Nonequilibrium Fluctuation-Induced Transport

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Ratchetlike devices can rectify symmetric, unbiased nonequilibrium noise resulting in fluctuation-induced currents. We study some simple models to investigate the dependence of a nonequilibrium steady-state current on the characteristic features of the ratchet and the applied noise. It turns out that the magnitude and the direction of the induced current depend not only on the shape of the ratchet, but also on the statistics of the fluctuations.

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Feynman used a ratchet example to illustrate some implications of the Second Law of thermodynamics [1], in particular, that useful work cannot be extracted from equilibrium fluctuations. In a recent study [2], Magnasco has pointed out that the same restrictions do not apply to nonequilibrium noise: An asymmetric potential can rectify even *symmetric* fluctuations, leading to a "coherent" response from unbiased forcing [3]. One motivation to study such problems comes from molecular biophysics where ratchetlike mechanisms have been proposed to explain nature's efficiency in transporting large molecules in the absence of obvious appropriate potential or thermal gradients [4]. There, the nonequilibrium fluctuations have been conjectured to arise from the nearly irreversible consumption of chemical energy. Applications not withstanding, the basic ideas contained in Magnasco's observations have potentially far reaching implications and deserve further investigation.

Here we study a class of noise-driven ratchetlike systems with the specific goal of investigating the ingredients necessary for nonequilibrium fluctuation-induced transport, as well as the robustness of such phenomena to details of the models. For example, it is desirable to know if there is a degree of universality in these phenomena in limiting situations, say, near equilibrium. We present exact, perturbative, and Monte Carlo simulation results for noise-driven motion in a one-dimensional periodic potential. The (overdamped) state variable $X(t)$ moves in the periodic potential $V(x)$ under the influence of a heat bath at temperature T and the applied fluctuation force, a random process denoted $Z(t)$. The state variable then satisfies the stochastic differential equation

$$\frac{dX}{dt}=f(X)+\sqrt{2k_BT}\,\xi(t)+Z(t)\,, \qquad (1)$$

where $f(x)=-V'(x)$ is the deterministic force and thermal fluctuations are represented by $\xi(t)$, a mean zero Gaussian white noise process [5] with

$$\langle\xi(t)\xi(s)\rangle=\delta(t-s)\,. \qquad (2)$$

In the absence of the applied noise or if $Z(t)$ is another symmetric white noise process, the stationary state corresponds to a thermal equilibrium state satisfying the condition of detailed balance, in which case no net current is possible for any shape of the potential. On the other hand if the noise is unbiased and symmetric and the potential is symmetric, then by symmetry no net current can flow in the stationary state. If the applied force is not symmetric then the appearance of a current would not be surprising [6]. The interesting case from our point of view is where the static potential V is asymmetric and the fluctuations are symmetric but nonwhite, i.e., $Z(t)$ is correlated over time intervals that are long compared to the thermal fluctuation time scale. For the dynamics of Eq. (1), the resulting stationary state then no longer satisfies the condition of detailed balance; the symmetry of the noise may be broken, resulting in a nonvanishing probability current in the x domain.

We note that our analysis applies to general periodic potential shapes. The results and observations presented specifically for the stylized (piecewise linear) potential shown in Fig. 1 are not just artifacts of that simplification.

We consider the dynamics in Eq. (1) with noisy random forces $Z(t)$ that are Markov processes with infinitesimal generator denoted M_z. That is, the marginal probability density $p(z,t)$ of the noise process satisfies

$$\frac{\partial p(z,t)}{\partial t}=M_z p(z,t)\,. \qquad (3)$$

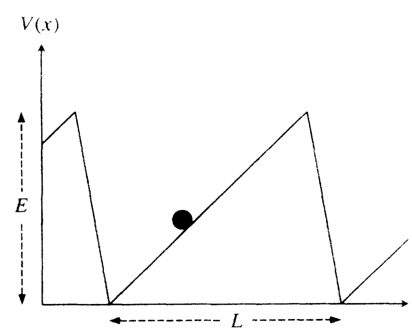

FIG. 1. A simple ratchetlike periodic potential.

