales and nanoscales.

As a working mechanical visualization of this model, one can use two overdamped and coupled Brownian particles, with positions u_1 and u_2 [so $u^{tr}=1/2(u_1+u_2)$ and $u^{int}=u_2-u_1$] moving in a periodic, symmetric potential $V(u+1)=V(u)=V(-u)$ and being driven by center-symmetric periodic forces $F_i=-F_i(t+T/2)i=1,2$ of period $T=2\pi/w$ [12]. In the deterministic limit, the equations of motion read

$$\dot{u}_1=-V'(u_1)-\partial_1 W(u_1,u_2)+F_1(t), \qquad (1)$$

$$\dot{u}_2=-V'(u_2)-\partial_2 W(u_1,u_2)+F_2(t). \qquad (2)$$

We impose on $W(u_1,u_2)$ the general condition of being a function of the relative distance $u^{int}=u_2-u_1$, so the partial derivatives with respect to u_1 and u_2 verify $\partial_1 W(u_1,u_2)=-\partial_2 W(u_1,u_2)$. We will consider the cases in which W is a convex and a nonconvex function of u^{int}.

Equations (1) and (2) remain invariant under the symmetry transformations $(u_1,u_2,t)\rightarrow(-u_2,-u_1,t+T/2)$ provided that $F_1(t)=F_2(t)$ and $(u_1,u_2)\rightarrow(-u_2,-u_1)$ if $F_1(t)=-F_2(t)$. With this proviso one can easily show that any averaged ''directional motion'' in phase space is necessarily (and straightforwardly) null : if there exists a solution of Eqs. (1) and (2) with nonzero velocity, by symmetry we can find another solution with the same velocity but opposite sign, so no net motion can be observed when averaging over the phase space. Directional motion in this strong sense can only occur if the inequality $F_1(t)\neq \pm F_2(t)$ holds, regardless of the specific form (convex or nonconvex) of the interaction potential W. Taking $F_i(t)$ from the class of functions $F(t)=F_{ac}\sin(\omega t+2\pi\delta)$ [the simplest periodic center-symmetric function $F(t)=-F(t+T/2)$], there are two ways of breaking the symmetry of this system [$F_1(t)\neq \pm F_2(t)$].

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(i) $\max_t F_1(t) \neq \max_t F_2(t)$.

(ii) $\delta_1 \neq \delta_2 \bmod \frac{1}{2}$.

That is, applying forces on each particle with (i) different amplitude or (ii) different phase. We will focus on the limit cases for each situation: we will consider $F_{ac}^{(1)}(t)=0$ and $F_{ac}^{(2)}(t)\neq 0$ as well as $\delta_1=0$ and $\delta_2\neq 0$. Any other situation verifying the condition $F_1(t)\neq \pm F_2(t)$ is just a combination of these two possibilities.

In particular, most numerics have been performed with the simplest choices

$$V(u)=\frac{Q}{(2\pi)^2}\cos(2\pi u), \quad W(u_1,u_2)=\frac{K}{2}[(u_2-u_1)-l_0]^2.$$
(3)

The convexity of W and the dissipative character of the dynamics have the important consequence that the partial order among initial conditions is preserved (monotonicity property or ''no-passing rule'' [13]). The monotonicity property says that if at a time $t=t_0$ two initial conditions $\mathbf{u},\mathbf{v}$ verify that $u_1(t_0)<v_1(t_0)$ and $u_2(t_0)<v_2(t_0)$, then for any time $t>t_0$ the inequalities $u_1(t)<v_1(t)$ and $u_2(t)<v_2(t)$ hold. This property leaves small room for deterministic complexities of this nonintegrable dynamics. For example, the asymptotic mean velocity of all trajectories in the phase space is unique, and vibrating pinned solutions (closed orbits) cannot coexist with mobile ones. The choice of $W(u_1,u_2)$ implies another symmetry relation: the system remains invariant under the transformation $(u_1,u_2,l_0)\rightarrow(-u_1,-u_2,1-l_0)$. That is, if we have a mobile solution of Eqs. (1) and (2) for a value l_0 we have another mobile solution with opposite velocity for $1-l_0$. For fixed values of (Q,K,l_0) we have approximated numerically to optimal accuracy the function $\mathcal{J}(F_{ac},\omega)$ where $\mathcal{J}$ is defined as the asymptotic flow in phase space $\mathcal{J}=\langle \dot{u}^{tr}\rangle$.

