PHYSICAL REVIEW LETTERS

VOLUME 84 | 10 JANUARY 2000 | NUMBER 2

Backward-to-Forward Jump Rates on a Tilted Periodic Substrate

M. Borromeo
Dipartimento di Fisica and Istituto Nazionale di Fisica Nucleare, Università di Perugia, I-06100 Perugia, Italy

F. Marchesoni
Istituto Nazionale di Fisica della Materia, Università di Camerino, I-62032 Camerino, Italy
and Department of Physics, University of Michigan, Ann Arbor, Michigan 40109-1120
(Received 4 August 1999)

Driven diffusion of a Brownian particle along a one-dimensional lattice is investigated numerically on decreasing its damping constant. The notions of multiple jumps, jump reversal, and backward-to-forward rates are discussed in detail. In particular, we conclude that in the underdamped limit backward jumps are suppressed relative to forward jumps more effectively than previously assumed. The dependence of such a drive-controlled mechanism on the damping constant and the temperature is interpreted analytically.

PACS numbers: 05.40.Jc, 02.50.Ey, 05.50.+q, 05.60.Cd

The decay of an asymmetric metastable state, represented, for instance, by the tilted potential wells of Fig. 1, plays a crucial role in the theories of chemical reactions [1] and lattice defects [2], to mention two among the most historically sigificant examples. Moreover, forced Brownian motion on periodic substrates [like the one-dimensional potential illustrated in Fig. 1(c)] provides an archetypal model of transport in condensed phase, notable examples being resistively shunted Josephson junctions [3], superionic conductors [4], plasma accelerators [5], adsorbates on crystal surfaces [6], and polymers diffusing at interfaces [7]. Brownian diffusion in the overdamped limit is by now a fully understood stochastic process, whose application to physical systems can be worked out in great detail [8,9]. *Low damping* diffusion, instead, while accounting for most inertial effects observed in real experiments—think of *I-V* characteristics of shunted Josephson junctions [9–11], dislocation losses in metals [12], dissipation in threshold devices [13], etc.—gives rise to more complicated transport mechanisms, whose description is not completed, yet, despite Risken's monumental work [8].

An equilibrium chemical reaction is often modeled as an escape process that takes place in a two-well potential [1]. As the reaction proceeds from the left to the right, or vice versa, one defines the corresponding mean-first-passage time (MFPT) T_R, or T_L, for the chemical coordinate $x(t)$ to overcome the barrier at x_0 from the left, or the right, respectively [14]. A simple combination of these two Kramers times yields the equilibrium reaction rate $\lambda = T_R^{-1} + T_L^{-1}$. For very large values of the damping constant (Smoluchowski approximation) T_R and T_L can be computed analytically with great accuracy; in particular, one easily proves that $T_L/T_R \simeq \exp(-\Delta V/kT)$, where $\Delta V/kT$ is the reaction-to-thermal energy ratio.

On turning the bistable potential in Fig. 1(a) upside down, we obtain a metastable asymmetric well (Duffing oscillator) with identical decay rate λ. The isospectrality of the discrete transformation connecting the two problems is discussed in Ref. [8]. The asymmetric Duffing well can be interpreted as a two-exit MFPT model: The escape time $T_0 = \lambda^{-1}$ is uniquely defined irrespective of the actual exit point, x_L or x_R, chosen by the coordinate $x(t)$ to exit the well. Correspondingly, one introduces the probabilities $p_\pm$ for the exit event to occur through x_R or x_L, respectively. In the overdamped limit, the backward-to-forward rate (BFR) p_-/p_+ boils down to the Arrhenius factor $\exp(-\Delta V/kT)$ [14]. The spectral symmetry of the two escape problems of Fig. 1(a) is thus made even stronger in the overdamped limit by the additional identity $p_-/p_+ = T_L/T_R$ (for a numerical verification see Fig. 2).

