The Effect of Focusing and Caustics on Exit Phenomena in Systems Lacking Detailed Balance

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Abstract

We study the trajectories followed by a particle subjected to weak noise when escaping from the domain of attraction of a stable fixed point. If detailed balance is absent, a *focus* may occur along the most probable exit path, leading to a breakdown of symmetry (if present). The exit trajectory bifurcates, and the exit location distribution may become 'skewed' (non-Gaussian). The weak-noise asymptotics of the mean escape time are strongly affected. Our methods extend to the study of skewed exit location distributions in stochastic models without symmetry.

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A particle moving in a force field, but weakly perturbed by external noise, will spend most of its time near stable fixed points of the force field. But the particle will occasionally undergo a *large fluctuation*: it will leave the basin of attraction of one such point, and enter that of another. The timescale on which such fluctuations occur grows exponentially in the low-noise limit.

In this limit, the particle typically follows a *unique trajectory* in its final, successful escape attempt; transverse deviations from this path become increasingly unlikely as the noise strength goes to zero. This trajectory is referred to as the most probable escape path (MPEP), and its properties govern the asymptotic behavior of the mean escape time. In our earlier work [13, 14] we suggested the possibility of a *focusing singularity*: as one moves out along the MPEP, transverse fluctuations become increasingly less stable, leading to a breakdown of stability before the boundary of the basin is reached. This hitherto unexplored phenomenon has profound consequences for the particle's escape behaviour. It frequently occurs when the force field is nonconservative, or in general when detailed balance is absent. Its wide prevalence has not previously been recognized.

In this Letter we study a simple example to demonstrate the effects of focusing singularities on exit phenomena. We show that when such a singularity occurs, the MPEP *bifurcates* (in the simplest case), leading to a type of broken symmetry. This transition affects not only the prefactor of the mean first passage time (MFPT) to the boundary, but also, its *exponential dependence on the noise*. It may induce an unusual 'skewed' (non-Gaussian) distribution of exit points on the boundary.

For simplicity we restrict ourselves to the case of an overdamped classical point particle moving in two dimensions and subject to additive isotropic white noise $\boldsymbol{w}(t)$. In the overdamped case the deterministic forces acting on the particle are described by a drift field $\boldsymbol{u}(\boldsymbol{x})$, so that

$$dx_i(t) = u_i(\boldsymbol{x}(t))\,dt + \epsilon^{1/2}\,dw_i(t), \quad i = 1, 2 \tag{1}$$

with ϵ the noise strength. The corresponding Fokker-Planck equation for the probability density is

$$\dot{\rho} = (\epsilon/2)\nabla^2\rho - \boldsymbol{\nabla}\cdot(\rho\boldsymbol{u}). \tag{2}$$

We shall employ the technique of matched asymptotic expansions described in Refs. [13, 14]. We impose absorbing boundary conditions on the 'separatrix' (the boundary of the basin) and study the behavior, as $\epsilon \to 0$, of the quasistationary density $\rho_1(x,y)$, *i.e.*, the slowest decaying eigenmode of the Fokker-Planck operator. In the low-noise limit, the properties of ρ_1 can be used to calculate both the MFPT and the distribution of exit points [13].

We specialize to the case of a drift field with a stable fixed point at $(x_S, 0)$, whose basin of attraction is the entire right-half plane. We assume symmetry about the x-axis, and that there is only one fixed point on the y-axis: a saddle point at $(0, 0)$. A simple drift field with this structure is

$$\boldsymbol{u}(x, y) = (x - x^3 - \alpha x y^2,\ -\mu y - x^2 y). \tag{3}$$

This force field is conservative, *i.e.*, is the gradient of a potential, only if $\alpha = 1$. Nonetheless for any $\mu > 0$ the field conforms to the assumptions, with $x_S = 1$. The symmetry of $\boldsymbol{u}$ suggests that the MPEP, which must connect $(x_S, 0)$ and the saddle, lies along the x-axis, and for small $\alpha > 0$ that is the case [14]. The case when exit occurs over an *unstable* fixed point [13] is also of interest; additional phenomena may emerge there because focusing on the separatrix (rather than the MPEP) can occur. We defer that case to a later paper.

