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Forced Thermal Ratchets

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We consider a Brownian particle in a periodic potential under heavy damping. The second law forbids it from displaying any net drift speed, even if the symmetry of the potential is broken. But if the particle is subject to an external force having time correlations, detailed balance is lost and the particle can exhibit a nonzero net drift speed. Thus, broken symmetry and time correlations are sufficient ingredients for transport.

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There are situations in which an ambient noise cannot be reduced; for instance, sufficiently small “machines” immersed in water at room temperature, such as proteins. In this Brownian realm, all laws of thermodynamics still apply but the theoretical constructs through which we learned to understand and interpret them may no longer be valid. We will address one such case, inspired by motor proteins.

Proteins are unlike the technologies we are familiar with; for instance, the size of the elementary unit, the amino acid, is fixed. Whenever some higher amount of complexity is needed, it becomes necessary to increase overall size. This becomes clear when we look at prokaryotic and eukaryotic cells. Prokaryotes are “primitive” cells without a nucleus (mostly bacteria), while eukaryotes (the cells in all multicellular organisms) are more sophisticated and complex cells; they are also an order of magnitude larger. Size increases pose a problem, for if all transport mechanisms are entirely diffusion driven then diffusive scaling implies that increasing the size of a cell by a factor of 20 entails slowing down its metabolism by a factor of 400. Nature solved this problem most elegantly by endowing the interior of eukaryotic cells with a network of highways (made of polymerized proteins such as tubulin and actin). On these highways, certain protein motors can move and transport vesicles containing chemicals (kinesin and dynein walk on tubulin; myosin walks on actin) [1]. These molecules consume energy while walking. They not only walk but also exert forces, like the myosin-actin structures in our muscles; they also consume

energy in order to exert a force.

When attempting to understand these motors, we must take into account that they live in the Brownian domain. This domain can be unintuitive. We are accustomed to our macroscopic world, where the energy barriers used to impose constraints and forces are much larger than the thermal energy; the “escape times” for thermal activation to permit jumps across these energy barriers are effectively infinite. But in the Brownian domain these barrier heights are a few times kT and the escape times are quite finite. The consequences are strange. In the macroscopic world, energy need not be spent to support a force; any object resting on a table is an obvious example. But in the Brownian domain, a hypothetical microscopic object on a microscopic table will not rest but rather dance around until it reaches the end of the table and falls off. If we wish to confine this object to the table top, we are obliged to pick it up from the floor and place it again on the table, thereby spending some energy. This is of course not a permanent solution: the object will keep falling. In order to exert a force, energy needs to be spent constantly. This means that constructions such as the Carnot cycle are meaningless in this domain; pistons cannot be pushed quasistatically without continuously spending energy, for the handle of the piston will constantly slip off our grasp. In order to understand biological motors it seems desirable to devise some simple scheme that can serve as a benchmark, much like the Carnot cycle serves our understanding of actual car motors.

I will propose now one such scheme, an extension of the

“ratchet and pawl” engine which Feynman used, in his *Lectures*, to illustrate the meaning of the second law [2]. Feynman shows that the core of the second law is that such a ratchet machine will not provide work or net motion when immersed in a single thermal bath. I will show that this only happens for an ideal thermal bath, one in which time correlations are negligible, and that the ratchet can extract energy (for free) out of the time correlated pieces of a colored (nonwhite) thermal bath. The ratchet works as a *mechanical diode*, capable of rectifying an input; it cannot, however, rectify “white” thermal noise alone.

It is worth noting that in the mesoscopic domain thermal noise will be correlated on times smaller than the Smoluchowski time [3], but since the damping terms will not be local in time, detailed balance, and thus the second law, can still be kept, as shown in [4]. But in our situation, barrier heights are order $10kT$, and hence not really mesoscopic. For proper comparison, time scales for motor proteins are around 10^{-2} s, while the Smoluchowski time is $< 10^{-10}$ s. The behavior of a motor protein is Brownian but not mesoscopic, and hence the appropriate Langevin equation is first order (local) in time. We will assume this context throughout this Letter; our results are invalid outside it.

We will call a “ratchet” a periodic potential $V(x)$ which has a broken parity symmetry, together with a Langevin equation of the form

$$\dot{x} = f(x) + \xi(t) + F(t), \quad (1)$$

where x (a cyclic coordinate) describes the state of the ratchet, $f(x) \equiv -\partial_x V(x)$ is a force field due to the potential, $\xi(t)$ is Gaussian noise obeying $\langle \xi(t)\xi(s) \rangle = 2kT\delta(t-s)$, and F is a “driving force” which may be stochastic. There is a large body of theory which has been devoted to the dynamics of Langevin equations and their associated Fokker-Planck equations [3,5-7] and to their behavior in the presence of external forces [8,9] or colored noise sources [4,10].

