Giant enhancement of diffusion and particle selection in rocked periodic potentials

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Abstract. – We investigate the motion of an overdamped Brownian particle in a periodic potential with weak thermal noise and a time-periodic unbiased (*i.e.* $\langle F(t)\rangle = 0$) external driving force $F(t)$. By introducing appropriate "waiting-periods", where $F(t)$ vanishes, an arbitrarily strong enhancement of diffusion in a *symmetric* potential is possible. In *asymmetric* periodic potentials (ratchets) the net flux of particles can be directed in both directions, even in the *absence* of thermal noise. For finite temperatures we observe and explain additional, pure-noise–induced flux reversal phenomena.

Directed transport induced by unbiased driving forces in periodic structures with broken spatial symmetry (ratchets) has been investigated in the context of photovoltaic and photorefractive effects already for several decades [1]. Independent of such precursors, considerable interest in this scheme resurfaced with both theoretical [2] and experimental [3] recent activities that relate to the operation of Brownian machinery and molecular motors. On the other hand, the exploration of diffusive transport in completely symmetric, driven systems is still at its beginning [4-7]. In this letter we cover both modes of transport within a common model that allows a quite detailed analytical treatment. In addition, it should be possible to realize this set-up experimentally. In a first part, we modify the setup from [5, 6] so as to achieve a controlled selective enhancement of diffusion that in principle can be made *arbitrarily strong.* In the second part of our paper we introduce a new variant of the so-called "rocking ratchet" [8,9] for which the flux of particles can be directed in both directions even in the absence of thermal fluctuations, and which exhibits additional pure-noise–induced flux reversals as well.

Control of diffusion. – We consider an overdamped Brownian particle with coordinate $x(t)$ whose dynamics is governed by the Langevin equation

$$\eta\dot{x}(t) = -V'(x(t)) + F(t) + \sqrt{2kT\eta}\,\xi(t) \ . \tag{1}$$

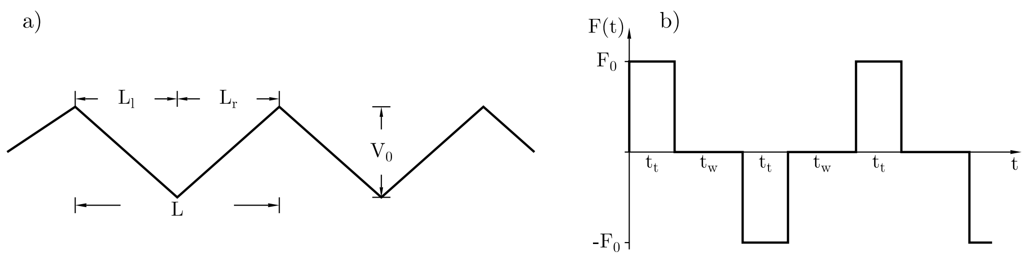

Fig. 1. – a) Sawtooth potential $V(x)$ with period L and barrier height V_0. The lengths of the piecewise linear parts to the left and right of each potential minimum are denoted as $L_\mathrm{l} = aL$ and $L_\mathrm{r} = (1-a)L$, respectively. Depicted is the symmetric case $L_\mathrm{l} = L_\mathrm{r}$. b) Time-periodic, piecewise constant driving force $F(t)$ with model parameters F_0 ("tilt"), t_t ("tilting-time"), and t_w ("waiting-period").

Here, η is the viscous friction coefficient, $V(x)$ is a periodic potential, $F(t)$ is an external driving force, and $\xi(t)$ are thermal fluctuations (at temperature T) modeled by unbiased δ-correlated Gaussian noise. The quantity of central interest is the diffusion coefficient

$$D := \lim_{t\to\infty} \{\sigma^2(t)/2\,t\}, \qquad \sigma(t) := \sqrt{\langle x^2(t)\rangle - \langle x(t)\rangle^2}\ . \tag{2}$$

For free Brownian motion, *i.e.* $V'(x) \equiv 0$ and $F(t) \equiv 0$, one finds from (1), (2) that

$$D_\mathrm{free} = kT/\eta\ . \tag{3}$$

The same result (3) is recovered for *any kind* of driving $F(t)$ as long as $V'(x) \equiv 0$. As far as non-trivial potentials $V(x)$ are concerned, we focus on the simplest case of a *symmetric* sawtooth profile with period L and barrier height V_0 (fig. 1a) and a time-periodic driving force $F(t)$ with three states F_0, 0, and $-F_0$. As illustrated in fig. 1b, time segments of length t_t with a constant tilt $F(t) = \pm F_0$ are separated by "waiting-periods" t_w with vanishing $F(t)$. Further, we henceforth restrict ourselves to weak thermal noise, $kT \ll V_0$.

