Mean First Passage Time and the Lifetime of a Metastable State

P. Talkner

Institut für Theoretische Physik, Universität Basel, Switzerland

Dedicated to Professor Harry Thomas on the occasion of his 60th birthday

The escape rate from quite general metastable states is calculated by means of the mean first passage time. Our result generalizes the known expression for transition rates in equilibrium systems in a very natural way. Possible limitations of its validity are discussed.

1. Introduction

In equilibrium and, more frequently, in nonequilibrium situations a system governed by deterministic nonlinear evolution laws may have different locally stable states. In general, the presence of noise renders these states unstable. It is both of principle and practical interest to know at which time scales the influence of noise becomes important. In the frequently occurring case of weak noise a clear cut separation of time scales shows up: on a short scale relaxation processes take place which are almost uneffected by the noise, followed by an intermediate scale which becomes larger with decreasing noise strength, on which the decay of unstable states take place, and, finally, on the largest scale transitions between metastable states occur [1]*.

This paper investigates the rates at which these transitions occur.

For their determination two methods have been developed, namely, the calculation of a rate as the ratio of a probability flux over a barrier and a population of a well [2–4], and, on the other hand, by the determination of the mean time after which a trajectory passes the separatrix between two neighbouring metastable states, i.e. by means of a mean first passage time (m.f.p.t.) [5, 6]. Reference 7 may serve as a review of the present state of the art.

In this paper I will utilize the second method. In the next section, the qualitative behaviour of the m.f.p.t. is discussed. Its constant part is expressed in terms of a stationary probability density of the process and in terms of the gradient of the formfactor of the m.f.p.t. at the separatrix [5, 6].

In Sect. 3 the contribution of the attractor to the rate is elaborated by means of a WKB ansatz for the stationary probability density. Because this approximation is only used in a local neighbourhood of the attractor and, in Sect. 4, of a saddle located at the separatrix the pertinent problems with a global use of the WKB approximation [8] do not spoil these considerations. In Sect. 4 the contribution of the saddle is analysed and the final expression for the rate is given. In Sect. 5 I investigate the special case of a point as an attractor and a limit cycle as a saddle in which case a further evaluation of the rate can be performed. Possible limitations of this theory are discussed in Sect. 6.

2. The Constant Part of the Mean First Passage Time and the Rate

I suppose that a set of first order autonomous differential equations

$$\dot{\mathbf{x}}^{i} = K^{i}(\mathbf{x}), \qquad \mathbf{x} = (x^{1}, x^{2}, \dots, x^{n}) \in \Gamma$$
(2.1)

describes the deterministic motion of a system in configuration space Γ , and that this set of differential equations has an attractor A with a domain of attraction Ω smaller than Γ . The boundary $\partial \Omega$ constitutes a separatrix which is supposed to be smooth.

^{*} Of course, there is a microscopic time scale which shrinks with decreasing noise, on which the noise impresses small irregularities on the otherwise deterministic motion

If the system is perturbed by Gaussian white noise the sojourn time within Ω is finite, even if the noise is arbitrarily small.

The perturbed motion is described by the Fokker Planck operator

$$L = -\frac{\partial}{\partial x^{i}} \left(K^{i}(\mathbf{x}) + \varepsilon l^{i}(\mathbf{x}) \right) + \frac{\varepsilon}{2} \frac{\partial^{2}}{\partial x^{i} \partial x^{j}} D^{ij}(\mathbf{x}), \qquad (2.2 a)$$

with the adjoint

$$L^{+} = (K^{i}(\mathbf{x}) + \varepsilon l^{i}(\mathbf{x})) \frac{\partial}{\partial x^{i}} + \frac{\varepsilon}{2} D^{ij}(\mathbf{x}) \frac{\partial^{2}}{\partial x^{i} \partial x^{j}}, \qquad (2.2b)$$

where $\varepsilon D^{ij}(\mathbf{x})$ is the diffusion matrix with a positive but small noise strength ε , and with $D^{ij}(\mathbf{x})$ bounded, and where $\mathbf{l}(\mathbf{x})$ denotes the noise induced drift.

