# Active elastic dimers: self-propulsion and current reversal on a featureless track

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We present a Brownian inchworm model of a self-propelled elastic dimer in the absence of an external potential. Nonequilibrium noise together with a stretch-dependent damping form the propulsion mechanism. Our model connects three key nonequilibrium features – position-velocity correlations, a nonzero mean internal force, and a drift velocity. Our analytical results, including striking current reversals, compare very well with numerical simulations. The model unifies the propulsion mechanisms of DNA helicases, polar rods on a vibrated surface, crawling keratocytes and Myosin VI. We suggest experimental realizations and tests of the model.

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Directed motion without an imposed external gradient in a homogeneous, isotropic environment is seen not only in living systems [1] but also in agitated granular matter [2, 3]. Can these apparently diverse systems be understood in a unified manner? We argue here that they can, and present a model which applies, suitably interpreted, to the movement of helicases on DNA [4], the directed motion of macroscopic polar rods lying on a vertically vibrated surface [2], the crawling of keratocytes which contain treadmilling actin [5] and the walking of processive motors [6] such as Myosin VI on actin filaments [7]. While not losing sight of the application to particular organisms or devices, our focus is on the general principles governing propulsion by rectification of an unbiased input active noise in a homogeneous medium.

In all the systems mentioned above, macroscopic directed motion of the center-of-mass (CM) arises via a coupling to internal coordinates, as a result of two crucial features – an asymmetrical environment for the internal coordinates and external energy input. Unlike in traditional "Brownian ratchet models" [8] of directed motion, the asymmetry of interest in the above systems is *internal* to the motile objects, and does not lie in an external periodic potential. Our approach is distinct from that of [9] where the external potential plays a central role, and also differs from the dynamical systems approach of [10]. The present model is similar in spirit to [11, 12] but simpler, and differs in several important details as seen below. We find an unexpected range of possible behaviors, especially in the dependence of the motion on the details of the nonequilibrium noise.

Our model self-propelled object is a dimer whose two heads are coupled by a spring, in a homogeneous, dissipative, noisy environment. The damping coefficients of the heads depend on the relative coordinate or *strain*. The noise on the particles is made of two parts – a *thermal* part whose strength is determined by a fluctuation-dissipation relation with the strain-dependent damping, and a nonequilibrium or *active* part, with strength independent of the damping, which represents the external energy input.

Our results are as follows: (i) The steady-state average of the CM velocity is in general nonzero and exhibits counter-intuitive reversals of direction as a function of the strengths and characteristics of the drive and the dampings. (ii) The steady state displays two other key nonequilibrium features: the mean internal force as well as the the equal-time correlation of the relative coordinate to the CM velocity are both nonzero. (iii) Active noise *alone* will not result in propulsion, even in the presence of an asymmetric internal potential; the strain-dependent damping is an essential ingredient. (iv) The preceding results, obtained by perturbative analytical solution of our model Langevin equations, with the coefficient of the stretch-dependent damping as a small parameter, are confirmed in detail by direct numerical solution of the equations of motion of the particles.

The heads of the dimer are two point masses $m_i$, $i = 1, 2$, with positions $x_i(t)$ at time $t$ and relative coordinate $x \equiv x_1 - x_2$ connected by a spring potential $U(x)$, with a minimum at $x_m$, and acted upon by viscous damping and noise with a nonequilibrium component. Thus the Langevin equations of the particles, in the Itô interpretation, are

$$m_i \dot{v}_i + \alpha_i(x) v_i = -\partial_i U + \sqrt{2\alpha_i(x) k_B T}\, f_i + \sqrt{A_i}\, \zeta_i \quad (1)$$

where $v_i$ are the velocities of the two heads, the overdot indicates a time-derivative, $\partial_i \equiv \partial/\partial x_i$, $\alpha_i(x)$ are damping coefficients which depend on the internal coordinate $x$, the terms containing the unit-strength, independent Gaussian white noise sources $f_i(t)$ and $\zeta_i(t)$ encode thermal and nonequilibrium agitation respectively, $k_B$ and $T$ are Boltzmann's constant and the thermodynamic temperature, and $A_i$ is a measure of the external energy input. We consider stretch-dependent dampings with $\alpha_i(x) > 0$ to ensure positive dissipation. For calculational convenience and concreteness we consider smooth spring potentials, but the qualitative results of our model

hold for any confining $U$.

Before solving (1), some general features are worth noting. The noise-averaged internal velocity $\langle \dot{x} \rangle = 0$ in the steady state, as long as $U$ confines $x$ so that such a steady state exists. Now consider the special case where the $\alpha_i$ are independent of $x$. By inspection of (1), we see then that the individual velocities $\langle v_i \rangle = 0$ even for a non-centrosymmetric $U(x)$, despite the presence of the nonequilibrium noises $\zeta_i$, and even for the "two-temperature" [13] case $A_1/\alpha_1 \neq A_2/\alpha_2$. Stretch-dependent damping is crucial to produce drift of the CM coordinate in this model.

