LIFETIME OF A METASTABLE STATE AT WEAK NOISE

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The mean time for a trajectory of a randomly perturbed system to leave a domain of attraction is determined in leading order of weak noise. Considerable simplifications are obtained if a WKB type expansion applies to the solution of the stationary Fokker-Planck equation.

1. INTRODUCTION

In the study of various equilibrium and nonequilibrium phenomena such as first order phase transitions, chemical reactions, optical bistability and electronic systems, the lifetime of a metastable state plays a decisive role: e.g., it determines nucleation rates, chemical reaction rates, the quality of optical switches and of electronic systems. Often it determines the long time behaviour of the system.

The metastability of a state arises as an interplay of nonlinear deterministic and weak stochastic forces. Under the influence of the deterministic force alone the metastable state would be one of several stable states. The stochastic force is negligible during most of the time, except for those rare events where the force becomes large enough to drive the system into another state. It is quite evident that the rate of these transitions is just the inverse of the mean lifetime of the metastable state, and one may show that the lifetime is exponentially distributed at weak noise.

Such rates were evaluated by Kramers [1] for a Brownian particle moving in a one-dimensional potential. Generalizations to Brownian motion in higher dimensions are due to Landauer et al. [2] and Langer [3]. In the considered models the metastable states are always point attractors of the deterministic forces; moreover the systems are supposed to reach thermal equilibrium for $t \to \infty$.

Under even stronger restrictions, the path integral method was used to calculate transition rates [4, 5]. An attempt to reformulate and generalize Kramers' rate calculation was recently presented by Gardiner [6].

A different approach is to calculate the mean lifetime of the metastable state rather than the rate. In this case the problem can be formulated without any special assumptions about the metastable state or about the probable transition path; even the exit points from the domain of attraction and the stationary distribution are not a priori restricted. The domain of attraction of the metastable state is conveniently imagined to be surrounded by an absorbing boundary. Then the mean time of absorption is just half the lifetime of the metastable state. For a continuous Markov process i.e. with stochastic forces proportional to Gaussian white noise, the mean time of absorption is the solution of a boundary value problem of an inhomogeneous second order differential equation [7, 8]. In one dimension it can be solved exactly for an arbitrary strength of the stochastic force [7]. In higher dimensions analytical solutions are not usually known and the standard numerical procedures inappropriate for small noise. However, the smallness of the noise which is inherent in the notion of metastability can be utilized to reduce the problem to first finding the solution of the homogeneous differential equation on a thin boundary layer and second solving the stationary Fokker-Planck equation on the domain of attraction of the metastable state [9]. The general solution of the boundary layer problem was given recently by the present authors [10].

In this paper the expression for the mean exit time is briefly rederived in Sect 2, and in Sect 3 more explicit results are obtained by use of a WKB-type solution of the stationary Fokker-Planck equation. This kind of solution reduces all occurring integrals to the saddle-point type, moreover it indicates where the transitions preferably take place.

2. THE MEAN ABSORPTION TIME

We suppose that a set of first order autonomous differential equations

$$\dot{x}^1 = K^1(x), x = (x^1, x^2, \ldots, x^n) \in \Gamma$$

(1)

describes the deterministic motion of the system in configuration space $\Gamma$, and that this set of differential equations has a connected but otherwise arbitrary attractor with a domain of attraction $\Omega$ smaller than $\Gamma$. The boundary $\partial \Omega$ is supposed to be smooth. If the system is perturbed by white noise the duration of stay within $\Omega$ is ge-
generally finite, even if the noise is arbitrarily weak.

The perturbed motion is described by the Fokker-Planck operator \( L \)

\[
L = -\frac{\partial^2}{\partial x^2} + \frac{1}{2} \frac{\partial}{\partial x} + \frac{1}{2} \frac{\partial}{\partial j} \frac{\partial^2}{\partial j^2} (x)
\]

(2a)

with the adjoint

\[
L^* = K^i(x) \frac{\partial}{\partial x} + \frac{1}{2} \epsilon \frac{\partial}{\partial x} (x) \frac{\partial}{\partial j} (x)
\]

(2b)

where \( \epsilon \) \( D^i j (x) \) is the diffusion matrix, \( D^i j (x) \) is bounded and \( \epsilon \) measuring the strength of the noise is positive and small.

