## PROCEEDINGS OF SPIE



SPIE—The International Society for Optical Engineering

# Noise in Complex Systems and Stochastic Dynamics

Lutz Schimansky-Geier Derek Abbott Alexander Neiman Christian Van den Broeck Chairs/Editors

2–4 June 2003 Santa Fe, New Mexico, USA



### Throwing ropes in the dark: the case of oscillating barriers

Jörg Lehmann<sup>a</sup>, Peter Reimann<sup>b</sup>, and Peter Hänggi<sup>a</sup>

<sup>a</sup>Institut für Physik, Universität Augsburg, Universitätsstraße 1, D-86135 Augsburg, Germany <sup>b</sup>Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, D-33615 Bielefeld, Germany

#### ABSTRACT

We present a novel path-integral method for the determination of time-dependent and time-averaged reaction rates in *multidimensional*, periodically driven escape problems at weak thermal noise. The so obtained general expressions are evaluated explicitly for the situation of a sinusoidally driven, damped particle with inertia moving in a metastable, piecewise parabolic potential. A comparison with data from Monte-Carlo simulations yields a very good agreement with our analytic results over a wide parameter range.

Keywords: Noise-activated escape, periodic-driving, path-integral technique

#### 1. INTRODUCTION

Thermally activated escape problems in the presence of an explicit time-dependent driving are at the root of many timely transport processes. Typical examples comprise the control of chemical reactions with tailored laser pulses, 1,2 ion transport through voltage-gated channels, 3 the pumping and shuttling of particles in Brownian environments, 4-9 or the amplification of weak information-carrying signals via the phenomenon of Stochastic Resonance, 10-13 to name only a few. In the absence of such a time-dependent driving and for the case of weak thermal noise the escape time is governed - as commonly known - by an exponentially leading Arrhenius factor. 14-16 Pioneered by Kramers 17 and extended to arbitrary dimensions in the works, 18-21 this scheme, however, meets formidable difficulties under far from thermal equilibrium conditions. This is so because of an extremely complex interplay between the global properties of the metastable potential and the nonlinear noisy The subject of our present paper is one of the simplest and experimentally most natural such non-equilibrium descendants of Kramers' original escape problem, 17 namely the thermally activated escape of a Brownian particle over a potential barrier in the presence of periodic driving which modulates both the corresponding potential well region and the activation barrier. While most previous attempts have been restricted to weak, 25-27 slow, 28, 29 or fast 25, 28, 30 driving, we have addressed in recent analytical explorations 31, 32 by means of a path-integral technique the most challenging intermediate regime of moderately strong and moderately fast driving for a one-dimensional, overdamped escape problem. Closely related to our recent works are the subsequent appealing efforts in Ref., 33 wherein on uses instead the method of singular perturbation theory in the weak noise limit — a so termed WKB approximation — which, however, also has been restricted to cover only the overdamped, one-dimensional case. The scheme in Ref. 33 yields results which are consistent with the findings in Ref. 31, 32; but it remains on a more formal and implicit level compared to ours.

The objective of this study is to extend these recent works of time-dependent rate theory put forward in Refs. 31-33 to the case of many dimension of the underlying stochastic process. In particular, we shall consider the generic case of a driven inertial Brownian motion dynamics. Furthermore, we shall derive for weak noise asymptotically exact results in analytically closed form for the escape of an inertial, sinusoidally driven Brownian particle in a metastable, piecewise parabolic potential in the regime of moderate forcing strengths and forcing frequencies. A comparison with data from Monte-Carlo simulations yields very good agreement over a wide parameter range.

We anticipate here that the following presentation is on purpose kept rather concise. While we are confident that the general idea of our approach remains more transparent in this way, it is nevertheless advisable to consult the detailed discussion of the one-dimensional, overdamped (i.e. no inertial) dynamics in Ref.<sup>32</sup> for a more thorough and in-depth understanding. It must be pointed out, however, that our present generalization to many dimensions in addition requires several conceptually new steps and features as compared to the one-dimensional overdamped case.

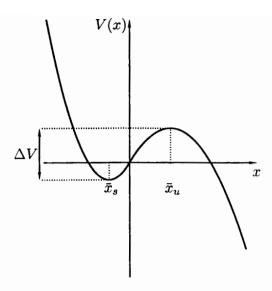


Figure 1. Sketch of a typical metastable potential V(x), namely the piecewise parabolic potential (66) with  $\Delta V = 0.9$ ,  $m\omega_s^2 = 0.6$ , and  $m\omega_u^2 = -0.3$  in arbitrary, dimensionless units.

In Sect. 2, we describe the model under investigation and define both the instantaneous and the time-averaged escape rate. The path-integral formalism and its evaluation for weak-noise is described in Sect. 3. Its application to the escape problem is demonstrated in Sect. 4. Our general findings are then evaluated and discussed explicitly for the case of the driven Kramers problem with a piecewise parabolic potential in Sect. 5. Concluding remarks are given in Sect. 6.

#### 2. THE ESCAPE PROBLEM

#### 2.1. The general Model

The starting-point of our investigations is the following model for the d-dimensional Brownian motion of a particle with coordinates  $\mathbf{x}(t)$  in a time-dependent force field  $\mathbf{F}(\mathbf{x},t)$ :

$$\dot{\mathbf{x}}(t) = \mathbf{F}(\mathbf{x}(t), t) + \sqrt{2\epsilon} \,\mathsf{B}\,\boldsymbol{\xi}(t) \;. \tag{1}$$

Here, bold quantities denote d-dimensional vectors, while  $d \times d$ -matrices are represented by sans-serif fonts. The d-dimensional Gaussian uncorrelated, white noise  $\xi(t)$  is defined by the relations (i, j = 1, 2, ..., d)

$$\langle \xi_i(t) \rangle = 0 , \quad \langle \xi_i(t) \, \xi_j(t') \rangle = \delta_{ij} \, \delta(t - t') ,$$
 (2)

where  $\delta_{ij}$  is the Kronecker delta and  $\delta(t)$  Dirac's  $\delta$ -distribution. The additive coupling of the noise to the stochastic dynamics is determined by the matrix B, which we assume to be non-singular.

We restrict ourselves to the case of a time-periodic driving, i.e.  $\mathbf{F}(\mathbf{x},t) = \mathbf{F}(\mathbf{x},t+T)$  for a certain period T. Furthermore, we assume that the deterministic dynamics, i.e. Eq. (1) for  $\epsilon = 0$ , possesses exactly one stable periodic orbit  $\mathbf{x}_s(t) = \mathbf{x}_s(t+T)$  with a time-dependent domain of attraction A(t). All other deterministic orbits, which start outside of A(t) and its boundary  $S(t) := \partial A(t)$  are assumed to diverge in the long time limit. The boundary S(t) then acts as a separatrix between these two kinds of deterministic solutions. Moreover, we require that there is exactly one unstable periodic orbit  $\mathbf{x}_u(t) = \mathbf{x}_u(t+T)$ , which then moves with the separatrix, i.e.  $\mathbf{x}_u(t) \in S(t)$  for all times t. Finally, all other deterministic solutions starting in a neighborhood of the unstable periodic orbit on the separatrix are assumed to be bounded. All these assumptions can usually be taken for granted in typical periodically driven escape problems of practical interest.

A particularly prominent example is the Kramers problem,  $^{17}$  namely the escape of a particle with mass m out of the bottom well of a static potential as cartooned in Fig. 1. Under the additional influence of an additive sinusoidal driving this corresponds to the stochastic dynamics

$$m\ddot{x} + \eta\dot{x} = -V'(x) + A\sin(\Omega t) + \sqrt{2\eta k_B T} \,\xi(t) \ . \tag{3}$$

Here,  $\eta$  is the viscous friction coefficient,  $k_B$  Boltzmann's constant, T the temperature and  $\Omega = 2\pi/T$  the angular frequency of the driving. We can rewrite the second order equation (3) in the form of Eq. (1), if we identify

$$\mathbf{x} := \begin{pmatrix} x \\ v \end{pmatrix} , \quad \mathbf{F}(\mathbf{x}, t) := \begin{pmatrix} v \\ \frac{1}{m} F(x, t) - \gamma v \end{pmatrix} , \quad \mathbf{B} := \frac{\sqrt{\eta}}{m} \begin{pmatrix} \delta & 0 \\ 0 & 1 \end{pmatrix} , \quad \epsilon := k_B T , \tag{4}$$

where we have introduced the one-dimensional force field  $F(x,t) := -V'(x) + A\sin(\Omega t)$  and the frequency  $\gamma := \eta/m$ . Furthermore, we have added an auxiliary noise source of a strength proportional to  $\delta$  to ensure that B is non-singular. Eventually, we shall consider the limit  $\delta \to 0$ , in which Eq. (4) reduces to the original dynamics (3). Figure 2 depicts the stable and unstable periodic orbits, the domain of attraction A(t), and the separatrix S(t) for a representative metastable potential.

