

Rates and mean first passage times

Reinhard Müller, Peter Talkner, Peter Reimann

Angaben zur Veröffentlichung / Publication details:

Müller, Reinhard, Peter Talkner, and Peter Reimann. 1997. "Rates and mean first passage times." *Physica A* 247 (1-4): 338–56. [https://doi.org/10.1016/S0378-4371\(97\)00390-7](https://doi.org/10.1016/S0378-4371(97)00390-7).

Rates and mean first passage times

Reinhard Müller^{a,1}, Peter Talkner^{a,*}, Peter Reimann^b

^a *Paul Scherrer Institut, CH-5232 Villigen, Switzerland*

^b *Institut für Physik, Universität Augsburg, Memminger Str. 6, D-86135 Augsburg, Germany*

Abstract

The relation between mean first passage times T and transition rates Γ in noisy dynamical systems with metastable states is investigated. It is shown that the inverse mean first passage time to the separatrix of the noiseless system may deviate from twice the rate not only because in general the deterministic separatrix is not the locus in the state space from which a noisy trajectory goes to either side with equal probability. A further cause of a deviation from the often assumed relation $\Gamma T = 1/2$ between rates and mean first passage times is given if the noisy dynamics is discontinuous, i.e. shows jumps with finite probability. Then the value of the splitting probability at the separatrix does not fix the value of ΓT since the system need not visit the separatrix during a transition from one to the other side. Most important, for discontinuous processes the deviation from the $\Gamma T = \frac{1}{2}$ rule survives even in the weak noise limit. A mathematical relation for the product of the rate and the mean first passage time is proposed for Markovian processes and numerically confirmed for a particular one-dimensional noisy map.

1. Introduction

The noise-induced escape from a deterministically stable state is a problem encountered in many different fields of natural sciences [1–3]. In many cases of practical interest, the strength of the noise is sufficiently small such that a separation of time scales applies, i.e., the typical escape time is much larger than any other characteristic time scale of the problem. The rare escape events then happen randomly with an exponential probability distribution in time. Thus, a meaningful rate exists and completely

* Corresponding author. Tel.: +41 56 310 2077; fax: +41 56 310 4412; E-mail: talkner@psi.ch.

¹ Permanent address. Universität Leipzig, Institut für Theoretische Physik, Augustusplatz 10/11, D-04109 Leipzig, Germany.

characterizes the statistics of the escapes. Various analytic and numeric methods to determine escape rates have been developed, most notably Kramers' flux over population method and the reactive flux method, see [1] for a review. All of them require the knowledge of the (quasi-) invariant density inside the deterministic basin of attraction under study. While in equilibrium systems one can utilize the Boltzmann distribution, the determination of this density becomes a highly non-trivial task for systems far from thermal equilibrium, for instance in the notorious colored noise problem [4].

Instead of characterizing the escape process by a rate one may also invoke mean first passage time (MFPT) concepts [1]. In this case, the average time which is needed to reach a prescribed boundary around the deterministically stable state from a given seed inside this boundary is determined. If the boundary is chosen sufficiently far outside the deterministic basin boundary (deterministic separatrix) and the seed sufficiently far inside, then the MFPT will coincide with the inverse rate for asymptotically weak noise. Alternatively, one may choose that particular boundary from which the system either falls back to the initial state or directly reaches the final state with the same probability, the so-called stochastic separatrix [5,6]. In the limit of vanishing noise it coincides with the deterministic separatrix. In systems which move continuously, e.g. diffusion processes in continuous time, the rate is given by the inverse of twice the MFPT across the stochastic separatrix [5–7].

In the present paper we demonstrate that this “one-half” rule no longer holds, but rather the rate exceeds the inverse of twice the MFPT across the stochastic separatrix for a large class of systems exhibiting discontinuous jumps during their time evolution. For these systems the one-half rule is also not recovered in the asymptotic limit of weak noise. We propose a general relation that connects the MFPT to an almost arbitrarily chosen boundary with the escape rate of the considered state. In view of the considerable complications of the MFPT concept in the context of colored noise [4], we restrict ourselves to white noise. We further mention that though the determination of the (quasi-) invariant density is seemingly avoided in the above-mentioned methods to derive the rate via the MFPT across an appropriate boundary, the actual technical difficulties turn out to be comparable or even more subtle both for equilibrium and non-equilibrium systems.

An example for the above-mentioned class of systems with a discontinuous-time evolution are processes driven by shot noise. Such processes are of importance for the description, e.g., of photomultipliers and other electronic devices [8,9]. The energy of a molecule in a dilute gas also changes discontinuously due to random collisions with other gas molecules. This represents an important, often rate-determining process in gas-phase reactions [10]. Yet another example, for which a discontinuous-time evolution arises automatically, are noisy dynamics in discrete time. For instance, for a periodically driven noisy system, the map that relates the actual state of the system with the state after one period of the driving force defines such a noisy dynamics in discrete time in a natural way [11,12]. In contrast to their continuous time counterparts, such systems are generically far from equilibrium already in one dimension [13]. Correspondingly, they share many characteristic features with higher-dimensional non-equilibrium systems in

continuous time but are often easily tractable both analytically and numerically. For noisy one-dimensional maps, rates have been determined by the same methods which are known for continuous-time processes. In particular, the flux over population method [12,14–16], the reactive flux method [17], and the MFPT concept [18,19] have been successfully adapted.

The paper is organized as follows. In Section 2 we formulate the above-mentioned general relation between the rate and the MFPT across an arbitrary boundary in terms of the so-called splitting probability and the density of exit points that applies for both continuous and discontinuous escape processes. For the sake of simplicity, we will explicitly deal here only with one-dimensional overdamped systems, but generalizations are immediate. For the common thermally driven overdamped escape problem in continuous time a proof of the proposed relation is given in Appendix A. In the remainder of the paper we focus on discrete time systems. Section 3 outlines the theoretical means which are needed to determine the various quantities entering the proposed relation for a one-dimensional Markov process in discrete time. In Section 4, for a particular noisy map numeric results are compared with approximate analytic expressions for these quantities. Finally, the proposed relation is numerically confirmed within an expected range of validity. The observed deviations are exponentially small in the Arrhenius factor entering the rate. Appendix B reviews the continuous-time limit of noisy maps. The paper closes with a summary in Section 5.

