LIFETIME OF A METASTABLE STATE AT LOW NOISE

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The mean time for the trajectory of a randomly perturbed system to leave a domain of attraction is determined in the limit of weak noise. The method applies for the decay of metastable states and it generalizes results of nucleation theory.

The rate of decay of a metastable state is a key element in the analysis of various physical phenomena, such as the dynamics of first-order phase transitions, of chemical reactions and of multistable systems in optics, electronics etc. The state of these systems is supposed to be determined by macrovariables, governed by a Fokker–Planck equation. In order that metastability shows up we assume that the noise is weak, and we focus on the leading terms when the noise intensity (ϵ) goes to zero. In this limit decay rates were evaluated by Kramers [1] and for higher-dimensional systems by Landauer et al. and Langer [2]. Their approach, based on a current-carrying solution of the stationary Fokker–Planck equation, has been used e.g. in nucleation theory. However, its applicability seems to be restricted to systems with detailed balance and with essentially one single transition state (saddle point). These restrictions can be dropped in the framework of another approach, the idea of which consists of surrounding the domain of attraction of the metastable state by an absorbing boundary and to consider the mean time until "absorption" occurs. The resulting equation for the mean first passage time is exact for any noise strength ϵ. In one dimension it can be solved analytically [3], and in the multidimensional case with a gradient drift field and with unit diffusion it was solved in the limit $\epsilon \to 0$ by Matkovsky and Schuss [4]. Steps towards the discussion of more general equations were made by Schuss [5].

For the general case we establish a formula for the leading term of the mean first passage time, involving a solution of the stationary Fokker–Planck equation on the domain of attraction of the metastable state.

We assume that an autonomous dynamical system in phase space Γ

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

has a connected attractor with a domain of attraction $\Omega \subset \Gamma$. The boundary $\partial\Omega$ is supposed to be smooth. If the system (1) is pertrubed by white noise the duration of stay within Ω is generally finite, even if the noise is arbitrarily weak.

The perturbed motion is described by the Fokker–Planck operator L

$$L = -\partial_i K^i(x) + \tfrac{1}{2}\epsilon \partial_i \partial_j D^{ij}(x) , \tag{2a}$$

with the adjoint

$$L^+ = K^i(x)\partial_i + \tfrac{1}{2}\epsilon D^{ij}(x)\partial_i\partial_j . \tag{2b}$$

The mean exit time $t(x)$ from the starting point $x \in \Omega$ is given by [3]

$$L^+ t = -1 , \quad \text{with } t = 0 \text{ on } \partial\Omega . \tag{3}$$

By integrating eq. (3) with a function $w(x)$ that satisfies

$$Lw = 0 , \tag{4}$$

one obtains

$$\frac{\epsilon}{2} \int_{\partial\Omega} \mathrm{d}S_i w D^{ij} \partial_j t = -\int_{\Omega} \mathrm{d}^n x \, w . \tag{5}$$

For small diffusion ($\epsilon \to 0$) a trajectory starting within

Ω will typically first approach the attractor and stay within its neighbourhood for a long time (compared with time constants of the deterministic motion), until it is carried back to the boundary by the noise. Therefore $t(x)$ assumes the same (large) value T everywhere in Ω, except for a thin layer $\Delta\Omega$ along the boundary, where the small diffusion is still sufficient to cause a direct exit. Accordingly

$$t(x) = Tf(x) \quad \text{with } f(x) \approx 1 \text{ for } x \in \Omega - \Delta\Omega \tag{6}$$

and

$$T = -\int_{\Omega} \mathrm{d}^n x\, w \Bigg/ \frac{\epsilon}{2} \int_{\partial\Omega} \mathrm{d}S_i\, w D^{ij} \partial_j f . \tag{7}$$

Since $T = \mathrm{O}(\exp \epsilon^{-1})$ [6], and since $\Delta\Omega$ shrinks to $\partial\Omega$ for $\epsilon \to 0$ which will be confirmed below, eq. (3) becomes

$$L^+ f \approx 0 \quad \text{in } \Delta\Omega , \quad \text{with } f = 0 \text{ on } \partial\Omega \quad \text{and } f \approx 1 \text{ on the inner boundary of } \Delta\Omega . \tag{8}$$