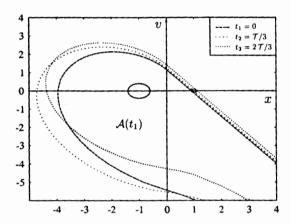


Figure 2. Phase space diagram for a typical metastable potential with additive sinusoidal driving (3), namely the piecewise parabolic potential (66) with  $\bar{x}_s = \omega_u^2 = -1$ ,  $\bar{x}_u = \omega_s^2 = m = \Delta V = \Omega = 1$ ,  $\eta = 0.5$ , A = 0.2. Solid line: Stable (left) and unstable (right) periodic orbit. Dashed lines: Separatrix at different times  $t_1 = 0$ ,  $t_2 = T/3$ , and  $t_3 = 2T/3$ . Grey area: Domain of attraction  $A(t_1)$  of stable periodic orbit  $x_s(t)$  at time  $t_1$ .

A fully equivalent description of the stochastic dynamics (1) is provided by the Fokker-Planck equation<sup>34</sup> for the probability distribution  $p(\mathbf{x}, t)$  of an ensemble of particles  $\mathbf{x}(t)$ ,

$$\frac{\partial}{\partial t} p(\mathbf{x}, t) + \nabla \cdot \mathbf{j}(\mathbf{x}, t) = 0 , \qquad (5)$$

where the probability current density is given by

$$\mathbf{j}(\mathbf{x},t) := \mathbf{F}(\mathbf{x},t) \, p(\mathbf{x},t) - \epsilon \, \mathsf{D} \nabla p(\mathbf{x},t) \tag{6}$$

with the positive semidefinite diffusion matrix  $D := BB^T$ .

#### 2.2. Escape rates

If we now consider our stochastic dynamics (1) for finite noise-strengths  $\epsilon$ , it is well-known that a particle x(t) starting in  $\mathcal{A}(t)$  will be able to escape out of this basin. To quantify this escape of particles, we first introduce the population  $P_{\mathcal{A}}(t)$  in  $\mathcal{A}(t)$ :

$$P_{\mathcal{A}}(t) := \int_{\mathcal{A}(t)} \mathbf{d}^d \mathbf{x} \ p(\mathbf{x}, t) \ . \tag{7}$$

A natural definition of an "instantaneous rate"  $\Gamma(t)$  for such escape events is then given by the relative decrease of this population per unit time, <sup>31, 32</sup>

$$\Gamma(t) := -\dot{P}_{A}(t)/P_{A}(t) . \tag{8}$$

We remark that — except for transients at early times — this quantity is independent of the initial conditions at time  $t = t_0$ , provided we start with a distribution that is concentrated within the basin  $\mathcal{A}(t)$ . We thus make the convenient choice  $p(\mathbf{x}, t_0) = \delta(\mathbf{x} - \mathbf{x}_s(t_0))$ . Furthermore, on the time scale of these transients,  $\Gamma(t)$  will approach a time-periodic limit, permitting a meaningful definition of the time-averaged rate

$$\bar{\Gamma} := \frac{1}{\mathcal{T}} \int_{t}^{t+\mathcal{T}} \mathrm{d}t' \, \Gamma(t') \ . \tag{9}$$

In the sequel of the present paper we will deduce analytic expressions for both the instantaneous and the time-averaged rate in the limit of small noise-strength  $\epsilon$ .

To make progress in this direction, we first note that for weak noise  $\epsilon$  the typical time scale of the escape events  $1/\bar{\Gamma}$  is well separated from the time scale of the just mentioned transients.<sup>14</sup> We can thus approximate  $P_{\mathcal{A}}(t)$  by its initial value  $P_{\mathcal{A}}(t_0) = 1$  in the denominator of Eq. (8). Using the Fokker-Planck equation (5) and the divergence theorem, the instantaneous rate reads

$$\Gamma(t) = \int_{S(t)} d^{d-1} \mathbf{n} \cdot [\mathbf{j}(\mathbf{x}, t) - \dot{\mathbf{x}} p(\mathbf{x}, t)] .$$
(10)

Here, the integration is over the entire time-dependent separatrix S(t) and  $\mathbf{n}$  denotes their outer normal vector. Furthermore, the time derivative in  $\dot{\mathbf{x}}$  refers to the t-dependence of the points on this separatrix, which is determined by the deterministic equation of motion, *i.e.* Eq. (1) with  $\epsilon = 0$ . Taking this and the definition (6) of the current density into account, one obtains the general result

$$\Gamma(t) = -\epsilon \int_{S(t)} d^{d-1} \mathbf{n} \cdot \mathsf{D} \nabla p(\mathbf{x}, t) . \tag{11}$$

As expected on naive grounds, a crossing of the separatrix is possible via a diffusive process only.

#### 3. PATH INTEGRALS AND THE SADDLE-POINT APPROXIMATION

Let us briefly summarize the path integral description of the dynamics generated by a stochastic differential equation (1). It is well-known from the literature<sup>22-24, 35-43</sup> that one can represent the conditional probability density  $p(\mathbf{x}_f, t_f | \mathbf{x}_0, t_0)$  to find the particle at time  $t_f$  at position  $\mathbf{x}_f$  if it has started at time  $t_0$  at position  $\mathbf{x}_0$  as weighted sum over all paths between these two points,

$$p(\mathbf{x}_f, t_f | \mathbf{x}_0, t_0) = \int_{\mathbf{x}(t_0) = \mathbf{x}_0}^{\mathbf{x}(t_f) = \mathbf{x}_f} \mathcal{D}\mathbf{x}(t) e^{-S[x(t)]/\epsilon} . \tag{12}$$

Here, S[x(t)] is the effective action or the Onsager-Machlup functional, i.e.

$$S[x(t)] := \int_{t_0}^{t_f} \mathrm{d}t \, L(\mathbf{x}(t), \dot{\mathbf{x}}(t), t) , \qquad (13)$$

with the corresponding Lagrangian

$$L(\mathbf{x}, \dot{\mathbf{x}}, t) := \frac{1}{4} \left[ \dot{\mathbf{x}} - \mathbf{F}(\mathbf{x}, t) \right] \cdot \mathsf{D}^{-1} \left[ \dot{\mathbf{x}} - \mathbf{F}(\mathbf{x}, t) \right] . \tag{14}$$

We remark that a prepoint-discretization scheme<sup>41-43</sup> (not to be confused with the Ito-scheme in stochastic calculus<sup>34</sup>) has been implicitly adopted in the path integral (12) implying the measure  $1/\sqrt{\det(4\pi \epsilon \Delta t D)}$ . Other

"discretization schemes" 41-43 would give rise to a somewhat modified path-integral formalism but would — of course — lead to identical results as far as the actual stochastic dynamics (3) is concerned.

It should be clear that in general an exact evaluation of the path integral (12) is impossible. Nevertheless, it represents an advantageous starting-point for a systematic weak-noise approximation: For small  $\epsilon$ , the main contributions to the path integral (12) stem from the surrounding of action minimizing paths. Carrying out a infinite-dimensional saddle-point approximation around these paths, one arrives at

$$p(\mathbf{x}_f, t_f | \mathbf{x}_0, t_0) = \sum_k \frac{e^{-\phi_k(\mathbf{x}_f, t_f)/\epsilon}}{\left[\det(4\pi \epsilon \, \mathbf{Q}_k^*(t_f))\right]^{\frac{1}{2}}} \left[1 + \mathcal{O}(\epsilon)\right], \tag{15}$$

where the sum runs over all paths  $\mathbf{x}_{k}^{*}(t)$  that (locally) minimize the action (13). These obey the Hamiltonian dynamics, defined by the Hamiltonian

$$H(\mathbf{x}, \mathbf{p}, t) := \mathbf{p} \cdot \mathsf{D} \, \mathbf{p} + \mathbf{p} \cdot \mathbf{F}(\mathbf{x}, t) \ . \tag{16}$$

The corresponding canonical equations assume the form

$$\dot{\mathbf{x}}_{k}^{*}(t) = \mathbf{F}(\mathbf{x}_{k}^{*}(t), t) + 2 \,\mathsf{D}\,\mathbf{p}_{k}^{*}(t)$$

$$\dot{\mathbf{p}}_{k}^{*}(t) = -\left(\nabla \mathbf{F}(\mathbf{x}_{k}^{*}(t), t)\right)^{T} \mathbf{p}_{k}^{*}(t) . \tag{17}$$