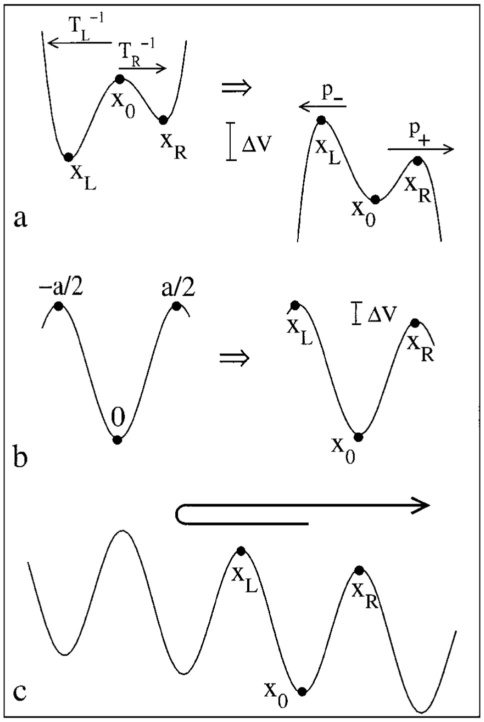

FIG. 1. Asymmetric one-dimensional potential wells. (a) Upside-down inversion of a tilted quartic double-well potential. Note that the energy barrier difference ΔV is the same before and after the transformation. (b) Cosine potential well for zero and finite tilt. The tilt shifts the position of the barriers and the well bottoms, i.e., $x_{R,L} = \pm(a/2 \pm x_0)$ and $x_0 = (a/2\pi)\arcsin(aF/2\pi\omega_0^2)$, where ω_0^2 is the cosine amplitude. (c) Tilted washboard potential, as obtained by continuously connecting replicas of the tilted cosine well in (b). The exit trajectory depicts a jump reversal.

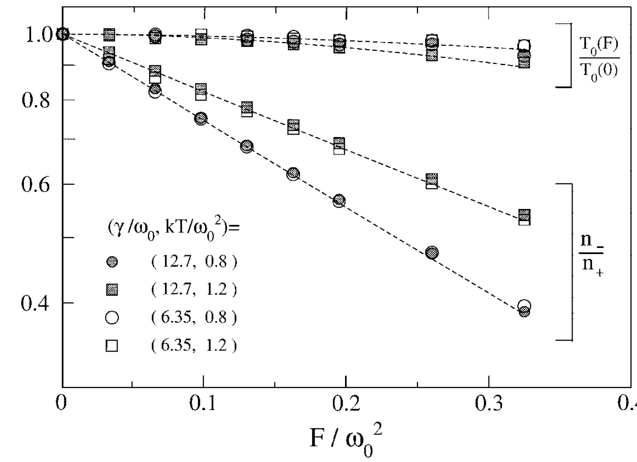

FIG. 2. Exit event statistics in the overdamped limit for different kT/ω_0^2 and γ/ω_0 values. All simulation results are given in dimensionless units. Dashed lines represent the MFPT predictions for $T_0(F)/T_0(0)$ (upper curves) and p_-/p_+ (lower curves), respectively. Note that in the overdamped limit no γ dependence of the plotted ratios is expected.

In the opposite limit of vanishingly small damping constant, the explicit calculation of the escape times T_R or T_L over the barrier of the two-well potential, though more complicated [8,9], leads again to the same Arrhenius law, $T_L/T_R \simeq \exp(-\Delta V/kT)$, as in the Smoluchowski approximation. Furthermore, the isospectrality property of the inverted potentials holds good in the presence of inertial effects, too (i.e., for finite values of the damping constant). This means that we are left with the ultimate task of determining to what extent the decay through the forward channel (with probability p_+) is more likely than through the backward one (with probability p_-).

This brings us to the central question addressed in this Letter: How does a BFR like p_-/p_+ depend on the damping constant? Here, we anticipate the main conclusion of this work, that, at variance with T_L/T_R, the ratio p_-/p_+ gets strongly suppressed in the underdamped limit; such an asymmetry controlled mechanism turns out to be much more effective than recognized in the earlier literature [9–11].