2. A relation between the rate and the mean first passage time to a dividing point

We consider an overdamped Brownian particle with coordinate x under the simultaneous action of a deterministic force field with two stable and one unstable fixed points and of a weak fluctuating force that is white (independent of the past) and additive (independent of the actual time and position x). In continuous time t such a process is governed by a Langevin equation of the form

$$\dot{x}(t) = -U'(x(t)) + \xi(t), \quad (2.1)$$

where $U(x)$ is a bistable potential with two wells (local minima) at $x = a < 0$ and $x = b > 0$ and a barrier (local maximum) at $x = 0$. An example is the quartic potential $U(x) = x^4/4 - x^2/2$. The white noise $\xi(t)$ may for instance be δ -correlated Gaussian fluctuations, $\langle \xi(t) \xi(s) \rangle = 2D \delta(t - s)$, of a strength D that is small in comparison with the potential barrier height. Another possibility would be shot noise, i.e., $\xi(t)$ consisting of a string of random, say, positive δ -spikes compensated on an average by a constant negative bias. Both the amplitudes of and the time between successive spikes have an exponential distribution. The noise is small if either the average amplitude is small or the average time between the spikes is large. Note that any other white noise $\xi(t)$ in continuous time can be composed by a suitable superposition of white Gaussian and shot noise “building blocks” [20].

Turning to discrete time, the Brownian particle is governed by the Langevin equation

$$x_{n+1} = f(x_n) + \xi_n, \quad (2.2)$$

where n denotes the time. The deterministic map $f(x)$ is monotonically increasing with a single unstable fixed point at $x = 0$ separating the basins of attraction of the stable fixed points at $x = a$ and $x = b$. The white noise ξ_n is given by independent, equally distributed random numbers with a probability distribution $P(\xi)$. A common choice is the Gaussian distribution

$$P(\xi) = (\pi\varepsilon)^{-1/2} e^{-\xi^2/\varepsilon}, \quad (2.3)$$

where ε measures the noise strength and is assumed to be small. The discrete-time escape problem for more general distributions $P(\xi)$ has been treated, e.g., in Refs. [21–23].

Due to the weak noise assumption, a Brownian particle [Eq. (2.1) or (2.2)] spends most of its time in close neighborhoods of the deterministic attractors at $x = a$ and $x = b$. Occasionally, it undertakes excursions out of these regions, ending either again close to the initial attractor (unsuccessful escape attempt) or close to the opposite one (successful escape attempts). As pointed out in Section 1, successful escapes from a to b can be characterized by a rate Γ_a that equals the inverse MFPT $T_b(a)$ which the particle needs on average to get from a to b

$$\Gamma_a = T_b(a)^{-1}. \quad (2.4)$$

Similarly, backward transitions from b to a occur at a rate $\Gamma_b = T_a(b)^{-1}$. The crucial ingredient for the subsequent discussion is the observation that for sufficiently small noise strength the typical duration of a single-escape attempt (successful or not) is negligibly short in comparison with the sojourn times close to one of the deterministic attractors between two successive attempts [24].

Next we introduce a dividing point q that satisfies

$$a < q \leq b \quad (2.5)$$

and does not belong to the neighborhood of a where the particle initially resides. The particle needs the MFPT $T_q(a)$ on average to cross q for the first time. The position $x \in [q, \infty)$ of the particle immediately after having crossed the dividing point q is characterized by a probability distribution $p_{a,q}(x)$, the so-called density of exit points. For a process with continuous trajectories (e.g. Eq. (2.1) with Gaussian white noise $\xi(t)$) the density of exit points is a Dirac δ -function, $p_{a,q}(x) = \delta(x - q)$. For any other kind of Markovian process [Eq. (2.1) or (2.2)] the density of exit points $p_{a,q}(x)$ is non-trivial, see Section 3.1 and 4 for a more detailed discussion of an example in discrete time, according to Eq. (2.2). From any point $x \geq q$ where the particle has entered the interval $[q, \infty)$ for the first time it will proceed with a certain probability $\pi_{a,b}(x)$ into the close neighborhood of b without returning into the vicinity of a before. This so-called splitting probability [25] $\pi_{a,b}(x)$ is 1 for $x \geq b$ but non-trivial for $q \leq x < b$, see

Sections 3.2 and 4, for an example. Since we assumed white noise $\xi(t)$, the probability that a particle reaches the vicinity of b once it has crossed the dividing point q equals $\int_q^\infty dx p_{a,q}(x) \pi_{a,b}(x)$, independent of the particle's past. Taking into account once more that the duration of each escape attempt is negligible, we arrive at our central relationship

$$\Gamma_a = T_q(a)^{-1} \int_q^\infty dx p_{a,q}(x) \pi_{a,b}(x). \quad (2.6)$$

For the backward rate Γ_b we expect an analogous relation to hold. Because of the normalization of the probability of exit points, the integral in Eq. (2.6) is larger than or equal to the minimum of the splitting probability within the range of integration. Both for the continuous processes defined by Eq. (2.1) and discrete time processes [Eq. (2.2)] with additive noise and monotonic maps $f(x)$ the splitting probabilities appearing in the integral [Eq. (2.6)] are minimal at the lower limit $x = q$. This yields the following inequality:

$$\Gamma_a \geq \pi_{a,b}(q) T_q(a)^{-1}. \quad (2.7)$$

In particular, the product of the rate and the MFPT to the stochastic separatrix is at least 0.5, since then we have $\pi_{a,b}(q) = 0.5$ by definition.

As already mentioned, for a process with continuous trajectories the density of exit points shrinks to a δ -function at the exit point and Eq. (2.6) yields

$$\Gamma_a = \pi_{a,b}(q) T_q(a)^{-1} \quad (2.8)$$

In particular, if q lies on the stochastic separatrix, the inverse rate is twice the MFPT to this point. In the case of a continuous Markov process, Eq. (2.1), i.e. a one-dimensional Smoluchowski process, Eq. (2.8) can be verified by inspection, see Appendix A. In the sequel we closely investigate Markovian processes in discrete time which always have discontinuous trajectories.