Furthermore, the boundary conditions

$$\mathbf{x}_{k}^{*}(t_{0}) = \mathbf{x}_{0} \quad , \quad \mathbf{x}_{k}^{*}(t_{f}) = \mathbf{x}_{f} .$$
 (18)

follow immediately from Eq. (12). The value of the action  $\phi_k(\mathbf{x}_f, t_f)$  of a path  $\mathbf{x}_k^*(t)$  is then given by

$$\phi_k(\mathbf{x}_f, t_f) := S[\mathbf{x}_k^*(t_f)] = \int_{t_0}^{t_f} \mathrm{d}t \, \mathbf{p}_k^*(t) \cdot \mathsf{D} \, \mathbf{p}_k^*(t) \,, \tag{19}$$

where we have suppressed in favor of notational brevity the dependence on the initial condition  $\mathbf{x}_0$  at time  $t_0$ . It is noteworthy to point out that in Eq. (16) the momentum enters both quadratically and linearly: the latter linear contribution mimics a magnetic field-like, time-dependent vector potential contribution. For later use, we also recall the well-known result from classical mechanics<sup>44</sup> that the derivative of the extremal action with respect to its endpoint  $\mathbf{x}_f$  equals the canonical conjugate momentum at time  $t_f$ ,

$$\mathbf{p}_{k}^{\star}(t_{f}) = \frac{\partial \phi_{k}(\mathbf{x}_{f}, t_{f})}{\partial \mathbf{x}_{f}} . \tag{20}$$

The yet unspecified prefactor term  $Q_k^*(t_f)$  in (15) is given by the solution at time  $t_f$  of the following second order differential equation

$$\ddot{\mathbf{Q}}_{k}^{\star}(t) - \nabla \mathbf{F}(\mathbf{x}_{k}^{\star}(t), t) \dot{\mathbf{Q}}_{k}^{\star}(t) - \dot{\mathbf{Q}}_{k}^{\star}(t) \mathbf{Q}_{k}^{\star}(t)^{-1} \mathbf{D} (\nabla \mathbf{F}(\mathbf{x}_{k}^{\star}(t), t))^{T} \mathbf{D}^{-1} \mathbf{Q}_{k}^{\star}(t) 
+ \left\{ \nabla \mathbf{F}(\mathbf{x}_{k}^{\star}(t), t) \mathbf{D} (\nabla \mathbf{F}(\mathbf{x}_{k}^{\star}(t), t))^{T} \mathbf{D}^{-1} - \mathbf{D} (\nabla \mathbf{F}(\mathbf{x}_{k}^{\star}(t), t))^{T} \mathbf{D}^{-1} \nabla \mathbf{F}(\mathbf{x}_{k}^{\star}(t), t) 
- \frac{\mathrm{d}}{\mathrm{d}t} \left[ \nabla \mathbf{F}(\mathbf{x}_{k}^{\star}(t), t) + \mathbf{D} (\nabla \mathbf{F}(\mathbf{x}_{k}^{\star}(t), t))^{T} \mathbf{D}^{-1} \right] + 2 (\mathbf{D} \mathbf{p}_{k}^{\star}(t)) \cdot (\nabla \nabla \mathbf{F}(\mathbf{x}_{k}^{\star}(t), t)) \right\} \mathbf{Q}_{k}^{\star}(t) = 0 \quad (21)$$

with initial conditions

$$Q_k^*(t_0) = 0 , \quad \dot{Q}_k^*(t_0) = D .$$
 (22)

The derivation of Eqs. (21,22) in the framework of the time-discretized version of the path integral (12) proceeds along the same general lines as in the one-dimensional case presented in Ref..<sup>32</sup> However, the rather technical details are beyond the scope of the present paper.

Though in principle, the prefactor  $Q_k^*(t_f)$  is completely determined by Eqs. (21,22), it will turn out to be more convenient to consider the following quantity:

$$\mathsf{G}_{k}^{\star}(t) := \frac{1}{2} \left[ \mathsf{D}^{-1} \, \dot{\mathsf{Q}}_{k}^{\star}(t) \, \mathsf{Q}_{k}^{\star}(t)^{-1} - (\nabla \mathbf{F}(\mathbf{x}_{k}^{\star}(t), t))^{T} \, \mathsf{D}^{-1} - \mathsf{D}^{-1} \, \nabla \mathbf{F}(\mathbf{x}_{k}^{\star}(t), t) \right] \, . \tag{23}$$

With the help of Eq. (21) one can then verify that  $G_k^*(t)$  fulfills for  $t > t_0$  the matrix Riccati equation

$$\dot{\mathsf{G}}_{k}^{*}(t) = -2\,\mathsf{G}_{k}^{*}(t)\,\mathsf{D}\,\mathsf{G}_{k}^{*}(t) - (\nabla\mathbf{F}(\mathbf{x}_{k}^{*}(t),t))^{T}\,\mathsf{G}_{k}^{*}(t) -\,\mathsf{G}_{k}^{*}(t)\,\nabla\mathbf{F}(\mathbf{x}_{k}^{*}(t),t) - \mathbf{p}_{k}^{*}(t)\cdot\nabla\nabla\,\mathbf{F}(\mathbf{x}_{k}^{*}(t),t) \ .$$

$$(24)$$

However, as can be inferred from Eqs. (22,23), there is no well defined initial condition for  $G_k^*(t)$  at time  $t_0$ . Instead, we have to content ourselves with the relations

$$\lim_{t \to t_0} \left[ \mathsf{G}_k^*(t) \, \mathsf{Q}_k^*(t) \right] = \frac{1}{2} \, 1 \quad \text{and} \quad \mathsf{G}_k^*(t_0)^{-1} = 0 \; . \tag{25}$$

By tracing over both sides of Eq. (23) one obtains a linear first order differential equation for the determinant  $\det Q_k^*(t)$  from Eq. (15):

$$\frac{\mathrm{d}}{\mathrm{d}t} \det \mathsf{Q}_k^{\star}(t) = 2 \operatorname{Tr} \left[ (\nabla \mathbf{F}(\mathbf{x}_k^{\star}(t), t))^T + \mathsf{D} \, \mathsf{G}_k^{\star}(t) \right] \det \mathsf{Q}_k^{\star}(t) \ . \tag{26}$$

The initial condition  $\det Q_k^*(t_0) = 0$  follows immediately from Eq. (22).

#### 4. EVALUATION OF THE ESCAPE RATE FOR WEAK NOISE

For small noise strengths  $\epsilon$ , we can now insert the saddle-point approximation (15) into the rate expression (11). After some calculational steps (for details, we refer the reader to<sup>45</sup>), we obtain

$$\Gamma(t_f) = \frac{1}{\sqrt{2^{d+1}\pi\epsilon}} \sum_{k} \frac{\mathbf{p}_k^*(t_f) \cdot \mathsf{D} \, \mathbf{p}_k^*(t_f) \, e^{-\phi_k(\mathbf{x}_{\mathsf{sep}}(\mathbf{s}_k^*, t_f), t_f)/\epsilon}}{\sqrt{\mathbf{p}_k^*(t_f) \cdot \mathsf{G}_k^*(t_f)^{-1} \, \mathbf{p}_k^*(t_f) \, \det \mathsf{Q}_k^*(t_f) \, \det \mathsf{G}_k^*(t_f)}} \left[ 1 + \mathcal{O}(\epsilon) \right]. \tag{27}$$

Here, the parameter values  $s_k^*$  are determined by an extremal condition, which assumes the form

$$\frac{\partial \phi_k(\mathbf{x}_{\text{sep}}(\mathbf{s}_k^*, t_f), t_f)}{\partial s_{k,\nu}^*} = \mathbf{p}_k^*(t_f) \cdot \frac{\partial \mathbf{x}_{\text{sep}}(\mathbf{s}_k^*, t_f)}{\partial s_{k,\nu}^*} = 0 \quad (\nu = 1, \dots, d-1) . \tag{28}$$

#### 4.1. The action minimizing paths

To proceed further in the evaluation of the rate formula (27), it is necessary to gain more insight about the nature of the action minimizing paths  $\mathbf{x}_k^*(t)$ , whose dynamics is governed by the Hamiltonian equations (17) supplemented by the boundary conditions (18). In view of our choice for the initial conditions (cf. discussion after Eq. (8)) and our result (27), the latter assume the form

$$\mathbf{x}_{k}^{*}(t_{0}) = \mathbf{x}_{s}(t_{0}) \quad , \quad \mathbf{x}_{k}^{*}(t_{f}) = \mathbf{x}_{sep}(\mathbf{s}_{k}^{*}, t_{f})$$
 (29)

where the parameter values  $s_k^*$  are restricted by the relations (28).

For given values of  $t_0$  and  $t_f$ , in the generic case only one of the solutions  $\mathbf{x}_k^*(t)$  of this boundary problem will represent a global minimum of the action (19). Denoting this path for the moment by  $\mathbf{x}_k^*(t)$ , it is clear that for large time differences  $t_f - t_0$  owing to the form of the action (13) and (14) this path  $\mathbf{x}_k^*(t)$  will spent most of its time near a deterministic trajectory, i.e.,  $\dot{\mathbf{x}}_k^*(t) \approx \mathbf{F}(\mathbf{x}_k^*(t), t)$ . With regard to the boundary conditions (29), this means that after its start at time  $t_0$  the path will closely follow the stable periodic orbit  $\mathbf{x}_s(t)$  for some time. Subsequently it switches over into the vicinity of the separatrix S(t), thereby accumulating the main part of its action, to remain there until its end at time  $t_f$ . With respect to the position of the end point on the separatrix, if we assume that ultimately all deterministic trajectories on the separatrix converge to the unstable periodic orbit

 $\mathbf{x}_{u}(t)$ , the same will also hold true for the path  $\mathbf{x}_{k}^{\star}(t)$ , which will thus end nearer and nearer to  $\mathbf{x}_{u}(t)$  the more ime it is able to spend in a close vicinity of the separatrix. Since the duration of the sojourns near the periodic rbits is long compared to that of the transition in between, the path  $\mathbf{x}_{k}^{\star}(t)$  is often called an "instanton" in the iterature.

