COMPUTATION OF TRANSPORT IN BROWNIAN RATCHETS

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1 Introduction

In Brownian ratchets the presence of random fluctuations (noise) can lead to directed diffusion in a periodic potential under nonequilibrium conditions, i.e. to a net unidirectional current. Such processes are thought to underlie macromolecular transport in biological cells and muscle contraction, and they provide a possible basis for nanoscale machinery.

In flashing ratchets, where the periodic potential changes discontinuously between two different configurations, transport can occur even under white noise because the nonequilibrium conditions are created by the configurational changes, and the net current is then relatively easy to calculate [1]. In correlation ratchets, on the other hand, the potential is fixed and the nonequilibrium conditions are typically created by the presence of non-white (coloured) noise or, as in the case that we will consider, by white noise with an additional periodic force. The caculation of the current then presents a much more challenging problem. In the present paper we describe how methods for controlling the direction and the amplitude of such currents are being investigated via numerical solution of a variational problem and by digital Monte-Carlo simulation.

Under these conditions, the physical situation is closely related to *resonant activation* – a periodic field-induced resonant reduction of the lifetime of a metastable state, originally observed in a current-biased Josephson junction [2]. The latter observation stimulated a wide-ranging discussion [3, 4, 5, 6] of the old theoretical problem of escape from a potential well in the presence of a nonadiabatic driving field. Surprisingly, measured field-induced corrections to the log of the activation rate, $\ln W$, were found [6] to be $\propto A$ over a wide range of field amplitude A, in marked contrast with the $\propto A^2$ implied by the intuitively appealing physical picture of field-induced heating.

The recently introduced logarithmic susceptibility (LS) [7, 8] is in principle capable of accounting for these observations. It also predicts new mechanisms of resonant rectification and the occurrence of a current reversal with changing parameters where the motion occurs in a spatially periodic asymmetric potential, i.e. in a ratchet. To check these ideas, the model we investigate is

$$\ddot{x} + 2\Gamma\dot{x} + U'(x) = A\cos(\Omega t) + \xi(t), \qquad (1)$$
$$\langle\xi(t)\rangle = 0, \quad \langle\xi(t)\xi(0)\rangle = 4k_B T\Gamma\delta(t),$$

where $U(x + L) = U(x)$ is a ratchet potential of form $U(x) = \alpha\sin(x) + \beta\sin(2x + \phi)$, and $\xi(t)$ is noise which, in a thermal system, corresponds to the temperature T. A similar model was recently considered in the contexts of quantum ratchets with $x(t)$ being the coordinate operator (restricted to the adiabatic limit) [9] and voltage rectification by a SQUID ratchet (restricted to the overdamped limit) [10].

We wish to find the period-averaged activation rates $W^\pm$ for transitions to the right $(+)$ and to the left $(-)$, the net current i.e. the rate of rectification of fluctuations $J = L(W^+ - W^-)$, and the activation energies $S^\pm$. In the $T \to 0$ limit noise-induced escape from a potential well is governed by the slowest decaying eigenmode of the Fokker-Planck operator corresponding to (1). In this limit

