The Kramers Problem: Beyond Quasi-Stationarity

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Abstract. Noise-induced escape from a metastable potential is considered on time-scales preceding the formation of quasi-equilibrium within the metastable part of the potential. It is shown that the escape flux may then depend exponentially strongly, and in a complicated manner, on time and friction.

INTRODUCTION

In his seminal work [1], Kramers considered the noise-induced flux from a single metastable potential well i.e. he considered a stochastic system

$$\ddot{q} + \Gamma \dot{q} + dU/dq = f(t),$$
$$\langle f(t) \rangle = 0, \quad \langle f(t)f(t') \rangle = 2\Gamma T \delta(t - t'),$$

(1)

which was put initially into the bottom of a metastable potential well $U(q)$ and then he calculated the quasi-stationary probability flux beyond the barrier. There have been many developments and generalizations of the Kramers problem (see [2,3] for reviews) but both he and most of those who followed him considered just the *quasi-stationary* flux, i.e. the flux established after the formation of a quasi-stationary distribution within the well (up to the barrier). The quasi-stationary flux is characterized by a slow exponential decay, an Arrhenius dependence on temperature T, and a relatively weak dependence on friction Γ:

$$J_{qs}(t) = \alpha_{\text{escape}} e^{-\alpha_{\text{escape}}t}, \qquad \alpha_{\text{escape}} = Pe^{-\frac{\Delta U}{T}},$$

(2)

where P depends on Γ and T in a non-activation manner.

But how does the flux evolve from its zero value at the initial moment to its quasi-stationary value at time-scales exceeding the time t_f for the formation of

quasi-equilibrium? It is obvious that the answer may depend on initial conditions. The most natural are those corresponding to the stable stationary state of the noise-free system i.e. $(q = q_{\text{bottom}}, \dot{q} = 0)$ where q_{bottom} is the coordinate of the bottom of the potential well. Just such an initial state is assumed in this paper[1]. If the noise is switched on suddenly (e.g. if the thermal isolation of a frozen system is broken) then the time evolution of the escape flux from the noise-free metastable initial state is highly relevant. It might seem natural that the evolution from zero to the quasi-stationary value should be *smooth*. Such an assumption might also seem to have been confirmed recently by Schneidman [4] who found that, for both the strongly underdamped and overdamped cases, the escape flux from a single metastable well grows with time t smoothly, at $t \sim t_f$. But does this exhaust the problem? We prove theoretically, and demonstrate experimentally, that there are two generic situations when the escape flux[2] behaves in a different manner.

The theoretical approach which we use for this is the method of *optimal fluctuation* (c.f. e.g. [5]) within which an escape rate is sought in the form

$$\alpha_{\text{escape}} = P e^{-\frac{S}{T}} \tag{3}$$

where the action S does not depend on T; the prefactor P does depend on T, but relatively weakly. The action S is related to a certain optimal fluctuation which, in turn, corresponds to the *most probable escape path* (MPEP).

Theoretical results are verified by computer and electronic simulations.

SHORT TIME-SCALES

The quasi-stationary flux is formed by optimal fluctuations which bring the system from the bottom of the (initial) well to a relevant saddle for an *optimal time*

$$t_{\text{opt}} \sim \frac{1}{\min(\Gamma, \omega_0)} \ln(\frac{\Delta U}{T}), \tag{4}$$

where ω_0 is the frequency of eigenoscillation in the bottom of the well.

At much shorter time-scales,

$$t \ll t_{\text{opt}}, \tag{5}$$

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[1] Note that, for the relatively large time-scales considered below in the section for the multi-well case (c.f. Fig. 2), such a restriction is not essential: the results remain valid for any initial distribution within one well. The case of arbitrary initial conditions, for the smaller time-scales as considered in the next section (c.f. Fig. 1), will be explored elsewhere.