The mean time $t(\mathbf{x})$ at which a trajectory starting at $\mathbf{x} \in \Omega$ reaches the separatrix $\partial \Omega$ for the first time, i.e. the m.f.p.t. is given by [9]:

$$L^+ t(\mathbf{x}) = -1 \qquad \mathbf{x} \in \Omega, \tag{2.3a}$$

$$t(\mathbf{x}) = 0 \qquad x \in \partial \Omega. \tag{2.3b}$$

For small noise, $\varepsilon \to 0$, a trajectory starting within Ω will typically first approach the attractor and stay within its neighbourhood for a long time compared with the time constants of the deterministic motion, until an occasional fluctuation drives it to the boundary. Hence, the m.f.p.t. $t(\mathbf{x})$ assumes the same large value T everywhere in Ω , except for a thin layer $\Delta\Omega$ along the boundary $\partial\Omega$ where the small noise is still sufficient to cause a direct exit. Accordingly, one may define a function $f(\mathbf{x})$ which is unity in the inner part of Ω :

$$t(\mathbf{x}) = Tf(\mathbf{x}), \tag{2.3a}$$

$$f(\mathbf{x}) = 0 \quad \text{for } \mathbf{x} \in \partial \Omega, \tag{2.3b}$$

$$f(\mathbf{x}) \simeq 1$$
 for $\mathbf{x} \in \Omega \smallsetminus \Delta \Omega$. (2.3c)

Because T is exponentially large in ε^{-1} and because $\Delta\Omega$ shrinks to $\partial\Omega$ for $\varepsilon \to 0$ the inhomogeneity in the equation for $f(\mathbf{x})$ following from (2.3a) can be neglected on the boundary layer:

 $L^{+}f(\mathbf{x}) = 0 \qquad \mathbf{x} \in \Delta\Omega, \tag{2.4a}$

$$f(\mathbf{x}) = 0 \qquad \mathbf{x} \in \partial \Omega, \tag{2.4b}$$

$$f(x) \simeq 1 \qquad x \in \Omega \smallsetminus \Delta \Omega. \tag{2.4c}$$

I will come back to these equations below.

The constant part T of the mean first passage time may be expressed in terms of a stationary solution w of the Fokker Planck equation

$$Lw = 0, \tag{2.5}$$

and in terms of the gradient of f on $\partial \Omega$ [5, 6]

$$T = -\frac{\int d^{n} x w}{\int \int dS_{i} w D^{ij} \frac{\partial f}{\partial x^{j}}},$$
(2.6)

where dS denotes the oriented surface element on $\partial \Omega$. The rate r at which the metastable state A is left is simply given by (see Appendix)

$$r = \frac{1}{2T}.$$

3. The Probability for Staying at the Attractor

For the stationary solution of the Fokker Planck equation I choose the ansatz

$$w(\mathbf{x}) = z(\mathbf{x}, \varepsilon) e^{-\boldsymbol{\Phi}(\mathbf{x})/\varepsilon}$$
(3.1)

where the potential $\Phi(\mathbf{x})$ is independent of ε and the prefactor $z(\mathbf{x}, \varepsilon)$ is assumed to be a smooth function of \mathbf{x} even in the limit $\varepsilon \to 0$. From (2.2a), (2.5) one finds that in leading order in $\varepsilon \Phi(\mathbf{x})$ and $z(\mathbf{x}) = z(\mathbf{x}, 0)$ obey the following first order differential equations [10]

$$K^{i}\frac{\partial\Phi}{\partial x^{i}} + \frac{1}{2}D^{ij}\frac{\partial\Phi}{\partial x^{i}}\frac{\partial\Phi}{\partial x^{j}} = 0, \qquad (3.2)$$

$$\begin{bmatrix} K^{i} + D^{ij} \frac{\partial \Phi}{\partial x^{j}} \end{bmatrix} \frac{\partial z}{\partial x^{i}} + \begin{bmatrix} \frac{1}{2} D^{ij} \frac{\partial^{2} \Phi}{\partial x^{i} \partial x^{j}} + \frac{\partial K^{i}}{\partial x^{i}} - \left(l^{i} - \frac{\partial D^{ij}}{\partial x^{j}}\right) \frac{\partial \Phi}{\partial x^{i}} \end{bmatrix} z = 0.$$
(3.3)

From (3.2) it follows that the potential Φ decreases along the trajectories of the deterministic system [11]

$$\left. \frac{\mathrm{d}\Phi}{\mathrm{d}t} \right|_{\dot{x}^{i}=K^{i}} = -\frac{1}{2} D^{ij} \frac{\partial\Phi}{\partial x^{i}} \frac{\partial\Phi}{\partial x^{j}} \leq 0, \tag{3.4}$$

where the positivity of the diffusion matrix has been used. Therefore, Φ is a Lyapunov function of the deterministic motion.