In Figs. 1(a) and 1(b) the $\mathcal{J}(F_{ac})$ profiles at typically low ($\omega=2\pi\times 0.01$) and high frequencies ($\omega=2\pi\times 0.1$) for $F_1(t)=0$ and $F_2(t)=F_{ac}\sin(\omega t)$ [case (i) —different amplitudes] are shown for the values $(Q,K,l_0)=(2,1,1/4)$. As can be seen from Fig. 1(a), the complex stairlike structure of the relation $\mathcal{J}(F_{ac})$ for low frequencies is qualitatively indistinguishable from those exhibited by single-particle rocking ratchets (asymmetric potential). However, when the frequency is increased, the direction of motion for fixed l_0 can be either positive or negative [Fig. 1(b)], something which cannot occur in deterministic single-particle rocking ratchets. The primary structure of mobility bands in F_{ac} separated by vibrating pinned solutions is well understood in terms of saddle-node bifurcations signaling the onset of global flow in phase space. Figure 1(c) shows the bifurcation diagram of pinned (vibrating) solutions. ϕ represents the mean value over a period of the external force of the traslational variable, $\phi=\langle u^{tr}\rangle_T$. Thick lines represent stable orbits whereas thin ones represent unstable ones. This bifurcation diagram neatly determines the intervals of motion in F_{ac} as well as the local sign of $\mathcal{J}$ in both interval's edges. The numerical inspection of the scaling of intermittencies density is one of a type-I
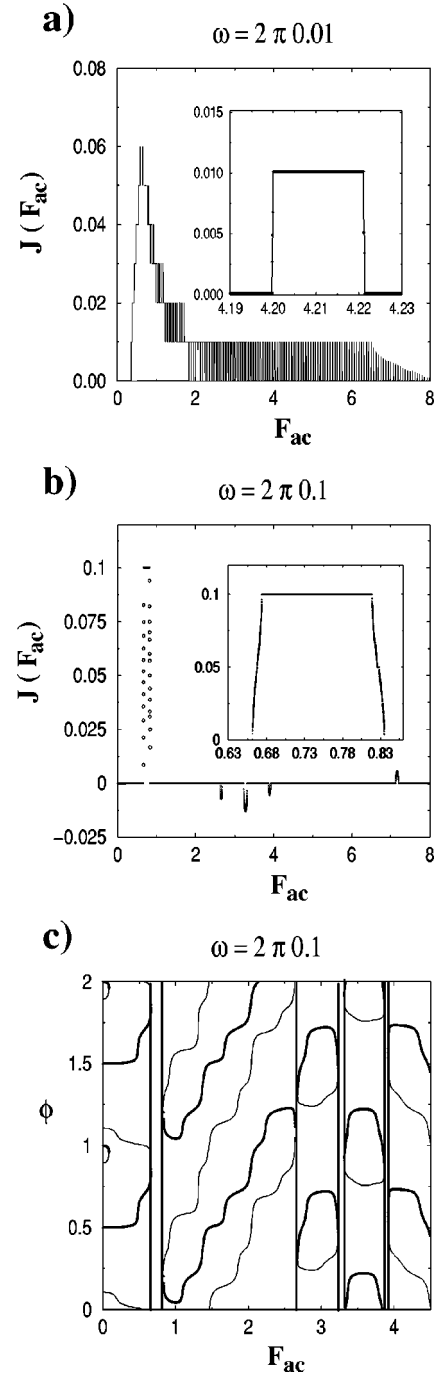

FIG. 1. (a) and (b) Flow as a function of the amplitude of the external force F_{ac} at two different frequency values. (c) Bifurcation diagram using the mean value over a period of u^{tr} $\phi=\langle u^{tr}\rangle_T$ as relevant magnitude for $\omega=2\pi\times 0.1$. Intervals between vertical lines correspond to mobility bands in F_{ac}.

intermittency scenario (associated here with quasiperiodicity and frequency locking), giving the staircase aspect of $\mathcal{J}(F_{ac})$ close to the mobility onset.