Away from both the stable point and the separatrix, ρ_1 can be approximated by a WKB form [14, 17]

$$\rho_1(x, y) \sim K(x, y) \exp\left(-W(x, y)/\epsilon\right). \tag{4}$$

$K(x, y)$ satisfies a transport equation, and $W(x, y)$ an eikonal (Hamilton-Jacobi) equation: $H(\boldsymbol{x}, \boldsymbol{\nabla} W) = 0$, with $H(\boldsymbol{x}, \boldsymbol{p}) = \frac{1}{2}\boldsymbol{p}^2 + \boldsymbol{u}(\boldsymbol{x}) \cdot \boldsymbol{p}$ the Wentzell-Freidlin Hamiltonian [8]. So for any point (x, y) in the basin of attraction of $(x_S, 0)$, $W(x, y)$ will be the action of a zero-energy classical trajectory, governed by this Hamiltonian, extending from $(x_S, 0)$ to (x, y). In general, computation of $W(x, y)$ will require a minimization over the set of zero-energy trajectories terminating at (x, y). MPEPs are accordingly the zero-energy trajectories from $(x_S, 0)$ to $(0, 0)$ of least action. The MPEP action is the exponential growth rate, in the low-noise limit, of the MFPT.

For non-gradient drift fields $\boldsymbol{u}$, it will be a common occurrence for two or more classical trajectories emanating from $(x_S, 0)$ to cross at some point. The locus of these points (equivalently, the set of points reachable from $(x_S, 0)$ *viâ* more than one zero-energy trajectory) is known as a *caustic* [5, 10, 16]. A *focus* is a critical point from which a caustic emanates. Pictorial examples of this are given in Refs. [5, 6, 14]. In these examples the caustics are found far from fixed points, MPEPs, or separatrices and have little effect on exit phenomena. However they may constitute regions of anomalous probability density, since the WKB expansion breaks down there [16].

Our concern here is what happens when a focus appears on the MPEP itself, making the action W non-unique at following points. Because the MPEP is initially assumed to lie along the

x-axis, we study the validity of the WKB approximation by introducing the expansion

$$W(x,y) = f_0(x) + f_2(x)y^2 + o(y^2). \tag{5}$$

Physically, $f_2(x)^{-1/2}\epsilon^{1/2}$ is the transverse lengthscale within which $\rho_1(x,y)$ is nonnegligible. $f_2(x)$ satisfies a nonlinear Riccati equation, described in Refs. [13, 14].

We begin by considering the drift field of (3) when $\mu = 1$. For all $\alpha < 4$, we find numerically that f_2 remains positive and finite from $x = 1$ to $x = 0$, converging to 1 as the origin is approached. (Because the origin is a fixed point of $\boldsymbol{u}$, it is formally reached in infinite time; see the discussion in Ref. [14]). However when $\alpha = 4$, f_2 converges to *zero*, signalling the appearance of a transverse 'soft mode,' or instability. (This is accompanied by a divergence of the prefactor K in (4).) For all $\alpha > 4$, f_2 reaches zero at *positive* x, and then plunges to $-\infty$ in *finite* time (hence at strictly positive x). This signals the presence of a singularity in W.

Fig. 1(a) displays this graphically. As one moves from $(1,0)$ toward the origin, the iso-action curves become non-convex at the point where f_2 goes negative. They become increasingly pinched near the x-axis, leading to a cusp singularity at $(x_F,0)$, where f_2 diverges. Beyond this point W remains continuous, but is not continuously differentiable across the x-axis. It must be computed by minimizing over trajectories, and different trajectories are employed as $y \to 0^+$ and $y \to 0^-$.

Fig. 1(b) makes this clear; it shows the zero-energy classical trajectories, derived from the Wentzell-Freidlin Hamiltonian by integrating Hamilton's equations. As x is decreased from 1, off-axis trajectories eventually reconverge on the axis, signalling that $(x_F,0)$ is a focus. (It is not hard to show this analytically, but we omit the proof here.) Every point $(x,0)$ with $x < x_F$, including the saddle point at the origin, is reachable by *three* zero-energy trajectories: the original x-axis MPEP, and two symmetrically placed off-axis trajectories, with lesser (degenerate) actions.

The dependence of the focus x_F on α, for the particular drift field (3), is of some interest. When $\alpha = 4$, $x_F = 0$. As α increases beyond 4, x_F increases continuously from zero but never reaches x_S. When $\alpha = 9$, a new focus appears at the origin so that *two* foci occur on the x-axis. Both of these move to larger x as α increases. We have found numerically that a new focus appears at $\alpha = n^2$, $n = 2,3,4,\ldots$, but have not yet explored in detail the set of zero-energy trajectories when multiple foci occur. We restrict ourselves below to the case of a single focus, *i.e.*, if $\mu = 1$ we consider only $4 < \alpha < 9$. If $\mu \neq 1$ the range of allowed values of α will differ.