[2] Our major results are not sensitive to the concrete definition of the flux. It could e.g. be the full flux through a boundary or just a first passage flux; the boundary may e.g. be a given coordinate (as in [1,3]), or a boundary of a basin of attraction (relevant to an escape rate), or the boundary of a close vicinity to another attractor (relevant to inter-well transition rates).
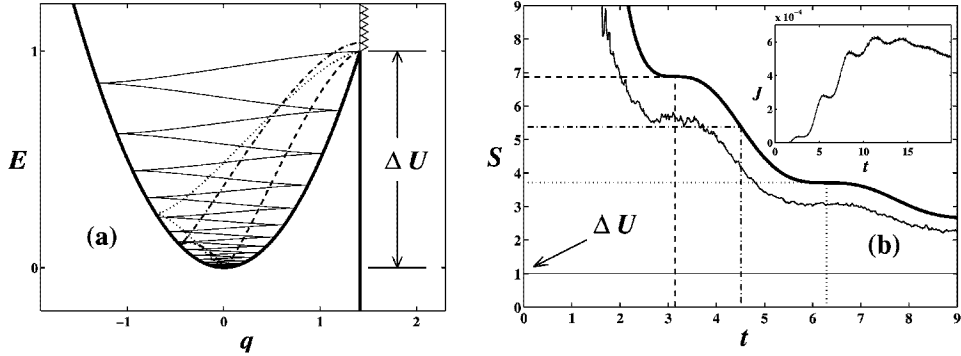
FIGURE 1. (a) Examples of MPEPs (plotted in the energy-coordinate plane $E - q$ where $E = \dot{q}^2/2 + U(q)$) for an escape from the bottom of the metastable well $U(q) = q^2/2$ at $q < \sqrt{2}$ (thick solid line) to beyond the barrier at $q = \sqrt{2}$ ($U(q) = -\infty$ at $q > \sqrt{2}$, which is equivalent to the absorbing wall indicated by triangles), at $\Gamma = 0.05$; (b) the corresponding theoretical (thick solid line) and experimental (thin jagged line) dependences of the action S on the escape time t. The dashed and dotted lines indicate: in (b) the 1st and 2nd inflection point with $dS/dt = 0$; and in (a) the corresponding MPEPs. The thin solid line shows: in (b) the large-time asymptote level equal to the barrier height ΔU; and in (a) the corresponding MPEP (which is the time-reversal of the noise-free trajectory from the top of the barrier into the bottom of the well). The dash-dotted line shows in (a) the MPEP corresponding to some arbitrarily chosen time $t = 4.51$ (see (b)) and demonstrates, in particular, that the escape velocity is generally non-zero. The inset shows the experimental dependence of the flux on time, for $T = 1.0$.

the flux is necessarily formed by optimal fluctuations strongly differing from those of duration $t_{\rm opt}$, and the smaller t the more marked this difference becomes. Thus, in the range (5), S is dependant on t. Moreover, we can show rigorously that if $\Gamma < \Gamma_c$ where Γ_c is typically equal to $2\omega_0$ then $S(t)$ is a *step-wise* function: see the example[3] in Fig. 1. The vertical and horizontal positions of the center of the step $S(t)$ number n (counted from the left) equal respectively $\Delta U \omega_0/(n\pi\Gamma)$ and $n\pi/\omega_0$, provided $n\pi\Gamma \ll \omega_0$. Generally, when the shape of the potential well departs from parabolicity, the equalities turn into approximations. Thus, in the range (5), J depends exponentially strongly both on Γ and on t (c.f. the inset).