the activation rate should, to leading order, take the WKB form $W^{\pm} \propto \exp(-S^{\pm}/k_B T)$ where $S^{\pm}$ is the activation energy [11]. We have investigated the system (1) for several sets of parameters. Here we present results for the particular shape of potential $U(x) = 0.1\sin(x) + 0.049\sin(2x + 0.2)$ with $\Gamma = 0.1$. It is shown by the bold curve in Fig. 1.
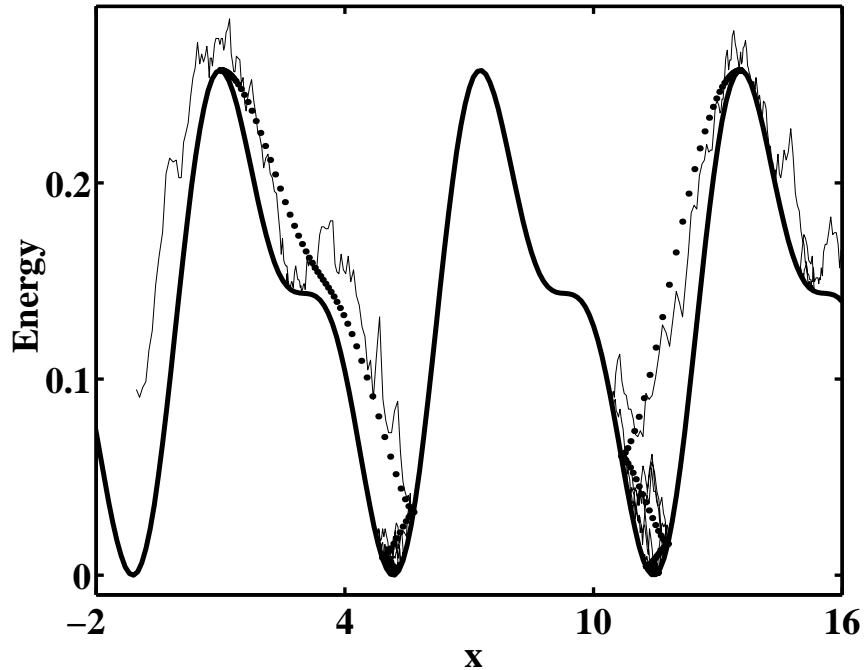

Figure 1: Escapes (thin full curves) to the right and to the left within the potential (bold curves), for $A = 0.03$, $T = 0.013$, $\Omega = 0.35$. Relaxational trajectories are shown by dotted lines. The time interval between dots is fixed: the slowing down effect during escape to the left is revealed as an increased dot density near the point of inflection.

2 Numerical simulations

The numerical simulations used a predictor-corrector method of integration and a high-speed pseudo-random generator [12] for the increment Δx. The simulation ran continuously, and the period-averaged rates of escape $W^{\pm}$ were determined from measurements of the mean times $\langle t \rangle$ to reach the bottom of the neighboring potential well (so that the probability of returning to the vicinity of original well was negligibly small). The activation energies $S^{\pm}$ were then extracted from the measured temperature dependences of $W^{\pm}$ (e.g. inset of Fig. 2). The main results are shown by the data plotted in Figs. 2 and 3. There are several points to be noted. First, the simulations have yielded *linear* dependences on the amplitude A of the field-induced corrections $\delta S^{\pm}$ to the activation energy $S^{\pm}$ over a wide range of parameters (Fig. 3), as expected from the LS theory; but there are deviations from linearity at large and very small A. Secondly, $\delta S^{\pm}$ are clearly *different* for transitions to the right and to the left, immediately implying a rectification of the fluctuations (see below). Thirdly, the *resonant* character of the field-induced activation is clearly demonstrated (filled circles in Fig. 2) for transitions to the right, though less convincingly for those to the left (diamonds). Finally, the shape of the former resonance curve is highly asymmetric: $\delta S^{\pm}$ tend (Fig. 2) at low frequencies towards the constant values corresponding to the change of the activation barrier in the static field whereas, for high frequencies, $\delta S^{\pm}$ drop to 0 relatively fast; the data are consistent with, but do not resolve, a weak additional peak at frequencies close to 1.
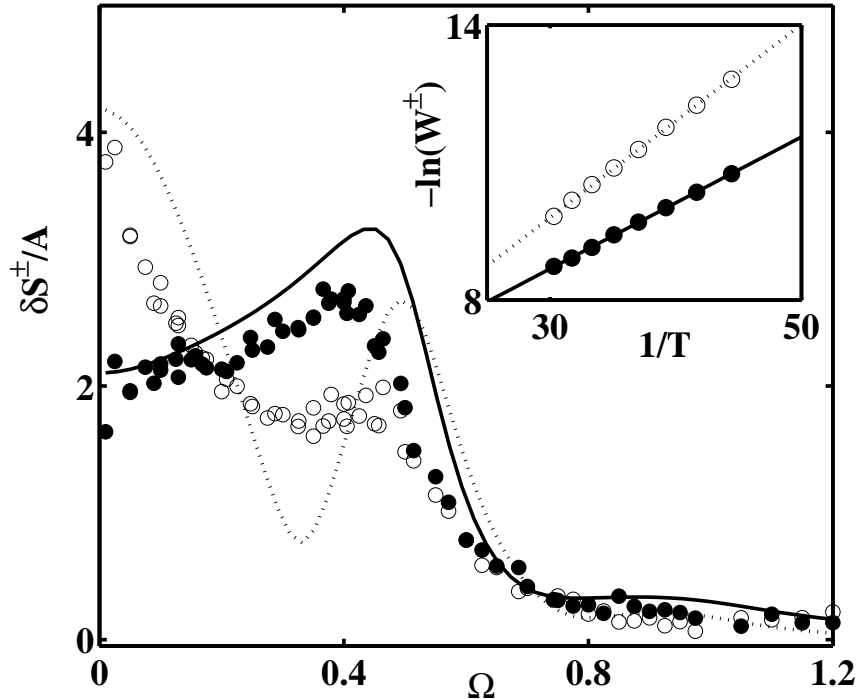
Figure 2: Dispersion of $\delta S^{\pm}/A$ determined by numerical simulation for transitions to the right ($\bullet$) and left (o), compared with the LS theory (bold and dotted curves). Data were recorded with: (i) $A = 0.03$, for $0.025 < T < 0.037$; (ii) $A = 0.035$, for $0.022 < T < 0.031$. Inset: dependence of $-\ln W^{\pm}$ on T^{-1} for $\Omega = 0.01$ and $A = 0.35$. The solid and dotted lines represent linear fits.