Upon encountering a single focus, the MPEP *bifurcates*. The path of minimum classical action

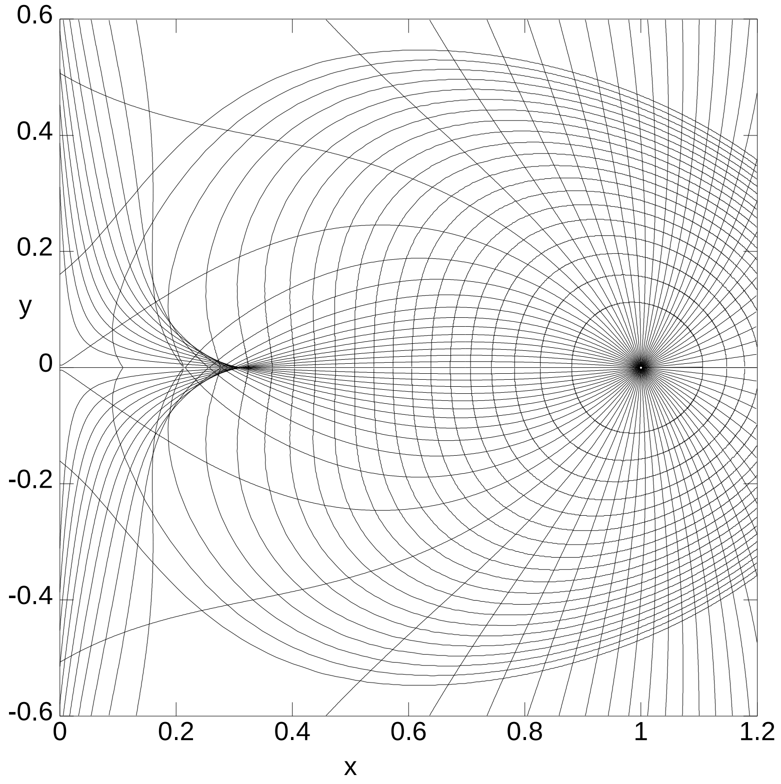

Figure 1: (a) The curves of constant action W surrounding the stable fixed point $(x_S, 0) = (1, 0)$, revealing the presence of a singularity in W at $(x_F, 0) \approx (0.3, 0)$. Here $\mu = 1$ and $\alpha = 5$. (b) The classical trajectories of zero energy, emanating from $(1, 0)$, from which the iso-action curves are computed. The two MPEPs are the off-axis trajectories incident on $(0, 0)$.

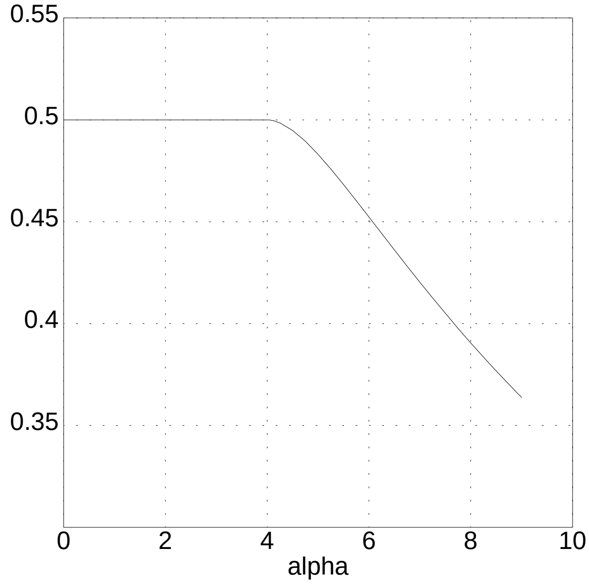

Figure 2: The action of the MPEP(s) for the drift field (3), as a function of the parameter α when $\mu = 1$. The MPEP extends along the x-axis only if $\alpha \leq 4$, and no focus is present.

— hence, the MPEP — to any point $(x, 0)$ with $x > x_F$ from $(x_S, 0)$ remains the x-axis. For $x < x_F$, however, the former MPEP (*i.e.*, the x-axis) remains an extremum of the action but is no longer a local minimum [16]. There are two new MPEPs, related by $y \to -y$. The symmetry has been broken: the drift field and the equations of motion are symmetric about the x-axis, but each MPEP is not.