The mean time \( t(x) \) at which a trajectory starting at \( x \in \Omega \) reaches the boundary \( \partial \Omega \) for the first time is given by [8]

\[
L^* t = -1, \quad t(x) = 0 \quad \text{for} \quad x \in \partial \Omega
\]

(3)

By integrating eq. (3) with a solution \( w \) of the stationary Fokker-Planck equation

\[
Lw = 0
\]

which is integrable on \( \Omega \) one obtains by the Gaussian theorem

\[
\frac{\epsilon}{2} \int_{\partial \Omega} d^m x \frac{\partial^i}{\partial x^i} \frac{\partial^j}{\partial x^j} t = -\int_{\partial \Omega} d^m x \cdot w
\]

(5)

where \( d^m x \) is the oriented surface element on \( \partial \Omega \). Note that there is no boundary condition imposed on \( w \) and that consequently \( w \) is not uniquely specified.

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

\[
t(x) = T f(x), \quad f(x) = 0 \quad \text{for} \quad x \notin \Omega
\]

(6)

for \( x \in \Omega \setminus \Delta \Omega \)

Since \( T \) is exponentially large in \( \epsilon^{-1} \) [11] and since clearly \( \Delta \Omega \) shrinks to \( \partial \Omega \) for \( \epsilon \to 0 \) (a quantitative estimate will be given below) the inhomogeneity in the equation for \( f(x) \) following from eq. (3) becomes negligible on the boundary layer \( \Delta \Omega \):

\[
\frac{\epsilon}{2} \frac{\partial^2}{\partial x^2} f(x) + \frac{1}{2} \frac{\partial}{\partial x} (x) \frac{\partial}{\partial j} (x) f(x) = 0 \quad \text{for} \quad x \in \Delta \Omega
\]

(7)

With eq. (5) \( T \) may be expressed in terms of \( \omega \) and of the gradient of \( f \) on \( \partial \Omega \):

\[
T = -\int_{\partial \Omega} d^m x / \frac{\epsilon}{2} \int_{\partial \Omega} d^m x \frac{\partial}{\partial j} (x) (x)
\]

(8)

To solve eq. (7) we make for \( f(x) \) the ansatz

\[
f(x) = \sqrt{\frac{\epsilon}{\pi \epsilon}} \int_0^\infty dz \exp \left(-\frac{z^2}{2\epsilon}\right).
\]

(9)

The function \( \rho(x) \) introduced thereby satisfies

\[
K^i(x) \frac{\partial}{\partial x} + \frac{1}{2} \epsilon \frac{\partial}{\partial x} (x) \frac{\partial}{\partial j} (x) \rho(x) = 0
\]

(10)

as follows from (7) in leading order of \( \epsilon \to 0 \). Since on \( \partial \Omega \) the normal component of the drift field \( x \) vanishes, eq. (10) admits a \( \rho(x) \) vanishing on \( \partial \Omega \). Next we suppose that in a coordinate system in the boundary with one axis \( (r) \) along \( d^m s \) on \( \partial \Omega \) \( (r=0) \) on \( \partial \Omega \) and \( r > 0 \) in \( \Omega \) and with all other axes lying in \( \partial \Omega \), the \( r \)-component of the drift vanishes linearly in \( r \)

\[
x^r = g \quad r \quad g > 0
\]

(11)

which represents the typical behaviour of a force field near a separatrix. Then near \( \partial \Omega \) the function \( \rho(x) \) is given by

\[
\rho = ar
\]

(12)

where \( a \) is a function on \( \partial \Omega \) which obeys the equation

\[
ga + \frac{K^a(x)}{a} = \frac{1}{2} B_{rr} a^2 = 0
\]

(13)

with \( a = 1, \ldots, n-1 \) denoting coordinates on \( \partial \Omega \). Note that at the stationary points on the separatrix \( a \) is simply given by

\[
a = \sqrt{2g/B_{rr}}.
\]

(14)

The characteristic system of the partial differential equation (13) consists of the deterministic system (1) restricted to the separatrix and the equation

\[
a + \frac{K^a(x)}{a} = \frac{1}{2} B_{rr} a^2 = 0
\]

(15)