If we consider now the limiting case  $t_0 \to -\infty$  and  $t_f \to \infty$  (in the following abbreviated as  $t_f - t_0 \to \infty$ ), here exists a well defined limit of  $\mathbf{x}_k^*(t)$ , in the sense that this path follows ever closer the periodic orbits, while etaining the shape of the intermediate segment. At the same time, its action  $S[\mathbf{x}_k^*(t)]$  converges from above to a nite value. We observe that in the limit  $t_f - t_0 \to \infty$  owing to the time-periodicity of the force field  $\mathbf{F}(\mathbf{x},t)$  the ction  $S[\mathbf{x}_k^*(t+nT)]$  is the same for all integers n. In other words, the global minimum of the action becomes ountable infinitely degenerate. However, one can still safely assume that these minima are well separated in he space of all the paths appearing in (12), provided that the driving is neither too weak, too slow nor too fast. These limiting cases are thus not covered by our theory. We remind the reader of the situation in the static ase, where the global minimum is also degenerate. However, while the degeneracy there is continuous in time Goldstone mode), we are dealing here with a discrete degeneracy.

As a consequence of the fact that the minimizing paths  $\mathbf{x}_k^*(t)$  remain well separated, our rate-formula (27) becomes asymptotically exact for any (arbitrary but fixed) finite values of the driving amplitude and period as he noise strength  $\epsilon$  tends to zero. Apart from this fact that in the limit  $\epsilon \to 0$  the  $\mathcal{O}(\epsilon)$  correction in the saddle point approximation (15) and thus in (27) vanishes, a more detailed quantitative statement seems difficult. On he other hand, for a given (small) noise strength  $\epsilon$ , we have to exclude extremely small driving amplitudes and extremely long or short driving periods since this would lead us effectively back to the static (undriven) escape problem, which requires a completely different treatment (especially of the (quasi-) Goldstone mode<sup>27, 38, 39, 46–48</sup>) han in (15). Put differently, in any of these three asymptotic regimes, the error  $\mathcal{O}(\epsilon)$  from (15,27) becomes very arge.

For the following, we introduce the symbol  $\mathbf{x}_{\text{opt}}^{\star}(t)$  for the limit of the path  $\mathbf{x}_{k}^{\star}(t)$  for  $t_{f} - t_{0} \to \infty$ , always teeping in mind that this path is only defined modulo time shifts by integer multiples of the driving period  $\mathcal{T}$ . The corresponding action is defined analogously by

$$\phi_{\text{opt}} := S[\mathbf{x}_{\text{opt}}^*(t)] \ . \tag{30}$$

Furthermore, all other quantities related to  $\mathbf{x}_{opt}^{\star}(t)$  inherit the subscript "opt", for instance  $\mathbf{p}_{opt}^{\star}(t)$  to name only one.

Coming back to the case of finite times  $t_0$  and  $t_f$ , we expect that as precursors of the limit  $t_f - t_0 \to \infty$  there xist besides the global minimum  $\mathbf{x}_k^*(t)$  additional, relative minima  $\mathbf{x}_k^*(t)$  with an only slightly larger action. After a suitable relabeling, each of them closely resembles an appropriately shifted "master path"  $\mathbf{x}_{\text{opt}}^*(t+kT)$  see Fig. 3). For finite  $t_f - t_0$ , we have a finite number of the order  $t_f - t_0/T$  of such paths. Thus, again without estriction of generality, we can assume that the sum in the rate formula (27) runs from 0 to a maximal value  $K(t_f, t_0)$ :

$$0 \le k \le K(t_f, t_0) = \mathcal{O}((t_f - t_0)/\mathcal{T}) \ . \tag{31}$$

Especially, the path  $\mathbf{x}_0^*(t)$  is the one that stays as long as possible in the vicinity of the stable periodic orbit  $\mathbf{x}_s(t)$  and starts with its transition towards the separatrix at the latest possible moment.

#### 4.2. Linearization scheme around periodic orbits

The discussion in the last section has shown that the paths  $\mathbf{x}_k^*(t)$  spend most of their time near the periodic orbits  $\mathbf{x}_{s,u}(t)$  of the deterministic dynamics. Thus, we may gain further insight in their behavior if we linearize the time-dependent force field around these orbits:

$$\mathbf{F}(\mathbf{x},t) \approx \mathbf{F}(\mathbf{x}_{s,u}(t),t) + \nabla \mathbf{F}(\mathbf{x}_{s,u}(t),t)(\mathbf{x} - \mathbf{x}_{s,u}(t)) . \tag{32}$$

Within this approximation, the Hamiltonian equations (17) assume the form

$$\Delta \dot{\mathbf{x}}_{k}^{*}(t) = \nabla \mathbf{F}(\mathbf{x}_{s,u}(t), t) \, \Delta \mathbf{x}_{k}^{*}(t) + 2 \, \mathbf{D} \, \mathbf{p}_{k}^{*}(t) 
\dot{\mathbf{p}}_{k}^{*}(t) = -\left(\nabla \mathbf{F}(\mathbf{x}_{s,u}(t), t)\right)^{T} \, \mathbf{p}_{k}^{*}(t) ,$$
(33)

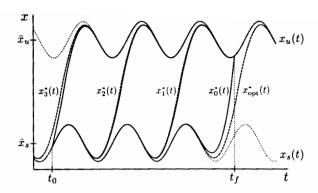


Figure 3. Action minimizing paths  $x_k^*(t)$ ,  $k=0,\ldots,K(t_f,t_0)=3$  (solid) and corresponding master paths  $x_{\text{opt}}^*(t+k\mathcal{T})$  (dashed) between stable and unstable periodic orbits (dotted). Depicted is the one-dimensional, overdamped case d=1 with an additively, harmonically driven piecewise parabolic potential from Ref..<sup>31, 32</sup>

where we have introduced the deviations from the periodic orbits,

$$\Delta \mathbf{x}_k^*(t) := \mathbf{x}_k^*(t) - \mathbf{x}_{s,u}(t) . \tag{34}$$

As we shall see later, for the evaluation of the rate formula (27), one only needs the solution for the momentum equation in the second line of Eq. (33). According to Floquet's theory,<sup>49</sup> this solution can be obtained from the eigenvalues and the left eigenvectors of the eigenvalue problem

$$\left[\frac{\mathrm{d}}{\mathrm{d}t} + \nabla \mathbf{F}(\mathbf{x}_{s,u}(t), t)\right] \Phi_{s,u}^{\alpha}(t) = \lambda_{s,u}^{\alpha} \Phi_{s,u}^{\alpha}(t) , \quad \Phi_{s,u}^{\alpha}(t + T) = \Phi_{s,u}^{\alpha}(t) , \quad \alpha = 1, \dots, d$$
 (35)

together with the corresponding right eigenvectors  $\Phi_{s,u}^{\dagger,\alpha}(t)$ , *i.e.* the solutions of Eq. (35) with  $(\nabla \mathbf{F}(\mathbf{x}_{s,u}(t),t))^T$ . Upon proper normalization of these eigenvectors at equal times, *i.e.* 

$$\Phi_{s,u}^{\dagger,\alpha}(t) \cdot \Phi_{s,u}^{\beta}(t) = \delta_{\alpha\beta} , \qquad (36)$$

we are able to write the solution for the momentum equation as

$$\mathbf{p}_{k}^{\star}(t) = \sum_{\alpha} e^{-\lambda_{s,u}^{\alpha}(t-t_{1})} \, \mathbf{\Phi}_{s,u}^{\alpha}(t_{1}) \cdot \mathbf{p}_{k}^{\star}(t_{1}) \, \mathbf{\Phi}_{s,u}^{\dagger,\alpha}(t) , \qquad (37)$$

where  $t_1$  are arbitrary reference times for which the linearization (32) is valid. Since for the master path we have  $\Delta \mathbf{x}_{\mathrm{opt}}^{\star}(t) \to 0$  for  $t \to \pm \infty$ , it follows with Eq. (33) that  $\lim_{t \to \pm \infty} \mathbf{p}_{\mathrm{opt}}^{\star}(t) = 0$ . Consequently, we must require  $\mathrm{Re} \, \lambda_u^{\alpha} > 0$  ( $\mathrm{Re} \, \lambda_s^{\alpha} < 0$ ) for all  $\alpha$  with  $\Phi_{u,s}^{\alpha}(t_1) \cdot \mathbf{p}_{\mathrm{opt}}^{\star}(t_1) \neq 0$ . In the following, we denote sums over this subset of eigenvectors by an apostrophe on the sum sign.