The new (curved) MPEPs, and their common action, are easily computed numerically. Since their action is the exponential growth rate of the MFPT, the bifurcation greatly affects the low-noise asymptotic behavior. In Fig. 2 we plot the classical action of the MPEP(s) between the stable and hyperbolic points (and therefore the asymptotic slope of the MFPT *vs.* $1/\epsilon$ on a log-log plot) *vs.* α for the case $\mu = 1$ in the drift field (3). The onset of focusing at $\alpha = 4$ is evident. The MFPT prefactor, one can show, is also singular at $\alpha = 4$.

To study the effects of focusing on the exit location distribution near the saddle, we set up a covariant formalism for computing the WKB behavior of ρ_1 along a curved MPEP. The Hamilton-Jacobi equation is

$$0 = H(x^i, p_i) = \tfrac{1}{2} D^{ij} p_i p_j + u^i(\boldsymbol{x}) p_i, \tag{6}$$

where $p_i = \partial W / \partial x^i$, an index is summed over when repeated, and the diffusion tensor $\boldsymbol{D}$ may be anisotropic (but we consider only isotropic $\boldsymbol{D}$ here). We adopt the notation $p_{i,j} = \partial p_i / \partial x^j$; note that $W_{,ij} = p_{i,j}$. By twice differentiating the Hamilton-Jacobi equation we arrive at the evolution equation for the second derivatives of W along any zero-energy trajectory:

$$\dot{W}_{,ij} = -D^{kl} W_{,ki} W_{,lj} - u^k{}_{,i}\, W_{,kj} - u^k{}_{,j}\, W_{,ki} - u^l_{,ij} p_l \tag{7}$$

where the dot signifies a derivative with respect to transit time along the trajectory.

Eq. (7) describes the evolution of fluctuations in all directions of the action along the MPEP, and represents a generalization of our previously derived nonlinear Riccati equation [13, 14] (to which it reduces when $i = j = y$ and the MPEP is along the x-axis). Similarly, the covariant generalization of our transport equation for K is [17]

$$\dot{K}/K = -u^i_{,i} - \tfrac{1}{2} D^{ij} W_{,ij}. \tag{8}$$

It is amusing to note that the diffusion tensor plays a role similar to that of a metric tensor, with additive noise (constant $\boldsymbol{D}$) corresponding to flat space, while multiplicative noise introduces an effective curvature [9].

In the vicinity of the stable and hyperbolic fixed points ($t \to -\infty, \infty$ above) the momentum and therefore the inhomogeneous term of (7) vanish. We see that in these limits we must solve an algebraic Riccati equation

$$D^{kl} W_{,ki} W_{,lj} + u^k{}_{,i}\, W_{,kj} + u^k{}_{,j}\, W_{,ki} = 0. \tag{9}$$

Eq. (9) was also derived by Ludwig and Mangel in the context of stochastic ecology [12, 15]. The quasistationary density in the far field of the 'diffusive' lengthscale, of size $O(\epsilon^{1/2})$, surrounding each fixed point is accordingly (up to a constant factor)

$$\rho_1(\boldsymbol{x}) \sim \exp\left[-(\boldsymbol{x} - \boldsymbol{x}_0)\boldsymbol{C}^{-1}(\boldsymbol{x} - \boldsymbol{x}_0)/2\epsilon\right] \tag{10}$$

where $\boldsymbol{x}_0 = (x_S, 0)$ or $(0, 0)$, and the inverse covariance matrix $\boldsymbol{C}^{-1} = (C^{-1})_{ij} = W_{,ij}$ is determined by the matrix equation (9). $\boldsymbol{C}^{-1}$ will be positive definite at the stable point, but not at the saddle point.

Our procedure is to compute $W(\boldsymbol{x})$ and $K(\boldsymbol{x})$ by (numerically) integrating the coupled equations (7) and (8) along the curved MPEP. Close to the two fixed points, we match to a quasistationary density which (a) is a solution of the Fokker-Planck equation, and (b) matches with (10) on the

$O(\epsilon^{1/2})$ lengthscale.

We find that the asymptotic behavior of exit phenomena falls into three qualitatively different categories depending on whether the parameter μ in the drift field is greater than, less than, or equal to 1. This is because in the vicinity of the saddle at the origin, $\boldsymbol{u} \approx (x, -\mu y)$. In this linearized field Hamilton's equations are easily solved. (All trajectories possess a reflection symmetry about the x-axis; when we refer to a trajectory in the first quadrant, note that it has a mirror image in the fourth.) The zero-energy trajectory which approaches the origin from above follows a curve $y \propto x^{\mu}$; hence the MPEP asymptotically approaches the x-axis for $\mu > 1$, the y-axis for $\mu < 1$, and comes in at a fixed angle for $\mu = 1$. [Cf. Fig. 1(b).] We consider these cases in turn.