In the absence of thermal noise, this system behaves the way we expect a ratchet to behave. If we attempt to “advance” the ratchet, there will be a minimum force necessary to overcome the barriers. A large enough force in the opposite direction will also move it. Hence there are two characteristic forces: one to make the ratchet

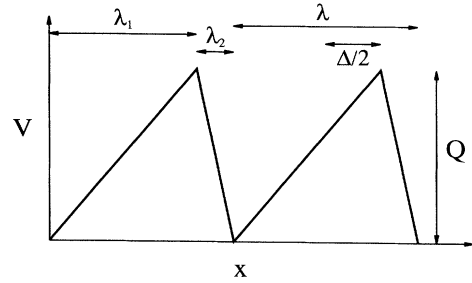


FIG. 1. A plot of the piecewise linear potential $V(x)$ as a function of position x . The width of each segment is called λ_1 and λ_2 . The period of the potential is $\lambda = \lambda_1 + \lambda_2$ and the symmetry breaking amplitude is $\Delta = \lambda_1 - \lambda_2$.

move in its preferred direction, and one to make it move in the opposite direction. More formally, under a simple force like $F(t) = A \sin(\omega t)$, there will be two threshold values for the amplitude A , equal to $\max_x f(x)$ and $-\min_x f(x)$. The role of symmetry breaking is to make these values different. When A lies below these two, the ratchet will not move. When it lies between them, the ratchet will work as we intuitively expect it to: to one side only. When the second threshold is exceeded, we are overdriving the ratchet which will then backslide, reducing its efficiency.

In the presence of the thermal source, the probability densities induced by the above equation obey a Fokker-Planck equation in the form of a conservation law for probability [3,7]: $\partial_t P + \partial_x J = 0$, where $P(x,t)$ is the probability density of the state being at x at time t , and $J(x,t)$ is a probability current obeying

$$2J = -kT\partial_x P + (f + F)P. \quad (2)$$

If we request stationary solutions when F is a constant, we can choose the potential V to be piecewise linear (see Fig. 1), and the equation above can be solved analytically for J as a function of F , because Eq. (2) becomes piecewise linear. Assuming a value of the probability density at the left of one period of the ratchet, we can propagate this to the right edge through this equation; requiring that the solution at the end of the period be equal to that at the beginning of the period we obtain an equation for P_0/J ; requiring the solution to be normalized we can solve for J to get

$$J(F) = \frac{P_2^2 \sinh(\lambda F/2kT)}{kT(\lambda/Q)^2 \{ \cosh[(Q - \Delta F/2)/kT] - \cosh(\lambda F/2kT) \} - (\lambda/Q) P_1 P_2 \sinh(\lambda F/2kT)}, \quad (3)$$

$$P_1 = \Delta + \frac{\lambda^2 - \Delta^2}{4} \frac{F}{Q}, \quad P_2 = \left[1 - \frac{\Delta F}{2Q} \right]^2 - \left[\frac{\lambda F}{2Q} \right]^2.$$

If we think of forcing with a slow forcing $F(t)$ of period T , the average current will be

$$J_{\text{aver}} = \frac{1}{T} \int_0^T J(F(t)) dt.$$

This can be calculated analytically for a slow square wave of amplitude A as the even part of Eq. (3):

$$J_{\text{sqr}} = \frac{1}{2} [J(A) + J(-A)].$$

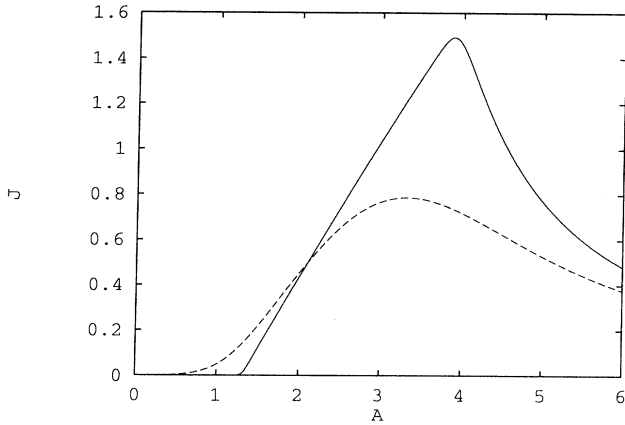


FIG. 2. Plot of $J_{sqr}(A)$; low temperature ($kT=0.01$, full lines) and medium temperature ($kT=0.1$, dashed lines).

Please see Fig. 2, where the solution is plotted for low and medium temperatures.