With respect to the prefactor quantities  $G_k^*(t)$  and  $\det Q_k^*(t)$ , we first observe that within the linearization (32) the matrix Riccati equation (24) assumes the form

$$\dot{\mathsf{G}}_{k}^{*}(t) = -2\,\mathsf{G}_{k}^{*}(t)\,\mathsf{D}\,\mathsf{G}_{k}^{*}(t) - (\nabla\mathbf{F}(\mathbf{x}_{s,u}(t),t))^{T}\,\mathsf{G}_{k}^{*}(t) - \mathsf{G}_{k}^{*}(t)\,\nabla\mathbf{F}(\mathbf{x}_{s,u}(t),t) \ . \tag{38}$$

A transformation to the inverse matrix  $G_k^*(t)^{-1}$  yields the linear matrix differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t} \left[ \mathsf{G}_{k}^{*}(t)^{-1} \right] = 2 \,\mathsf{D} + \mathsf{G}_{k}^{*}(t)^{-1} \left( \nabla \mathbf{F}(\mathbf{x}_{s,u}(t),t) \right)^{T} + \nabla \mathbf{F}(\mathbf{x}_{s,u}(t),t) \,\mathsf{G}_{k}^{*}(t)^{-1} , \tag{39}$$

where the initial condition is given by Eq. (25) as

$$G_k^*(t_0)^{-1} = 0. (40)$$

Furthermore, multiplication of Eq. (38) with  $G_k^*(t)^{-1}$  shows that

$$\operatorname{Tr}\left[\dot{\mathsf{G}}_{k}^{\star}(t)\mathsf{G}_{k}^{\star}(t)^{-1}\right] = -2\operatorname{Tr}\left[\left(\nabla\mathbf{F}(\mathbf{x}_{s,u}(t),t)\right)^{T} + \mathsf{D}\,\mathsf{G}_{k}^{\star}(t)\right] . \tag{41}$$

With the help of the linearized version of Eq. (26) we then find for the last two terms of the product appearing in the denominator of our rate expression (27) the result

$$\det \mathsf{G}_{k}^{*}(t) \det \mathsf{Q}_{k}^{*}(t) = \mathrm{const.} =: \mu_{s,u} \ . \tag{42}$$

Note that while  $\mu_s$  is fixed for all paths  $\mathbf{x}_k^*(t)$  by the initial condition (25) to the value  $\mu_s = 2^{-d}$ ,  $\mu_u$  depends both on the index k and on the explicit form of the time-dependent force field  $\mathbf{F}(\mathbf{x},t)$ . Later on, we only need  $\mu_u$  for the master path, which we denote by

$$\mu_{\text{opt}} := \lim_{t \to \infty} \det \mathsf{G}^{\star}_{\text{opt}}(t) \det \mathsf{Q}^{\star}_{\text{opt}}(t) \ . \tag{43}$$

The rest of the product in the denominator of (27) can be rewritten by using the equation of motion (39) for  $G_k^*(t)^{-1}$  together with the Hamiltonian equation (33) for  $\mathbf{p}_k^*(t)$ . This yields

$$\frac{\mathrm{d}}{\mathrm{d}t} \left[ \mathbf{p}_k^*(t) \cdot \mathsf{G}_k^*(t)^{-1} \, \mathbf{p}_k^*(t) \right] = 2 \, \mathbf{p}_k^*(t) \cdot \mathsf{D} \, \mathbf{p}_k^*(t) \tag{44}$$

or equivalently in integrated form

$$\mathbf{p}_{k}^{\star}(t) \cdot \mathsf{G}_{k}^{\star}(t)^{-1} \, \mathbf{p}_{k}^{\star}(t) = \mathbf{p}_{k}^{\star}(t_{1}) \cdot \mathsf{G}_{k}^{\star}(t_{1})^{-1} \, \mathbf{p}_{k}^{\star}(t_{1}) + 2 \int_{t_{1}}^{t} \mathrm{d}t' \, \mathbf{p}_{k}^{\star}(t') \cdot \mathsf{D} \, \mathbf{p}_{k}^{\star}(t') \,. \tag{45}$$

For the master path  $\mathbf{x}^*_{\text{opt}}(t)$ , the integral on the right hand side of the last equation has to converge in the limit  $t \to \infty$  in order that the action  $\phi_{\text{opt}}$  assumes a finite value. Hence, the quantity on the left hand side is also well defined in this limit and we obtain for  $t \to \infty$  after a subsequent renaming  $t_u \to t$ 

$$\mathbf{p}_{\text{opt}}^{\star}(t) \cdot \mathsf{G}_{\text{opt}}^{\star}(t)^{-1} \, \mathbf{p}_{\text{opt}}^{\star}(t) = q_{\text{opt}} - \mathbf{p}_{\text{opt}}^{\star}(t) \cdot \mathsf{A}_{u}(t) \, \mathbf{p}_{\text{opt}}^{\star}(t) \tag{46}$$

Here we have exploited Eq. (37) for the master path and furthermore introduced the abbreviations

$$q_{\text{opt}} := \lim_{t \to \infty} \mathbf{p}_{\text{opt}}^*(t) \cdot \mathsf{G}_{\text{opt}}^*(t)^{-1} \, \mathbf{p}_{\text{opt}}^*(t) \,, \tag{47}$$

$$\mathsf{A}_{u}(t) := 2 \sum_{\alpha\beta}^{\prime} \mathbf{\Phi}_{u}^{\alpha}(t) \mathbf{\Phi}_{u}^{\beta}(t)^{T} \int_{t}^{\infty} \mathrm{d}t' \, e^{-(\lambda_{u}^{\alpha} + \lambda_{u}^{\beta})(t'-t)} \mathbf{\Phi}_{u}^{\dagger,\alpha}(t') \cdot \mathsf{D} \, \mathbf{\Phi}_{u}^{\dagger,\beta}(t') \,. \tag{48}$$

Note that owing to the time-periodicity of the Floquet solutions,  $A_u(t)$  is also a periodic function of t:

$$A_{u}(t + kT) = A_{u}(t) \quad \text{for all times } t. \tag{49}$$

#### 4.3. Approximation in terms of the master path

After having gained sufficient insight into the nature of the paths  $\mathbf{x}_k^*(t)$ , we now come back to the evaluation of the rate expression (27). The main idea is to approximate all quantities related to the paths  $\mathbf{x}_k^*(t)$  in terms of the corresponding master path, since, as discussed in Sect. 4.1, both resemble each other closely. However, while the boundary conditions for the master path are  $\mathbf{x}_{\text{opt}}^*(t) - \mathbf{x}_s(t) \to 0$  for  $t \to -\infty$  and  $\mathbf{x}_{\text{opt}}^*(t) - \mathbf{x}_u(t) \to 0$  for  $t \to \infty$ , the paths  $\mathbf{x}_k^*(t)$  have to satisfy Eq. (29). From the results of our previous work,<sup>32</sup> we know that while we can safely neglect these deviations at the initial time  $t_0$ , the boundary at time  $t_f$  has to be treated more carefully. First, we modify the upper boundary condition for  $\mathbf{x}_{\text{opt}}^*(t)$  by requiring that

$$t_k := t_f + kT , \quad \mathbf{x}_k := \mathbf{x}_{\text{opt}}^*(t_k) \tag{50}$$

are the new end time and end point, respectively. In other words, we simply truncate the path  $\mathbf{x}_{\text{opt}}^*(t+kT)$  corresponding to  $\mathbf{x}_k^*(t)$  at the time  $t_f$ . Obviously, this new path still satisfies the Hamiltonian equations (17) and is thus an extremizing path. The value of its action follows from the definitions (19) and (30) as

$$\phi_{\text{opt}}(\mathbf{x}_k, t_k) := \int_{-\infty}^{t_k} dt \ \mathbf{p}_{\text{opt}}^{\star}(t) \cdot \mathsf{D} \, \mathbf{p}_{\text{opt}}^{\star}(t) = \phi_{\text{opt}} - \int_{t_0}^{\infty} dt \ \mathbf{p}_{\text{opt}}^{\star}(t) \cdot \mathsf{D} \, \mathbf{p}_{\text{opt}}^{\star}(t) \ . \tag{51}$$

Next, we express the action (19) of the path  $\mathbf{x}_k^*(t)$  by expanding the one belonging to the associated master path  $\mathbf{x}_{\mathrm{opt}}^*(t+kT)$  in powers of the difference  $\delta\mathbf{x}_k^*(t_f) := \mathbf{x}_k^*(t_f) - \mathbf{x}_{\mathrm{opt}}^*(t_k) = \Delta\mathbf{x}_k^*(t_f) - \Delta\mathbf{x}_{\mathrm{opt}}^*(t_k)$  between their endpoints,

$$\phi_{k}(\mathbf{x}_{\text{sep}}(\mathbf{s}_{k}^{\star}, t_{f}), t_{f}) = \phi_{\text{opt}}(\mathbf{x}_{k}, t_{k}) + \frac{\partial \phi_{\text{opt}}(\mathbf{x}_{k}, t_{k})}{\partial \mathbf{x}_{k}} \cdot \delta \mathbf{x}_{k}^{\star}(t_{f}) + \cdots$$
 (52)