For a stiff enough spring, the dimer will explore small values of $x$ so that $\alpha_i(x) \simeq \gamma_0 + \gamma_i x$ where, for simplicity and with only trivial loss of generality, we have taken the $x$-independent part of the dampings on the two heads to be equal. Averaging over the noise in (1), we find

$$\frac{\langle v_i \rangle}{(\gamma_1 + \gamma_2)} = \frac{\langle U'(x) \rangle}{\gamma_0(\gamma_1 - \gamma_2)} = -\frac{\langle x v_i \rangle}{2\gamma_0} \qquad (2)$$

where the prime denotes differentiation with respect to $x$. This relation connects three key quantities – mean drift velocity, correlation of internal coordinate and drift velocity, and mean internal force – each of which can be nonzero only away from thermal equilibrium. In particular, we see that a nonzero mean internal force (a force dipole [14]) is linked to $xv_i$ correlations, and that either leads to drift if the damping is stretch-dependent ($\gamma_i \neq 0$). The above relation also elucidates the manner in which an internal asymmetry in $x$ leads to macroscopic directed motion: the drift velocity and the internal coordinate are correlated in the presence of a nonequilibrium driving force.

Before analyzing our model in detail we examine four examples where internal frictional asymmetry and nonequilibrium noise lead to directed motion.

(i) Structural studies [15] together with the findings of a recent molecular simulation [4] of the PcrA helicase motor on single stranded DNA are of particular interest: its protein domains 1A and 2A contract around ATP and catalyze its hydrolysis which then actively stretches them apart. Stretch-dependent damping as in our Eq. (1) is encoded in the fact that in the ATP-bound (free) state 1A has a higher (lower) barrier to motion than 2A. The periodic potential in [4] is centrosymmetric, and serves only to provide the barriers that define the mobility. Holding the relative coordinate out of equilibrium, in this case by maintaining a disequilibrium between ATP and ADP + $P_i$, results in motion in the direction of 2A.

(ii) Polar granular rods on a vertically vibrated, horizontal plate were studied in [2]. The two ends of the rod have different friction, so damping depends on the tilt, which is the internal coordinate of interest. The nonequilibrium agitation being uncorrelated to this frictional asymmetry, the CM of the rod translates.

(iii) In the crawling of cells or cell-fragments driven by "treadmilling actin" [5], the relevant internal coordinate is the instantaneous degree of polymerization, averaged over all filaments. This quantity is maintained in a nonequilibrium steady state by the balance between ATP-aided polymerization at the leading edge, and passive depolymerization at the trailing edge. This leads to more focal adhesions at the front of the cell. The stretched cell thus detaches primarily at the rear, resulting in net translatory motion.

(iv) In the motion of Myosin VI [7] the detachment of the forward head is inhibited by the extension of the linker connecting it to the rear head. The differential binding of the forward head depending on the extension of the linker mimics our stretch-dependent damping, and ATP hydrolysis provides the energy source.

Our model thus provides a unifying understanding of four quite distinct self-propelled systems.

To understand qualitatively how the dimer walks, consider the case where the nonequilibrium noise and the stretch-dependent damping (with a simple form interpolating smoothly between $\Gamma$ for $x > 0$ and $\Gamma' < \Gamma$ for $x < 0$) act only on one head of the dimer, say particle 1. Let particle 2 have a fixed damping coefficient lying between $\Gamma$ and $\Gamma'$. Suppose the active noise consists of discrete dimer-stretching events separated by intervals whose mean $\tau$ is much larger than the relaxation time $\tau_d$ of the dimer. Then, if noise compresses (stretches) the dimer, particle 1 retracts faster (slower) than particle 2, leading to translation of the CM in the direction of particle 1. Suppose instead the active noise consists of a succession of small impulses, at intervals $\tau \ll \tau_d$ (effectively white noise as in this paper), then the dimer is kicked many times before it can relax. Head 1, whose damping increases with stretch, will accumulate a smaller displacement than head 2, so that the net displacement will be in the direction of head 2. This latter behavior is in fact what our calculations and numerical studies find. A purely equilibrium thermal white noise, with variance equal to $2k_BT$ times the stretch-dependent damping, will of course fail to produce any net motion, because increases in the noise amplitude compensate precisely for the enhanced damping.