We may also look at the above solution as a function of temperature. For high amplitudes of the forcing, near overdrive, the presence of temperature always degrades the efficiency of the ratchet. However, for low and moderate forcing, increasing temperature will result first in a rise and then a fall in this efficiency (see Fig. 3). There is a region of the operating regime where the efficiency is optimized at finite temperatures around $Q/6$.

These are results for a particular ratchet in a particular type of forcing. In order to establish that there is some degree of robustness in the system, we will perform numerical computations [11] for a different ratchet in non-quasistatic forcing. The ratchet we will use is

$$f(x) = e^{\alpha \cos x} / J_0(i\alpha) - 1,$$

which is a smooth approximation to a periodic set of Dirac δ s, with width $\alpha^{-1/2}$ and period 2π . We will set $\alpha=16$.

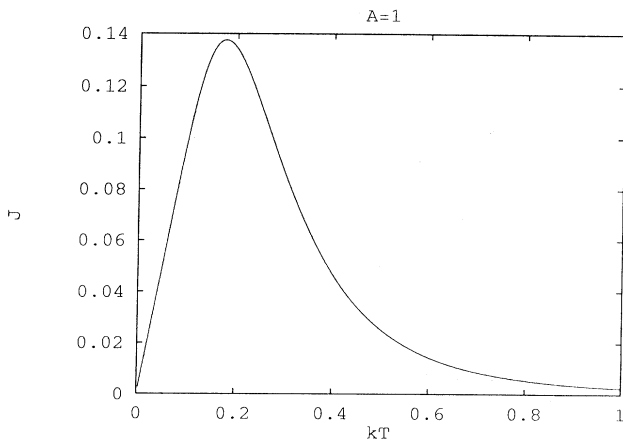


FIG. 3. Plot of J_{sqr} at fixed $A=1$ as a function of kT/Q .

We will employ three different types of forcing: a sine wave $F_s(t) = A \sin(\omega t)$, a "synthetic noise" made by recursively frequency modulating a carrier,

$$F_{FM}(t) = A \sin\{\omega t + B \sin[\omega \phi t + B \sin(\omega \phi^2 t + \dots)]\},$$

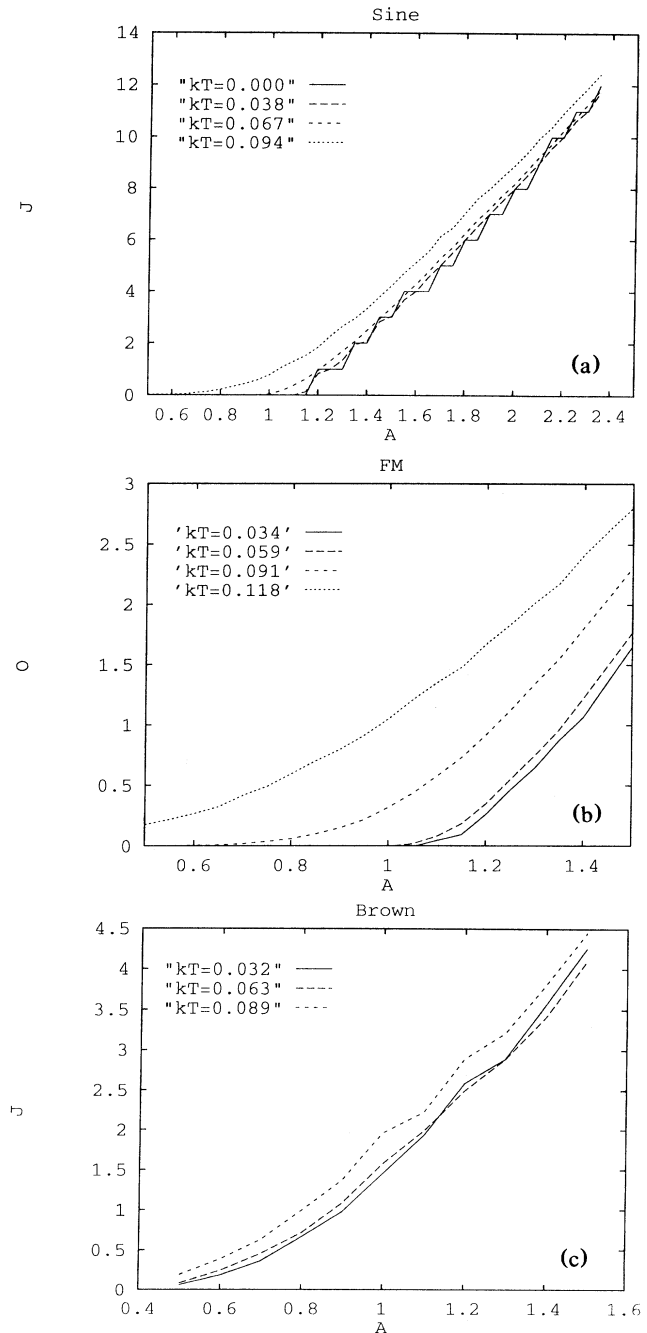


FIG. 4. Numerical data. (a) Sine forcing, (b) FM forcing, (c) Brown noise. All data points were computed by averaging over 400 random walkers, each of these evolved for 100 "periods" of the forcing. Notice that the curves are still quite noisy.