$\mu > 1$: Very near the saddle point at $(0,0)$, this case resembles the case of unbroken symmetry described in Ref. [14]. The action there can be approximated as $W(x,y) \approx -x^2 + \mu y^2$. The prefactor K simply tends to a nonzero constant. Because the MPEPs approach the origin asymptotically close to the x-axis, matching in the vicinity of the saddle remains the same as in the unbroken case. Up to a constant factor, the quasistationary density ρ_1 on the $x, y = O(\epsilon^{1/2})$ lengthscale will be

$$\left[\exp(x^2/2\epsilon)\, y_2(\tfrac{1}{2}, x\sqrt{2/\epsilon})\right] \exp(-\mu y^2/\epsilon) \tag{11}$$

where $y_2(\frac{1}{2}, \cdot)$ is the odd parabolic cylinder function [1] of index $\frac{1}{2}$. This agrees with (10) in the far field, and falls to zero as $x \to 0$ due to absorption of probability. The exit location distribution will be asymptotically Gaussian, with standard deviation $\epsilon^{1/2}/\sqrt{2\mu}$, as in the unbroken case. We stress, however, that in this and the following two cases the exponential dependence of the MFPT on the noise depends on proper identification of the α-dependent off-axis MPEPs, as does the prefactor.

$\mu < 1$: Here the MPEP approaches the origin asymptotically along the y-axis. However, the *momentum* of the MPEP asymptotically aligns itself along the x-axis. (This is true in all three cases.) This can easily be seen by solving Hamilton's equations of motion near the origin. Because the quadratic fluctuations of the action around the MPEP are perpendicular to the momentum, we have the unusual situation where 'transverse' fluctuations of the escaping particle around the MPEP become asymptotically aligned with the MPEP itself: they become longitudinal. The quasistationary density and exit location distribution are, moreover, spread over an anomalously large region. Absorption takes place in a boundary layer of width $O(\epsilon^{1/2})$, but because the MPEP approaches the origin along a curve $y \propto x^{\mu}$ the appropriate lengthscale in the y-direction is $y = O(\epsilon^{\mu/2})$, not $y = O(\epsilon^{1/2})$.

This becomes clear when $W(x,y)$ and $K(x,y)$ are approximated near the origin. Integrating the evolution equation (7), in the linear approximation, yields

$$W(x,y) \approx -2x(|y|/A)^{1/\mu} + (|y|/A)^{2/\mu} \tag{12}$$

where A is the limit of the ratio y/x^μ along the MPEP as it approaches the origin. Since $\mu < 1$, this action is of higher order than quadratic in the displacements x, y. Equivalently, the inverse covariance matrix $\boldsymbol{C}^{-1}$ of (10) *vanishes*. This vanishing is always allowed [$W_{,ij} \equiv 0$ is a solution of the algebraic Riccati equation (9)] but it occurs only when $\mu < 1$, leading to an anomalously large lengthscale. The behavior of the prefactor K may be computed from (8); along the MPEP, it is asymptotically proportional to $x^{1-\mu}$. This is an unusual situation: strictly speaking, the 'frequency factor' [11, 14] $K(0,0)$ equals zero, yet all physical exit quantities remain nonzero and finite. The MFPT prefactor, however, turns out not to be anomalous; it is independent of ϵ.

To compute the exit location density and the MFPT asymptotics, an expression for the quasi-stationary density ρ_1 on the $x = O(\epsilon^{1/2})$, $y = O(\epsilon^{\mu/2})$ lengthscale is needed. It is easily seen to be (up to a constant factor)

$$|y|^{(1/\mu)-1} \sinh[2x(|y|/A)^{1/\mu}/\epsilon] \exp[-(|y|/A)^{2/\mu}/\epsilon] \tag{13}$$

which both solves the Fokker-Planck equation to leading order, and matches up with the WKB approximation (4) when W is given by (12) and $K \sim x^{1-\mu}$ along the MPEP. Since the exit location probability density is proportional to $\partial_n \rho_1$, *i.e.*, $\partial\rho_1/\partial x(x = 0)$, this gives an asymptotic exit location distribution $f(y)\,dy$ on the y-axis, with