The second term on the right hand side can be rewritten as  $\mathbf{p}_{\text{opt}}^{\star}(t_k) \cdot \Delta \mathbf{x}_k^{\star}(t_f) - \mathbf{p}_{\text{opt}}^{\star}(t_k) \cdot \Delta \mathbf{x}_{\text{opt}}^{\star}(t_k)$ . Here, the first scalar product is zero, as can been seen as follows: We know that the endpoint  $\mathbf{x}_k^{\star}(t_f)$  lies one the separatrix  $\mathcal{S}(t_f)$  and thus a deterministic solution  $\mathbf{x}_{\text{det}}(t)$  starting at time  $t_k$  from  $\mathbf{x}_{\text{det}}(t_k) = \mathbf{x}_k^{\star}(t_f)$  will for all times stay on  $\mathcal{S}(t)$ . Its deviation from the unstable periodic orbit is denoted by  $\Delta \mathbf{x}_{\text{det}}(t)$ . Within our linearization (32) one can then readily verify with the help of the dynamical equation (33) that  $\mathbf{d}[\mathbf{p}_{\text{opt}}^{\star}(t) \cdot \Delta \mathbf{x}_{\text{det}}(t)]/\mathrm{d}t = 0$ . Hence, this scalar product is a constant of motion and we can infer that

$$\mathbf{p}_{\mathrm{opt}}^{\star}(t_k) \cdot \Delta \mathbf{x}_k^{\star}(t_f) = \mathbf{p}_{\mathrm{opt}}^{\star}(t_k) \cdot \Delta \mathbf{x}_{\mathrm{det}}(t_k) = \lim_{t \to \infty} \left[ \mathbf{p}_{\mathrm{opt}}^{\star}(t) \cdot \Delta \mathbf{x}_{\mathrm{det}}(t) \right] = 0 . \tag{53}$$

Here, the last equality follows from the boundedness of  $\mathbf{x}_{\text{det}}(t)$  near the saddle point (cf. the discussion below Eq. (2)) together with  $\mathbf{p}_{\text{opt}}^{\star}(t) \to 0$  for  $t \to \infty$ .

The second scalar product,  $\mathbf{p}_{\text{opt}}^{\star}(t_k) \cdot \Delta \mathbf{x}_{\text{opt}}^{\star}(t_k)$ , can be determined by a similar consideration: The linearized Hamiltonian dynamics (33) yields

$$\frac{\mathrm{d}}{\mathrm{d}t} \left[ \mathbf{p}_{\mathrm{opt}}^{\star}(t) \cdot \Delta \mathbf{x}_{\mathrm{opt}}^{\star}(t) \right] = 2 \, \mathbf{p}_{\mathrm{opt}}^{\star}(t) \cdot \mathsf{D} \, \mathbf{p}_{\mathrm{opt}}^{\star}(t) \,, \tag{54}$$

and since again this scalar product has to vanish in the limit  $t \to \infty$ , we obtain

$$\mathbf{p}_{\text{opt}}^{\star}(t_k) \cdot \Delta \mathbf{x}_{\text{opt}}^{\star}(t_k) = -2 \int_{t_k}^{\infty} dt \ \mathbf{p}_{\text{opt}}^{\star}(t) \cdot \mathsf{D} \, \mathbf{p}_{\text{opt}}^{\star}(t) \ . \tag{55}$$

Altogether, the approximation (52) for the value of the action of the path  $\mathbf{x}_{k}^{*}(t)$  thus takes the form

$$\phi_k(\mathbf{x}_{sep}(\mathbf{s}_k^*, t_f), t_f) = \phi_{opt} + \int_{t_f}^{\infty} dt \ \mathbf{p}_{opt}^*(t + kT) \cdot \mathsf{D} \ \mathbf{p}_{opt}^*(t + kT) + \cdots$$
 (56)

The k-dependence of the exponential term in the rate expression (27) is thus reduced to a simple sum of exponential factors as given by the time-dependence (37) of the integrand in (56). With respect to the prefactor terms in the rate expression (27), we already now from the results of our previous work<sup>32</sup> that up to corrections of the order  $\mathcal{O}(|\mathbf{p}_{opt}^*(t_k)|^2)$  we can directly substitute all quantities belonging to the path  $\mathbf{x}_k^*(t)$  by those of the corresponding master path  $\mathbf{x}_{opt}^*(t+kT)$ . Consistently, we also neglect the terms on the right hand side of Eq. (46), which are of the same order.

#### 4.4. Rate formula

After the discussion in the previous section, it is just a matter of collecting everything in order to arrive at the central result of the present work, namely the asymptotic value of the instantaneous escape rate,

$$\Gamma(t) \simeq \sqrt{\epsilon} \, \alpha_{\rm opt} \, e^{-\phi_{\rm opt}/\epsilon} \kappa_{\rm opt}(t, \epsilon) \ .$$
 (57)

Here, we have introduced the quantities

$$\alpha_{\text{opt}} := \left[ 2^{d+1} \pi \, \mathcal{T}^2 \lim_{t \to \infty} \mathbf{p}_{\text{opt}}^{\star}(t) \cdot \mathsf{G}_{\text{opt}}^{\star}(t)^{-1} \, \mathbf{p}_{\text{opt}}^{\star}(t) \, \det \mathsf{Q}_{\text{opt}}^{\star}(t) \, \det \mathsf{G}_{\text{opt}}^{\star}(t) \right]^{-\frac{1}{2}} , \tag{58}$$

$$\kappa_{\text{opt}}(t,\epsilon) := \mathcal{T} \sum_{k=0}^{K(t,t_0)} \frac{\mathbf{p}_{\text{opt}}^*(t+k\mathcal{T}) \cdot \mathsf{D} \, \mathbf{p}_{\text{opt}}^*(t+k\mathcal{T})}{\epsilon} \, \exp\left[-\frac{1}{\epsilon} \int_t^\infty dt' \, \, \mathbf{p}_{\text{opt}}^*(t'+k\mathcal{T}) \cdot \mathsf{D} \, \mathbf{p}_{\text{opt}}^*(t'+k\mathcal{T})\right] \, . \tag{59}$$

With the help of Eqs. (37, 48) and the time-periodicity of the Floquet solutions  $\Phi_u^{\alpha}(t)$  we can rewrite the last expression as

$$\kappa_{\text{opt}}(t,\epsilon) = \mathcal{T} \sum_{k=0}^{K(t,t_0)} \frac{\mathbf{b}_{\text{opt}}(t) \cdot \mathsf{B}_k(t)^T \, \mathsf{D} \, \mathsf{B}_k(t) \, \mathbf{b}_{\text{opt}}(t)}{\epsilon} \, \exp \left\{ -\frac{\mathbf{b}_{\text{opt}}(t) \cdot \mathsf{B}_k(t)^T \, \mathsf{A}_u(t) \, \mathsf{B}_k(t) \, \mathbf{b}_{\text{opt}}(t)}{2 \, \epsilon} \right\} , \quad (60)$$

$$\mathsf{B}_{k}(t) := \sum_{\alpha}' e^{-\lambda_{u}^{\alpha}kT} \Phi_{u}^{\dagger,\alpha}(t) \Phi_{u}^{\alpha}(t)^{T} = \mathsf{B}_{k}(t+T) \;, \tag{61}$$

$$\mathbf{b}_{\mathrm{opt}}(t) := \lim_{\hat{t} \to \infty} \sum_{\alpha}' e^{-\lambda_{u}^{\alpha}(t-\hat{t})} \, \mathbf{\Phi}_{u}^{\alpha}(\hat{t}) \cdot \mathbf{p}_{\mathrm{opt}}^{\dagger}(\hat{t}) \, \mathbf{\Phi}_{u}^{\dagger,\alpha}(t) \; . \tag{62}$$

Since  $B_k(t)$  in (61) is a sum of terms that exponentially decrease with k, there is a competition in the sum (60) between a pre-exponential factor which quickly decreases with k and an exponential term increasing with k. The main contribution to this sum thus comes from a few k values around a number  $\hat{k}(t)$  that is for small noise strength  $\epsilon$  much larger than 0 but at the same moment, for large enough  $t_f - t_0$ , still much smaller than  $K(t_f, t_0)$ . Hence, up to an exponentially small error in  $\epsilon$ , we can extend the summation range in Eq. (60) and thus in Eq. (59) to all integers k. This allows us to identify two important features of the time-dependence of  $\kappa_{\text{opt}}(t, \epsilon)$ . To prove the first one, the time-periodicity

$$\kappa_{\text{opt}}(t + \mathcal{T}, \epsilon) = \kappa_{\text{opt}}(t, \epsilon) ,$$
(63)

we merely have to shift the summation index in Eq. (59) by 1. For asymptotic times and small noise strengths, the instantaneous escape rate (57) is thus, as expected, a periodic function of the time t. To establish the second property, we use furthermore that the pre-exponential term in Eq. (59) is just the negative time-derivative of the expression in the exponential. Again up to an exponentially small correction, we then obtain

$$\frac{1}{\mathcal{T}} \int_{t}^{t+\mathcal{T}} dt' \, \kappa_{\text{opt}}(t', \epsilon) = 1 \ . \tag{64}$$