3. The discrete-time model

We exemplify in more quantitative detail the general arguments from the preceding section for a discrete-time dynamics [Eq. (2.2)] with weak Gaussian white noise [Eq. (2.3)]. Because of the independence of the random force ξ_n at different times n the resulting process x_n is Markovian and, hence, completely determined by an initial density $W_0(x)$ of finding the particle at time $n = 0$ at x , and the conditional density $P(x, n|y)$ of finding the particle n time-steps later at x if it started exactly at y . The time evolution of the conditional density can be described equally well by the forward equation, i.e.,

$$P(x, n+1|y) = \int_{-\infty}^{\infty} dz P(x|z) P(z, n|y) \quad (3.1)$$

or the backward equation

$$P(x, n+1|y) = \int_{-\infty}^{\infty} dz P(x, n|z)P(z|y). \quad (3.2)$$

The initial condition complementing these recursion relations in n is given by

$$P(x, 0|y) = \delta(x - y). \quad (3.3)$$

The single-step transition probability $P(x|y) = P(x, 1|y)$ follows from Eq. (2.2) and (2.3) as

$$P(x|y) = (\pi\varepsilon)^{-1/2} \exp\{-(x - f(y))^2/\varepsilon\}. \quad (3.4)$$

In terms of this transition probability one readily sees that the MFPT across an arbitrary boundary q when starting from any $x < q$ satisfies the following integral equation [19]:

$$T_q(x) - 1 = \int_{-\infty}^q dy T_q(y)P(y|x). \quad (3.5)$$

Choosing either $q = 0$ or $q = b$ gives integral equations for the MFPT across the unstable fixed point (deterministic separatrix) or the inverse escape rate, respectively, see Eq. (2.4). In order to verify our central relationship, Eq. (2.6), we first have to address in more detail the density of exit points $p_{a,q}(x)$ and the splitting probability $\pi_{a,b}(x)$, which is done in the following two subsections.

We close with the remark that the noisy map dynamics, Eq. (2.2) and (2.3) approaches a continuous time dynamics, Eq. (2.1), with Gaussian white noise when the time steps τ between iterations shrink to zero and at the same time the deterministic map approaches a continuous dynamics and the noise strength ε decreases proportionally to τ (for details see Appendix B). Apart from a special case treated in Section 4, it is only in the limit $\tau \rightarrow 0$ that analytic progress for the MFPT from Eq. (3.5) seems possible, see also [19].

3.1. Density of exit points

In order to determine the density of exit points of particles starting at a point y beyond a separating point, $q > y$, we modify the original process by making the part of the x -axis with $x \geq q$ absorbing. In this way the particle is hindered to continue moving once it has crossed q . The density of exit points then coincides with the density of particles sticking on the interval $[q, \infty)$ when all particles have escaped from $(-\infty, q)$. The conditional density $P_q(x, n|y)$ of finding the particle, which starts at y , after n steps at a value $x < q$ obeys a forward equation similar to Eq. (3.1) with the only difference that because of the absorption of the interval $[q, \infty)$ the integral

extends only over the remaining part of the x -axis. In other words

$$P_q(x, n+1|y) = \int_{-\infty}^q dz P(x|z) P_q(z, n|y) \quad (3.6)$$

with the initial condition, Eq. (3.3). At each time $n+1$ the following fraction $p_q(x, n+1|y)$ of particles reaches a position $x > q$:

$$p_q(x, n+1|y) = \int_{-\infty}^q dz P(x|z) P_q(z, n|y). \quad (3.7)$$

Once the particle has left the interval $(-\infty, q)$ it sticks forever where it has entered $[q, \infty)$ and contributes to the density of exit points at the point x

$$\begin{aligned} p_{y,q}(x) &= \sum_{n=0}^{\infty} p_q(x, n+1|y) \\ &= \int_{-\infty}^q dz P(x|z) g_q(z, y), \end{aligned} \quad (3.8)$$

where we interchanged the order of integration and summation and introduced the function $g_q(x, y)$ reading

$$g_q(x, y) = \sum_{n=0}^{\infty} P_q(x, n|y). \quad (3.9)$$

In order to determine the density of exit points $p_{y,q}(x)$ from Eq. (3.8) and (3.4) we are left to calculate $g_q(x, y)$. Summing the forward Eq. (3.6) over all n we obtain the following equation for $g_q(x, y)$ from Eq. (3.9):

$$g_q(x, y) - \delta(x - y) = \int_{-\infty}^q dz P(x|z) g_q(z, y). \quad (3.10)$$

Eq. (3.10) allows two interpretations of the quantity $g_q(x, y)$: First, $g_q(x, y)$ is the Greens function belonging to the forward Eq. (3.6), and second, it is the stationary solution of the process defined by the noisy map Eqs. (2.2) and (2.3) with an absorbing interval $[q, \infty)$ and with a source of particles at y that compensates the loss due to the outflow over the point $x = q$. In passing we mention that the MFPT $T_q(y)$ coincides with the x -integral of $g_0(x, y)$ over the negative x -axis [1,26]

$$T_q(y) = \int_{-\infty}^q dx g_q(x, y). \quad (3.11)$$

This expression for the MFPT can be interpreted as the ratio of the population to the flux which both follow from the flux carrying density $g_q(x, y)$. Note that with the total source strength also the flux over the point $x = q$ is unity.

In view of Eq. (3.11) it is clear that the solution of the integral Eq. (3.10) for $g_q(x, y)$ is not easier than the original MFPT problem, Eq. (3.5). While there is little hope for a general analytic solution, the limiting case of continuous time is worth a closer look both from analytic and numeric viewpoints. In the limit of continuous time $\tau \rightarrow 0$, the integral Eq. (3.10) approaches the boundary value problem, Eq. (B.10), see Appendix B. The latter has the following solution:

$$g_q^{(0)}(x, y) = \frac{1}{D\tau} \int_{\max\{y, x\}}^q dz \exp \left\{ -\frac{U(x) - U(z)}{D} \right\}. \quad (3.12)$$

For finite τ this solution may serve as a first approximation from which a systematic improvement can be obtained by turning Eq. (3.10) into an iteration and using $g_q^{(0)}(x, y)$ as starting point. The n th iteration step then reads

$$g_q^{(n)}(x, y) = \delta(x - y) + \int_{-\infty}^q dz P(x|z) g_q^{(n-1)}(z, y). \quad (3.13)$$

One can show that the iteration converges towards the uniquely defined solution of the integral Eq. (3.10) [27]. We note that though the starting function $g_q^{(0)}(x, y)$ vanishes by construction at $x = q$, all iterations yield a finite value there, see also [19].