In Fig. 2(c) an example of the $\mathcal{J}(F_{ac})$ profile for $F_1(t)=F_{ac}\sin(\omega t)$, $F_2(t)=F_{ac}\sin(\omega t+2\pi\delta)$ [case (ii) —different phase] with $(\omega,\delta)=(2\pi\times 0.05,0.35)$ $[Q,K,l_0=(2,1/2,1/4)$ shows clearly the complex alternation of positive and negative flows in the phase space. Again the mobility bands in
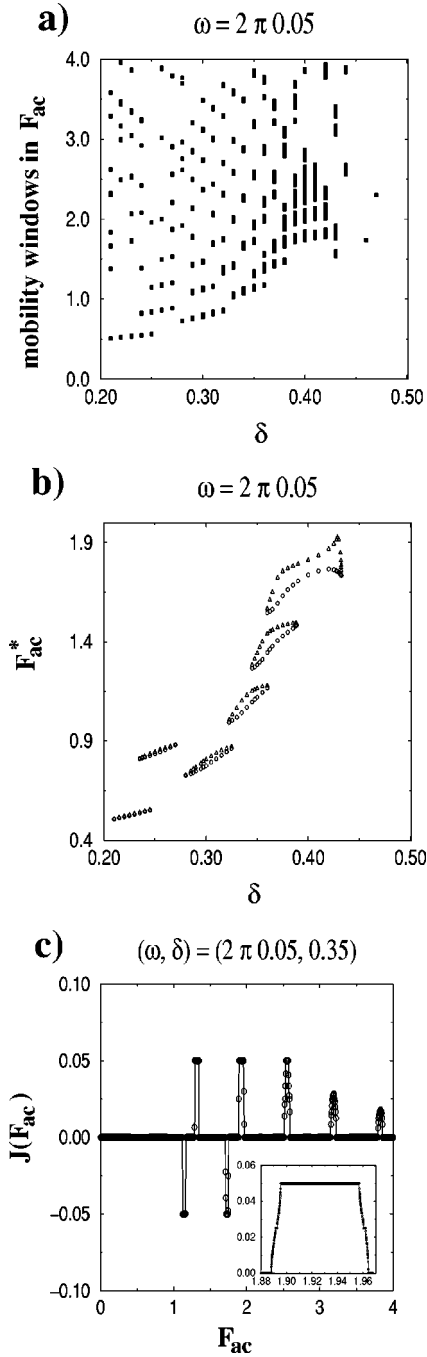
a) $\omega = 2\pi\, 0.05$

b) $\omega = 2\pi\, 0.05$

c) $(\omega, \delta) = (2\pi\, 0.05, 0.35)$

FIG. 2. (a) Mobility bands in F_{ac} at $\omega = 2\pi \times 0.05$ as a function of the phase difference δ. (b) Lower and upper values of F_{ac} for the first mobility band as a function of δ. (c) Dependence of the velocity with F_{ac} for $(\omega, \delta) = (2\pi \times 0.05, 0.35)$.

F_{ac}, when (ω, δ) remains fixed, appear after the collision of stable and unstable orbits by means of a saddle-node bifurcation. In Fig. 2(a) we have plotted for $\omega = 2\pi \times 0.05$ the width in F_{ac} of the mobility bands at different values of δ. Figure 2(b) shows the values of F_{ac} where the first and second bifurcations occur, that is, the smaller value of F_{ac} where the stable and unstable orbits collide (depinning transition) and the nearest value where they emerge again (pinning transition), which determines the width of the first mo-
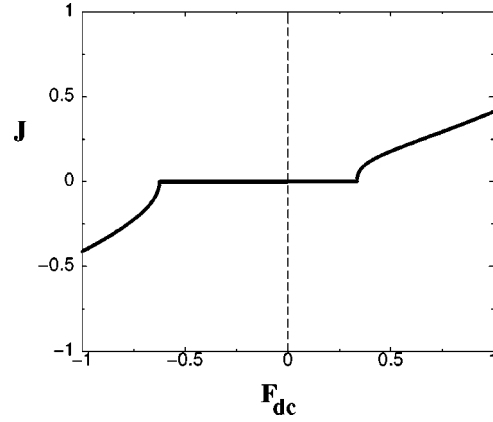

FIG. 3. Flux $\mathcal{J}$ in the presence of a constant force: it can be clearly seen that the depinning force is smaller in the ''driver'' particle direction (positive one).

bility band. As usual, very simple dynamics reveal astonishingly complex phase diagrams whenever time and length scale competition plays a role.

We want to stress that the rectification mechanisms in the models presented here are completely different from other rocking ratchet systems with internal degrees of freedom (dof) [10], where the symmetry is broken *ab initio* by the asymmetric potential $V(u)$. The only system with a symmetric environment for the traslational dof. in which symmetry breaking comes through the internal dof. is the flashing system (as oposed to rocking) studied by Porto *et al.* [11]. We also remark that the rectification mechanisms for the cases numerically studied in the preceeding paragraphs show some differences: in case (i) we observe directional motion even at the adiabatic limit (slow varying forces) whereas in case (ii) directional motion occurs only at finite frequencies. When applying forces with different amplitudes, the ratchet effect lies in the fact that one particle acts as a cargo, so it is easier to move the system in the ''driver'' particle direction than in the other. In Fig. 3 it can be clearly seen that the depinning force is smaller in the driver's direction than in the other. When applying different phases, the ratchet effect is more subtle: the combined effect of phase value and strength F_{ac} determines which particle plays the role of cargo and which one the role of driver. The absence of the adiabatic limit for this case (ii) precludes the use of time-independent schemes for understanding rectification in an intuitive way. In Fig. 4 two trajectories corresponding to both limit situations [cases (i) and (ii) above] analyzed are drawn. Although our system is a rocking ratchet, there is an alternative view in which, looking at the equations of motion for the traslational variable u^{tr},