As an important consequence of this fact one finds that for sufficiently small ε the integral over Ω in the expression (2.6) for the constant part T of the m.f.p.t. is dominated by the attractor and its vicinity. Let $(s^{\alpha}, y^{i}), \alpha = 1, ..., m_{A}, i = 1, ..., n - m_{A}$, be a coordinate system, where the s^{α} denote coordinates at the attractor and the y^{i} coordinates transversal to the attractor, and where m_{A} denotes the dimension of the attractor. I assume that the drift $\mathbf{K}(\mathbf{x})$ near A may be expanded about $y^i = 0$:

$$K^{\alpha}(\mathbf{s}, \mathbf{y}) = k_{A}^{\alpha}(\mathbf{s}) + q_{Ai}^{\alpha}(\mathbf{s}) y^{i} + O(|y|^{2}), \qquad (3.5 a)$$

$$K^{i}(\mathbf{s}, \mathbf{y}) = B^{i}_{Aj}(\mathbf{s}) y^{j} + O(|y|^{2}), \qquad (3.5 b)$$

where K^{α} and K^{i} denote the components of the drift in the s^{α} and y^{i} direction, respectively.

Due to its Lyapunov property the potential Φ is constant at the attractor A. I assume that Φ and z can be expanded about $y^i = 0$, too:

$$\Phi(\mathbf{s}, \mathbf{y}) = \Phi_A + \frac{1}{2} \, \varphi_{ij}^A(\mathbf{s}) \, y^i \, y^j + O(|y|^3), \tag{3.6}$$

$$z(\mathbf{s}, \mathbf{y}) = z_{\mathcal{A}}(\mathbf{s}) + O(|y|). \tag{3.7}$$

From (3.2), (3.3) one obtains in leading order in y

$$k_A^{\alpha} \frac{\partial \varphi_{ij}^A}{\partial s^{\alpha}} + B_{Ai}^k \varphi_{kj}^A + \varphi_{ik}^A B_{Aj}^k + \varphi_{ik}^A D_A^{kl} \varphi_{lj}^A = 0, \qquad (3.8)$$

and

$$k_{A}^{\alpha} \frac{\partial z_{A}}{\partial s^{\alpha}} + \left[\frac{1}{2} D_{A}^{ij} \varphi_{ij}^{A} + \frac{\partial k_{A}^{\alpha}}{\partial s^{\alpha}} + B_{Ai}^{i}\right] = 0.$$
(3.9)

Multiplying (3.8) with the inverse $(\varphi_{ij}^A)^{-1}$ and taking the trace yields

$$k_A^{\alpha} \frac{\partial \det \varphi^A}{\partial s^{\alpha}} (\det \varphi^A)^{-1} + 2B_{Ai}^i + D_A^{ij} \varphi^A_{ij} = 0, \qquad (3.10)$$

where det denotes the determinant and where the following identity has been used

$$\operatorname{tr}\left\{\varphi^{A-1} \frac{\partial \varphi^{A}}{\partial s^{\alpha}}\right\} = \frac{\partial \det \varphi^{A}}{\partial s^{\alpha}} (\det \varphi^{A})^{-1}.$$
(3.11)

With (3.10), (3.9) can be simplified further to yield

$$\frac{\partial}{\partial s^{\alpha}} \left\{ k_A^{\alpha} \, z_A (\det \varphi^A)^{-\frac{1}{2}} \right\} = 0. \tag{3.12}$$

This means that $z_A(\mathbf{s}) (\det \varphi^A(\mathbf{s}))^{-\frac{1}{2}}$ is proportional to a probability density which is invariant under the deterministic motion restricted to the attractor.

In passing I note that Eq. (3.8) can be transformed to a linear equation for the inverse matrix $(\varphi_{ij}^A)^{-1}$

$$-k_A^{\alpha} \frac{\partial \varphi_A^{ij}}{\partial s^{\alpha}} + \varphi_A^{ik} B_{Ak}^j + B_{Ak}^i \varphi_A^{kj} + D_A^{ij} = 0, \qquad (3.13)$$

where φ_A^{ij} denotes a matrix element of the inverse matrix $(\varphi^A)^{-1}$.

In order to obtain uniquely defined solutions the differential equations (3.12), (3.13) have to be supplemented by the condition that φ_A and z_A are single

valued functions on A. In the case that the single valuedness is not sufficient to determine z_A uniquely, correction-terms of order ε have to be considered.