3.2. Splitting probability

The splitting probability $\pi_{a,b}(x)$ gives the fraction of all those particles that start at $x \in (a, b)$ and leave the interval at b without having visited a before. One obtains $\pi_{a,b}(x)$ by adding up the outgoing flux through the point b for all times n

$$\pi_{a,b}(x) = \sum_{n=0}^{\infty} \int_b^{\infty} dy \int_a^b dz P(y|z) P_{a,b}(z, n|x), \quad (3.14)$$

where $P_{a,b}(z, n|x)$ denotes the conditional density of the process with absorbing exterior of the interval (a, b) . It obeys the following backward equation

$$P_{a,b}(z, n+1|x) = \int_a^b du P_{a,b}(z, n|u) P(u|x). \quad (3.15)$$

The absorbing parts $(-\infty, a]$ and $[b, \infty)$ hinder the particles which have left (a, b) to come back in the interval. In this way, multiple counting of the same particle is excluded.

From the definition of the splitting probability, Eq. (3.14), and the backward Eq. (3.15) one obtains the following inhomogeneous integral equation for the

splitting probability:

$$\pi_{a,b}(x) - \int_b^\infty dy P(y|x) = \int_a^b dy \pi_{a,b}(y) P(y|x). \quad (3.16)$$

For the bistable noisy map, Eq. (2.2), where a and b are locally stable points separated by an unstable fixed point at $x = 0$ this equation can be further simplified in the weak noise limit. When the noise is weak a particle almost behaves according to the deterministic map; the typical deviations from the deterministic dynamics are small and large deviations are exponentially rare. In the present case that means that within the domain of attraction of the point a most of the noisy trajectories directly approach the point a except those which start in the vicinity of the unstable point $x = 0$ and may also go to b with some probability. Analogously, trajectories starting with a positive coordinate first reach the point b , again with the exception of trajectories starting near $x = 0$. Hence, the splitting probability is almost zero between a and 0 and almost unity between 0 and b . Within a small vicinity of 0 it continuously changes its value between these extremes. The smaller the noise strength the smaller is the region where $\pi_{a,b}(x)$ strongly varies. Within this region, the deterministic map as it enters the transition probability in Eq. (3.16) can be linearized and, moreover, the inhomogeneity in Eq. (3.16) can be neglected since it is exponentially small. The such simplified equation for the splitting probability in the vicinity of the unstable point $x = 0$ reads

$$\pi_{a,b}(x) = \int_{-\infty}^{\infty} \frac{dy}{\sqrt{\pi\varepsilon}} \pi_{a,b}(y) \exp \left\{ -\frac{(y - f'(0)x)^2}{\varepsilon} \right\}, \quad (3.17)$$

where $f'(0)$ denotes the derivative of the deterministic map at 0. We have extended the limits of integration to $\pm\infty$ since for the relevant small $|x|$ -values large $|y|$ -values contribute only with an exponentially small weight to the integral in Eq. (3.17). The solution of Eq. (3.17) satisfying the required asymptotic behavior for large positive and negative x reads [19]:

$$\pi_{a,b}(x) = \frac{1}{2} (1 + \operatorname{erf}(x/l_\varepsilon)), \quad (3.18)$$

where $\operatorname{erf}(z) = 2\pi^{-1/2} \int_0^z dt \exp\{-t^2\}$ denotes the error function, and $l_\varepsilon = \sqrt{\varepsilon/(f'(0)^2 - 1)}$ the noisy length-scale at the unstable fixed point $x = 0$. This expression is a reliable approximation of the exact solution of Eq. (3.16) if the non-linear contributions of the map $f(x)$ can be neglected on a distance of a few l_ε about $x = 0$. Corrections can be obtained by means of a perturbation theory for Eq. (3.16) in an analogous way as finite barrier corrections in the Kramers rate problem in continuous time [7].

4. Piecewise linear noisy maps

As particular examples of discrete-time dynamics of noisy maps we consider Eqs. (2.2) and (2.3) with symmetric piecewise linear maps having stable fixed points at $a = -b = -1$ given by

$$f(x) = \begin{cases} sx - (1 - s) & \text{for } x \leq -x_m, \\ ux & \text{for } -x_m \leq x \leq x_m, \\ sx + (1 - s) & \text{for } x_m \leq x, \end{cases} \quad (4.1)$$

where $\pm x_m$ with $x_m = (1 - s)/(u - s)$ denote the matching points of the linear pieces of the map. The stability properties of the fixed points and the monotonicity of $f(x)$ require $u > 1$ and $0 \leq s < 1$, see Fig. 1.

For the present class of maps an analytic expression is known for the escape rates $\Gamma_{-1} = \Gamma_1 = \Gamma$ for arbitrary fixed values of u and s in the asymptotic limit of small noise [14,17],

$$\Gamma = \sqrt{\varepsilon/[4\pi\phi]} e^{-\phi/\varepsilon}, \quad (4.2)$$

where ϕ is given by

$$\phi = (u^2 - 1)(1 - s^2)/(u^2 - s^2). \quad (4.3)$$

On the contrary, there exist no analytic expressions for the MFPT to the unstable fixed point at $x = 0$ except for values of the parameters u and s close to unity, i.e., in the neighborhood of the limiting case of continuous time, see Ref. [19], and another extreme case with $s = 0$ and $u = \infty$. In the latter case, the integral Eq. (3.5) has a degenerate kernel [27] and can readily be solved. One finds for arbitrary q and $x \leq q$

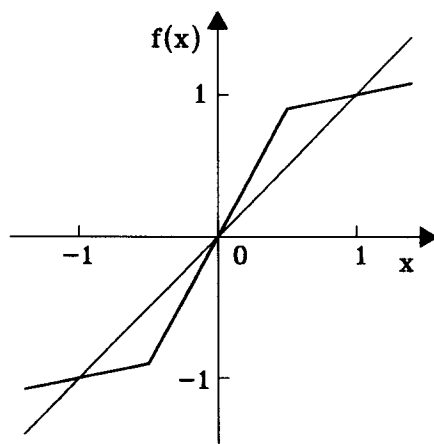


Fig. 1. Piecewise linear map as given by Eq. (4.1) with $s = 0.2$ and $u = 1.8$.