The question above has a natural counterpart in the characterization of stationary transport along a tilted washboard potential [like that created in Fig. 1(c) by connecting continuously the individual asymmetric wells of Fig. 1(b)]. As shown in Refs. [15–19], an underdamped Brownian particle falls down a tilted periodic substrate by performing multiple jumps, that is, over many a potential barrier. A particle trapped into a certain potential well can exit it by jumping either to the right (forward) or to the left (backward); moreover, no matter what side it jumps, the particle can get retrapped either to the right or to the left from its starting well or, equivalently, it may reverse its velocity on the jumping process. Thus, more different (though related) definitions of BFR may be introduced to which our question, as of their damping constant dependence, applies.

Our simulation code is based on a standard one-step collocation algorithm for the integration of stochastic differential equations. To allow an easier comparison of BFRs from decay and transport processes we simulated the Langevin equation (in rescaled units)

$$\ddot{x} = -\gamma\dot{x} - \omega_0^2 \sin x + F + \xi(t)\,, \qquad (1)$$

where the force terms on the right-hand side (rhs) represent, respectively, a viscous damping with constant γ, a spatially periodic, tilted substrate described by the potential

$$V(x,F) = \omega_0^2(1 - \cos x) - Fx \qquad (2)$$

[see Fig. 1(c)], and a stationary Gaussian noise with zero mean $\langle\xi(t)\rangle = 0$ and autocorrelation function $\langle\xi(t)\xi(0)\rangle = 2\gamma kT\delta(t)$. At low temperatures, $kT \ll \omega_0^2$, the system (1) undergoes a sudden locked-to-running transition as the tilt amplitude is increased above a certain threshold $F_2 \simeq 3.36\omega_0\gamma$; correspondingly, the stationary current $\langle\dot{x}\rangle$ jumps from exponentially small intensities for $F < F_2$ to a free-fall asymptotic value F/γ for $F > F_2$ [8,19].

On imposing absorbing boundary conditions at x_L and x_R, the MFPT out of a single potential well can be computed with arbitrarily high statistics. As a caveat we remind the reader that the simulation outcome may depend (weakly at low temperature) on the choice of the initial conditions—for simplicity we set $x(0) = x_0$, $\dot{x}(0) = 0$. Periodic boundary conditions at x_L and x_R are required to simulate a stationary probability current; however, the jump statistics is sensitive to the definition of particle trapping. Here, we agree to consider the diffusing particle as trapped in the well centered at x_0, if it has sojourned in the unit cell (x_L, x_R) for a time lapse not shorter than $(2\gamma)^{-1}$, the relaxation time of the energy variable $E(x,\dot{x}) = \dot{x}^2/2 + V(x,0)$ [8]. Our initial conditions for the decay of a metastable state and the trapping criterion for the stationary jumping dynamics are consistent with one another as shown in Fig. 4(a), below.

Decay of an asymmetric well.—Figures 2, 3(a), and 4(a) summarize the statistics of the decay process out of an asymmetric metastable state. In the overdamped limit of Fig. 2 the BFR p_-/p_+ is clearly independent of the damping constant and vanishes with increasing the tilt amplitude F according to the (leading order) Arrhenius law

$$p_-/p_+ = \exp(-aF/kT) \tag{3}$$

with $a = 2\pi$. For the sake of a comparison we also plotted the MFPT predictions for the ratios $T_0(F)/T_0(0)$ and p_-/p_+ versus F: as expected, the agreement is very close [14].

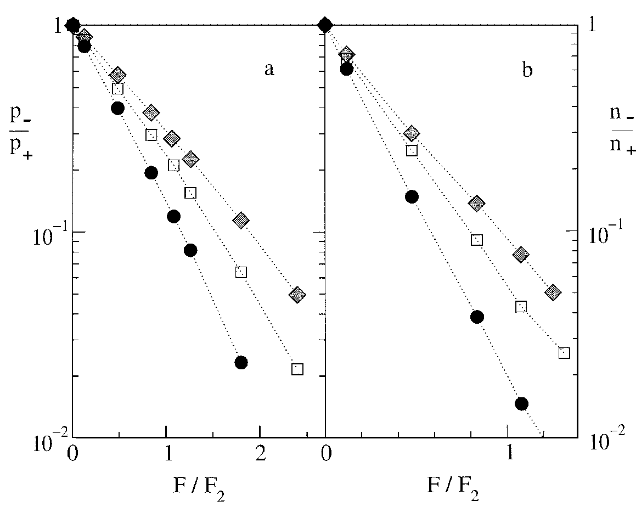

FIG. 3. Backward-to-forward rates for the decay of an asymmetric well p_-/p_+ (a) and in the stationary flow regime n_-/n_+ (b) at different temperatures $kT/\omega_0^2 = 1.2$ (diamonds), 0.8 (squares), and 0.4 (circles).