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Then the joint probability density for the position variable $X(t)$ and the fluctuation variable $Z(t)$, $\rho(x,z,t)$, satisfies the Fokker-Planck master equation

$$\frac{\partial\rho(x,z,t)}{\partial t}=\frac{\partial}{\partial x}\left\{-f(x)-z+k_BT\frac{\partial}{\partial x}\right\}\rho(x,z,t)+M_z\rho(x,z,t)\,, \tag{4}$$

supplemented with periodic boundary conditions on $[0,L]$ in x, and the appropriate boundary conditions for z. The fluctuation's marginal density and the position variable's marginal density, $r(x,t)$, are related to the joint density by

$$p(z,t)=\int\rho(x,z,t)dx \tag{5}$$

and

$$r(x,t)=\int\rho(x,z,t)dz\,, \tag{6}$$

and the x-space probability current is

$$J(x,t)=\left\{f(x)-k_BT\frac{\partial}{\partial x}\right\}r(x,t)+\int z\rho(x,z,t)dz\,. \tag{7}$$

In the absence of the nonequilibrium fluctuations (i.e., if either $Z\equiv0$ or Z is unbiased white noise for this simple model) the system achieves an equilibrium state satisfying detailed balance, characterized by the condition $J\equiv0$.

Now we consider symmetric, mean zero, exponentially correlated fluctuation forces. In the stationary state the fluctuation process $Z(t)$ satisfies $\langle Z(t)\rangle=0$ and

$$\langle Z(t)Z(s)\rangle=(D/\tau)e^{-|t-s|/\tau}\,, \tag{8}$$

where τ is the correlation time of the noise and D is its intensity. The power spectrum for such processes is a Lorentzian of width τ^{-1}. In the limit of vanishing τ the correlation function reduces to a delta function and the power spectrum becomes flat, corresponding to white noise. By "symmetric" we mean that the marginal distribution $p(z,t)$ is a symmetric function of z. There are many stochastic processes—even many Markov processes—with the first and second order statistics considered here, and we focus on three specific examples that are amenable to analysis.

The first and simplest example is the symmetric dichotomous Markov process, also known as the random telegraph signal. This process takes on two values, $\pm\sqrt{D/\tau}$, staying in one state for an exponentially distributed time before switching to the other state for another independent identically distributed time, and so on. The marginal density of this process takes the form

$$p(z,t)=P_+(t)\delta(z-\sqrt{D/\tau})+P_-(t)\delta(z+\sqrt{D/\tau})\,, \tag{9}$$

where the probabilities $P_\pm(t)$ satisfy

$$\frac{d}{dt}\begin{bmatrix}P_+\\P_-\end{bmatrix}=\frac{1}{2\tau}\begin{bmatrix}-1&1\\1&-1\end{bmatrix}\begin{bmatrix}P_+\\P_-\end{bmatrix}. \tag{10}$$

For this noise the $T=0$ problem can be solved exactly, in closed form.

The second example is the Ornstein-Uhlenbeck process, the unique Gaussian Markov diffusion process. It has continuous sample paths and corresponds to low-pass filtered Gaussian white noise. Its marginal density satisfies the Fokker-Planck equation

$$\frac{\partial p(z,t)}{\partial t}=\frac{1}{\tau}\frac{\partial}{\partial z}\left\{z+\frac{D}{\tau}\frac{\partial}{\partial z}\right\}p(z,t) \tag{11}$$

with vanishing boundary conditions as $z\to\pm\infty$. We cannot solve the full problem exactly for the Ornstein-Uhlenbeck process, but we can compute the current in perturbation theory about the equilibrium white noise $(\tau\to0)$ limit.

The third example is a whole family of stochastic processes known as "kangaroo processes" [7], parametrized by a probability distribution $q(z)$. Here, the process $Z(t)$ waits at some value in the support of q for an exponentially distributed time, and then jumps to a level chosen independently according to the distribution q, where it waits for another independent identically distributed time before jumping again, etc. The marginal density for the kangaroo process evolves according to

$$\frac{\partial p(z,t)}{\partial t}=-\frac{1}{\tau}\left\{p(z,t)-q(z)\int p(z',t)dz'\right\}, \tag{12}$$

where $q(z)$ is the stationary distribution which we take to be symmetric with second moment D/τ. (If q is a discrete two-level distribution, then Z is equivalent to the dichotomous process. If q is a Gaussian then Z is Gaussian and Markovian, but it is *not* the Ornstein-Uhlenbeck process.) We cannot solve the full problem exactly with the kangaroo process but we can compute the $O(\tau)$ contribution to the current. The kangaroo process is a particularly valuable example because of the variety of statistics available in the choice of $q(z)$.