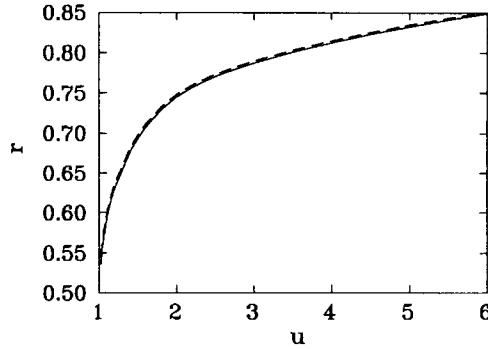


Fig. 2. The product r_T of the transition rate Γ_a given by Eq. (2.4) and the MFPT $T_0(-1)$ obtained from numerical solutions of the integral Eq. (3.5) with $q = b$ and $q = 0$, respectively, for a piecewise linear noisy map, Eqs. (2.2,2.3,4.1) with $s = 0$ as a function of u (solid line). The noise strength ε is chosen such that the Arrhenius factor is kept fixed at $\phi/\varepsilon = 5$; see Eq. (4.3). The broken line shows the integral expression r_p , see Eqs. (2.6,4.5). The value of r_p is slightly larger than that of r_T because in Eq. (2.6) the duration of escape attempts has been neglected.

that

$$T_q(x) = \left(\int_{\min\{q,0\}}^{\infty} \frac{dy}{\sqrt{\pi\varepsilon}} e^{-(y+1)^2/\varepsilon} \right)^{-1} \Theta(-x) + \left(1 - \int_0^q \frac{dy}{\sqrt{\pi\varepsilon}} e^{-(y-1)^2/\varepsilon} \right)^{-1} \Theta(x), \quad (4.4)$$

where $\Theta(x)$ denotes the theta-function. Note that the rate resulting from Eq. (4.4) coincides in leading order in the noise strength ε with the expression given by Eq. (4.2). Further note that the MFPTs with negative x do not depend on the dividing point q provided $q \geq 0$. Consequently, for $u = \infty$, the product of the rate and the MFPT to a point $q \geq 0$ is one. For $u \rightarrow 1$ this product approaches the value of the splitting probability at $x = q$ which is $1/2$ for $q = 0$ because of the symmetry of the considered maps.

We numerically solved the integral equations (3.5) for $q = 0$ and $q = 1$ by means of the Nyström method [28]. As a result, the ratio $r_T = T_0(-1)/T_1(-1) = \Gamma_{-1}T_0(-1)$ is shown in Fig. 2 for maps with $s = 0$ as a function of the other map parameter u . The noise strength ε was chosen such that the Arrhenius factor ϕ/ε has a constant value. The deviations from the value $\frac{1}{2}$ set in strongly for values of u which differ only slightly from unity. For large values of u the ratio gradually approaches one.

Using the same numeric method we solved the integral Eq. (3.10) for the Greens function and compared it for small time-steps τ to the continuous-time result, Eq. (3.12), and the first iteration of Eq. (3.13), see Fig. 3. As an independent control we integrated the numeric solution of the integral Eq. (3.10) over all $x \leq q$ and found within the numeric accuracy perfect agreement with the MFPT time to q in accordance with Eq. (3.11).

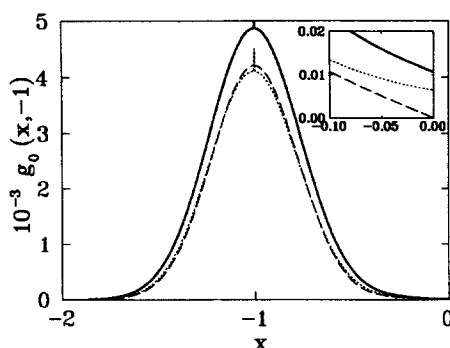


Fig. 3. Green function $g_0(x, -1)$ obtained as numerical solution of Eq. (3.10) (solid line), the continuous-time approximation $g_0^{(0)}(x, -1)$, from Eq. (3.12) (broken line), and the first iteration $g_0^{(1)}(x, -1)$ of Eq. (3.13) (dotted line) for the piecewise linear noisy map, Eqs. (2.2), (2.3) and (4.1) with $s = 0.8$, $u = 1.2$, $\varepsilon = 0.04$ and $\tau = 0.2$ corresponding to $D = 0.05$, see Eqs. (B.1) and (B.2). The inset shows a magnification of the same three functions near the boundary at $x = 0$.

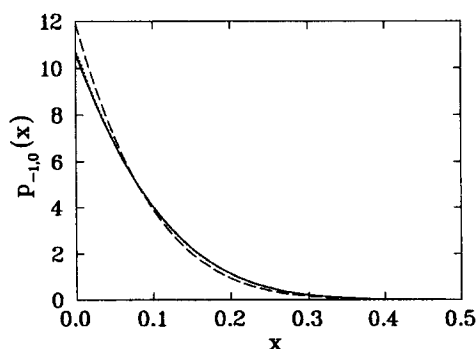


Fig. 4. Distribution of exit points resulting from the numerically exact Green's function $g_0(x, -1)$ (solid line), the continuous-time approximation $g_0^{(0)}(x, -1)$ (broken line), and the first iteration $g_0^{(1)}(x, -1)$ by means of Eq. (3.8) (dotted line) for the same parameter values as in Fig. 3. The two functions $g_0^{(0)}(x, -1)$ and $g_0^{(1)}(x, -1)$ have been multiplied by factors 2.458 and 1.677, respectively, in order that they are properly normalized to one.