3   Discussion

We can account for these results by recalling that, when the temperature is small, a transition between the potential wells occurs as the result of a large rare fluctuation. Because of the constraint on the particle dynamics imposed by the deterministic equations of motion, there is a special energetically optimal way [13] for the fluctuations to drive the particle to the top of the potential barrier, known as the most probable escape path (MPEP). This path is experimentally observable [14, 15]. In thermal equilibrium, it is the time-reversed deterministic relaxational path $x^{\pm}(t)$ down to the potential minimum at x_s, starting from the left ($-$) or right ($+$) adjacent maximum at $x_u^{\pm}$ [13, 14, 15] (see Fig. 1). Thus, $x^{\pm}(t)$ are given by the solutions of the deterministic equation

$$\ddot{x}^{\pm} - 2\Gamma\dot{x}^{\pm} + U'(x^{\pm}) = 0, \tag{2}$$
$$x^{\pm}(t) = x_u^{\pm} \text{ for } t = 0, \quad x^{\pm}(t) = x_s \text{ for } t = +\infty,$$

and the activation energy for escape is equal to the difference between the maximum and minimum values of the potential, $S_0 = U(x_u^{\pm}) - U(x_s)$.

The periodic driving force breaks time-reversal symmetry and, in general, the *nonequilibrium* MPEP then has to be found numerically by solution of e.g. a variational problem [7]. According to the LS theory[7, 8], if the driving field is not too strong, the deviation of the path away from $x^{\pm}(t)$ can be neglected (see Fig. 1 and the discussion below). To leading order, the changes in activation energy are given by the maximal work the force does on the system as it moves along the *equilibrium* paths so that, for (1)