The underdamped limit reveals more interesting properties: (i) The ratio p_-/p_+ decays exponentially with F but at a much faster rate than previously assumed, namely,

$$p_-/p_+ = \exp[-F/F_e(T,\gamma)] \tag{4}$$

with $F_e \ll kT/a$ [see Fig. 3(a)]. (ii) The tilt constant F_e scales like $\sqrt{\gamma T}$ as displayed in Fig. 4(a). (iii) The above properties apply to the BFR out of a trapping well in the stationary flow regime, too. Even more remarkably, the tilt constant $F_e(T,\gamma)$ is numerically the same for the two problems, at least for the initial conditions and trapping criterion adopted in the present simulation.

The analytical estimate for $F_e(T,\gamma)$ plotted in Fig. 4(a) was obtained through a simple rate argument. As proven by Risken and co-workers [8], the excitable energy states that contribute to the stationary current along a tilted cosine potential all belong to a thin $(x,\dot{x})$ phase-space (or "skin") layer with upper energy bound $2\omega_0^2$ (the energy barrier of the cosine potential) and width $kT\sqrt{aF_1/2kT}$ [with $F_1 = (4/\pi)\omega_0\gamma$ and $a = 2\pi$]. Exiting a potential well to the left, that is, against the external force F, implies wasting an additional energy aF off the available layer energy; hence, the exponential law (4) with

$$F_e(T,\gamma) = \frac{kT}{a}\sqrt{\frac{aF_1}{2kT}}\,. \tag{5}$$

Jumps in the stationary flow regime.—A more practical definition of BFR in the presence of a stationary flow

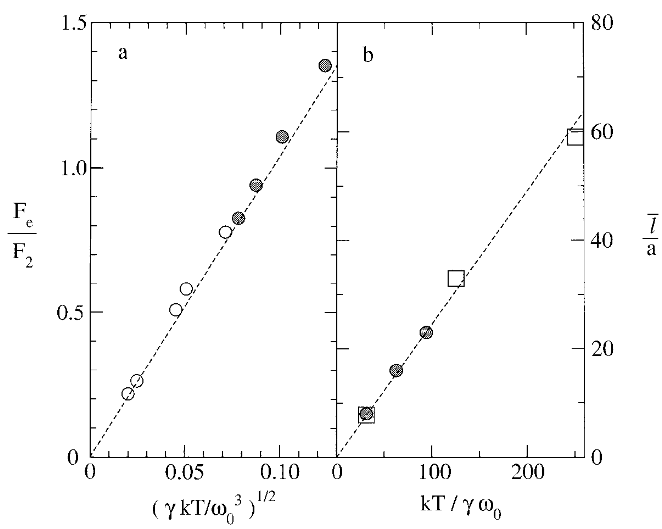

FIG. 4. Theoretical interpretation of the BFR decay. (a) The tilt constant $F_e(T,\gamma)$ that fits the BFR data for the decay of a metastable state (solid circles) and of a trapped particle in the stationary flow regime (open circles). The open circles have been obtained by varying γ/ω_0 with $kT/\omega_0^2 = 0.8$, the solid circles by varying kT/ω_0^2 at $\gamma/\omega_0 = 1.27 \times 10^{-2}$. The dashed line represents the fitting laws (4) and (5). (b) The average trajectory length $\bar{l}$ in units of a for $F = 0$ and different values of kT/ω_0^2 (with $\gamma/\omega_0 = 1.27 \times 10^{-2}$, solid circles) and different values of γ/ω_0 (with $kT/\omega_0^2 = 0.8$, open squares). The dashed line represents the fitting law (7).