Since the gradient of \( f \) on \( \partial \Omega \) is proportional to \( a \), the constant part \( T \) of the absorption time becomes

\[
T = \sqrt{\frac{2\pi}{\epsilon}} \int_{\partial \Omega} d^m x / \int_{\partial \Omega} d^m x \frac{\partial}{\partial j} (x) (x)
\]

(16)

It is thus expressed in terms of the solution \( \omega \) of the stationary Fokker-Planck equation, the boundary \( \partial \Omega \), and the function \( f \) essentially determined by the deterministic dynamics on \( \partial \Omega \). We recall that \( w \) need not fulfill any boundary conditions. Our next aim will be to utilize this for the further evaluation of eq. (16).
3. WB EXPANSION OF THE STATIONARY FOKKER PLANCK EQUATION

For $\varepsilon \to 0$ the solution of the stationary Fokker Planck equation with natural boundary conditions will tend to $\phi$-functions concentrated at the attractors of the deterministic motion. If next a point attractor, the deterministic motion can be linearized this solution will locally become a Gaussian with variance proportional to $V_{\varepsilon}$. We assume that this $\varepsilon$ dependence is still obeyed for nonlinear systems in leading order

$$\dot{\phi}(z) = \left( x, \varepsilon \right) e^{-\gamma z} \tag{17}$$

where $\phi(z)$ is independent of $\varepsilon$ and $z(x,\varepsilon)$ can be expanded in a power series in $\varepsilon$, from which in the following only the lowest order term will be kept. For a process obeying detailed balance this is exact. Note the analogy to the WKB expansion in quantum mechanics: The Schrödinger and the Fokker-Planck equations are both second order differential equations, which in the classical and deterministic limit, respectively, have vanishing coefficients of the second order differential operators. Moreover (17) is the precise analogue of the WKB wave function.

From eq. (4) we find that in leading order in $\varepsilon$ $\phi(z)$ and $z(x,\varepsilon)$ obey first order differential equations [12]

$$\dot{x} = \phi_z \tag{18}$$

$$\dot{z} = (\phi_z, z) + \left( \phi_{zz} + \phi_{zz} \right) \dot{z}$$

Since $\phi_z$ is a nonnegative matrix from (18) it follows that $\phi$ decreases along the trajectories of the deterministic dynamics (1) [13]

$$\frac{d\phi}{d\varepsilon} - \frac{1}{2} D_{ij} \phi_{ij} < 0 \tag{20}$$

Therefore $\phi$ is a Lyapunov function of the deterministic motion. This shows that for $\varepsilon \to 0$ the ansatz converges to $\phi$-functions at the deterministic attractors as desired.

Near a point attractor, at which the drift is supposed to vanish linearly, as $K_k z = b_k^i z^i$,

$$\phi \text{ varies quadratically }$$

$$\phi(x) = \phi_0 + \frac{1}{2} \phi_{ij} x^i x^j \tag{22}$$

It follows from (1) that the matrix $\phi_{ij}$ of the second derivatives is determined by

$$D_{ij} - \phi_{ij} + b_k^j e_k^i + b_k^i e_k^j = 0 \tag{23}$$

where $D_{ij}$ is taken at the attractor. The inverse of the matrix $\phi_{ij}$, obeys a linear inhomogeneous equation which may be solved by standard methods. In the same way the curvature of $\phi$ may be determined at a hyperbolic point of the drift field $K$ which corresponds to a saddle-point of $\phi$ because of the Lyapunov property (20). For a limit cycle a similar method applies for the calculation of the matrix $\phi_{ij}$ of second derivatives transvers to the limit cycle [14]. This matrix determines $\phi$ in a linear neighbourhood of the limit cycle. To calculate $\phi$ it is most convenient to interpret $\phi$ as the action of a reversible system with the Hamiltonian

$$H = \frac{1}{2} D_{ij} p_i p_j + K_k p_k \tag{24}$$

in a 2$n$-dimensional phase space. Clearly, with

$$P_1 = \frac{1}{2} p_i \phi_{ij} \tag{25}$$

eq.(16) is recovered as the Hamilton Jacobi equation of a system with the Hamiltonian (24) moving on the "energy"-hypersurface $H = 0$. Consequently, the characteristic system of eq.(18) is given by the canonical equations of the Hamiltonian (24):

$$x^i = -\frac{\partial H}{\partial y_i} \tag{26}$$

$$P_1 = -\frac{\partial H}{\partial x_1} = -\left( b_k^i \delta_k^j \right) P_{kj} P_j - \left( b_k^i \right) \tag{27}$$