If $F_0 < 2V_0/L$, particles obeying (1) spend most of their time near some minimum of the potential $V(x)$ and only very rarely exhibit thermally activated hopping between different minima. As a consequence [10], the diffusion coefficient (2) is exponentially smaller than for free diffusion (3). To discuss the opposite case, $F_0 > 2V_0/L$, we consider an initial particle distribution at time $t = 0$ with a very narrow peak at a minimum of the potential $V(x)$, say at $x = 0$. As long as $t \le t_\mathrm{t}$, we have $F(t) \equiv F_0$, so the peak moves to the right under the action of the deterministic forces and also broadens slightly due to the weak thermal noise in (1). The deterministic time t_n at which the peak crosses the n-th maximum of $V(x)$ at $x = (n-1/2)L$ while $F(t) = F_0$ is acting, reads

$$t_n = \frac{\eta L^2}{2}\left(\frac{n}{LF_0 - 2V_0} + \frac{n-1}{LF_0 + 2V_0}\right)\ , \qquad n = 1, 2, 3, \ldots \tag{4}$$

If now t_t just matches one of those times t_n, then the original single peak is split into two equal parts and if the subsequent "waiting-interval" t_w with $F(t) \equiv 0$ is sufficiently long (*i.e.* $t_\mathrm{w} > L^2\eta/4V_0$) the two parts will proceed towards the respective nearest minimum of $V(x)$ at $x = (n-1)L$ and $x = nL$. The result is *two* very sharp peaks after half a period $t = t_\mathrm{t} + t_\mathrm{w}$ of the driving force $F(t)$. Similarly, after a full period $\tau := 2(t_\mathrm{t} + t_\mathrm{w})$ one obtains *three* narrow peaks at $x = -L$, 0, L with weights 1/4, 1/2, 1/4, respectively. For the variance (2) this implies $\sigma^2(\tau) = L^2/2$. In the same way one sees that after n periods $\sigma^2(n\tau) = nL^2/2$, yielding for the diffusion coefficient (2) the temperature-independent (extremal) result

$$D = L^2/8(t_\mathrm{t} + t_\mathrm{w}) \ . \tag{5}$$

In the case that t_t does *not* match any of the t_n from (4) (but still $t_\mathrm{w} > L^2\eta/4V_0$), the initial single peak is split after half a period $t = t_\mathrm{t} + t_\mathrm{w}$ into two peaks with unequal weights. If t_t is sufficiently different from any t_n and the thermal fluctuations are sufficiently weak, one of those two peaks has negligible weight. Consequently, after a full period almost all particles will return to $x = 0$. The diffusion coefficient (2) is therefore very small, in particular much smaller than for free diffusion (3). The next question is how much t_t may deviate from t_n in order that the resulting diffusion coefficient (2) is still comparable to the peak-value (5). A straightforward calculation leads to the following estimate for the mismatch $\Delta t_n = |t_\mathrm{t} - t_n|$ corresponding to half the peak-value (5):

$$\Delta t_n \approx (2kT\eta L^2 t_n)^{1/2}/(LF_0 - 2V_0) \ . \tag{6}$$

We remark that if t_t becomes very large, then even an initially sharply peaked distribution of particles will spread out over several periods L during such a long "tilting-time" t_t under the influence of the thermal fluctuations. The peak then gets split into more than two pieces with appreciable weights and our above arguments have to be modified accordingly. To keep things under control we exclude this case in the following. Because this condition is equivalent to excluding that neighboring peaks of D merge, one arrives with (4), (6) in terms of this merging condition at $t_\mathrm{t} \ll L^2\eta/8kT(1 + 2V_0/LF_0)^2$.