For the dichotomous Markov process, in the zero temperature case and provided $D/\tau>\sup_x|f(x)|$, the exact stationary current is

$$J=(1-e^{\phi(L)-\phi(0)})/Q\,, \tag{13}$$

where

$$\phi(x)=-\frac{1}{D}\int_0^x\frac{f(y)dy}{1-\tau f(y)^2/D} \tag{14}$$

and

$$Q=\int_0^L\frac{e^{-\phi}}{D/\tau-f^2}\int_0^L\left[\frac{1}{\tau}-V''\right]e^{\phi}-(1-e^{\phi(L)-\phi(0)})\int_0^L dy\frac{e^{-\phi(y)}}{D/\tau-f(y)^2}\int_0^y\left[\frac{1}{\tau}-V''\right]e^{\phi}. \tag{15}$$

The current as a function of the noise intensity D is plotted in Fig. 2 for some specific parameter values. There is an "optimal" noise strength which maximizes this noise-induced current. This result illustrates the fact that coherent, asymmetric motion can be extracted from unbiased, symmetric *nonequilibrium* fluctuations. Note that for the ratchet potential as shown in Fig. 1, the current is positive (to the right) in accord with the considerations in Ref. [2].

The specific factors responsible for the fluctuation-induced current are not altogether transparent in the full solution in Eqs. (13)–(15). Near the white noise limit —i.e., near an equilibrium state—the solution can be expanded as a power series in the noise correlation time. To first order we find

$$J \approx \frac{\tau}{D} \frac{\int_0^L f(x)^3 dx}{\int_0^L e^{+V/D} \int_0^L e^{-V/D}}, \tag{16}$$

indicating a current proportional to τ (which in these cases is a measure of the "distance from equilibrium") and depending in a particularly simple way on the asymmetry in the static potential. Even though V is periodic, so the integral of f over the period vanishes, the integral of f^3 does not generally vanish. The steeper slopes in V are emphasized by the integral of f^3, which for a shape like that in Fig. 1 results in a positive value for J. The first term in the small τ expansion is also plotted in Fig. 2 for comparison with the exact curve.

It is reasonable to conjecture that the near-equilibrium functional dependence on the noise-induced current on τ, f, V, and D is typically of the form in Eq. (16), although

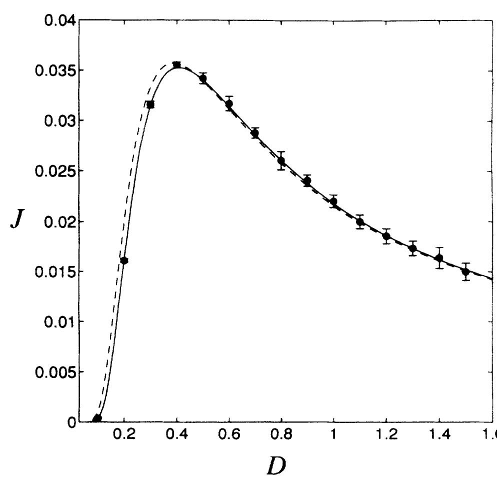

FIG. 2. Fluctuation-induced current for dichotomous Markov noise vs noise strength, at $T=0$, from Eqs. (13)–(15) (solid line). In this plot the potential barrier height $E=1$ in units of D, the period is $L=1$, and the ($\pm$) forces are piecewise constant on 20% (+) and 80% (−) of the interval, respectively. The correlation time is $\tau=0.001$ in this plot. The first-order approximation from Eq. (16) is also shown (broken line), as are the results of direct Monte Carlo simulation (discrete data).

perhaps with numerical prefactor adjustments.

In the case where $Z(t)$ is the Gaussian diffusion process, the Ornstein-Uhlenbeck process, no full exact solution is known, but the current can be computed as a power series in $\tau^{1/2}$ in a singular perturbation expansion [8]. The $O(\tau^{1/2})$ term vanishes identically, and the first nontrivial terms appear at $O(\tau)$. The net result of the $T=0$ calculation to $O(\tau)$ for the Ornstein-Uhlenbeck noise, though, is

$$J \approx 0. \tag{17}$$

This result is not inconsistent with the conjecture in the paragraph above—it is just that the prefactor is zero [9].

For the kangaroo process a similar short τ singular perturbation expansion can be carried out for general stationary distributions $q(z)$, and the result at $T=0$ is

$$J = \left[2 - \frac{\langle z^4 \rangle}{\langle z^2 \rangle^2}\right] \frac{\tau}{D} \frac{\int_0^L f(x)^3 dx}{\int_0^L e^{+V/D} \int_0^L e^{-V/D}} + O(\tau^2), \tag{18}$$

where $\langle z^n \rangle$ are the moments of the noise process:

$$\langle z^n \rangle = \int z^n q(z) dz. \tag{19}$$

The current in Eq. (18) has the same form as Eq. (16), modified with a prefactor depending on the noise statistics through the "flatness," the ratio of the fourth moment to the square of the second moment. The rub is that the flatness can take on any value between 1 and ∞, depending on the choice of q. When the statistics of the nonequilibrium noise are such that the flatness is greater than 2 the *sign* of the current changes. For example, a Gaussian distribution has flatness 3, so the first-order fluctuation-induced current for the Gaussian kangaroo process is exactly the negative of the dichotomous noise case (the minimum flatness distribution).

