Negative resistance and anomalous hysteresis in a collective molecular motor

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A spatially extended model for a collective molecular motor is presented. The system is driven far from equilibrium by a quenched additive noise. As a result, it exhibits anomalous transport properties, namely, negative resistance and a clockwise hysteresis cycle. The phase diagram and the region of negative resistance are calculated using a Weiss mean field theory. Intuitive explanations of the anomalous transport properties as well as details of its energetics are given.

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I. INTRODUCTION

The study of noise in nonequilibrium systems has revealed a rich collection of constructive effects. Three celebrated examples are noise induced phase transitions in spatially extended systems, where noise can induce macroscopic order and spatial patterns [1–3]: molecular motors or ratchets, where nonequilibrium fluctuations can help to rectify thermal noise inducing a systematic motion in a Brownian particle [4–8]; and stochastic resonance, where noise can improve the response of a system to a given signal [9].

Nonequilibrium noise induced phase transitions are formally identical to equilibrium phase transitions and critical phenomena. In fact, a simple Weiss mean field theory, combined with stochastic calculus, is currently the simplest and most powerful analytical tool to predict qualitatively the phase diagrams of these systems [1]. As in equilibrium, a noise induced phase transition of second order can be interpreted as a spontaneous symmetry breaking.

On the other hand, molecular motors consist of single Brownian particles moving in asymmetric potentials and subject to some source of nonthermal fluctuations. Here the asymmetry of the potential seems to be a necessary ingredient to have systematic motion.

Recently, Reimann et al. [10] nicely combined ideas from noise induced phase transitions with those from molecular or Brownian motors. In their work, they devised a system of many Brownian particles where a multiplicative noise induces a spontaneous symmetry breaking, and the corresponding asymmetry is used by the system to rectify fluctuations, exactly as in a Brownian ratchet. As expected, they found a ratchet effect in a system whose dynamics is completely symmetric [11].

However, the system considered has a much more intriguing and unexpected behavior regarding its response to an external force. An external force compels the system to choose one of the asymmetric macroscopic phases. Therefore, the symmetry breaking is no longer spontaneous. Since this symmetry breaking induces the systematic motion of the Brownian particles through a nontrivial ratchet effect, it turns out that the asymmetry created by the force can induce a motion against the force, even for very small forces. In this way, the authors of Ref. [10] found that the system can have negative mobility or negative resistance.

The model also presents an anomalous hysteresis cycle. The combination of negative resistance for nonzero external force and spontaneous symmetry breaking for zero external force creates a hysteresis cycle when the force is modulated from negative to positive values. Due to the negative transport coefficient, the cycle has a clockwise orientation, just the opposite to the orientation of “normal cycles” in systems close to equilibrium.

To our knowledge, this is the first simple system exhibiting negative resistance. It is well known that one can build a circuit with negative resistance, but involving a number of components including a powered operational amplifier [12]. Systems with negative differential resistance—i.e., where current is a decreasing function of the external force—are also known [13].

The system studied in [10] is completely different. The mobility is nothing but the transport coefficient which relates the current to the force in the linear regime (i.e., for small forces). The Green-Kubo formula ensures that every transport coefficient is positive for a system close to equilibrium. In fact, the second law of thermodynamics implies that the transport coefficients are positive. Therefore, negative transport coefficients can be found only in systems far from equilibrium.

Negative resistance prompts the general question of how the Green-Kubo formula is modified when applied to systems far from equilibrium. The question is undoubtedly of great theoretical relevance in nonequilibrium statistical mechanics. Moreover, simple systems with negative transport coefficients will probably have a number of important technological applications.

All these considerations demand a further exploration of the phenomenon of negative resistance. In this paper we study another model that also exhibits negative resistance. Our model has an important difference with respect to the one studied by Reimann et al. the nonequilibrium noise is quenched and additive. We determine its phase diagram with mean field techniques, as well as the region of negative resistance. An interesting feature of the phase diagram is the presence of reentrant transitions, which seems to be common in noise induced phase transitions [1,2,14]. Furthermore, we
The paper is organized as follows. In Sec. I, we introduce the model and its mean field analysis. We then present in Sec. II the phase diagram and in Sec. III the results concerning negative resistance and anomalous hysteresis. Section IV is devoted to discussing the energetics of the model. Finally, in Sec. V we give an intuitive explanation of the above results and summarize the main conclusions of the work.