Summing up, under the assumptions that $F_0 > 2V_0/L$, $t_\mathrm{w} > L^2\eta/4V_0$, $kT \ll V_0$, and $t_\mathrm{t} \ll L^2\eta/8kT(1{+}2V_0/LF_0)^2$ the appearance of peaks in the diffusion coefficient (3) is predicted when t_t matches t_n from (4). The height of the peaks is given by (5) and their width by $2\Delta t_n$ from (6). Outside those peak regions, a D-value much smaller than D_free from (3) is predicted. Note that such a multi-peak structure of D is not only expected upon variation of t_t but also by keeping t_t fixed and varying any other parameter entering t_n from (4), as for instance the friction coefficient η.

By means of the dimensionless quantities

$$\tilde{F}_0 := F_0 L/V_0 \ , \qquad \tilde{t}_\mathrm{t} := t_\mathrm{t} V_0/\eta L^2 \ , \qquad \tilde{t}_\mathrm{w} := t_\mathrm{w} V_0/\eta L^2 \tag{7}$$

and upon noting the condition that $\tilde{F}_0 > 2$, $\tilde{t}_\mathrm{w} > 1/4$, $kT \ll V_0$, and $\tilde{t}_\mathrm{t} \ll V_0/8kT(1{+}2/\tilde{F}_0)^2$, the position of the peaks (4) can be rewritten as

$$\tilde{t}_n := t_n V_0/\eta L^2 = n/(2\tilde{F}_0 - 4) + (n-1)/(2\tilde{F}_0 + 4) \tag{8}$$

and with (3), (5) the corresponding peak-values of D take the form

$$D/D_\mathrm{free} = V_0/8kT(\tilde{t}_\mathrm{t} + \tilde{t}_\mathrm{w}) \ . \tag{9}$$

Finally, the scaled approximate width $\tilde{\Delta}_n := 2\Delta t_n V_0/\eta L^2$ of the n-th peak can be read off from (6) as

$$\tilde{\Delta}_n \approx (8\tilde{t}_n kT/V_0)^{1/2}/(\tilde{F}_0 - 2) \ . \tag{10}$$

These predictions (8)-(10) for the diffusion coefficient D as a function of the scaled "tilting-time" $\tilde{t}_\mathrm{t}$ agree very well with the numerical simulations depicted in fig. 2a. Especially, with increasing n the peaks become approximately equidistant, their height decreases like $1/n$, and their width increases like $\sqrt{n}$. Thus, for large enough times $\tilde{t}_\mathrm{t}$ the peaks actually merge and the diffusion coefficient D approaches a constant asymptotic value. As can be conjectured already from fig. 2a, this asymptotic D-value, corresponding to a fixed static tilt $F(t) \equiv F_0$ or

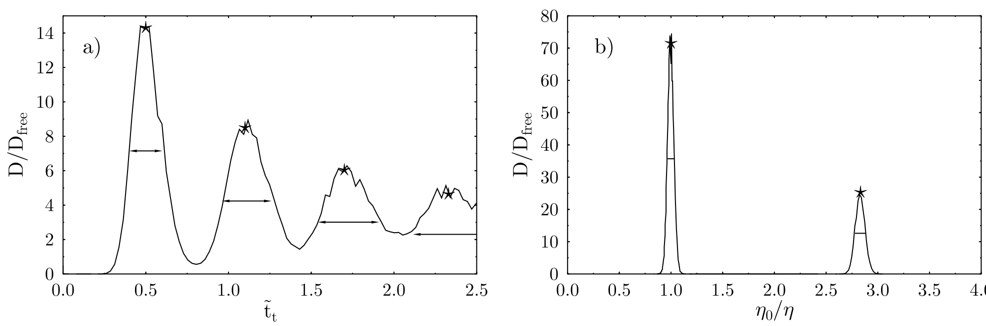

Fig. 2. – a) Diffusion coefficient (2) in units of $D_{\rm free}$ from (3) *vs.* scaled "tilting-time" $\tilde{t}_{\rm t}$ (7) from numerical simulations of the stochastic dynamics (1). The wiggles reflect the statistical uncertainty due to the finite though extensive number of realizations. The relevant dimensionless parameters (cf. (7)) are $kT/V_0 = 0.01$, $\tilde{t}_{\rm w} = 0.375$, and $\tilde{F}_0 = 3$. The theoretical predictions for the location and height of the peaks (8), (9) are indicated by stars, and their approximate widths at half-height (10) by arrows. b) Diffusion coefficient *vs.* friction coefficient from simulations of (1) with $kT/V_0 = 0.005$ and $\tilde{F}_0 = 22$. The (unscaled) times $t_{\rm t}$ and $t_{\rm w} = 13\,t_{\rm t}$ are both kept at fixed values and also define η_0 via $\eta_0 = (2LF_0 - 4V_0)/L^2 t_{\rm t}$. The scaled times (7) are thus varying as $\tilde{t}_{\rm t} = \tilde{t}_{\rm w} = \eta_0/\eta$. Theoretical predictions are indicated analogous to a). Note that the absolute heights (*i.e.* not in units of $D_{\rm free}$) are the same for all peaks.