Analytical expressions for the inchworm speed, the average internal force and related statistical descriptors of the motion can be obtained in a perturbative treatment, expanding the damping coefficients to leading order in $x$. The value of this approach is that it elucidates the separate and essential roles of the $x$-dependent damping and the nonequilibrium noises, and shows the connection of the mean drift speed to the mean internal force and correlations of $x$ with the CM velocity $V$. We choose $m_i = m$ and take a harmonic internal potential $U(x) = \frac{1}{2}ax^2$. This simplifies considerably the perturbation theory calculations that follow, without losing any of the essential physics. We also assume that the active noise is absent

for $t < 0$ and that at $t = 0$, the variables $x$, $\dot{x}$ and $V$ are at equilibrium at temperature $T$. A formal solution for $V(t)$ and $x(t)$ can be written, using the propagators from the linearized version of the equations (1), treating all the nonlinearities as source terms, from which we approximate the solutions to successive orders in perturbation theory. Since we are interested in *velocities* and their correlations with position coordinates, we find it convenient to retain inertia, particularly in the numerical calculation, so as to avoid ambiguities in solving our stochastic differential equations [16]. Our numerical studies are, however, entirely in the overdamped regime.

Numerical simulations were performed using an Euler-Maruyama scheme [17]. For simplicity, we take $x$-dependent damping on only one of the particles, say the particle 1, while the other particle has a constant value of the damping coefficient ($\gamma_2 = 0$). Specifically, we choose $\alpha_1(x) = \frac{1}{2}\left[(\Gamma + \Gamma') + (\Gamma - \Gamma')\tanh(x/w)\right]$, where $w$ is the width over which the strain-dependent damping changes over between the two extreme values of $\Gamma$ and $\Gamma'$. In this particular form, we have $\gamma_0 = (\Gamma + \Gamma')/2$ and $\gamma_1 = (\Gamma - \Gamma')/2w$. We scale masses, lengths and times by $m$, $x_m$ and $m/\gamma_0$ respectively and use a constant dimensionless time step of $\Delta t = 10^{-2}$. Averages are reported over $n = 10^6$ realizations of the noise. We choose plausible values of $a = 0.05$, $k_BT = 0.01$ based on those quoted in [4] for the dimeric PcrA helicase and take $(\Gamma + \Gamma') = 2$ in dimensionless units. To vary $\gamma_1$, we fix a value of $w$ and change $(\Gamma - \Gamma')$.

The linearized version of the equations (1), retaining the nonequilibrium noise, can be solved exactly. To this order, the noise averaged steady state values of the CM velocity and the internal force vanish. However, the equal time correlators have a distinct contribution from the nonequilibrium noise. In particular, the steady state value of the equal time correlator between the internal coordinate and the CM velocity is

$$\langle xV\rangle_0 = \frac{(A_1 - A_2)}{4(\gamma_0^2 + am)}. \qquad (3)$$

where the subscript 0 indicates the order in perturbation theory. Notice that $\langle xV\rangle_0$ is proportional to $\Delta T_{neq} \equiv (A_1 - A_2)/\gamma_0$, which has a precise interpretation as the difference in the effective temperatures of the nonequilibrium noise terms of the two heads constituting the dimer. At thermal equilibrium, by contrast, all equal-time correlations between $x$ and $V$ must vanish. The nonzero correlation (3) between $x$ and $V$ leads to nonzero steady-state averages for $V$ and $x$ at first order in perturbation theory through (2). Note from (2) and (3) that a nonzero mean drift velocity and mean internal force require $\gamma_i \neq 0$, i.e., stretch-dependent friction, in addition to the two-temperature scenario just described.

From equation (2), we notice that since $x \to -x$ and $v_i \to -v_i$ is a symmetry of the equation, $\langle xv_i\rangle$ must be even in the $\gamma_i$. A calculation of the equal time correlator

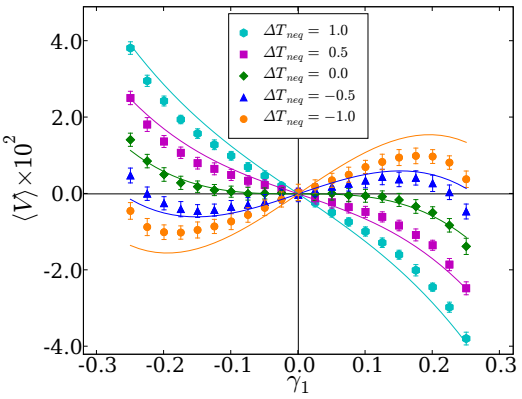


FIG. 1: (Color online) CM velocity as a function of the stretch dependent damping coefficient $\gamma_1$ for various $\Delta T_{neq}$ with $\gamma_2 = 0$ and $w = 4.0$. $\Delta T_{neq}$ was changed by fixing the value of $A_1 = 1.0$ and varying $A_2$. The solid lines are the corresponding perturbation theory calculations from equation (4).