II. THE MODEL: MEAN FIELD ANALYSIS

Our model consists of \( N \) coordinates \( x_i \) obeying the following dimensionless Langevin equations:

\[
\dot{x}_i = F_0(x_i) + \eta_i + F + \frac{D}{N} \sum_{j=1}^{N} \sin(x_j - x_i) + \xi_i(t). \tag{1}
\]

They can be interpreted as overdamped and interacting particles subject to a local force \( F_0(x) \), additive fluctuations \( \eta_i + \xi_i(t) \), and an external force \( F \). The system can also model a field \( x_i \) defined on a lattice and following a local dynamic given by \( F_0(x) \) \[1\].

The coupling term between particles is called the Kuramoto interaction and plays a synchronizing role. It is a simple choice of periodic interaction, widely used in the theory of weakly coupled oscillators \[15\]. This theory has been applied to oscillatory chemical systems that can be described as assemblies of limit-cycle oscillators, as well as to collective rhythms in living organisms, resulting from cooperative interactions among cellular oscillators \[15,16\]. For the local force we take

\[
F_0(x) = -\sin x + W \sin 2x, \tag{2}
\]

which derives from the 2\( \pi \)-periodic and symmetric local potential,

\[
V_0(x) = -\cos x + \frac{W}{2} \cos 2x, \tag{3}
\]

\( W \) being a positive constant. Depending on the value of \( W \), \( V_0(x) \) presents the following behavior: if \( W < 1/2 \), it has one stable equilibrium point within a period, whereas if \( W > 1/2 \), it has two symmetric stable equilibrium points inside the same period (see Fig. 1). Throughout the paper, we set \( W = 0.75 \). Thus, the potential has two wells and is a periodic version of a Ginzburg-Landau potential that exhibits spontaneous symmetry breaking.

\( F \) is a constant external force and \( \xi_i(t) \) are uncorrelated Gaussian white noises, which account for thermal fluctuations:

\[
\langle \xi_i(t) \xi_j(t') \rangle = \sigma^2 \delta_{ij} \delta(t - t'). \tag{4}
\]

Finally, \( \eta_i \) are quenched Gaussian noises, which are the source of nonequilibrium in the system. They are, in fact, site dependent fluctuations of the external force \( F \). We assume that they have zero mean value and are spatially uncorrelated:

\[
\rho_\eta(z) = \frac{1}{\sqrt{2\pi \sigma_z^2}} e^{-z^2/(2\sigma_z^2)}, \tag{5}
\]

\[
\langle \eta_i \eta_j \rangle = \delta_{ij} \sigma_z^2. \tag{6}
\]

These noises are also uncorrelated with \( \xi_i(t) \). Note that this spatial disorder corresponds to the quenched limit of the Ornstein-Uhlenbeck process.

To implement the Weiss mean field theory, note first that the coupling term in Eq. (1) can be rewritten as

\[
\sin(x_j - x_i) = \cos x_i \sin x_j - \sin x_i \cos x_j. \tag{7}
\]

Summing over \( j = 1, \ldots, N \) and dividing by \( N \), one has

\[
\frac{1}{N} \sum_{j=1}^{N} \sin(x_j - x_i) = s \cos x_i - c \sin x_i, \tag{8}
\]

where \( s \) and \( c \) are, respectively, the averages of the sine and cosine of the field.