$F(t) \equiv -F_0$, is larger than $D_{\rm free}$! A more detailed study of this remarkable behavior will be the subject of a forthcoming paper.

Of particular interest is the dependence of the diffusion coefficient D upon the friction coefficient η, corresponding to the situation in which different types of particles are moving in the same rocked periodic potential (1). Of course, particle interactions must still be negligible and —for eqs. (4)-(6) to be applicable— the range of η-values has to respect the restrictions $t_{\rm w} > L^2\eta/4V_0$ and $t_{\rm t} \ll L^2\eta/8kT(1+2V_0/LF_0)^2$. As fig. 2b demonstrates, the dynamics (1) can indeed act as an extremely selective device for separating different types of particles by controlled colossal enhancement of diffusion. Note that eqs. (3), (9) in combination with $\tilde{t}_{\rm w} > 1/4$ and $\tilde{t}_{\rm t} > 0$ imply the inequality $D/D_{\rm free} < V_0/2kT$, which goes over into an equality for $\tilde{t}_{\rm w} \to 1/4$ and $\tilde{F}_0 \to \infty$. In combination with (10) it follows that the peaks in the diffusion coefficient D can in fact be made arbitrarily narrow and high by a proper choice of parameters! One possibility is to decrease the temperature, another to increase V_0 at fixed T while at the same time keeping F_0L/V_0 large. Similarly as for the friction coefficient η, particles can also be separated, *e.g.*, according to their electrical charge since this implies different values of the "coupling-parameters" V_0 and F_0. A practical realization of such a particle separation device (1) along the lines of the beautiful previous experiments [3] should be rather straightforward.

Our findings are robust against various modifications of the model in (1). For instance, more realistic potentials $V(x)$ and driving forces $F(t)$ may be chosen, inertia effects may be included, or more than one spatial dimension may be taken into account. The latter opens interesting perspectives, *e.g.*, to manipulate reaction-diffusion systems. We further note that the symmetries of $V(x)$ and $F(t)$ simplify matters but are not absolutely necessary and that also fluctuations $\xi(t)$ other than of thermal origin will do the job. The indispensable ingredients are strict periodicity in space and time [11] and sufficiently long "waiting-periods" $t_{\rm t}$ with $F(t) \equiv 0$ between subsequent "tilting-times" with non-vanishing $F(t)$. The latter requirement is the crucial difference between our model and the otherwise closely related studies [5, 6].

Not only does our model admit a much better qualitative and quantitative understanding of the basic physical mechanisms but —more importantly— it also seems that only weak-to-moderately pronounced enhancement of the diffusion coefficient D can be obtained with a sinusoidal driving $F(t)$ as considered in [6].

Selective control of current in asymmetric potentials. – Our above reasoning can also be applied to *asymmetric* sawtooth potentials with two different lengths of the potential slopes, $L_\mathrm{l} = aL$ and $L_\mathrm{r} = (1-a)L$ (fig. 1a). As demonstrated in [8,9], with such a "rocking ratchet", a net particle flux can be produced by a deterministic periodic force of zero average. In the deterministic case ($T = 0$) the flux becomes a very complicated function of the model parameters, but for a given potential $V(x)$ and a sinusoidal driving force $F(t)$ it exhibits strictly the same sign [8]. While this deterministic behavior is now well understood, the numerically observed appearance of so-called flux reversals in the presence of thermal noise [8] has up to this date never been satisfactorily explained. Our model also shows a quite complicated but different deterministic behavior; especially deterministic flux reversals are now possible (cf. fig. 3a). Additionally, pure-noise–induced reversals are observed as well.