As a next step, the distribution of exit points was numerically determined by means of Eq. (3.8) from the numerically exact Green's function and its various approximations, see Fig. 4. It turns out, that the distributions resulting from the approximate Green's functions are not properly normalized to one. If, however, this is done by hand, good agreement with the numerically exact results is achieved. When the approximate Green's functions are renormalized by the same factor a much better agreement with the numerically exact Green function results in the relevant region near the boundary at $x = 0$, see Fig. 5. It is a typical feature of a rate process that the form of a current carrying distribution as is the Green function is much faster approached than its total equilibrium population.

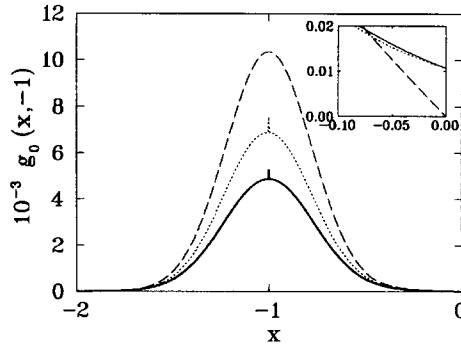


Fig. 5. Same as in Fig. 3 with the only difference that the approximate Green's functions are renormalized by the same factors that give normalized distributions of exit points.

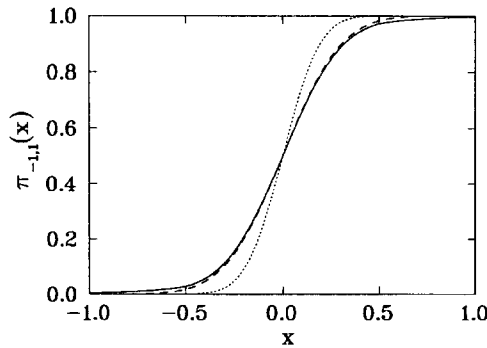


Fig. 6. Splitting probability $\pi_{-1,1}(x)$ resulting from a numerical solution of the integral Eq. (3.16) (solid line) compared to the approximation, Eq. (3.18) (broken line) for the noisy piecewise linear map Eqs. (2.2), (2.3) and (4.1) with $s = 0.8$, $u = 1.2$ and $\varepsilon = 0.05$. For the same s and u but the smaller $\varepsilon = 0.02$ the numerically exact and approximate curves fall on top of each other (dotted line).

In Fig. 6 the approximation of the splitting probability by an error-function, Eq. (3.18) is compared to a numerically exact solution of the integral Eq. (3.16), again obtained by means of the Nyström method. The numerically exact splitting probability, somewhat slower, approaches the asymptotic values 0 and 1 for large negative and positive x -values, respectively, than the error-function, Eq. (3.18). In the vicinity of the unstable point $x = 0$ the agreement of the numerically exact and the approximate solution of Eq. (3.18) is very good.

Using the numerically exact distribution of exit points and splitting probability we calculated the following integral:

$$r_p = \int_q^\infty dx p_{-1,q}(x) \pi_{-1,1}(x). \quad (4.5)$$

In Fig. 7, r_p is compared to the respective expressions obtained from the approximate expressions of $p_{-1,q}(x)$ and $\pi_{-1,1}(x)$ for small time steps τ at a fixed value of D as

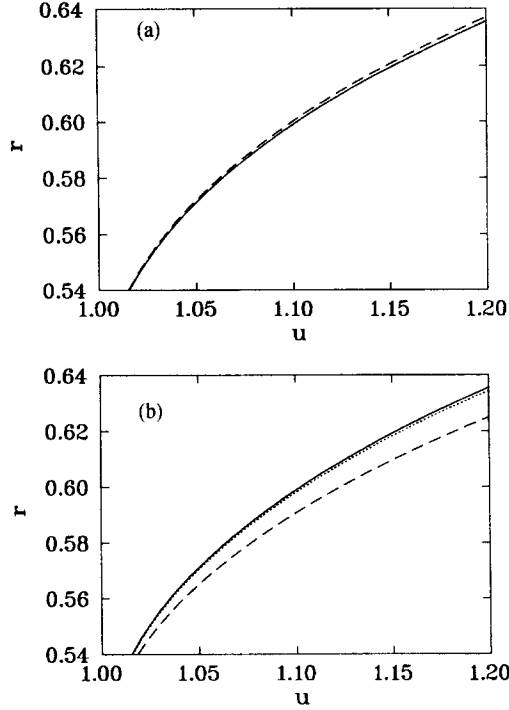


Fig. 7. (a) Integral expression r_p calculated with the numerically exact splitting probability and density of exit points (solid line) and with the approximation, Eq. (3.18) for the splitting probability (broken line) for the noisy piecewise linear map, Eqs. (2.2), (2.3) and (4.1) for $D = \varepsilon/(4\tau) = 0.05$, $\tau = u - 1$, and $s = \tau + 1$ as a function of u , see also Appendix B. The resulting Arrhenius factor $\phi/\varepsilon = 5(1 - \tau^2/4)$ is almost constant for small τ . (b) Numerically exact integral expression r_p (solid line) and the same integral with the product of the exact splitting probability and the distribution of exit points as it results after proper renormalization from the Smoluchowski equation (broken line) and from the first iteration of Eq. (3.13) (dotted line) for the same parameter values as in (a).

a function of u , see Appendix B. The largest deviation is obtained if the renormalized continuous-time approximation, Eq. (3.12) of the Green's function is used. The first iteration according to Eq. (3.13) leads to a considerable improvement. The error function approximation leads also to a very good approximation of r_p .

In Figs. 2 and 8 the ratio of the MFPTs r_T and the integral r_p are compared with each other. According to the proposed relation, Eq. (2.6), r_T and r_p should coincide. The observed deviation is indeed small. The relative deviation between r_p and r_T is shown in Fig. 9 for fixed map parameters u and s as a function of the Arrhenius factor ϕ/ε . We find that the error is positive and down to an Arrhenius factor of 1.5 it is exponentially small in the Arrhenius factor. Both these observations are in accordance with the neglect of small time contributions in Eq. (2.6). This means that within the realm of rate description the proposed relation, Eq. (2.6), between rates and MFPTs is exact.