In the thermodynamic limit, \( N \to \infty \), one can write the following Langevin equation for the field \( x \) at a generic site of the lattice (notice that now we drop the lattice index):

\[
\dot{x} = F_{\text{eff}}(x; \eta) + \xi \tag{9}
\]

where the effective force acting on \( x \) is given by

\[
F_{\text{eff}}(x; \eta) = F_0(x) + F + \eta + D(s \cos x - c \sin x), \tag{10}
\]

with \( c = \langle \cos x \rangle \) and \( s = \langle \sin x \rangle \). This effective force acting on \( x \) can be derived from an effective potential:

\[
V_{\text{eff}}(x; \eta) = V_0(x) - x(F + \eta) - D(s \sin x + c \cos x), \tag{11}
\]

which is no longer periodic, but has the following tilt property:

\[
V_{\text{eff}}(x + 2\pi; \eta) - V_{\text{eff}}(x; \eta) = \Delta V_{\text{eff}}(\eta) = -2\pi(F + \eta). \tag{12}
\]

Equation (8) is not a closed equation due to the presence of parameters \( c \) and \( s \). However, it can be closed in the stationary regime using the self-consistency equations

\[
c = \int_0^{2\pi} \rho(x; s, c) \cos(x) dx, \tag{13}
\]
\[ s = \int_{0}^{2\pi} \rho(x;s,c) \sin(x) \, dx, \]

where \( \rho(x;s,c) \) is the stationary probability density that can be obtained by proceeding as follows.

The stationary Fokker-Planck equation corresponding to the Langevin equation (8) for a given value of the noise \( \eta = z \) reads

\[ \frac{\partial}{\partial x} \left[ F_{\text{eff}}(x;z) \rho(x;z) \right] - \frac{\sigma^2}{2} \frac{\partial^2}{\partial x^2} \rho(x;z) = 0 \]

and its solution is the conditional stationary probability density \( \rho(x|z) \). A first integration of Eq. (13) yields

\[ F_{\text{eff}}(x;z) \rho(x|z) - \frac{\sigma^2}{2} \frac{\partial}{\partial x} \rho(x|z) = J(z), \]

where \( J(z) \) is the current of the process \( x(t) \) obeying the Langevin equation (8) with \( \eta = z \). The solution of Eq. (14) satisfying normalization and periodic boundary conditions is

\[ \rho(x|z) = N(z) \int_{x}^{x+2\pi} \exp \left[ 2 \left( V_{\text{eff}}(x',z) - V_{\text{eff}}(x;z) \right)/\sigma^2 \right] \, dx', \]

where \( N(z) \) is a normalization constant. The current \( J(z) \) is given by the expression

\[ J(z) = \frac{\sigma^2}{2} N(z) \left( 1 - e^{-2\Delta V_{\text{eff}}(z)/\sigma^2} \right). \]

Finally, the total probability density reads

\[ \rho(x;s,c) = \int_{R} \rho_{g}(z) \rho(x|z) \, dz, \]

which is the one that must be used in the self-consistency equations (12).

The total current \( J \) can be calculated using

\[ J = \int_{R} J(z) \rho_{g}(z) \, dz, \]

and both \( J(z) \) and \( J \) depend on \( c \) and \( s \), which are obtained from Eq. (12).

**III. PHASE DIAGRAM**

Let us first focus on the case \( F = 0 \). As expected, the symmetric state \( s = 0 \) is always a solution of the self-consistency equations. Note that in that case, if \( F = 0 \), \( J(z) = -J(-z) \) and, consequently, the total current becomes null. However, if \( W > 1/2 \), there are regions in the space of parameters where that solution becomes unstable and two stable asymmetric solutions with \( s \neq 0 \) appear for \( F = 0 \). It turns out that, for these asymmetric or ordered phases, the current is also different from zero. Therefore both \( s \) and \( J \) can be used as order parameters for the order-disorder phase transitions in our system.

The phase boundary that separates the region where \( J = 0 \) from the region where \( J \neq 0 \) is given by the solution of the following equations:

\[ e = \int_{0}^{2\pi} \rho(x;s,c)_{|x=0} \cos(x) \, dx, \]

\[ 1 = \int_{0}^{2\pi} \frac{\partial \rho(x;s,c)}{\partial s}_{|x=0} \sin(x) \, dx. \]