$$S^{\pm} = S_0 + \delta S^{\pm}, \quad \delta S^{\pm} = -A|\tilde{\chi}(\Omega)|,$$
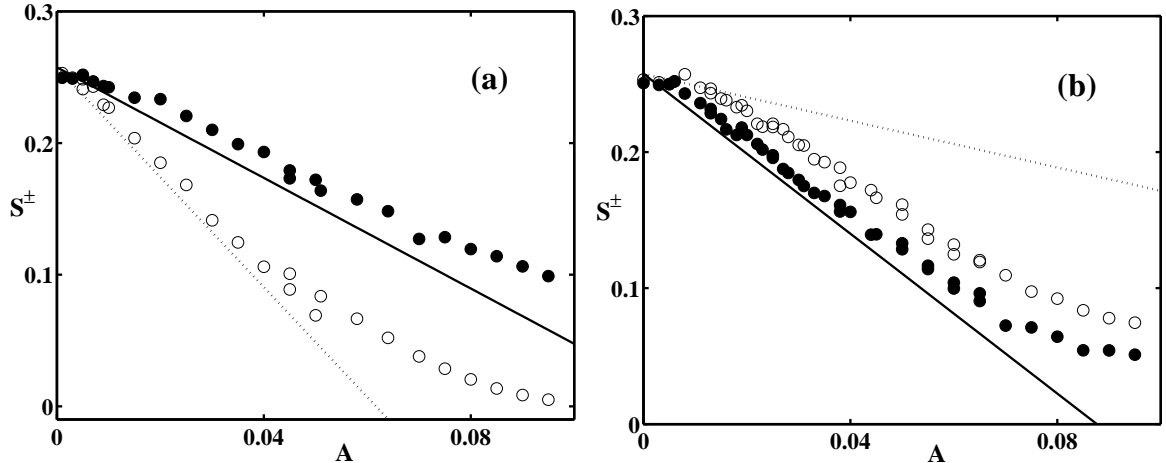
Figure 3: Dependence of the activation energy S on the amplitude A of the drive determined by numerical simulations with $0.016 < T < 0.031$ for (a) $\Omega = 0.01$; (b) $\Omega = 0.35$. The lines indicate the LS theory. Other parameters and symbols are as in Fig. 1.

$$\tilde{\chi}(\Omega) = \int_{-\infty}^{\infty} dt \, \chi^{\pm}(t) e^{i\Omega t}, \quad \chi^{\pm}(t) = -\dot{x}^{\pm}(t). \tag{3}$$

Thus the susceptibility $\tilde{\chi}(\Omega)$ is given by the Fourier transform of the velocity $\dot{x}^{\pm}(t)$ of the system when travelling along the MPEP in the absence of driving. Since $\delta S^{\pm}$, i.e. the changes of the *logarithms* of the escape rates $W^{\pm}$, are proportional to A and are expressed in terms of the system characteristics in equilibrium the coeficient of proportionality is called the *logarithmic susceptibility* [7, 8] by analogy with standard linear susceptibility.

The WKB-like activation law for the escape probabilities (see above) means that, although $\delta S^{\pm}$ are small, the field-induced corrections to the escape probabilities depend upon the field amplitude exponentially strongly in the limit $T \to 0$. When the system fluctuates close to an unstable periodic state, it will remain there for a time exceeding the field period. Thus, in contrast to the adiabatic case, the transition probability is not synchronized with the field, and does not depend on time [16].

Calculations based on (2) yield the full and dotted curves in Figs. 2 and 3. It is evident that all the main qualitative features of the simulations are reproduced by the LS theory. For transitions to the right, there is good agreement between experiment and simulation over the full frequency range. For transitions to the left there is of course good agreement in the adiabatic range (Fig. 3(a)), apart from a small offset associated with the prefactor, but definite disagreement (Fig. 3(b)) for higher frequencies corresponding to the range for which there is a marked deviation of the dispersion of $\delta S^{-}/A$ from the theoretical curve (c.f. Fig. 2). The deviation from a linear dependence of $\delta S^{\pm}$ on A at small amplitudes was also observed in earlier experiments [6], but an explanation in terms of the dependence of the prefactor on noise amplitude was given only recently [16]: for the theory to be applicable without corrections, the field-induced changes to the activation energy must be larger that the uncertainty due to the finiteness of the temperature. This idea is being tested experimentally by measurement of $\delta S^{\pm}$ in different temperature ranges. The deviation from $\delta S^{\pm} \propto A$ at large A is caused mainly from going beyond the range of applicability ($\delta S^{\pm} \ll S^{\pm}$) of the theory.