Inserting the asymptotic rate expression (57) into the definition (9) for the time-averaged rate and using the last identity, we thus arrive at the second main result of the present work, namely

$$\tilde{\Gamma} \simeq \sqrt{\epsilon} \, \alpha_{\rm opt} \, e^{-\phi_{\rm opt}/\epsilon} \, .$$
 (65)

Hence, the noise-strength dependence of the time-averaged rate is of the form of an Arrhenius-type, exponentially leading term times an  $\epsilon$ -dependent prefactor. Note that for a system in thermal equilibrium *i.e.* for a time-independent force field  $\mathbf{F}(\mathbf{x})$ , the escape rate is given by an exponentially leading Arrhenius factor, which contains the barrier against the escape, multiplied by an  $\epsilon$ -independent prefactor, which depends only on local properties of the force field at the barrier and in the well.<sup>19</sup> In comparison with this structure of the equilibrium rate, we observe two crucial differences in (65). First, in the present, non-equilibrium situation, both the effective potential barrier in the exponential and the prefactor depend in a non-trivial way on global properties of the force field  $\mathbf{F}(\mathbf{x},t)$ , and can thus in general only be determined by means of a numerical computation. Second, the non-equilibrium case exhibits an  $\epsilon$ -dependence of the prefactor.

## 5. EXPLICIT RESULTS FOR A METASTABLE PIECEWISE PARABOLIC POTENTIAL

While, in general, one has to resort to numerical methods for the evaluation of the rate expression (57), in the special case of a particle moving in a one-dimensional piecewise parabolic potential with an additive sinusoidal driving (3) a complete analytical treatment is possible. In the following, we work out the simplest such example with two parabolic pieces, and compare the so obtained analytical predictions with numerical results from a Monte-Carlo simulation of the stochastic dynamics (3).

Let us thus consider the force field deriving from the piecewise parabolic potential of the form

$$V(x \le 0) = \frac{1}{2} m \omega_s^2 \left[ (x - \bar{x}_s)^2 - \bar{x}_s^2 \right]$$

$$V(x \ge 0) = \frac{1}{2} m \omega_u^2 \left[ (x - \bar{x}_u)^2 - \bar{x}_u^2 \right] ,$$
(66)

where  $\bar{x}_s < 0$  and  $\bar{x}_u > 0$  denote the position of the potential minimum and maximum, respectively, with corresponding curvatures

$$m\omega_s^2 > 0$$
 and  $m\omega_u^2 < 0$ . (67)

Note that within our notation  $\omega_u$  is an imaginary number. To ensure the continuity of the corresponding force field F(x,t),

$$F(x \le 0, t) = -m \,\omega_s^2 \,(x - \bar{x}_s) + A \sin(\Omega \,t) F(x \ge 0, t) = -m \,\omega_u^2 \,(x - \bar{x}_u) + A \sin(\Omega \,t) ,$$
(68)

at the point x=0, we have to impose the additional restriction  $\omega_s^2 \bar{x}_s = \omega_u^2 \bar{x}_u$ . Selecting as independent model parameters  $\omega_s^2$ ,  $\omega_u^2$ , and the static potential barrier  $\Delta V := V(\bar{x}_u) - V(\bar{x}_s)$ , the fixed points  $x_{s,u}$  can be expressed through

$$\omega_s^2 \,\bar{x}_s = \omega_u^2 \,\bar{x}_u = -\sqrt{\frac{2\,\Delta V}{m} \,\frac{\omega_s^2 \,|\omega_u|^2}{\omega_s^2 + |\omega_u|^2}} \,. \tag{69}$$

We restrict ourselves to the case that that the periodic orbits  $x_{s,u}(t)$  do not cross the point x=0, i.e.

$$x_s(t) < 0 < x_u(t) \tag{70}$$

for all times t, which is granted if and only if the conditions

$$A^{2} < m^{2} \left[ \gamma^{2} \Omega^{2} + (\Omega^{2} - \omega_{s,u}^{2})^{2} \right] \bar{x}_{s,u}^{2}$$
(71)

are fulfilled for both the "s" and the "u" indices. Furthermore, we demand that the master path  $x_{opt}^*(t)$  crosses the point x = 0 exactly once, say at time  $t_1$ ,

$$x_{\text{opt}}^{\star}(t) = 0 \iff t = t_1$$
 (72)

Under these conditions, the action of the master path reads

$$\phi_{\text{opt}} = \Delta V \left[ 1 - \left| \frac{A^2 \,\omega_s^2 \,\omega_u^2 \,(\omega_s^2 + |\omega_u|^2)}{2 \,m \,\Delta V \,\nu^8} \right|^{1/2} \right]^2 \,, \tag{73}$$

where we have introduced the frequency  $\nu$ ,

$$\nu^4 := \left[ \left( \gamma^2 \Omega^2 + \left( \Omega^2 - \omega_s^2 \right)^2 \right) \left( \omega_u^4 + \Omega^2 \lambda_u^{-2} \right) \right]^{1/2} . \tag{74}$$

The periodic driving thus leads to an "effective potential barrier"  $\phi_{\rm opt}$  which is smaller than the static barrie  $\Delta V$  to which it reduces in the limits  $A \to 0$  or  $\Omega \to \infty$ . While  $\phi_{\rm opt}$  is monotonically decreasing with increasin

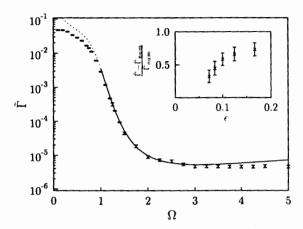


Figure 4. Time-averaged rate  $\bar{\Gamma}$  vs. driving frequency  $\Omega$  for  $\bar{x}_s = \omega_u^2 = -1$ ,  $\bar{x}_u = \omega_s^2 = m = \eta = \Delta V = A = 1, \epsilon = 0.1$  (dimensionless units). Crosses: Inverse mean first exit time from simulations of Eq. (3) (error bars: mean square deviation of mean value). Solid (dotted) line: Analytical prediction (65) (condition (72) not fulfilled). Inset: Convergence behavior of  $\bar{\Gamma}$  for  $\epsilon \to 0$  for fixed driving frequency  $\Omega = 5$  (all other parameters as in main panel).

driving amplitude A, the dependency on the driving frequency  $\Omega$  is more complicated. In particular one observes resonance behavior near the frequency  $\omega_s$  of the bottom well. For the prefactor  $\alpha_{\rm opt}$ , we arrive at

$$\alpha_{\text{opt}} = \left[ \frac{|A| \left[ \Omega^2 \lambda_u^{-2} - \omega_s^2 |\omega_u|^2 \right] + \sqrt{\frac{2 m \Delta V \nu^8}{\omega_s^{-2} + |\omega_u|^{-2}}}}{16\pi^3 |A| \lambda_u^{-2} \phi_{\text{opt}}} \right]^{1/2} . \tag{75}$$

We remark that the structure of the results (73) and (75) closely resembles those in the overdamped case, as obtained in Ref..<sup>31, 32</sup> In particular, this limiting case  $m \to 0$  is correctly reproduced by (73) and (75).

We have checked our above analytical predictions by comparing them with results from Monte-Carlo simulations of the stochastic dynamics (3), which yield the mean time  $\overline{t_{\rm exit}}$  necessary for an exit out of the driven well. The time-averaged rate is related to this quantity via<sup>50</sup>

$$\bar{\Gamma} = \left(\overline{t_{\text{exit}}}\right)^{-1} . \tag{76}$$

Since the necessary simulation times diverge exponentially with decreasing noise strength  $\epsilon$  (cf. (65) and (75)), the numerical determination of the mean exit time becomes impossible for extremely small  $\epsilon$ . For similar reasons, the numerical determination of the time-resolved rates  $\Gamma(t)$  is ruled out.

Figures 4–5 depict the time-averaged rate  $\bar{\Gamma}$  as a function of various system parameters. Parameter regions for which condition (72) is not fulfilled are indicated, which in particular applies for the case of weak damping  $\eta$  and the vicinity of the deterministic resonance at  $\Omega^2 = \omega_s^2 - \gamma^2/2$ , as discussed above. Outside of these regions, already for a noise strength of  $\epsilon = 1$ , the agreement between theory and simulation is very good.