is provided by the backward-to-forward jump rate ratio n_-/n_+. Here, $n_\pm$ denote the fractions of jumps that land to the right or left from the starting well. Note that the Brownian particle has a finite probability of ending its flight in the very same well from where it set out (closed loops); hence, $n_+ + n_- < 1$. In view of our trapping criterion such a BFR can be easily computed as a function of the applied tilt F for different temperature and damping constant values. Our numerical results are displayed in Fig. 3(b). In close analogy with the simulation of Fig. 3(a), our data for n_-/n_+ decay according to the exponential law $\exp[-F/F_j(t,\gamma)]$ with tilt constant F_j proportional to $\sqrt{\gamma T}$. More notably, we observed that over the entire range of (small) γ and T values we simulated, the numerical relation $F_j(T,\gamma) = (1/2)F_e(T,\gamma)$ holds with good accuracy (i.e., within less than 5%). This allows us to connect the two alternate definitions of BFR in the stationary flow regime, namely,

$$\frac{n_-}{n_+} = \left(\frac{p_-}{p_+}\right)^2. \tag{6}$$

This BFR property can be traced back to the well established fact that as the diffusing particle hits the top of a potential barrier (with almost zero speed [8–11]), it has still a 50% chance of jumping to the left (with rate n_-) or to the right (with rate n_+). This simple rate argument relates F_j and F_e to one another in agreement with the outcome of our simulation.

The two different BFR of Eq. (6) are a signature of the jump reversal mechanism described in Refs. [15–18]. In order to get a deeper insight in the steady-state jumping process we computed the normalized distributions of the jump lengths X and the corresponding trajectory lengths l connecting two trapping events. Our numerical results are displayed in Fig. 5 for three values of the tilt amplitude.

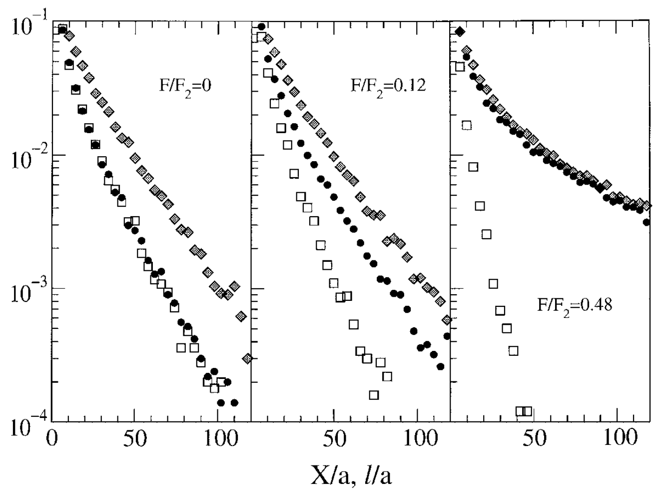

FIG. 5. Distribution of the trajectory lengths l (diamonds) and jump lengths X to the right (circles) and to the left (squares) for $kT/\omega_0^2 = 1.2$ and $\gamma/\omega_0 = 1.27 \times 10^{-2}$. The l distributions and the *sum* of both X distributions are normalized to unity.

More distributions have been obtained over wide temperature and damping constant ranges. It is apparent on inspection that the average jump lengths $\bar{X}_\pm$, to the right and to the left, respectively, are shorter than the average trajectory length $\bar{l}$. This implies that, as an effect of thermal fluctuations, a jumping particle, after exiting a trapping well in either direction, has a finite chance of reversing its velocity prior to getting trapped again.

We investigated the difference between $\bar{X}_\pm \equiv \bar{X}$ and $\bar{l}$ in the zero tilt case: The ratio $\bar{l}/\bar{X}$ tends to one linearly with decreasing the temperature. Moreover, we concluded that $\bar{l}$ is proportional to T and inverse proportional to γ; our data for $\bar{l}(T,\gamma)$ seem to follow closely the phenomenological law [see Fig. 4(b)]

$$\frac{\bar{l}}{a} = 2\,\frac{kT}{aF_1} \tag{7}$$

with $a = 2\pi$ and F_1 given in Eq. (5). Our estimate (7) for $\bar{l}$ means that a thermally diffusing particle (with average thermal energy kT [8–11]) can jump over $\bar{l}/a$ potential barriers by dissipating an energy amount of the order of $aF_1/2$ in each unit cell (note that a jumping particle performs only half a closed trajectory in the relevant skin layer [8]). Another important remark: The ratio on the rhs of Eq. (7), which also shows up in Eq. (5), is likely to be the true control parameter of the jump statistics. Finally, switching on the tilt F makes $\bar{X}_+$ grow exponentially at the expense of $\bar{X}_-$ until, as expected, $\bar{X}_- \simeq 0$ and $\bar{X}_+ \simeq \bar{l}$.