Perhaps the most interesting and important features of resonant activation in a spatially asymmetric potential are the predictions [7] of resonant rectification of the fluctuations and current reversal. The occurrence of these phenomena in the simulations can immediately be inferred from the frequency and amplitude dependences of the activation energies of transitions in opposite directions. Direct measurements of the rectification rate, i.e. of the net current, are indeed found [20] to exhibit both resonance and current reversal. As expected from the WKB approximation for the escape probabilities, the current rises exponentially with temperature.

But the efficiency of the rectification, defined as the net current J normalized by the sum of the currents in both directions, i.e. $(W^+ - W^-)/(W^+ + W^-)$, is better at lower temperatures [20]. Thus if we have e.g. to transport particles from one side of the ratchet to the other, as in the case of diffusion of cold rubidium atoms in an asymmetric optical lattice [17] or surface electromigration [18], the process works faster at higher temperatures, but more particles will then be travelling in the wrong direction. Neglecting the dependences of the prefactors on parameters and temperature, we have compared the efficiency of the rectification with theoretical predictions. The agreement is semi-quantitative: as expected, the effect is much weaker then predicted for the range of frequencies between 0.3 and 0.4 where deviations of δS^- from the theory are most pronounced.

In attempting to account for the disagreements between simulation and theory we note, first, that the transitions to the right and to the left were measured independently and that the temperature was low enough that the transition time was always exponentially smaller then the escape time. Thus the possibility of mutual interference between transitions to the right and to the left was excluded. We have also investigated possible effects of the stochastic layer near the saddles which can in principle annihilate the difference between left and right [21]: but, for our parameters, the effect is insignificant, and no direct transitions between saddles were observed. For the LS theory to be applicable, $k_B T$ has to be the smallest parameter of the problem. Thus for the fluctuations to "feel" the difference in the shape of the MPEP in opposite directions, $k_B T$ should be smaller than the characteristic energy loss between turning points of the MPEP, which $\propto \Gamma$. Temperatures above ~ 0.05 tend to eliminate the asymmetry of the transition rates, the selective effect of the potential is washed out, and the rectification rate falls (see also e.g. [19]). Even at lower temperatures, the sharp resonances predicted by the theory are found to be smeared out in the numerical simulations (dotted curve v. open circles data) in Fig. 2.

The data in Figs. 2 and Fig. 3(b) show that the effect of finite temperature is apparently different in the two directions. The origin of this difference must presumably lie in the dynamics of fluctuations along the actual escape trajectories (see Fig. 1) and is apparently associated with the potential barrier for transitions to the left having a point of inflection. It can be seen in Fig. 1 that the MPEP to the left moves very close to the potential and therefore experiences critical slowing down. The effect is local in coordinate, but it is not local in time. In this region even small deviations of the escape path away from $x^-(t)$ result in significant changes of activation energy and must be taken into account as corrections to (3). In general, one may expect the theory to work best in cases where (as for transitions to the right, c.f. Fig. 2) there are no very sharp features in the shape of the potential. For example, we would expect the theory to work without correction for the smooth asymmetric potential used in the experiments on the diffusion of cold rubidium atoms [17].

4 Conclusion

In conclusion, we have observed resonant rectification of fluctuations to yield transport for weakly damped motion in a Brownian ratchet. The LS theory provides a satisfactory description of the observed phenomena, but it can become only semi-quantitative near sharp features in the dispersion of $\delta S^\pm$, apparently because these are rounded by the necessarily finite noise intensity, or by the small deviations of the MPEP from the path in thermal equilibrium. Note that the effects considered here differ from resonant activation (in the sense of an optimal noise intensity) in an overdamped system with fluctuating potential barrier [22], and from rectification of fluctuations in an underdamped system with periodic temperature profile [23]. The work opens new possibilities for controlling the effectiveness of thermal ratchets. For example, it was noticed in [10] that voltage rectification by an overdamped SQUID ratchet decreases very fast (exponentially fast [24]) for high frequencies. Given that its equations of motion [10] are of the form (1) we suggest that the rectification mechanism

discussed above can be applied to e.g. high-frequency voltage rectification by a SQUID ratchet.

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