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[3] Although we present just one example (chosen for its simplicity), we emphasize that a step-wise dependence of $S(t)$ is typical for *any* potential, including those which possess a saddle or several wells, and that it remains valid for any reasonable boundary (c.f. footnote 2). We have developed a rigorous (and simple) procedure for obtaining a numerical solution provided the metastable part of the potential is a single well and the absorbing boundary is not too close to a saddle. A qualitative analysis shows that if the boundary is close enough to a saddle (or just includes it) then $S(t)$ possesses *folds* at certain critical values of t corresponding to switching between MPEPs of different topologies.
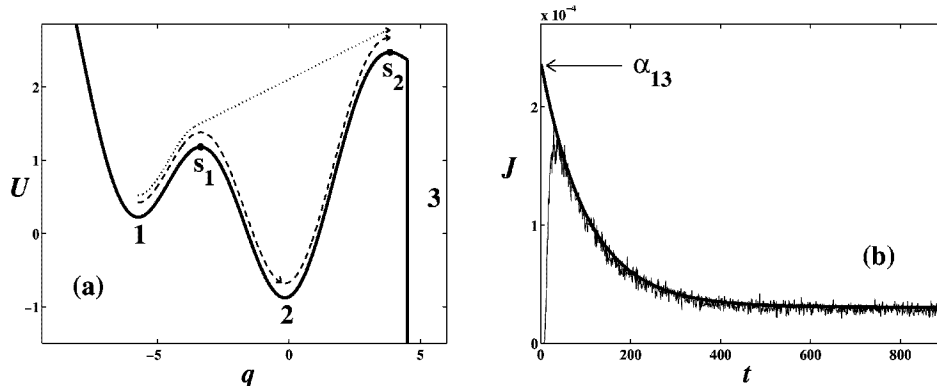
FIGURE 2. (a) a double-well metastable potential $U(q) = \begin{cases} 0.06(q+1.5)^2 - \cos(q) & \text{at} \quad q < q_l = 4.5, \\ -\infty & \text{at} \quad q > q_l, \end{cases}$ and schematically shown direct (dotted line) and indirect (dashed line) transitions $1 \to 3$ i.e. escapes from the well 1 beyond the coordinate q_l; (b) simulations of the escape flux $J(t)$ $1 \to q_l$ (thin jagged line) at $\Gamma = 0.15$, $T = 0.4$, compared with the approximation of $J(t)$ by Eq. (6) (thick full line); α_{12}, α_{21} and α_{qs} are calculated by the Kramers-Melnikov formula [3] while α_{13}, α_{23} are calculated by Eq. (7) with $m \approx 1.1$.

MULTI-WELL METASTABLE POTENTIAL

Unlike the single-well case, where the formation time of quasi-equilibrium is of the order of t_{opt} (4), its formation in the multi-well case (e.g. as in Fig. 2) proceeds via two distinct stages: first, quasi-equilibrium is formed within the initial well which as in the single-well case, takes $\sim t_{\text{opt}}$; secondly, quasi-equilibrium between wells becomes established which takes exponentially longer ($\sim t_{\text{opt}} \exp(\Delta U/T) \gg t_{\text{opt}}$ where ΔU means a minimal internal barrier). During the latter stage (as well as during the subsequent quasi-stationary stage), the flux $J(t)$ can be described via a solution of kinetic equations for the well populations, using the concept of constant inter-attractor[4] transition rates α_{ij} (c.f. [6]):

$$J(t) = \alpha_{13} e^{-\frac{t}{t_s}} + \alpha_{qs}\left(e^{-\frac{t}{t_{qs}}} - e^{-\frac{t}{t_s}}\right), \tag{6}$$

$$t_s \approx \alpha_{12}^{-1}, \qquad t_{qs} \approx \alpha_{qs}^{-1} \approx \alpha_{12}/(\alpha_{12}\alpha_{23} + \alpha_{21}\alpha_{13}),$$

$$T \ll U_{S_1} - U_1, \qquad t \gg t_{\text{opt}}.$$

The physical meaning of the two terms in (6) is easily understood (c.f. Fig. 2(b)). The first one corresponds to *direct* escapes (i.e. those ones which do not go via the bottom of well-2) and dominates before the quasi-equilibrium is established; whereas the second term, corresponding to indirect escapes, dominates in the ensuing quasi-stationary stage: it is the asymptotic part of this latter flux, $\alpha_{qs} \exp(-t/t_{qs})$, that is called the quasi-stationary flux.

Although the coefficients $\alpha_{12}, \alpha_{21}, \alpha_{qs}$ can readily be obtained from the Kramers-Melnikov theory [3], α_{13} and α_{23} cannot be found [3] in this way. One of us [7] has developed a theory of α_{13}, α_{23} based on the concept of optimal fluctuation:

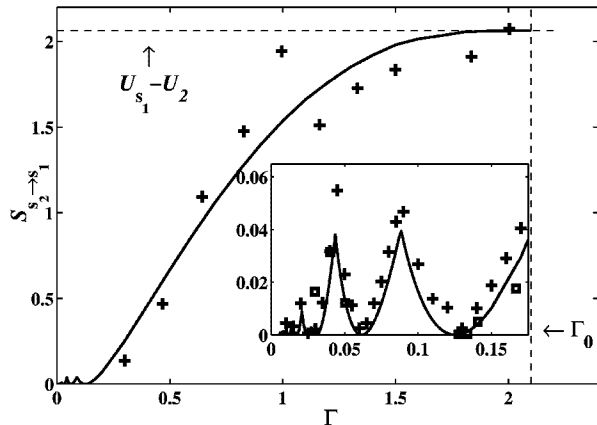[4] For the sake of brevity, we refer to region 3 as an "attractor" too.