In the present Letter we have investigated numerically the backward-to-forward jump diffusion of a Brownian particle on a one-dimensional periodic lattice. The analytic interpretation of the stationary jump statistics is meant here as instrumental to the full understanding of stochastic resonance [20] and thermal transport on a washboard potential subjected to a periodic bias [21]. Moreover, the dependence of the BFR on the damping constant and the temperature allows an alternate characterization of the complicated underdamped dynamics taking place on a periodic substrate [8,9].

[1] P. Hänggi, P. Talkner, and M. Borkovec, Rev. Mod. Phys. **62**, 251 (1990).
[2] F. R. N. Nabarro, *Theory of Crystal Dislocations* (Dover, New York, 1987).
[3] A. Barone and G. Paternó, *Physics and Applications of the Josephson Effect* (Wiley, New York, 1982).
[4] P. Fulde, L. Pietronero, W. R. Schneider, and S. Strässler, Phys. Rev. Lett. **35**, 1776 (1975).
[5] T. Katsouleas and J. Dawson, Phys. Rev. Lett. **51**, 392 (1983).
[6] J. W. M. Frenken and J. F. van der Veen, Phys. Rev. Lett. **54**, 34 (1985); B. Pluis *et al.*, Phys. Rev. Lett. **59**, 2678 (1987).
[7] G. I. Nixon and G. W. Slater, Phys. Rev. E **53**, 4969 (1996).

[8] H. Risken, *The Fokker-Planck Equation* (Springer, Berlin, 1984), Chap. 11; K. Voigtlaender and H. Risken, J. Stat. Phys. **40**, 397 (1985); H. Risken and K. Voigtlaender, J. Stat. Phys. **41**, 825 (1985).
[9] V. I. Melnikov, Phys. Rep. **209**, 1 (1991).
[10] E. Ben-Jacob, D. J. Bergman, B. J. Matkowsky, and Z. Schuss, Phys. Rev. A **26**, 2805 (1982); E. Ben-Jacob, D. J. Bergman, and Z. Schuss, Phys. Rev. B **25**, 519 (1982).
[11] M. Büttiker, E. P. Harris, and R. Landauer, Phys. Rev. B **28**, 1268 (1983); M. Büttiker and R. Landauer, Phys. Rev. B **30**, 1551 (1984).
[12] O. M. Braun, A. R. Bishop, and J. Röder, Phys. Rev. Lett. **79**, 3692 (1997); C. Cattuto and F. Marchesoni, Phys. Rev. Lett. **79**, 5070 (1997).
[13] M. Borromeo, G. Costantini, and F. Marchenoni, Phys. Rev. Lett. **82**, 2820 (1999).
[14] C. W. Gardiner, *Handbook of Stochastic Methods* (Springer, Berlin, 1983).
[15] R. Ferrando, R. Spadacini, and G. E. Tommei, Phys. Rev. E **48**, 2437 (1993).
[16] E. Pollak, J. Bader, B. J. Berne, and P. Thalkner, Phys. Rev. Lett. **70**, 3299 (1993).
[17] P. Jung and B. J. Berne, in *New Trends in Kramers' Theory,* edited by P. Talkner and P. Hänggi (Kluwer Academic, Dordrecht, 1995), p. 67.
[18] R. Ferrando, R. Spadacini, and G. E. Tommei, Phys. Rev. E **51**, 126 (1995).
[19] G. Costantini and F. Marchesoni, Europhys. Lett. **48**, 491 (1999).
[20] L. Gammaitoni, P. Hänggi, P. Jung, and F. Marchesoni, Rev. Mod. Phys. **70**, 223 (1998).
[21] F. Marchesoni, Phys. Lett. A **231**, 61 (1997).