Using (3.1), (3.6) and (3.7) the integral over Ω in (2.6) yields in leading order in ε :

$$\int_{\Omega} \mathbf{d}^{n} x \, w \simeq \mathrm{e}^{-\boldsymbol{\Phi}_{A/\varepsilon}} \int_{A} \mathrm{d}^{m_{A}} s \int \mathrm{d}^{n-m_{A}} \, y \, z_{A}(\mathbf{s}, \, \mathbf{y}) \, \mathrm{e}^{-\frac{1}{2\varepsilon} \, \varphi_{ij}^{A}(\mathbf{s}) \, y^{i} \, y^{j}}$$
$$\simeq p_{A}, \qquad (3.14)$$

where p_A is the probability that the systems is found in the linear neighbourhood of A:

$$p_A = \mathrm{e}^{-\Phi_{A/\varepsilon}} (2\pi\varepsilon)^{\frac{n-m_A}{2}} \int_A \mathrm{d}^{m_A} s z_A(\mathbf{s}) (\det \varphi^A(\mathbf{s}))^{-\frac{1}{2}}. \quad (3.15)$$

4. The Contribution of the Saddle and the Final Formula for the Rate

Due to the Lyapunov property of the potential Φ the surface integral in the expression (2.6) for the mean absorption time is dominated by the attractors of the deterministic system restricted to the separatrix. Of course, these attractors are always unstable in the direction transverse to the separatrix and, in the sequal, they will be referred to as saddles.

If there are different saddles on the separatrix the one with the smallest potential prevails. I assume that this relevant saddle is sufficiently smooth such that in its neighbourhood a coordinate system $(s^{\alpha}, y^{i}), \alpha$ = 1, ..., m_{S} , $i = 1, ..., n - m_{S}$ can be introduced. As in the case of the attractor, $(s^{\alpha}, y^{i} = 0)$ denotes a point at the saddle and y^{i} are coordinates transverse to the saddle. m_{S} denotes the dimension of the saddle. Again, as for the attractor, I expand both the drift, the potential and the prefactor in terms of the transverse coordinates y^{i} :

$$K^{\alpha}(\mathbf{s}, \mathbf{y}) = k_{S}^{\alpha}(\mathbf{s}) + q_{Si}^{\alpha}(\mathbf{s}) y^{i} + O(|y|^{2}), \qquad (4.1 a)$$

$$K^{i}(\mathbf{s}, \mathbf{y}) = B^{i}_{Sj}(\mathbf{s}) y^{j} + O(|y|^{2}), \qquad (4.1 \text{ b})$$

$$\Phi(\mathbf{s}, \mathbf{y}) = \Phi_{S} + \frac{1}{2} \,\varphi_{ij}^{S}(\mathbf{s}) \, y^{i} \, y^{y} + O(|y|^{3}), \tag{4.2}$$

$$z(\mathbf{s}, \mathbf{y}) = z_{\mathbf{s}}(\mathbf{s}) + O(|y|). \tag{4.3}$$

Consequently, I find the same equations for φ^S and z_S as for φ^A and z_A , respectively, with coefficients taken at the saddle rather than at the attractor:

$$k_{S}^{\alpha} \frac{\partial \varphi_{ij}^{S}}{\partial s^{\alpha}} + B_{Si}^{k} \varphi_{kj}^{S} + \varphi_{ik}^{S} B_{Sj}^{k} + \varphi_{ik}^{S} D_{S}^{kl} \varphi_{lj}^{S} = 0, \qquad (4.4)$$

$$k_{S}^{\alpha} \frac{\partial z_{S}}{\partial s^{\alpha}} + \left[\frac{1}{2} D_{S}^{ij} \varphi_{ij}^{S} + \frac{\partial k_{S}^{\alpha}}{\partial s^{\alpha}} + B_{Si}^{i}\right] z_{S} = 0.$$

$$(4.5)$$

In particular, there corresponds to Eq. (3.12)

$$\frac{\partial}{\partial s^{\alpha}} \left\{ k_{S}^{\alpha} z_{S} |\det \varphi^{S}|^{-\frac{1}{2}} \right\} = 0.$$
(4.6)

Note that det φ^s is negative because of the existence of exactly one unstable direction transverse to the separatrix $\partial \Omega$ at the saddle.

In order to determine this unstable direction I consider a linear combination r of the transverse coordinates

$$r = v_i(\mathbf{s}) \ y^i, \tag{4.7}$$

where the coefficients v_i are to be chosen such that the deterministic motion yields a time rate of change of r proportional to r itself with a positive proportionality factor λ_+ independent of s

$$\dot{r} = \lambda_+ r. \tag{4.8}$$

Combining (2.1), (4.1 a, b), (4.7), (4.8) yields a coupled set of linear first order partial differential equations for the coefficients $v_i(s)$

$$k_{S}^{\alpha} \frac{\partial v_{i}}{\partial s^{\alpha}} + B_{Si}^{j} v_{j} = \lambda_{+} v_{i}, \qquad \lambda_{+} > 0.$$

$$(4.9)$$

 λ_+ is an eigenvalue which must be determined together with the vector field $v_i(s)$ from (4.9).