For an asymmetric sawtooth potential the deterministic traveling times $t_{n,\mathrm{r}}$ from a potential minimum to the n-th neighboring maximum to the right in the presence of a constant tilt $F(t) \equiv F_0$ are different from the corresponding traveling times $t_{n,\mathrm{l}}$ to the left when $F(t) \equiv -F_0$. The results in scaled units (cf. (8)) read:

$$\tilde{t}_{n,\mathrm{r}} = \frac{n(1-a)^2}{\tilde{F}_0(1-a)-1} + \frac{(n-1)a^2}{\tilde{F}_0 a+1}, \qquad \tilde{t}_{n,\mathrm{l}} = \frac{na^2}{\tilde{F}_0 a-1} + \frac{(n-1)(1-a)^2}{\tilde{F}_0(1-a)+1}\ . \tag{11}$$

As a consequence, the displacement of particles to the right after the first half-period $t_\mathrm{t} + t_\mathrm{w}$ need not be identical to the displacement to the left during the second half-period. Under the assumption that $t_\mathrm{w} > L^2_{\mathrm{r,l}}\eta/4V_0$, guaranteeing strong localization about the minima of $V(x)$ after each half-period, a net *deterministic* displacement after a full period by an integer multiple (including 0) of L results, or equivalently, a net flux $\langle\dot{x}\rangle$ equal to a multiple of $L/2(t_\mathrm{t} + t_\mathrm{w})$. Discrete jumps in $\langle\dot{x}\rangle$ occur whenever t_t matches one of the traveling times (11). Note that any displacement to the right is ruled out for $\tilde{F}_0 < 1/(1-a)$ and to the left for $\tilde{F}_0 < 1/a$. Hence, for $a < 1/2$ (so-called "forward-ratchet") and very large t_t there is a net motion to the right if $1/(1-a) < \tilde{F}_0 < 1/a$, cf. fig. 3a. In clear contrast to the previously studied deterministic rocking ratchets [8,9] without a "waiting-time", a net flux in the opposite direction is possible as well: To see this, we consider a large driving force $\tilde{F}_0 \gg 1$. In this case the particle velocities while the potential is tilted to the right or left are very large and nearly the same. But since L_l is smaller than L_r, the particles can reach the left maximum more quickly than the corresponding right one, leading to a net flux in this direction for appropriate t_t, see the high-$\tilde{F}_0$ end in fig. 3a. The crucial point here is once again the strong localization of particles near the minima of $V(x)$ after each half period of the driving $F(t)$. In the absence of the "waiting-period" t_w, this property is lost and no deterministic net flux to the left becomes possible in a rocked "forward-ratchet" [8,9].

So far we were concerned with the purely deterministic behavior ($T = 0$). One effect of a small but finite amount of noise is that the discontinuities at the boundaries between the parameter regions of different flux in fig. 3a are smeared out. But in addition one can also find pure-noise–induced flux reversals. For instance, in the region

$$1/a < \tilde{F}_0 < 1/a(1-a)\ , \tag{12}$$

where the upper boundary $1/a(1-a)$ corresponds to the intersection point of $\tilde{t}_{1,\mathrm{l}}$ and $\tilde{t}_{1,\mathrm{r}}$ in fig. 3a, only zero or positive *deterministic* flux is possible upon variation of $\tilde{t}_\mathrm{t}$. However