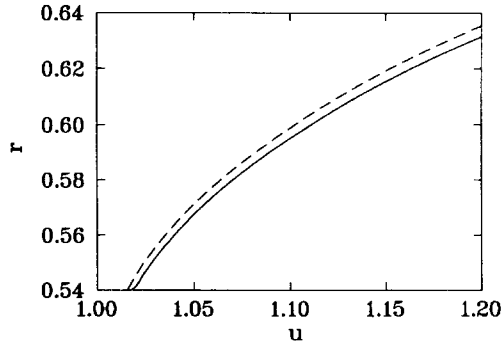


Fig. 8. Ratio of numerically exact MFPTs r_T (solid line) and the numerically exact integral expression r_p (broken line) for the same map as in Fig. 7 as a function of u .

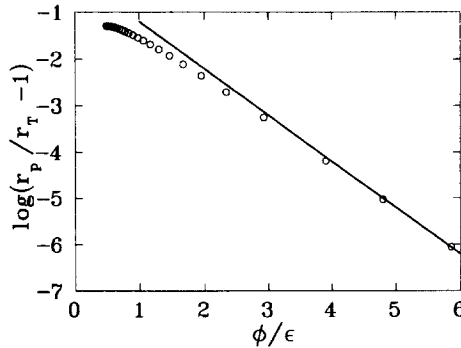


Fig. 9. The logarithm of the relative deviation of r_p and r_T for the noisy piecewise linear map, Eqs. (2.2), (2.3) and (4.1) for $s = 0.8$ and $u = 1.2$ as a function of the Arrhenius factor ϕ/ϵ . Note the straight line down to $\phi/\epsilon = 1.5$ with a slope of 1.

5. Summary

We investigated escape rates of metastable states and their relation to MFPTs of separating points located between the initial and final state for one-dimensional Markov processes. Even if the probabilities are equal to go from the separating point to either of the two metastable states, the product of the rate and the MFPT is, in general, larger than $\frac{1}{2}$. In other words, the fraction of successful crossings of a separating point q is in general larger than the splitting probability at this point. Only for continuous processes the two are the same.

In the weak noise limit the deterministic and stochastic separatrices become identical. So, for continuous processes the MFPT across the deterministic separatrix approaches $\frac{1}{2}$ the inverse rate. For discontinuous processes, however, this well known “one-half” relation is violated even in the weak noise limit. Prominent examples for this class of processes include shot noise driven dynamics, kinetics of gases, and noisy systems in discrete time.

We proposed that the product of the rate and the MFPT is given by the integral over the product of the splitting probability and the density of exit points. This relation is based on the two assumptions that the process is Markovian and a rate description is appropriate. The latter assumption implies that the actual time of a typical escape event irrespective of being successful or not is much shorter than the sojourn time in the vicinities of the metastable states and, hence, can always be neglected. The other assumption is crucial since the splitting probability and the density of exit points are uniquely defined only if the process is Markovian. Otherwise these quantities depend on the past history of the particle before it has jumped over the separating point q to x .

Using a particular class of discrete-time dynamics we numerically demonstrated that the proposed relation holds up to exponentially small deviations. They are caused by neglecting the short times that the particle needs either to fall back to its initial state or to proceed to the other side once it has managed to traverse the dividing point q . Assumptions of this type are inherent in rate theory and most rate laws at best are valid up to corrections that are exponentially small in the Arrhenius factor.

For the sake of simplicity we considered only one-dimensional Markovian processes. It is straightforward to formulate the proposed relation for general Markovian processes having metastable states. We are convinced that it will also hold in these cases. A simple generalization to non-Markovian processes is not obvious and even cannot be expected.

Appendix A. The product of rate and MFPT in the continuous-time limit

The MFPT of a particle moving in continuous time according to the Langevin Eq. (2.1) with Gaussian white noise $\xi(t)$, $\langle \xi(t) \xi(s) \rangle = 2D \delta(t-s)$, reads, see Ref. [1]:

$$t_q(a) = D^{-1} \int_a^q dx e^{U(x)/D} \int_{-\infty}^x dy e^{-U(y)/D}, \quad (\text{A.1})$$

where a is the starting point and q is the dividing point at which the time is taken. The double integral in Eq. (A.1) can be factorized into a product of two integrals if the distance of the upper and lower limit of the first integral is much larger than the noisy length-scale at the locally stable point a , i.e., if

$$q - a \gg \sqrt{D/U''(a)}. \quad (\text{A.2})$$

The MFPT then becomes

$$t_q(a) = n \int_a^q dx e^{U(x)/D} \quad (\text{A.3})$$

up to exponentially small corrections. Here, n denotes the population of the initial well reading

$$n = \int_{-\infty}^0 dx e^{-U(x)/D}. \quad (\text{A.4})$$

Using Eqs. (2.4) and (A.3) we obtain for the product of the rate Γ_a and the MFPT $T_q(a)$

$$\Gamma_a T_q(a) = \frac{\int_a^q dx e^{U(x)/D}}{\int_a^b dx e^{U(x)/D}}. \quad (\text{A.5})$$

The right-hand side of Eq. (A.5) solves, as a function of q , the same boundary value problem as the continuous-time splitting probability $\pi_{a,b}(q)$, see Eqs. (B.8) and (B.9). For uniqueness reasons, they must exactly coincide and, consequently, Eq. (2.8) is proved. Deviations from Eq. (2.8) must be expected when the condition (A.2) is not satisfied, i.e. if D is too large, or if D is small but the separating point q is not sufficiently remote from a .

Appendix B. Continuous-time limit

In this appendix we review the continuous-time limit of the noisy map, Eq. (2.2), see Ref. [19]. For this purpose we introduce the time-step τ of an iteration and consider the limit $n\tau = t$ for $\tau \rightarrow 0$ and $n \rightarrow \infty$. In order that a meaningful dynamics results in this limit, the deterministic part $f(x)$ of the noisy map must deviate from the identical map only by an amount that is proportional to τ ,

$$f(x) = x - \tau U'(x), \quad (\text{B.1})$$

where $U(x)$ is a potential and the prime denotes the derivative with respect to x . For the same reason, the noise strength ε has to be proportional to τ , i.e.

$$\varepsilon = 4D\tau, \quad (\text{B.2})$$

where D is independent of τ . In the limit $\tau \rightarrow 0$ the noisy map approaches the Langevin Eq. (2.1) with $\xi(t)$ being Gaussian white noise, $\langle \xi(t) \rangle = 0$, $\langle \xi(t)\xi(s) \rangle = 2D\delta(t-s)$.