In Fig. 2(a), we plot with a solid line the phase boundary on the \((\sigma_{z},D)\) plane for \( W = 0.75 \), \( \sigma = 1.25 \), and \( F = 0 \). Note that there are several reentrant phase transitions, both with the coupling \( D \) and with the intensity of the quenched noise \( \sigma_{z} \). We then have paths in the \((\sigma_{z},D)\) plane where the current appears and disappears through second order phase transitions. In Fig. 2(a) two arrows indicate different trajectories showing this behavior. The vertical arrow shows an increasing \( D \) trajectory with three phase transitions. The behavior of the current along that trajectory is shown in Fig. 2(b) for which \( \sigma_{z} = 3.975 \). We see that there are two values of \( D \) for which the current reaches local maxima. The opposite behavior is obtained when increasing \( \sigma_{z} \) for constant \( D \), as indi-
Mobility as a function of the intensity of the quenched noise, illustrated in Fig. 2(a) by a horizontal arrow. In Fig. 2(c), we have plotted the behavior of the total current as a function of the intensity $\sigma_z$ of the quenched noise for $D=8$. It can be seen that there are also three phase transitions and two optimal values of the noise intensity. This last phenomenon could be considered as a type of stochastic resonance [9].

IV. NEGATIVE MOBILITY AND ANOMALOUS HYSTERESIS

In this section we turn to the case $F \neq 0$ and discuss the transport properties of the system. We are interested in the response of the system to the external force as given by $J(F)$, i.e., the net current as a function of $F$.

The mean field theory explained above gives exact values of $J(F)$ for the globally coupled model, which are found to be in very good agreement with numerical simulations. In Fig. 3, we plot both analytical (solid line) and numerical (circles) values of $J(F)$ for $\sigma_z = 2$ and $D = 6$ [the rest of the parameters are the same as in Fig. 2(a)].

The curve crosses the origin, i.e., $J(0) = 0$. This was expected, since the point $(\sigma_z = 2, D = 6)$ lies in the region of zero current in Fig. 2(a). However, the behavior of $J$ for $F$ small but different from zero is striking: current and force have opposite signs, i.e., the particles move against the force. We call this phenomenon negative resistance, since the resistance is proportional to $F/J(F)$. Of course, the energy necessary for this motion is provided by the nonequilibrium fluctuations, as shown below.

At $F = 0$, the slope of the curve $J(F)$ is negative. In analogy with systems close to equilibrium, we call this slope

$$\mu = \left. \frac{\partial J}{\partial F} \right|_{F=0}$$

the mobility of the system, which can take negative values in our model.

The mean field theory allows us to find the value of $\mu$ analytically. Notice, however, that $\mu$ is defined only for values of $D$ and $\sigma_z$ lying in the region where $J(0) = 0$, i.e., in the disordered phase region in Fig. 2(a). In Fig. 2(a) the region with negative mobility is given by the band between the line of phase transitions (solid line) and the dashed line. Observe that, for constant $D$ and increasing $\sigma_z$, the sign of the mobility can even change twice. An example is given in Fig. 4, where we have plotted $\mu$ as a function of the intensity of the quenched noise $\sigma_z$.

The addition of an external force when the system exhibits a spontaneous symmetry breaking [region of $J \neq 0$ in Fig. 2(a)] yields a first order phase transition. For $F = 0$, the system has either positive or negative current. The sign, as in any equilibrium first order phase transition, depends on the history of the system, leading to a hysteresis cycle. One example is given in Fig. 5, where we plot analytical and numerical results of $J(F)$ for $\sigma_z = 5.5$ and $D = 10$. In the region of hysteresis, the self-consistency equations have three solutions, two stable (solid line) and one unstable (dashed line). The numerical results (circles) have been obtained by tuning the external force quasistatically from $F = -0.4$ to $F = 0.4$ and back to $F = -0.4$. The arrows indicate jumps in the value of the current.

Note that, since $J(F)$ is not a unique function for $F = 0$, the mobility cannot be defined. However, we still have negative resistance for small values of the external force. Moreover, the hysteresis cycle runs clockwise. This orientation is opposite to the one followed by “standard” hysteresis cycles.