$$\dot{u}^{tr} = \frac{Q}{2\pi} \sin(2\pi u^{tr}) \cos(\pi u^{int}) + \frac{1}{2}[F_1(t) + F_2(t)], \quad (4)$$

one can see for both situations, cases (i) and (ii), that the time dependence (periodic or quasiperiodic) of u^{int} allows the interpretation of the first term on the right-hand-side (rhs) as a flashing potential for u^{tr}. The directional motion can thus be
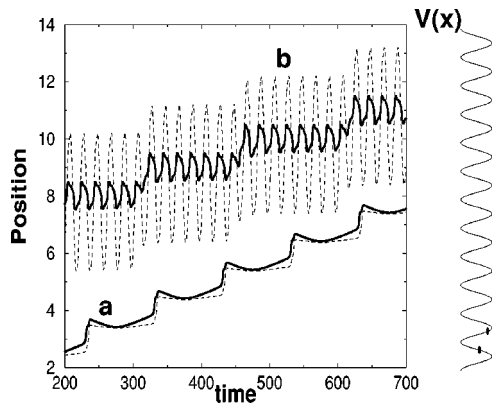
FIG. 4. Deterministic trajectories [$u_1(t)$ dashed line and $u_2(t)$ solid line] for the two models discussed. (a) corresponds to different amplitudes [case (i)] $(\omega, F_{ac}) = (2\pi \times 0.01, 0.35)$ and (b) to different phases [case (ii)] $(\omega, F_{ac}, \delta) = (2\pi \times 0.05, 1.284, 0.35)$.

seen as the result of the adequate synchrony between external force on u^{tr} and the periodic flashing potential.

When the convexity condition on the interaction potential $W(u_1, u_2)$ is removed and nonconvex interaction (such as double-well or Lennard-Jones) potentials are considered, the monotonicity property (which severely restricts the complexity of the dynamics) is lost, and generically the space is partitioned in basins of attraction corresponding to attractors with different asymptotic velocities. The description of the dynamics becomes thus more complex. The phase portrait shows, for certain regions of parameter values, chaotic attractors and there appear new bifurcations (other than that observed for the convex case: pitchfork, generic saddle-node, and stability interchange) as the parameters change. Anyway, the existence of net flow (i.e., a nonzero phase-space average of asymptotic velocities) in phase space is a generic property in wide regions of parameter space, as in the convex case.

We are dealing with rockinglike systems [3] where the rectification mechanism is completely deterministic, so when introducing noise $\xi_1(t)$ and $\xi_2(t)$ in Eqs. (1) and (2) [white Gaussian noise with correlation function $\langle \xi_i(t)\xi_j(s) \rangle = D\delta_{i,j}\delta(t-s)$, $i, j = 1, 2$, being $D = k_B T$ the diffusion coefficient] the mobility bands widen (fluctuation-induced depinning) and $\mathcal{J}$ decreases with increasing noise strength (within the deterministic mobility bands). Both phenomena are eas-

ily explained in the limit of small noise [14]. For high D the phenomenon of current reversal [15] arises too and when noise strength is high enough diffusive motion dominates and no directional motion can be observed.

The proteins of the kinesin superfamily are just composed of two globular ''*heads*'' (catalitic domains that move over the microtubule using the energy delivered in ATP hydrolysis). As mentioned before, recent experimental work suggests that the mechanism for directionality may rest on the characteristics of the flexible structure joining both domains. ATP-hydrolysis induces conformational changes in these proteins, that is, acts through their internal degrees of freedom that may provide the symmetry breaking needed for the directional motion along the microtubule. The detailed modeling of these conformational changes of the kinesin is beyond the scope of this work; nevertheless, the generic model discussed in this paper could help us to understand in the simplest mechanical terms the role of the internal degrees of freedom in molecular motors.

Rigorous results on general simple models like this could serve to guide or inspire new technological applications, especially in the field of nanotechnology. A simple nanoscale realization of the type of motors considered here would consist of clusters of entities (particles or macromolecular agregates) with different electrophoretic mobilities joined with the aid of ''flexible'' molecules or polymers. In order to reproduce the symmetric environment it will suffice to place this engine in a row of symmetric obstacles (electrodes, for instance). When applying an ac electric field, because of the difference in the electrophoretic mobilities, different periodic forces will act on each cluster, making it possible to observe directional motion.

In summary, the analysis of these minimal models convincingly demonstrates that the mirror symmetry breaking needed for directional motion to occur can act through an internal degree of freedom even though the overall position of the system experiences a symmetric environment.

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