$$f(y) \propto |y|^{(2/\mu)-1} \exp[-(|y|/A)^{2/\mu}/\epsilon] \tag{14}$$

So on the $O(\epsilon^{\mu/2})$ lengthscale to either side of the saddle, the exit location has a bimodal (symmetrized) Weibull distribution [4], with shape parameter $2/\mu$. (Equivalently, $|y|^{2/\mu}$ at exit time becomes *exponentially distributed* in the low-noise limit.) This 'skewing' phenomenon (the particle tending to exit to one side of a saddle, in a non-Gaussian way, rather than at the saddle itself) was discovered by Bobrovsky and Schuss [2], and has been further investigated [3, 7]. However, in our simple model we are able to work out the skewed exit location distribution exactly. Of course the scaling parameter $A = A(\alpha, \mu)$ must be determined numerically, by integrating Hamilton's equations. The physical interpretation of the exponential distribution remains unclear.

$\mu = 1$: As in the $\mu > 1$ case, absorption occurs on the $x, y = O(\epsilon^{1/2})$ lengthscale. But a new feature enters: the inverse covariance matrix $\boldsymbol{C}^{-1}$ is no longer uniquely determined by (9). There is a free parameter, which must be computed numerically by matching. The asymptotic expression for the exit location distribution involves parabolic cylinder functions. We defer the details.

We have dealt only with a drift field symmetric about some axis. Our results (excepting those relating to broken symmetry) and methods are more general and apply to drift fields without such symmetry. So they should apply, in particular, to the asymmetric models (with anisotropic $\boldsymbol{D}$) reviewed by Bobrovsky and Zeitouni [3]. For such models the MPEP will typically be curved even in the absence of focusing, and skewed exit distributions will frequently occur. But the presence of a focus will still be signalled by a breakdown in transverse fluctuations, at which point qualitatively new behavior will emerge. One amusing prospect is to study drift fields with a 'symmetry parameter.' As this is tuned through zero one might observe a jump in the exponential growth rate of the MFPT, much as a jump in magnetization results when an applied field passes through zero.

References

[1] M. Abramowitz and I. A. Stegun. *Handbook of Mathematical Functions*. Dover, New York, 1965.

[2] B. Z. Bobrovsky and Z. Schuss. A Singular Perturbation Approach for the Computation of the Mean First Passage Time in a Nonlinear Filter. *SIAM J. Appl. Math.* **42** (1982), 174–187.

[3] B. Z. Bobrovsky and O. Zeitouni. Some Results on the Problem of Exit from a Domain. *Stochastic Process. Appl.* **41** (1992), 241–256.

[4] R. S. Burington and D. C. May. *Handbook of Probability and Statistics with Tables*. McGraw-Hill, New York, second edition, 1970.

[5] V. A. Chinarov, M. I. Dykman, and V. N. Smelyanskiy. Dissipative Corrections to Escape Probabilities of Thermally Nonequilibrium Systems. *Physical Review E*, to appear, 1993.

[6] M. V. Day. Recent Progress on the Small Parameter Exit Problem. *Stochastics* **20** (1987), 121–150.

[7] M. V. Day. Cycling and Skewing of Exit Measures for Planar Systems. Preprint, 1993.

[8] M. I. Freidlin and A. D. Wentzell. *Random Perturbations of Dynamical Systems*. Springer-Verlag, New York/Berlin, 1984.

[9] R. Graham. Path Integral Formulation of General Diffusion Processes. *Z. Phys. B* **26** (1977), 281–290.

[10] M. C. Gutzwiller. *Chaos in Classical and Quantum Mechanics*. Springer-Verlag, New York/Berlin, 1990.

[11] R. Landauer and J. A. Swanson. Frequency Factors in the Thermally Activated Process. *Phys. Rev.* **121** (1961), 1668–1674.

[12] D. Ludwig. Persistence of Dynamical Systems Under Random Perturbations. *SIAM Rev.* **17** (1975), 605–640.

[13] R. S. Maier and D. L. Stein. Transition-rate Theory for Non-Gradient Drift Fields. *Phys. Rev. Lett.* **69** (1992), 3691–3695.

[14] R. S. Maier and D. L. Stein. The Escape Problem for Irreversible Systems. *Physical Review E*, to appear, 1993.

[15] M. Mangel and D. Ludwig. Probability of Extinction in a Stochastic Competition. *SIAM J. Appl. Math.* **33** (1977), 256–266.

[16] L. S. Schulman. *Techniques and Applications of Path Integration*. Wiley, New York, 1981.

[17] P. Talkner. Mean First Passage Times and the Lifetime of a Metastable State. *Z. Phys. B* **68** (1987), 201–207.