![FIG. 4. Mobility as a function of the intensity of the quenched noise $\sigma_z$ for $D=3.25$, $W=0.75$, and $\sigma=1.25$. Open circles indicate a change of sign in the mobility.](image)

![FIG. 5. Analytical (solid and dashed lines) and numerical (circles) values of the current vs the external force for $\sigma_z = 5.5$, $D = 10$, $W=0.75$, and $\sigma=1.25$. The arrows indicate jumps of the current in the simulations.](image)
In this section we discuss the energy transfer between the particles and their surroundings. The system exchanges energy with (a) a thermal bath producing the thermal fluctuations $\xi_i(t)$, (b) an external agent applying the force $F$, and (c) a second external agent which is the source of the external fluctuations $\eta_i$. In Fig. 6 we present a diagram of the energy transfers with their corresponding notations. In the following, $Q$, $E_{\text{in}}$, and $E_{\text{out}}$ refer to energy transfer per particle. Finally, the arrows in Fig. 6 indicate the direction of positive transfer. Thus, $E_{\text{in}}$ is the energy (per unit time and particle) that the external fluctuations introduce in the system, $E_{\text{out}}$ is the work done by the system against the external force which is the result of the rectification of fluctuations, and $Q$ is the dissipated heat.

To calculate these energy transfers, we recall that an external force $F$ on a Brownian particle develops a power $\dot{E}=F\langle v \rangle$, where $\langle v \rangle$ is the mean velocity of the particle. In our case, $\langle v \rangle=2\pi J$. Hence,

$$\dot{E}_{\text{out}}=-2\pi jF,$$

where the minus sign comes from the fact that $E_{\text{out}}$ is the power developed by the system against the force. The power developed by the external fluctuations is

$$\dot{E}_{\text{in}}=\left\langle \frac{1}{N} \sum_{i=1}^{N} \eta_i \langle v_i \rangle \right\rangle_{\text{disor}} = \langle \eta \langle v \rangle \rangle_{\text{disor}},$$

where $\langle \cdot \rangle_{\text{disor}}$ denotes an average over disorder configurations. Taking into account that $J(z)$ is the current conditioned to $\eta=z$, one finally has

$$\dot{E}_{\text{in}}=2\pi \int_{-\infty}^{\infty} zJ(z)\rho_{\eta}(z)dz.$$

Since the internal energy of the system is constant in the stationary regime, conservation of energy implies that the dissipated heat is [17]:

$$\dot{Q}=\dot{E}_{\text{in}}-\dot{E}_{\text{out}}.$$

The rate of entropy change in the bath is $\dot{S}_{\text{bath}}=N\dot{Q}/T$, where $T$ is the temperature of the bath ($k_B T=\sigma^2/2$). On the other hand, the entropy of the system is constant in the stationary regime. Therefore the total entropy production (again per particle) is

$$\dot{S}=\dot{S}_{\text{total}}.$$

and, according to the second law, the dissipated heat $\dot{Q}$ must always be positive.

Finally, the efficiency of the system can be defined as the ratio of the ‘rectified energy’ to the input energy, i.e.,

$$\varepsilon=\frac{\dot{E}_{\text{out}}}{\dot{E}_{\text{in}}}. $$

Figure 7 depicts (a) $\dot{Q}$, (b) $E_{\text{out}}$, and (c) the efficiency $\varepsilon$ as a function of the external force $F$ for $W=0.75$, $\sigma=1.25$, $\sigma_z=2$, $W=0.75$, and $\sigma=1.25$.

In Fig. 8, the same quantities as in Fig. 7 are presented, for a point lying in the region of anomalous hysteresis. The values of the parameters are $\sigma_z=5.5$, $D=10$, $W=0.75$, and
s = 1.25. Note that in this case, $\dot{Q}$, $\dot{E}_{\text{out}}$, and $\varepsilon$ present hysteresis. The dissipated heat $\dot{Q}$ has an interesting behavior: starting from negative values of the force, it increases but for a certain value of $F$ jumps down and then decreases.

In both cases, there is a value of the force for which the efficiency is maximum, as in other irreversible Brownian motors [18].