Note that the action $\phi$ grows on a solution of the canonical equations:

$$\frac{d\phi}{dt} = \frac{1}{2} \frac{d^2\phi}{dt^2} \tag{28}$$

Together with the Lyapunov property (20) of $\phi$ it follows that the solutions with $H = 0$ go away from the attractors of the drift field $K$. Since $H$ is invariant under the "time"-reversal symmetry

$$P_1 \rightarrow -P_1, \quad K_1 \rightarrow -K_1 \tag{29}$$

the solutions of the "time"-reversed eqs. (26, 27) go away from unstable points and finally approach an attractor of $K$. In this way one can easily find trajectories connecting e.g. hyperbolic points with attractors. For the difference of the action it follows

$$\Delta \phi = \frac{1}{2} dt \left( x^i \phi_{ij} \right) \tag{30}$$

Some comments are in order. Since both the drift field $K$ and the momentum $p$ vanish at a hyperbolic point one has to start the trajectory in the linear neighbourhood. Assuming that $\phi$ is of the form (12) eq. (25) yields the initial momentum. Since it needs an infinitesimal amount of "time" to reach the attractor, one must termi-
nate the trajectory at a point in the linear neighbourhood of the attractor. If \( \phi \) is such that of the form (22) one can correct the error made in the action. However, the assumptions about the action near the stationary points of the drift field \( \mathbb{K} \) need not be consistent with each other. In order to check the consistency one has to compare the moments following from the trajectory with those derived analytically from \( \phi \) in the linear neighbourhood of the attractor.

Next we discuss eq. (19) for the prefactor \( z(t) \). On a trajectory of the Hamiltonian system (26, 27) eq. (19) reduces to

\[
\dot{z}(\omega^2_1 P_{ij}^{12} - \omega^2_2 P_{ij}^{21}) + \frac{1}{2} \mu_{ij}(\omega^2_1, \omega^2_2) z = 0
\]

where \( \omega^2_1 \) and \( \omega^2_2 \) are known functions of \( t \). Since the second derivative of \( \phi \) can too be determined from the eqs. (26, 27) linearized about the considered trajectory as functions of \( t, z \) obeys an ordinary differential equation.

Finally we will apply the WKB expansion to the evaluation of the mean absorption time \( T \) given by eq. (16). First we notice that for the volume integral only the absolute minimum of \( \phi \) in \( \mathbb{A} \) prevails which due to the Lyapunov property (20) is taken on the attractor. For a point attractor \( \phi \) is typically given by eq. (22), and since at the attractor the prefactor \( z(\phi) \) is a slowly varying function compared with \( \exp(-\phi/\kappa) \) it can be put constant and only a Gaussian integral has to be performed. For attractors, limit cycles, and higher dimensional invariant tori again typically a quadratic approximation of \( \phi \) transfers to the attractor will be sufficient.

For the surface integral only the absolute minimum of \( \phi \) on \( \mathbb{A} \) prevails, which due to the Lyapunov property (20) are taken at the attractors of the drift field \( \mathbb{K} \) restricted to the separatrices.

Hence, isolated minima are taken at the hyperbolic points of \( \mathbb{K} \) and, thus, easy to find. At these points the separatrices can be replaced by its tangential plane and the function \( a \) is given by eq. (14). Since again the nonexponential part of the integrand varies slowly compared with \( \exp(-\phi/\kappa) \) it can be put constant, and assuming that \( \phi \) is quadratic there a Gaussian integral remains. In this case the difference of the action at the saddle point and the attractor can be determined by eq. (30) using a "time"-reversed path.

If the lowest minimum of \( \phi \) on \( \mathbb{A} \) is assumed at a limit cycle, the eq. (13) determining the function \( a \) reduces to an ordinary first order differential equation which can easily be integrated. Moreover \( \phi \) is a quadratic form in local coordinates over the limit cycle the mean time \( T \) can be calculated in the same way as discussed for the hyperbolic point.

For a \( d \)-dimensional attractor and a \( d \)-dimension-