At $\partial\Omega$ the normal component of the drift field vanishes. If it decays with power α ($\alpha > 0$, typically $\alpha = 1$), an ansatz satisfying eq. (8) in $\Delta\Omega$ is

$$f(x) = N \int_0^{\rho(x)} \mathrm{d}z\, \exp[-z^{\alpha+1}/(\alpha+1)\epsilon] , \tag{9a}$$

with

$$N^{-1} = \epsilon^{1/(\alpha+1)} (\alpha+1)^{-\alpha/(\alpha+1)} \Gamma[1/(\alpha+1)] , \tag{9b}$$

where in the limit $\epsilon \to 0$ $\rho(x)$ is determined by

$$K^i \partial_i \rho - \tfrac{1}{2} D^{ij} (\partial_i \rho)(\partial_j \rho) \rho^\alpha = 0 . \tag{10}$$

Bearing in mind that on $\partial\Omega$ the normal component of the drift vanishes, one can show that there always exists a solution of eq. (10) vanishing everywhere on $\partial\Omega$ and increasing towards the attractor. In eq. (7) only the gradient of that solution on $\partial\Omega$ is required, since

$$\partial_i f = N \partial_i \rho \quad \text{on } \partial\Omega . \tag{11}$$

Note, that the width of $\Delta\Omega$ is thus proportional to $\epsilon^{1/(\alpha+1)}$, as eq. (10) for ρ does not involve ϵ. In a coordinate system in the boundary layer $\Delta\Omega$ with one axis (r) along $\nabla\rho$ and with all other axes lying in $\partial\Omega$ [‡1], the normal component of the drift is by assumption

$$K^r = g r^\alpha \quad (g \text{ constant with respect to } r) , \tag{12}$$

and the gradient of ρ is obtained from eq. (10) as

$$\partial_r \rho = (2g/D^{rr})^{1/(\alpha+1)} \quad \text{on } \partial\Omega . \tag{13}$$

Inserting eqs. (13), (11) and (9b) into eq. (7) gives

$$T = (2/\epsilon(\alpha+1))^{\alpha/(\alpha+1)}\, \Gamma(1/(\alpha+1)) \times \left(-\int_{\Omega} \mathrm{d}^n x\, w \Bigg/ \int_{\partial\Omega} \mathrm{d}S_r\, w\, (D^{rr})^{\alpha/(\alpha+1)} g^{1/(\alpha+1)} \right) . \tag{14}$$

Clearly, for an integer α

$$g = (\alpha!)^{-1} (\partial_r)^\alpha K^r . \tag{15}$$

The mean first passage time is thus expressed in terms of the function w and of the boundary $\partial\Omega$. The transition states may form an arbitrary subset of $\partial\Omega$, and no assumptions have been made about the nature of the attractor. Once the boundary, which is supposed to be smooth, is known, D^{rr}, as well as g, are readily evaluated. For the function w one may choose any solution of the stationary Fokker–Planck equation. The irrelevance of boundary conditions for the mean first passage time will be proved elsewhere. A solution is trivially found when L admits detailed balance [7]. Then w takes the form

$$w(x, \epsilon) = N(\epsilon) z(x) \exp[-\phi(x)/\epsilon] , \tag{16}$$

for all $\epsilon > 0$, with ϕ and z independent of ϵ.

In fact only the leading term of w for $\epsilon \to 0$ is required, and, whether or not detailed balance holds, the expression (16) leads to an asymptotic expansion, analogous to the WKB or eikonal approximation [8,9]. The fact that this ansatz selects a subset of the possible solutions is immaterial in view of the above remark concerning boundary conditions, and even convenient since ϕ is a Lyapunov function for the system (1) [9]. For the boundary integral in eq. (14) only the absolute minimum of ϕ on $\partial\Omega$ prevails. If it is assumed at isolated points, the saddle point method applies. Due to the

[‡1] We require that the transformation to the new coordinates has an inverse in $\Delta\Omega$ including $\partial\Omega$. Then the exponent α in eq. (12) as well as the expression (14) for T are invariant.

Lyapunov property of ϕ these points are hyperbolic points of eq. (1) and, thus, easy to find. For the volume integral in eq. (14) only the absolute minimum of ϕ in Ω prevails, which, again due to the Lyapunov property, is taken on the attractor. Clearly, the Arrhenius law now follows from eqs. (14) and (16). It is easily verified that for $\alpha = 1$ the results of refs. [1,2,4] are recovered. A possible noise-induced drift [10] proportional to ϵ can be included in eqs. (2): it merely modifies the function w, more specifically, the function z in eq. (16).

As a concluding remark we note that the form (16) is general enough to admit limit cycles [11]. Whether it also applies for strange attractors is an interesting open question.

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