These results are not limited to the zero temperature model. The expansion can be carried out as well for the kangaroo process for temperatures $T>0$, and the first-order current is

$$J \approx \left[2 - \frac{\langle z^4 \rangle}{\langle z^2 \rangle^2}\right] \frac{\tau D^2}{(D+k_B T)^3} \times \frac{\int_0^L f(x)^3 dx}{\int_0^L e^{+V/(D+k_B T)} \int_0^L e^{-V/(D+k_B T)}}. \tag{20}$$

Finite temperature renormalizes the noise strength D in the exponents in the denominator, and it modifies the prefactor in a simple way: In the presence of nonzero *equilibrium* fluctuations, the current induced by low-amplitude *nonequilibrium* noise is proportional to D^2. The qualitative shape of the magnitude of J vs D curve is still as in Fig. 2 for $T>0$, and the same dependence of the sign of the current on the noise statistics is present.

Our prediction that the *direction* of the nonequilibrium fluctuation-induced current depends on the details of the statistics of the nonequilibrium fluctuations is a perturbative result, so it is desirable to check it by other means.

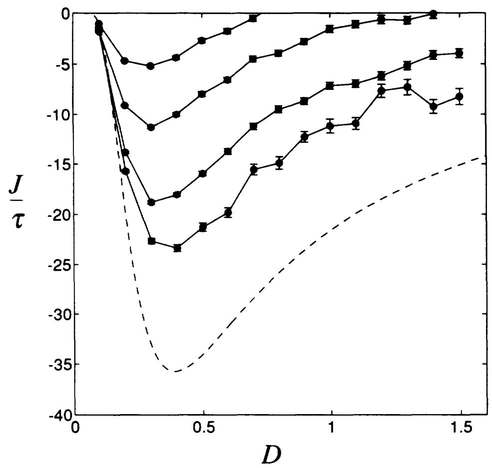

FIG. 3. Current per unit τ for Gaussian kangaroo process vs noise strength, to first order in τ, from Eq. (18) (broken line). The system parameters are the same as in Fig. 2, and the discrete points are, from top to bottom, Monte Carlo data for $\tau = 0.005$, 0.0025, 0.001, and 0.0005.

The problems outlined above may be studied via Monte Carlo methods, and we have carried out direct simulation of the stochastic differential equations for the cases of dichotomous fluctuations and Gaussian kangaroo noise. The data for the dichotomous noise case are shown in Fig. 2, a test case indicating the quality of the simulations. In Fig. 3 we plot the current per unit τ from Eq. (18) along with the data from Monte Carlo simulations for the Gaussian kangaroo process. The current induced by the Gaussian kangaroo noise is *opposite* in direction to that induced by the dichotomous noise, and as $\tau \to 0$ it appears to be converging to the first-order values predicted by the perturbative analysis.

We have constructed and analyzed theoretical examples of fluctuation-induced transport in nonequilibrium systems. For the models studied here, the nonequilibrium fluctuations give rise to a statistical stationary state of the system that lacks detailed balance. Although lack of detailed balance means precisely that the current does not vanish in phase space (x,z), it is the ratchet's mechanical rectification of *completely symmetric noise* in configuration space, i.e., in the x domain, that is of importance.

The direction of the current under the influence of large flatness noise might be understood as follows, at least in the case of a three-level noise process $[Z(t) \in \{\pm F, 0\}]$. Large flatness implies relatively large [say, $F \gg \sup_x |f(x)|$] fluctuations which are relatively rare. During the time between the large rare fluctuations, the particle becomes localized near a stable equilibrium of the periodic potential. When the large force is applied, the periodic force is negligible and the particle will be displaced—perhaps over a distance of several periods of the potential—in the direction of the noise force. When the noise changes back to $Z=0$, the particle finds itself with an essentially random phase within a period of V and the particle will move toward the nearest minimum of V. On average, the large displacements when $Z = \pm F$ yield no net displacement by the symmetry of the noise. Referring to potentials oriented as in Fig. 1, though, the relaxation process to the nearest minimum of V when $Z=0$ will preferentially be to the minimum on the left because its basin of attraction is larger than that of the minimum on the right. This mechanism is similar in spirit to that generating current in the presence of a fluctuating potential [10].

Whether or not nature takes advantage of this kind of effect at the subcellular level remains to be seen.

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