FIGURE 3. Dependence of the action for the transition $s_2 \to s_1$ on the damping constant Γ, at time-scales $t \gg t_{\mathrm{opt}}$, in the system (1) with $U(q)$ shown in Fig. 2(a). The solid line is calculated numerically from the theory [7]. The horizontal and vertical dashed lines indicate respectively the upper limit for $S_{s_2 \to s_1}$ and the value of Γ at which the cutoff of direct transitions $s_2 \to s_1$ and escapes $1 \to s_2$ occurs. The crosses and squares represent digital and analogue simulation data respectively. The inset shows an expanded plot of the region of small damping.

$$\alpha_{13,23} = \alpha_{qs}(1 + (\Omega_1 \Omega_2^{-1} \exp((U_1 - U_2)/T))^{\pm 1})/(1 + (m \exp(k S_{s_2 \to s_1}/T))^{\pm 1}), \quad (7)$$

where: Ω_1, Ω_2 are the frequencies of eigenoscillation in the bottom of wells 1, 2; $k = 1$ or -1 for ranges of Γ providing the noise-free relaxation from s_2 respectively into 2 or 1; the action $S_{s_2 \to s_1}$ for the transition $s_2 \to s_1$ is calculated from the theory [7]; and m is the only adjustable parameter, related to the prefactor.

As seen from Eq. (7) and Fig. 3, the rates α_{13} and α_{23} depend on friction exponentially strongly, at sufficiently small temperatures. Moreover, they oscillate[5] in the underdamped range, and α_{13} has a cutoff at a certain friction $\Gamma_0 \geq 2\Omega_2$ i.e. $\alpha_{13} = 0$ for $\Gamma \geq \Gamma_0$. The oscillations are related to an alternation between ranges of friction in which a noise-free trajectory from the external saddle s_2 goes into either well-1 or well-2: in accordance with the principle of detailed balance, the noise-induced escape $1 \to s_2$ is the time-reversal of $s_2 \to 1$, so that its probability is characterized by the Arrhenius factor if a noise-free trajectory $s_2 \xrightarrow{nf} 1$ exists; otherwise the probability is exponentially smaller. The cutoff at large Γ is related to the absence of turning points in the noise-free trajectories $s_1 \xrightarrow{nf} 2$, $s_2 \xrightarrow{nf} 2$.

CONCLUSIONS AND OPEN PROBLEMS

We conclude that: (i) escape from a metastable potential differs markedly after and before the formation of quasi-equilibrium within the metastable part of the

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[5] Typically, the scale of oscillation of S is small in comparison with $U_{s_2} - U_1$ (corresponding to the Arrhenius dependence on T) but, in some cases, it can equal or even exceed $U_{s_2} - U_1$ [7].

potential; (ii) at time-scales much less than the optimal duration of a fluctuation t_{opt}, the escape flux J grows exponentially strongly with time and, moreover, if the friction Γ is small, it does so in a *step-wise* manner and depends exponentially strongly on Γ; and (iii) if the metastable part of the potential consists of more than one well, then the formation of quasi-equilibrium takes an exponentially long period of time and the escape flux during the most of this period is formed from direct escapes and depends exponentially strongly on friction and, moreover, $J(\Gamma)$ undergoes oscillations in the underdamped range and may drop drastically if Γ exceeds a critical value $\Gamma_0 \geq 2\Omega_2$.

Open problems yet to be addressed include: (i) for the range $t \ll t_{\mathrm{opt}}$: (a) the transition from a smooth $S(t)$ (with inflection points only) to an $S(t)$ possessing folds, (b) additional features characteristic of the multi-well case, (c) the pre-exponential factor; (ii) the pre-exponential factor for inter-attractor transition rates in the multi-well case; and (iii) a generalization for non-potential systems for which, unlike potential systems where a switching between different MPEPs gives rise only to folds in $S(t)$, we anticipate the possibility of jumps in $S(t)$.

ACKNOWLEDGEMENTS

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