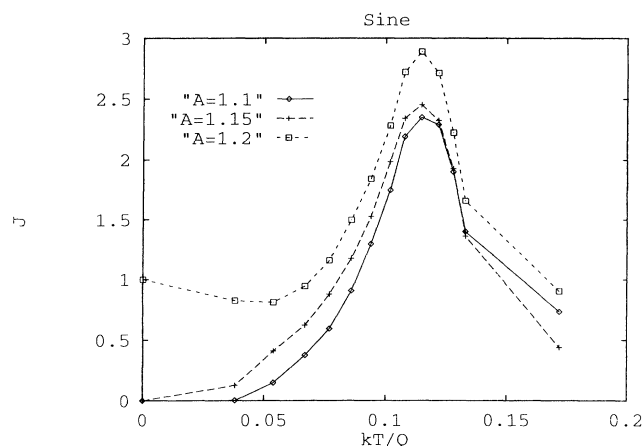


FIG. 5. Current vs kT for sine forcing. The other types of forcing show essentially the same structure.

and simple “brown” noise, defined through its own Langevin equation

$$\dot{F}_B = -\omega F_B + A^2 \xi'(t), \quad \langle \xi'(t) \xi'(0) \rangle = \delta(t),$$

and set $2\phi = \sqrt{5} - 1$, $B = 1$, and $\omega = 2\pi/100$. The results are always qualitatively the same, as shown in Fig. 4; the main difference is that brown noise always makes the ratchet work for any nonzero amplitude, even in the absence of temperature; for it has a nonzero probability of having an arbitrarily large amplitude for an arbitrarily long time. A minor difference is that the sine forcing, being strictly periodic, forces a quantization of the number of wells the particle can jump per period in the zero-temperature case. This results in a staircase that is rapidly smoothed out by temperature. We still see a “peak” in performance for nonzero A in the moderate forcing regime (Fig. 5). The forcing we have used here is “slow” in comparison with the natural relaxation time scales of the ratchet; we have not explored the “stochastic resonance” regime [8] or any issue related to “resonant activation” [9].

Finally, we want to make an observation on time correlated thermal sources. Let us write together the equations for the particle and the forcing:

$$\dot{x} = f(x) + F(t) + \xi(t),$$

$$\dot{F} = g(F) + \xi'(t).$$

We note that this can be written as a single two-dimensional Langevin equation forced with white noise

$$\dot{x} = h_x(x, y) + \xi(t), \quad h_x(x, y) = f(x) + y,$$

$$\dot{y} = h_y(x, y) + \xi'(t), \quad h_y(x, y) = g(y),$$

but the vector field \mathbf{h} is not curl-free, since $\partial_y h_x - \partial_x h_y = 1 - 0 = 1$ and hence this is *not* potential flow. There is an *active decoupling* of the equations involved here, since the forcing kicks the particle but the particle

cannot affect the forcing; the flow is thus not potential [12].

In summary, we have shown that all that is needed to generate motion and forces in the Brownian domain is loss of symmetry and substantially long time correlations. This mechanism is robust enough to survive the ambient “temperature” noise, even, in certain forcing regimes, being helped by it. Whether this principle can be applied to the motion of motor proteins is still under investigation. Even though an equation like (1) is certainly too naive to be of use for purposes of detailed modeling, its features seem to be present: both the biopolymers on which the motors walk and the geometry of motor attachment are heavily symmetry broken, and the biochemistry induces time correlations since (for instance) when adenosine triphosphate (ATP) or adenosine diphosphate (ADP) are attached to the motor, no other ATP can be bound. Thus, even though the arrival times of ATP molecules is a Poisson process, many of these molecules will not bind to the motor because the motor socket is already occupied; the *binding* times will be a Poisson process with “hard cores” (a sharp high frequency cutoff); rough estimates indicate [13] that under physiological conditions this hard core time represents a non-negligible fraction of the total time.

On the physics side, we have shown that a driving force with substantial time correlations (much beyond the Smolowchowski time) can destroy detailed balance and hence the second law. This is not because of “technical” issues, like obtaining a formidable-looking integrodifferential Fokker-Planck equation [7] or not being able to use certain inequalities [14]. It has a simple and definite physical meaning: symmetry breaking allows the system to extract energy out of the time-correlated pieces of the bath without “paying” for it.

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