In the simplest case, namely a saddle *point*, there is no s^{α} at all $(m_s=0)$, and (4.9) represents the algebraic eigenvalue equation of the linearized motion around the saddle point. Obviously, there exists exactly one positive eigenvalue λ_+ and one eigenvector v_i . $1/\lambda_+$ is the characteristic time of the escape from the saddle point.

In the case where the saddle consists of an unstable limit cycle, s has one component $(m_s = 1)$ which can be chosen as the arc length of the limit cycle. Equation (4.9) represents the adjoint Floquet equation of the linearized motion around the limit cycle. Due to the unstable direction transverse to the separatrix $\partial \Omega$ there exists exactly one positive Floquet index λ_+ and one corresponding eigenvector $v_i(s)$. Though I do not know of any theorems concerning existence and uniqueness of solutions of Eq. (4.9) for more complicated saddles than points and limit cycles, I presume that for any saddle on which k_x^{α} is ergodic and which has only one unstable direction, there exists exactly one solution with positive λ_+^{\star} .

In terms of the unstable direction r the surface integral in (2.6) reads in leading order in ε

$$\int_{\partial\Omega} \mathrm{d}S_i \, w \, D^{ij} \, \frac{\partial f}{\partial x^j} \simeq \int_{r=0} \mathrm{d}S_r \, w \, D^{rr} \, \frac{\partial f}{\partial r}, \qquad (4.10)$$

where, the separatrix $\partial \Omega$ near the saddle has been approximated by the tangential hypersurface r=0and where D^{rr} denotes the r, r-component of the diffusion

$$D^{rr}(\mathbf{s}) = v_i(\mathbf{s}) D^{ij}(\mathbf{s}, 0) v_j(\mathbf{s}).$$

$$(4.11)$$

In order to determine $\partial f/\partial r$ one has to solve Eq. (2.4a-c). For this purpose I make the ansatz [6]

$$f(\mathbf{s}, \mathbf{r}) = \sqrt{\frac{2}{\pi\varepsilon}} \int_{0}^{a(\mathbf{s})\mathbf{r}} \mathrm{d}u \, \mathrm{e}^{-u^{2}/2\varepsilon}, \qquad (4.12)$$

where the positive function $a(\mathbf{s})$ allows for an s-dependent thickness of the boundary layer $\Delta\Omega$ near the saddle. Note that this ansatz already fulfills the boundary conditions (2.4 b, c). From (2.4a) one obtains in leading order both in ε and r an equation for $a(\mathbf{s})$:

$$k_{S}^{\alpha} \frac{\partial a}{\partial s^{\alpha}} + \lambda_{+} a - \frac{1}{2} D^{rr} a^{3} = 0.$$
(4.13)

The transformation

$$b = a^{-2}$$
 (4.14)

yields the linear equation

$$k_{S}^{\alpha} \frac{\partial b}{\partial s^{\alpha}} - 2\lambda_{+} b + D^{rr} = 0.$$
(4.15)

From (4.4), (4.9) it follows that the negative r, r component of the inverse curvature of the potential Φ at the saddle fulfills Eq. (4.15), too

$$-k^{\alpha} \frac{\partial \varphi_{S}^{\prime\prime}}{\partial s^{\alpha}} + 2\lambda_{+} \varphi_{S}^{\prime\prime} + D^{\prime\prime} = 0, \qquad (4.16)$$

where

$$\varphi_S^{rr} = v_i \, \varphi_S^{ij} \, v_j \,. \tag{4.17}$$

Hence, (4.15), (4.16) yield

$$a = |\varphi_S^{rr}|^{-\frac{1}{2}}.\tag{4.18}$$

With (3.1), (4.2), (4.10) and (4.12) the surface-integral reads

$$\int_{\partial \Omega} dS_i w D^{ij} \frac{\partial f}{\partial x^j} \simeq -\sqrt{\frac{2}{\pi \varepsilon}} e^{-\Phi_{S/\varepsilon}}$$

$$\cdot \int_{r=0} dS_r z_S(\mathbf{s}, \mathbf{y}) e^{-\frac{1}{2} \varphi_{ij}^S y^i y^j} D^{rr}(\mathbf{s}, \mathbf{y}) a(\mathbf{s}).$$
(4.19)