For the integrals that enter the equations for the MFPT, Eq. (3.5) and the splitting probability, Eq. (3.16) one obtains the following expressions for small τ and any $x \in (x_1, x_2)$:

$$\int_{x_1}^{x_2} dy h(y) P(y|x) = h(x) + \tau L^+ h(x) + \mathcal{O}(\tau^2), \quad (\text{B.3})$$

while for $x = x_1$ or $x = x_2$

$$\int_{x_1}^{x_2} dy h(y) P(y|x) = \frac{1}{2} h(x) + \mathcal{O}(\tau^{1/2}), \quad (\text{B.4})$$

where L^+ is the backward Smoluchowski operator

$$L^+ = -U'(x) \frac{\partial}{\partial x} + D \frac{\partial^2}{\partial x^2}. \quad (\text{B.5})$$

and $h(x)$ an arbitrary smooth function on (x_1, x_2) . Using (B.3) we recover from Eq. (3.5) the equation for the MFPT time of a continuous-time process reading

$$L^+ t_q(x) = -1 \quad \text{for } x \in (-\infty, q), \quad (\text{B.6})$$

where $t_q(x) = \tau T_q(x)$ is the MFPT time measured in physical units. Taking $x = q$ and using Eq. (B.4) we find the usual absorbing boundary condition for the MFPT, i.e.

$$t_q(q) = 0. \quad (\text{B.7})$$

The inhomogeneity $\int_b^\infty dy P(y|x)$ of the equation for the splitting probability, Eq. (3.16), vanishes exponentially fast with $\tau \rightarrow 0$ for all values of x which are different from b . At $x = b$ the inhomogeneity has the value $1/2$. Hence, we recover a homogeneous backward equation for the splitting probability

$$L^+ \pi_{a,b}(x) = 0 \quad (\text{B.8})$$

with the following boundary conditions:

$$\pi_{a,b}(a) = 0 \quad \text{and} \quad \pi_{a,b}(b) = 1. \quad (\text{B.9})$$

Using the same kind of arguments we obtain from Eq. (3.10) the continuous-time limit of the equation for the Green's function reading

$$\begin{aligned} LG(x, y) &= -\delta(x - y) \quad \text{for } x, y \in (-\infty, q), \\ G(q, y) &= 0, \end{aligned} \quad (\text{B.10})$$

where $G(x, y) = \tau g(x, y)$ is the properly scaled Green's function in continuous time and

$$L = \frac{\partial}{\partial x} U'(x) + D \frac{\partial^2}{\partial x^2} \quad (\text{B.11})$$

denotes the forward Smoluchowski operator.

References

- [1] P. Hänggi, P. Talkner, M. Borkovec, Rev. Mod. Phys. 62 (1990) 251.
- [2] G.R. Fleming, P. Hänggi, Activated Barrier Crossing, World Scientific, Singapore, 1993.

- [3] P. Talkner, P. Hänggi, *New Trends in Kramers' Reaction Rate Theory*, Kluwer Academic publishers, Dordrecht, 1995.
- [4] P. Hänggi, P. Jung, *Adv. Chem. Phys.* 89 (1995) 239.
- [5] D. Ryter, *J. Stat. Phys.* 49 (1987) 751; *Physica A* 142 (1987) 103.
- [6] M.M. Klosek, B.J. Matkowsky, Z. Schuss, *Ber. Bunsenges. Phys. Chem.* 95 (1991) 331.
- [7] P. Talkner, *Chem. Phys.* 180 (1994) 199.
- [8] L. Mandel, E. Wolf, *Optical Coherence and Quantum Optics*, Cambridge University Press, Cambridge, 1995.
- [9] R.L. Stratonovich, *Topics in the Theory of Random Noise*, vol. I, Gordon and Breach, New York, 1963.
- [10] W. Forst, *Theory of Unimolecular Reactions*, Academic Press, New York, 1973.
- [11] L.E. Reichl, *J. Stat. Phys.* 70 (1993) 213.
- [12] P. Reimann, P. Talkner in *New Trends in Reaction Rate Theory*, Kluwer Academic Publishers, Dordrecht, 1995, p. 143.
- [13] P. Reimann, P. Talkner, *Phys. Rev. A* 44 (1991) 6348.
- [14] P. Reimann, P. Talkner, *Phys. Rev. E* 51 (1995) 4105.
- [15] P. Reimann, *J. Stat. Phys.* 82 (1996) 1467.
- [16] P. Reimann, *Phys. Rev. E* 49 (1994) 4938.
- [17] P. Reimann, R. Müller, P. Talkner, *Phys. Rev. E* 49 (1994) 3670.
- [18] C. Knessl, B.J. Matkowsky, Z. Schuss, C. Tier, *J. Stat. Phys.* 42 (1986) 169.
- [19] P. Talkner, P. Hänggi, E. Freidkin, D. Trautmann, *J. Stat. Phys.* 48 (1987) 231.
- [20] C. Van den Broeck, *J. Stat. Phys.* 31 (1983) 467.
- [21] P. Reimann, *Z. Naturf. A* 49 (1994) 1248.
- [22] P. Reimann, E. Lootens, *Europhys. Lett.* 34 (1996) 1.
- [23] P. Reimann, *J. Stat. Phys.* 85 (1996) 403.
- [24] M. Suzuki, *Adv. Chem. Phys.* 46 (1981) 195.
- [25] N.G. van Kampen, *Stochastic Processes in Physics and Chemistry*, North-Holland, Amsterdam, 1992.
- [26] T. Naeh, M.M. Klosek, B.J. Matkowsky, Z. Schuss, *SIAM J. Appl. Math.* 50 (1990) 595.
- [27] H. Hochstadt, *Integral Equations*, Wiley, New York, 1973.
- [28] W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, *Numerical Recipes*, Cambridge University Press, Cambridge, 1992.