To check the influence of the phase transitions on the energetics of the system we plot in Fig. 9 the dissipated heat $\dot{Q}$, the output energy $\dot{E}_{\text{out}}$, and the efficiency $\varepsilon$, as a function of $s$ for $F = 0.005$, $D = 8$, $W = 0.75$, and $\sigma = 1.25$.

\[(\langle \dot{x} \rangle = \langle F_{\text{eff}}(x; \eta) \rangle = F - s + 2W\langle \sin x \cos x \rangle. \quad (27)\]

Neglecting correlations and noting that $\langle \dot{x} \rangle = 2\pi J$, an approximated expression for the current can be written down as

\[J(F) = \frac{1}{2\pi}[F + s(2Wc - 1)]. \quad (28)\]

For $F = 0$, $s = 0$, and then $J(0) = 0$. If $s$ depends on $F$ as $s = \alpha F + o(F^2)$, then the mobility reads

\[\mu = \frac{1 + \alpha(2Wc - 1)}{2\pi}. \quad (29)\]

where $c$ is the average $\langle \cos x \rangle$ for $F = 0$. We see that, if $\alpha(1 - 2Wc) > 1$, $\mu$ becomes negative.

$\alpha$ can be considered as a susceptibility that measures the response of the mean value of the sine, $s$, to the force $F$. It is always positive and diverges at the critical point. Therefore, one should expect negative mobility in a region close to the line of critical points, exactly like the result depicted in Fig. 2(a).

However, the argument is by no means complete since we have to specify how $c$ and $\alpha$ depend on the parameters of the

VI. DISCUSSION AND CONCLUSIONS

Negative resistance can be explained with a simple approximation. By averaging Eq. (8) we obtain
model. In fact, second order phase transitions are not a necessary ingredient to have negative mobility [20].

Our model also provides a "mechanical" picture of how negative resistance arises. Notice first that a Brownian particle in a potential like the one depicted in Fig. 10, and affected by an external fluctuating force, will move to the left or, more generally, to the direction where the slope of the potential is lower [4]. The reason is that, due to the external force, jumps over the highest barrier of the potential to the left are more likely than jumps to the right.

In the case where the system does not break any symmetry the current is zero for $F=0$. Suppose that we apply a small positive force that pushes the particles to the right. The particles within each interval $[n\pi, (n+2)\pi]$ move to the right. Then, the shape of the potential that each individual particle experiences is similar to the one in Fig. 10. Now the external fluctuations come into play, inducing more jumps over the highest barrier of the potential to the left than to the right. Notice that the effect of the external force is the one expected: it induces a motion to the right within each interval. However, this effect, in combination with the local potential and the external fluctuations, makes jumps to the left more probable than to the right. The current is finally the result of this nonbalanced rates of jumps, which happens to be opposite to the applied force. This behavior obviously occurs only for weak enough forces.

When there is a symmetry breaking for $F=0$ the argument is very similar. Here, for $F=0$ the system can be in two different macroscopic states or phases, exactly like an equilibrium Ginzburg-Landau or Ising model. Any small force will drive the system to one of the two phases and the resulting current will have the opposite sign.

To summarize, we have presented a model of a spatially extended molecular motor with a periodic and symmetric local potential. The model exhibits anomalous transport properties, even though the external nonequilibrium fluctuations are as simple as quenched Gaussian noises. This simplicity has allowed us to solve the model analytically and provide intuitive explanations of the behavior of the system. The energetics of the model reveals that it works very far from equilibrium and that phase transitions do not induce a sensible decrease in the dissipated heat or, equivalently, in the entropy production.

Finally, the model that we have presented here can be interpreted as a collection of interacting oscillators, closely related to Kuramoto type models [15]; cf. [20] for a discussion on the relationship between the phase transitions discussed here and the synchronization and desynchronization phases in collective oscillators.

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[11] The absence of current in symmetric systems with convex interaction has been proven using the so called Middleton rule [21]. Our model (as well as that in Ref. [10]) has a nonconvex interaction potential, which seems to be a necessary ingredient for symmetry breaking transitions leading to nonzero currents.
[17] The same result for the dissipated heat could be obtained considering that the force $F + \eta_i$ derives from a linear potential $-(F + \eta_i)x_i$. In this interpretation, the energy of the system decreases and the only energy exchange is with the thermal bath.