204

^{*} If the saddle consists of different ergodic classes with respect to k_x^{s} to these classes there may belong different values of λ_+ . In this case each ergodic class has to be treated as a separate saddle

The minus sign results from the opposite directions of dS_i and $\partial r/\partial x^i$. It is most convenient to transform the surface integral $\int_{r=0}^{r=0} dS_r$ into the volume integral $\int d^{m_s} s \int d^{n-m_s} y \,\delta(r)$ and to use the Fourier representation of the δ -function. With (4.7) all integrals except those over the coordinates s^{α} are Gaussian ones, and, hence, easily performed. One finds after some algebra

$$\int_{\partial\Omega} \mathrm{d}S_i w D^{ij} \frac{\partial f}{\partial x^j}$$

$$\simeq -2(2\pi\varepsilon)^{\frac{n-m_s-2}{2}} \mathrm{e}^{-\boldsymbol{\varphi}_s/\varepsilon} \int_{\mathcal{S}} \mathrm{d}^{m_s} s \frac{z_s}{|\det \varphi^{\mathcal{S}}|^{\frac{1}{2}}} \frac{D^{rr} a}{|v_i \varphi_s^{ij} v_j|}.$$
(4.20)

Using (4.13) and (4.17) the second factor of the integrand in (4.20) yields

$$\frac{D^{rr}a}{|v_i\varphi_S^{ij}v_j|} = 2\lambda_+ + 2k^{\alpha}\frac{\partial}{\partial s^{\alpha}}\ln a.$$
(4.21)

With (4.6) the contribution of the second term in (4.21) can be transformed into an integral over the boundary of the saddle S

$$\int_{S} d^{m_{S}} s \frac{z_{S}}{|\det \varphi^{S}|^{\frac{1}{2}}} k_{S}^{\alpha} \frac{\partial}{\partial s^{\alpha}} \ln a$$

$$= \int_{\partial S} dS_{\alpha} k_{S}^{\alpha} \frac{z_{S}}{|\det \varphi^{S}|^{\frac{1}{2}}} \ln a.$$
(4.22)

However, either the saddle has no boundary, or if it has one, the drift k^{α} transverse to ∂S must vanish because S is an invariant set under the deterministic motion. In either case, the integral (4.22) vanishes. With the remaining term in (4.21) the surface integral (4.20) reads

$$\int_{\partial\Omega} \mathrm{d}S_i \, w \, D^{ij} \, \frac{\partial f}{\partial x^j} \simeq -\frac{2}{\pi \varepsilon} \, \lambda_+ \, p_S, \qquad (4.23)$$

where p_s is the probability for finding the system in the vicinity of the saddle if the unstable direction at the saddle is turned into a stable one by simply replacing det φ^s by its modulus:

$$p_{S} = (2\pi\varepsilon)^{\frac{n-m_{S}}{2}} e^{-\boldsymbol{\Phi}_{s}/\varepsilon} \int_{S} d^{m_{S}} S \frac{z_{S}(\mathbf{s})}{|\det \varphi^{S}(\mathbf{s})|^{\frac{1}{2}}}.$$
 (4.24)

From (2.6), (3.14) and (4.23) one finds for the constant part T of m.f.p.t.

$$T = \pi \lambda_{+}^{-1} \frac{p_A}{p_S}.$$
 (4.25)

This is the central result of the present work. It says that T is given by the time scale λ_{+}^{-1} on which the deterministic dynamical system goes away from the saddle, however, stretched by the relative frequence p_A/p_S of finding the system at the attractor rather than at the saddle. With (2.7), (4.25) one gets for the rate

$$r = \frac{\lambda_+}{2\pi} \frac{p_s}{p_A}.$$
(4.26)

For equilibrium systems the result of Langer [4] is recovered as p_S/p_A can be expressed in terms of the imaginary part of the free energy evaluated at the saddle in steepest descent approximation.

5. Escape Over a Limit Cycle

As an example I consider a dynamical system in a *n*-dimensional state space $(n \ge 2)$ with a point attractor and an unstable limit cycle in the separatrix constituting the saddle. In this case the dimension m_A of the attractor is zero and one finds from (3.15)

$$p_A = (2\pi\varepsilon)^{\frac{n}{2}} \frac{z_A}{(\det \varphi^A)^{\frac{1}{2}}} e^{-\Phi_{A/\varepsilon}}, \qquad (5.1)$$

where φ^A and Φ_A are defined according to (3.6). According to (3.8) φ^A is the solution of the algebraic equation

$$B_{Ai}^{k} \varphi_{kj}^{A} + \varphi_{ik}^{A} B_{Aj}^{k} + \varphi_{ik}^{A} D_{A}^{kl} \varphi_{lj}^{A} = 0.$$
(5.2)