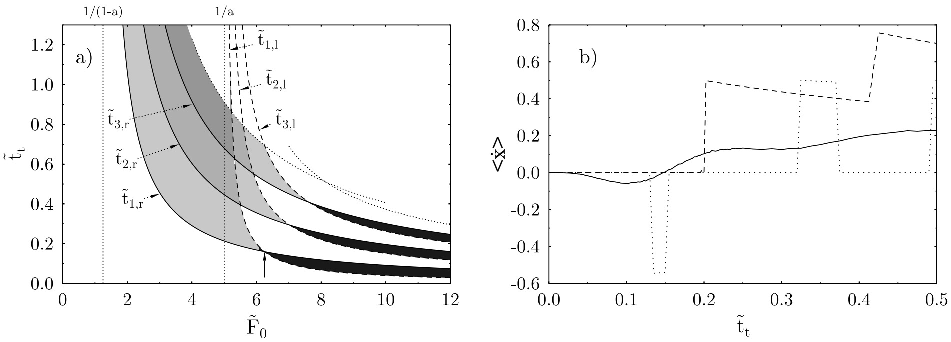

Fig. 3. – a) Scaled traveling times (11) to the right (solid) and left (dashed) *vs.* tilt $\tilde{F}_0$ for $n = 1, 2, 3$ and $a = 0.2$. In the ($\tilde{t}_t$-$\tilde{F}_0$) parameter plane these curves separate areas with different net particle flux for the deterministic dynamics (1) with $T = 0$. White areas denote regimes of zero flux, shaded areas correspond to positive valued flux and the black regions to negative flux values given in multiples of the "unit flux" $L/2(\tilde{t}_t + \tilde{t}_w)$. Additional shaded and black areas associated with $n = 4, 5, \ldots$ in the right upper part of the plot have been omitted. The dotted lines $\tilde{F}_0 = 1/(1-a)$ and $\tilde{F}_0 = 1/a$ refer to the asymptotics of the solid and dashed curves for large $\tilde{t}_t$, respectively. The arrow marks the intersection of $\tilde{t}_{1,r}$ and $\tilde{t}_{1,l}$ at $\tilde{F}_0 = 1/a(1-a) = 6.25$. b) Current $\langle \dot{x} \rangle$ in units of $L/(t_{1,r} + t_w)$ *vs.* scaled "tilting-time" $\tilde{t}_t$ for $a = 0.2$ and $\tilde{F}_0 = 5.2$ (solid and dashed lines). The solid line shows results from simulations of the stochastic dynamics (1) with $kT/V_0 = 0.1$ and the corresponding dashed line depicts the analytical solution for $T = 0$ as discussed below eq. (11). A pure-noise–induced flux reversal is observed for $0 < \tilde{t}_t < a(1-a) = 0.16$. The dotted line exemplifies a multiple *deterministic* current reversal for $\tilde{F}_0 = 6.5$.

if temperature fluctuations are included, the particles may also move to the left (cf. fig. 3b). This effect arises from the fact that the left slope is shorter than the right one. As long as $\tilde{t}_t < a(1-a)$, particles cannot deterministically cross any of the maxima of $V(x)$ but while $F(t) \equiv -F_0$ they can get closer to the left maximum than they get to the right maximum while $F(t) \equiv F_0$. Because the thermal broadening of the particle distribution during such excursions is equal in both cases, more particles will thermally cross the left than the right maximum of the potential, yielding a pure-noise–induced net flux to the left.

Our explanation for the noise-induced flux reversal should hold also for models without t_w; *i.e.* for high driving frequencies, such that particles do not move far away from the minima, and with sufficiently large driving forces such that the particles can thermally cross the maximum to the side of the steep, but short slope easier. As in these models no flux to the left occurs deterministically, this *noise-induced* flux reversal constitutes a general phenomenon (cf. [8]).

Conclusion. – The key ingredient of our model (1) turned out to be the introduction of "waiting time-intervals", in order to concentrate the particles near the potential minima after each half-period of the driving $F(t)$. This opens not only a simple way to understand various features of such a rocked periodic potential but also enables one to control selectively diffusive as well as directed transport in an extremely efficient way. Both for the diffusive and the directed transport, the underlying physical mechanism is rather simple. Symmetric periodic potentials, which without additional force $F(t)$ exponentially suppress thermal diffusion [10], can be used to greatly *enhance* the diffusion over its free value by an appropriate choice of parameters. Remarkably, the peak-diffusion values (6) do not depend on temperature but solely on parameters of the deterministic forces.

In asymmetric potentials the flux of particles can be directed deterministically either to the left or to the right. The addition of noise can induce a current reversal that is absent otherwise. Our asymmetric model can again be exploited for particle selection in various ways. By properly adjusting parameters, one type of objects may be forced to stay localized while the other ones moves. Likewise, both types may move in opposite directions.

The unraveled paradigmatic features of giant diffusion enhancement, and related, the selective control of sign and magnitude of rocking-induced current of this ratchet class, calls for intriguing applications in physics, chemistry and biomedical sciences, *e.g.* to speed up corresponding sluggish diffusion-controlled transport schemes.

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This work was supported by the GIF program "Microscopic Theory of Activated Rate Processes", the Deutsche Forschungsgemeinschaft (HA1517/13-2), and the Graduiertenkolleg GRK283 on "nonlinear problems in analysis, geometry, and physics".

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[11] Small deviations from strict periodicity are tolerable for not too small noise strengths. The peaks in D can then no longer be made arbitrarily sharp.