$\langle xV\rangle$ to next order in perturbation theory yields

$$\begin{aligned}\langle xV\rangle_2 &= C_0\,(\Delta T_{neq}) + C_1\,(\Delta T_{neq})^2\,(\gamma_1 + \gamma_2)^2 \\ &+ C_2\,(\Delta T_{neq})\,A\,(\gamma_1 - \gamma_2)^2 \\ &+ C_3\,(\Delta T_{neq})^2(\gamma_1^2 - \gamma_2^2) + C_4 A^2(\gamma_1^2 - \gamma_2^2) \qquad (4)\end{aligned}$$

where $A = A_1 + A_2$ and the $C_i$ are coefficients depending on $a$, $\gamma_0$ and $m$. Notice from the above equation that if both $\gamma_1 = \gamma_2$ and $\Delta T_{neq} = 0$, $\langle xV\rangle$ vanishes and hence there can be no motion of the CM coordinate at this order. The slope of the $V$ vs. $\gamma_1$ curve at the origin is proportional to the value of $\Delta T_{neq}$. Tuning the value of $\Delta T_{neq}$ changes the slope and hence the small $\gamma_1$ dependence of $V$. However at large $\gamma_1$, this effect becomes small and the $V$ goes as a power of $\gamma_1$. Thus there must be a current reversal at some $\gamma_1$. Equation (4) indeed predicts current reversals as a function of the $\gamma_i$ depending on the values of the $A_i$. Numerical simulation results confirm this (Fig. 1) and the current reversals agree reasonably with perturbation theory calculations.

With the increase in $A_i$, the CM velocity does not saturate in our simple model. This is because the harmonic spring can stretch indefinitely and thus the dimer can be in an infinite number of states defined by the relative coordinate $x$. A real molecular motor, on the other hand, cannot consume an indefinite number of ATP units and thus its velocity saturates with the increase in ATP concentration. Modifying $U(x)$ so that the effective range of $x$ is limited should give rise to a saturation of the CM velocity with increase in the input energy.

In the presence of an external load we find a linear relation, to lowest order in perturbation theory, between the steady state CM velocity and the applied force. The reason for a linear relation is that the applied external

force does not alter the mechanism of energy uptake in our simple model.

We also find a generalized efficiency [18] $\eta \approx 2m\gamma_0\langle V\rangle^2/A$ to leading order in perturbation theory, in the absence of an external load. With $\gamma_1 = 0.1$, $\gamma_2 = 0$ and $A_1 = 1.0$, $A_2 = 0.0$, we find $\eta \approx 0.2\%$.

The results above are for the case of a harmonic spring potential and a non-centrosymmetric $\alpha_i(x)$. A non-centrosymmetric $U(x)$ and a centrosymmetric $\alpha_i(x)$ also yields directed motion. Crucially, even in this case, the damping must be $x$-dependent for a nonzero drift velocity. A non-centrosymetric $U(x)$ alone does not lead to nonzero $\langle V\rangle$. We have confirmed this with an explicit numerical simulation.

A few words comparing our model to that of [11]. Although the idea of stretch-dependent damping is present in these papers, our model is much simpler in the way the separation of equilibrium and nonequilibrium forces are presented. In [11], stretch dependent damping is *induced* by activity whereas in our model it is present even in the absence of the nonequilibrium driving noise. It does not lead to directed motion because of the the strength of the equilibrium noise exactly balances the dissipation according to the fluctuation-dissipation theorem. Directed motion is induced by the acive noise whose strength is independent of the $\alpha_i(x)$. Also in our model, equation (2) explicitly clarifies the manner in which asymmetry in an internal degree of freedom is coupled to a macroscopic coordinate in the presence of nonequilibrium noise, and leads to directed motion. That this is also proportional to a nonzero average internal force highlights the nonequilibrium nature of the phenomenon.

A likely realization of this model is [19] in the form of a colloidal bead with a polymer tail. The damping on the CM of the polymer will depend significantly on its stretch, while that on the bead will not. Subjecting this composite colloid to nonequilibrium noise (chemical reactions, catalysis at its surface [20], fluctuating laser interference patterns) should cause it to drift in the direction of its instantaneous orientation. One-dimensional versions could be constructed using optical tweezers in a line trap geometry. This system could serve to test our theory.

Tests should focus on (2) as well as the phenomenon of current reversal (Fig. 1). In our model the dampings and their $x$-dependences are properties intrinsic to the dimer in the absence of active noise. Changing the strength of the active noise should change the numerators in (2), leaving the denominators unchanged, thus allowing a test of the two equalities in (2). Current reversals (Fig. 1) are best probed by altering the active noise levels on each head of the dimer.

Several natural generalizations of our model suggest themselves, and will be investigated in the near future. These include Poisson or other active noises, dimers moving in more than one dimension, coupled arrays or an elastic continuum of active particles [21], and coupling to hydrodynamic flow.

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