The saddle has the dimension $m_s = 1$. As already indicated above, λ_+ is the positive Floquet index of the linearized deterministic motion in the vicinity of the limit cycle. The prefactor $z_s(s)$ follows from (4.6):

$$z_{S}(s) = \frac{z_{S}L}{\int \mathrm{d}s \, \frac{|\det \varphi^{S}(s)|^{\frac{1}{2}}}{k_{S}(s)}} \, \frac{|\det \varphi^{S}(s)|^{\frac{1}{2}}}{k_{S}(s)}.$$
(5.3)

Where $L = \int ds$ denotes the length of the limit cycle. I have chosen the normalization z_s of $z_s(s)$ such that $w_s = z_s e^{-\phi_s/\epsilon}$ denotes the mean probability density on the limit cycle. Equations (5.3) and (4.21) yield for the probability p_s :

$$p_{S} = (2\pi\varepsilon)^{\frac{n-1}{2}} L \frac{\int \mathrm{d}s \, 1/k_{S}}{\int \mathrm{d}s \, \frac{|\det \varphi^{S}|^{\frac{1}{2}}}{k_{S}}}.$$
(5.4)

Obviously,

$$\left(\int \frac{\mathrm{d}s}{k_s}\right)^{-1} \int \frac{\mathrm{d}s}{k_s} \frac{|\det \varphi^s|^{\frac{1}{2}}}{(2\pi\varepsilon)^{(n-1)/2}}$$

represents the time average over one period of the limit cycle of the reciprocal area which is probed by the transverse degrees of freedom in Gaussian approximation at the noise level ε .

Combining (4.23), (5.1) and (5.5) yields the result

$$r = \frac{\lambda_+}{2\pi (2\pi\varepsilon)^{\frac{1}{2}}} \frac{(\det \varphi^A)^{\frac{1}{2}} L \int \frac{\mathrm{d}s}{k_s}}{\int \frac{\mathrm{d}s}{k_s} |\det \varphi^S|^{\frac{1}{2}}} \frac{z_s}{z_A} e^{-\frac{\Phi_s - \Phi_A}{\varepsilon}}.$$
 (5.5)

For d=2 this result coincides with the one given in [12].

6. Conclusions

In this work I have shown that for a large class of systems the lifetime of a metastable state is determined by the positive Lyapunov index characterizing the unstable motion at the saddle at which the exit takes place most probably and by the ratio of the stationary probabilities at the attractor and at the saddle. Both these probabilities are defined as the mean probability densities at the respective sets times the respective volumes which are probed in Gaussian approximation. In order to obtain a real volume the negative curvature of the potential at the saddle must be replaced by its modulus. This result for the rate seems to be of greater validity than the assumptions made in its derivation might indicate.

However, there are certain conditions which must be met. First of all, the noise must be sufficiently small, otherwise the mean first passage time fails to be constant almost everywhere on the domain of attraction and it does not determine the escape rate. Moreover, for the Gaussian approximations performed both at the attractor and the saddle the noise must be small, too. In this respect the saddle is more sensitive because there, the restriction of the potential to the separatrix may contain a direction in which the potential is almost constant and in which higher then quadratic terms of the transverse coordinates contribute even at a rather low noise level [13, 14].

Finally, I note that even for weak noise the mean time of the first passage of the separatrix need not determine the transition rate to a neighbouring state if, roughly speaking, the way down from the saddle to the final state is complicated in a way that back-scattering from points beyond the saddle to the attractor A cannot be neglected.* For example this is the case for a Brownian particle moving in a metastable potential at very low friction [2, 15]. In this case

the particle, once having crossed the saddle may undergo many revolutions until it thermalizes in one or the other state. In Ref. 13 one finds a very instructive numerical simulation of this behaviour. By definition, for the mean first passage time, the fate of a trajectory after the first crossing of the separatrix does not count, whereas the trajectory contributes to the rate until the final state has been reached.

For higher than two-dimensional nonequilibrium systems the separatrix may become very complicated. One can easily envisage situations in which it is not sufficient to know the mean first time at which the separatrix is reached by the trajectory, rather one should know when the separatrix has been left definitely. As is well known one copes with the problem of a Brownian particle at low friction by studying the diffusive motion of the energy (or action). Whether in the case of a complicated separatrix one can introduce appropriate slow quantities, in terms of which the determination of the rate can again be found from a m.f.p.t. is an interesting problem of future research.