Furthermore, as one can see in Fig. 4, the theory breaks down both for small and large driving frequencies  $\Omega$ , if the noise strength  $\epsilon$  is kept fixed. However, for  $\epsilon \to 0$ , we again observe the convergence of numerically determined rate towards the theoretical approximation (cf. inset of Fig. 4). This behavior is in full accordance with our predictions from Sect. 4.1.

#### 6. CONCLUSIONS

With the present work, we have generalized earlier results for the noise-activated escape in time-periodically driven one-dimensional overdamped systems to an arbitrary number of dimensions. The basic idea of the path-

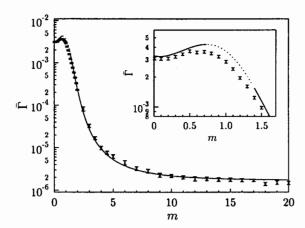


Figure 5. Time-averaged rate  $\bar{\Gamma}$  vs. particle mass m for  $\bar{x}_s = m\omega_u^2 = -1$ ,  $\bar{x}_u = m\omega_s^2 = \eta = \Delta V = A = \Omega = 1, \epsilon = 0.1$  (dimensionless units). Crosses: Inverse mean first exit time from simulations of Eq. (3) (error bars: mean square deviation of mean value). Solid (dotted) line: Analytical prediction (65) (condition (72) not fulfilled). Inset: Magnification of small m regime. Note that the deterministic resonance lies at  $m = \sqrt{1/2} \approx 0.707$ .

integral approach put forward is that it is necessary to sum over all local, nearby minima of the relevant action that contribute to the escape rate. For asymptotically weak noise, these minima are well separated in the space of all paths, and the contribution of each of them can be obtained by a standard saddle-point approximation of the path-integral. This behavior is in strong contrast to the undriven situation, where the occurrence of a (quasi-) Goldstone mode requires a more sophisticated treatment of the associated prefactor.

Our central results express the time-instantaneous rate (57) and the time-averaged rate (65) in terms of quantities belonging to a master path, which has in general to be obtained numerically as the solution of a minimization problem. However, the structure of the result already reveals two noteworthy, salient differences compared to the static case: both the exponentially leading Arrhenius factor and the prefactor not only depend on the relative barrier height and the local properties of the potential inside the well and at the barrier region, respectively, but in addition these two quantities depend as well sensitively on the global behavior of the time-dependent metastable potential. Additionally, a  $\sqrt{\epsilon}$ -dependence of the rate prefactor appears as a consequence of the non-equilibrium situation. Finally, we have been able to derive closed analytical rate expressions for a distinctive case, namely the sinusoidally driven Kramers problem with a metastable potential formed by two parabolas.

#### ACKNOWLEDGMENTS

This work has been supported by the Studienstiftung des deutschen Volkes (I.L.), the Graduiertenkolleg GRK-283, the Sonderforschungsbereich SFB-813 (P.R.).

#### REFERENCES

- 1. R. de Vivie-Riedle, H. Rabitz, K.-L. Kompa, special issue: Laser control of quantum dynamics, Chem. Phys. 267, Nos. 1-3 (2001).
- 2. M. Shapiro, Adv. Chem. Phys. 114, 123 (2000).
- E.H. Serpersu and T.Y. Tsong, J. Membr. Biol. 74, 191 (1983); J. Col. Chem. 259, 7155 (1984); D.S. Liu. R.D. Astumian, and T.Y. Tsong, ibid 265, 7260 (1990).
- 4. P. Hänggi and R. Bartussek in *Nonlinear Physics of Complex Systems*, Lecture Notes in Physics, Vol. 476, 294-308 (1996); J. Parisi, S.C. Müller, and W. Zimmermann (eds.), (Springer, Berlin, 1996.)
- 5. R.D. Astumian, Science 276, 917 (1997).

- 6. F. Jülicher, A. Ajdari, and J. Prost, Rev. Mod. Phys. 69, 1269 (1997).
- 7. P. Reimann, Phys. Rep. 361, 57 (2002).
- 8. P. Reimann and P. Hänggi, Appl. Phys. A 75, 169 (2002).
- 9. R.D. Astumian and P. Hänggi, Brownian Motors, Physics Today, 55, No. 11 (november), 33-39 (2002).
- 10. P. Jung and P. Hänggi, Phys. Rev. A 44, 8032 (1991).
- 11. L. Gammaitoni, P. Hänggi, P. Jung, and F. Marchesoni, Rev. Mod. Phys 70, 223 (1998).
- 12. K. Wiesenfeld and F. Moss, Nature 373, 33 (1995).
- 13. P. Hänggi, CHEMPHYSCHEM 3, 285 (2002).
- 14. P. Hänggi, P. Talkner, and M. Borkovec, Rev. Mod. Phys. 62, 251 (1990).
- 15. G.R. Fleming and P. Hänggi (editors), Activated barrier crossing; applications in Physics, Chemistry, and Biology, World Scientific, Singapore 1993.
- 16. P. Talkner and P. Hänggi (editors), New trends in Kramers' Reaction Rate Theory, Kluwer, Dordrecht 1995.
- 17. H.A. Kramers, Physica (Utrecht) 7, 284 (1940).
- 18. R. Landauer and J.A. Swanson, Phys. Rev. 121, 1668 (1961).
- 19. J.S. Langer, Ann. Phys. (N.Y.) 54, 258 (1969).
- 20. B.J. Matkowsky and Z. Schuss, SIAM J. Appl. Math. 33, 365 (1977).
- 21. P. Talkner, Z. Phys. B 68, 201 (1987).
- 22. R. Graham and T. Tél, Phys. Rev. A 31, 1109 (1985).
- 23. S.J.B. Einchcomb and A.J. McKane, Phys. Rev. E 51, 2974 (1995).
- 24. R.S. Maier and D.L. Stein, SIAM J. Appl. Math. 57, 752 (1997).
- 25. R. Graham and T. Tél, J. Stat. Phys. 35 729 (1984); 37 709 (1984).
- 26. P. Jung, Phys. Rep. 234, 175 (1993).
- V.N. Smelyanskiy, M.I. Dykman, and B. Golding, Phys. Rev. Lett. 82, 3193 (1999).
- 28. P. Jung, Z. Phys. B 76, 521 (1989).
- 29. P. Talkner, New J. Phys. 1, 4 (1999).
- 30. P. Reimann, R. Bartussek, R. Häußler, and P. Hänggi, Phys. Lett. A 215, 26 (1996).
- 31. J. Lehmann, P. Reimann, P. Hänggi, Phys. Rev. Lett. 84, 1639 (2000).
- 32. J. Lehmann, P. Reimann, P. Hänggi, Phys. Rev. E. 62, 6282 (2000).
- 33. R.S. Maier and D.L. Stein, Phys. Rev. Lett. 86, 3942 (2001).
- 34. H. Risken, The Fokker-Planck Equation, Springer, Berlin 1984.
- 35. D. Ludwig, SIAM Review 17, 605 (1975).
- 36. H.S. Wio, P. Colet, M. San Miguel, L. Pesquera, and M.A. Rodriguez, Phys. Rev. A 40, 7312 (1989).
- 37. M.I. Freidlin and A.D. Wentzell, Random Perturbations of Dynamical Systems, Springer, New York 1984.
- 38. U. Weiss and W. Häffner, p. 311 in Functional Integration, edited by J.P. Antoine and E. Tirapegui, Plenum, New York 1980.
- 39. B. Caroli, C. Caroli, and B. Roulet, J. Stat. Phys. 26, 83 (1981).
- 40. L.S. Schulman, Techniques and Applications of Path Integration, Wiley, New York 1981.
- 41. F. Langouche, D. Roekaerts, and E. Tirapegui, Functional Integration and Semiclassical Expansions, Vol. 10 of Mathematics and its Applications, D. Reidel, Dordrecht, Holland, Boston, USA 1982.
- 42. P. Hänggi, Z. Physik B 75, 275 (1989).
- 43. P. Hänggi, in: Path Integrals from meV to MeV: Tutzing 1992, edited by H. Grabert, A. Inomata, L.S. Schulman, and U. Weiss, (World Scientific, Singapore 1993), pp. 289-301.
- 44. H. Goldstein, Classical Mechanics, Addison-Wesley, Reading, Massachusetts, USA 1980.
- 45. J. Lehmann, P. Reimann, P. Hänggi, arXiv:cond-mat/0212117.
- 46. S. Coleman, in: The Whys of Subnuclear Physics, edited by A. Zichichi, (Plenum, New York, USA 1979), pp: 805-920.
- 47. U. Weiss, Phys. Rev. A 25, 2444 (1982).
- 48. U. Weiss, H. Grabert, P. Hänggi, and P. Riseborough, Phys. Rev. B 35, 9535 (1987).
- 49. G. Floquet, Ann. de l'Ecole Norm. Sup. 12, 47 (1883).
- 50. P. Reimann, G.J. Schmid und P. Hänggi, Phy. Rev. E 60, R1 (1999) Rapid Communication.