Appendix

The higher moments $t_n(x)$, n = 1, 2, ..., of the first passage time obey the following hierarchy of equations [16]

$$L^{+} t_{n}(\mathbf{x}) = -n t_{n-1}(\mathbf{x}) \qquad \mathbf{x} \in \Omega,$$

$$t_{n}(\mathbf{x}) = 0 \qquad \mathbf{x} \in \partial \Omega.$$

Provided that, as assumed throughout in this paper, Ω consists of a domain of attraction and that the noise is weak, the mean first passage time $t_1(\mathbf{x})$ attains a constant value T almost everywhere on Ω . Hence, the second moment $t_2(\mathbf{x})$ obeys the same equation as $t_1(\mathbf{x})$ except that the inhomogeneity is approximately -2T rather than -1. Therefrom one concludes for the second moment

$$t_2(\mathbf{x}) = 2T^2 \quad \mathbf{x} \in \Omega \smallsetminus \Delta \Omega$$

This argument may be repeated with the result

$$t_n(\mathbf{x}) = n! T^n \quad x \in \Omega \smallsetminus \Delta \Omega.$$

Consequently the probability density of the first passage time reads

$$p(t) = T^{-1} e^{-t/T}.$$

This is the waiting time distribution of a state A without memory [17]. Hence, disregarding backflow, the decay rate is T^{-1} . Actually, a transition occurs to the boundary which one may identify with a shortlived intermediate state. This state is left with equal

^{*} For a crude model of this situation see the Appendix

transition probabilities, $p \ge T^{-1}$, back to the initial state A or to the final state. If the final state is assumed to be absorbing, the rate at which the state A is depleted is simply $(2T)^{-1}$. Finally, I will discuss a simple model in which one has a chain of N intermediate states. The first one in this chain represents the separatrix and is fed by A at the rate T^{-1} . From each intermediate state there is an equal transition probability to its neighbouring states. If, again, the final state is absorbing, the rate at which A is depleted turns out to be $((1+N)T)^{-1} + O(N/pT)$. Hence, it is decreased roughly by a factor 2/(N+1) by the presence of the additional intermediate states.

References

- 1. Suzuki, M.: Systems far from equilibrium. In: Lecture Notes in Physics. Vol. 132, p. 48. Garrido, L. (ed.). Berlin, Heidelberg, New York: Springer 1980
- 2. Kramers, H.A.: Physica 7, 284 (1940)
- 3. Landauer, R., Swanson, J.A.: Phys. Rev. 121, 1668 (1961)
- 4. Langer, J.S.: Phys. Rev. Lett. 21, 973 (1986); Ann. Phys. (NY) 54, 258 (1969)
- Matkowsky, B., Schuss, Z.: SIAM J. Appl. Math. 33, 365 (1977);
 43, 673 (1983)

- Talkner, P., Ryter, D.: Phys. Lett. 88 A, 162 (1982); In: Noise in physical systems and 1/f noise. Savelli, M., Lecoy, G., Nougier, J.-P. (eds.). New York: Elsevier Science Publ. 1983 Talkner, P., Hänggi, P.: Phys. Rev. A 29, 768 (1984)
- 7. Hänggi, P.: J. Stat. Phys. 42, 105 (1986)
- Graham, R., Tél, T.: Phys. Rev. Lett. 52, 9 (1984) Jauslin, H.R.: J. Stat. Phys. 42, 573 (1986)
- 9. Dynkin, E.B.: Markov processes. Berlin, Heidelberg, New York: Springer 1965
- 10. Ludwig, D.: SIAM Rev. 4, 605 (1975)
- 11. Graham, R.: In: Stochastic nonlinear systems. Arnold, L., Lefever, R. (eds.). Berlin, Heidelberg, New York: Springer 1981
- 12. Matkowski, B., Schuss, Z.: SIAM J. Appl. Math. 42, 822 (1982)
- Straub, J.E., Borkovec, M., Berne, B.J.: J. Chem. Phys. 83, 3172 (1985); 84, 1788 (1986)
- 14. Talkner, P., Braun, H.B.: (to be published)
- Büttiker, M: Noise in nonlinear dynamical systems: theory, experiment, simulation. Moss, F., McClintock, P.V.E. (eds.). Cambridge: Cambridge Univ. Press (to appear)
- 16. Weiss, G.H.: Adv. Chem. Phys. 13, 1 (1967)
- 17. Weiss, G.H., Rubin, R.J.: Adv. Chem. Phys. 52, 364 (1983)

P. Talkner Institut für Physik Universität Basel Theoretische Physik Klingelbergstrasse 82 CH-4056 Basel Switzerland