Journal of Statistical Physics, Vol. 123, No. 4, May 2006 (© 2006)
DOI: 10.1007/s10955-006-9082-2

Last Passage Time Statistics for Barrier-Crossing Processes

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Received September 28, 2005; accepted January 25, 2006
Published Online: May 19, 2006

A concept of mean last passage time at the saddle point is proposed in order to compute both the lifetime and the escape rate of a particle in a metastable potential, where the backstreaming across the saddle point is taken into account. It is shown that the mean oscillating time around the saddle point is the longest one among all the time scales at high temperatures and the inverse of the mean last passage time at the saddle point is more close to the steady escape rate.

KEY WORDS: Mean last passage time, saddle oscillation, backstreaming, escape rate.

1. INTRODUCTION

How long does it take a randomly varying quantity to reach a given position firstly? How large is the rate for escaping the saddle point of a metastable well? The two questions are universal in the studies of unstable systems.(1,2) Usually, the steady escape rate of a particle in a metastable potential is approximated by the inverse of mean first passage time (MFPT) at an exit point.(3) The latter can be analytically derived without the steepest descent approximation in the overdamped case, only an absorbent boundary (exit point) is required to choose sufficiently far beyond the saddle point. The rate process is a phenomenon that takes place on a long time scale when compared to all the dynamic time scales characterizing the local stability.(2) It is both of principle and practical interest to know at which time scale the influence of noise becomes important, and also to clear what time scale is the longest one when the intensity of noise varies. For the existence of structures either in the power spectrum of noise(4,5) or in the

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potential,[6,7] the MFPT at the saddle point may consequently be less by several orders of magnitude than the reciprocal escape probability, for instance, a colored noise-driven particle can pass the saddle point of bistable potential several times, back and forth. This implies that the MFPT is not enough to investigate the surviving behavior of some complex unstable systems.[8,9] Thus a new time scale needs to be introduced, which is the mean last passage time (MLPT) at the saddle point. It describes the mean time required of a particle completely leaving the saddle point, if the particle starts from the metastable potential minimum. This is indeed the occupying life of the particle within the well. The difference between the MLPT and the MFPT is actually the mean oscillating time of the particle passing over the saddle point multi times. Furthermore, if the initial position of the particle is outside of the saddle point, the particle driven by fluctuation can enter the well of metastable potential. This is called noise-enhanced stability.[10] The oscillating time around the saddle point can be also applied to study such phenomenon.

We would like to point out that the difference between the escape rate defined at the saddle point by using test particles passing over the saddle point first time (i.e., the saddle point is chosen to be an absorbent boundary) and that defined at an exit point is regarded as a saddle-point *backstreaming*. If we take into account this quantity in the studies of escape dynamics, namely, test particles multiply pass over the saddle point back and forth as proposed in the present work, the steady escape rate can always be determined at the saddle point. The *backstreaming* should be used as a probe for investigating the characteristic behavior of unstable systems at the saddle point. Moreover, a potential application of the MLPT is help one to sort out some of problems with channel diffusion between constant concentration reservoirs in biological channels.[11,12]

In this paper, we propose a concept for the mean last passage time at the saddle point in order to investigate both the lifetime and the escape rate of a metastable system. The dependence of distributions of first passage time and last passage time on the initial condition is discussed. Time-dependent escape rate is numerically calculated at the saddle point rather than other exit points.

2. LAST PASSAGE TIME DISTRIBUTION

The equation for overdamped motion of a particle is written as

$$\gamma \dot{q}(t) = -\frac{\partial V(q)}{\partial q} + \sqrt{2\gamma T}\xi(t) \tag{1}$$

with $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\xi(t') \rangle = \delta(t - t')$, where γ is the friction coefficient, $V(q)$ is the potential, and T is the temperature.

Let us distinguish several time scales appearing in the MFPT at an exit point q_{ex} starting from the potential minimum q_0, i.e.,

$$\begin{aligned}\tau_{\text{MFPT}}(q_0 \to q_{\text{ex}}) &= \tau_{\text{MFPT}}(q_0 \to q_b) + \Delta\tau_b + \tau^*_{b\to\text{ex}} \\ &= \tau_{\text{MLPT}}(q_0 \to q_b) + \tau^*_{b\to\text{ex}} \end{aligned} \tag{2}$$

where $\tau_{\text{MLPT}}(q_0 \to q_b)$ is the mean last passage time at the saddle point q_b, $\tau^*_{b\to\text{ex}}$ denotes the mean saddle-to-exit descent time after the particle passes over the saddle point at the last time, and $\Delta\tau_b$ is called the mean oscillating time around the saddle point. The latter is the difference between the mean leaving time and mean arriving time of the particle at the saddle point and defined by

$$\Delta\tau_b = \tau_{\text{MLPT}}(q_0 \to q_b) - \tau_{\text{MFPT}}(q_0 \to q_b) \tag{3}$$

For simplicity, the metastable potential $V(q)$ is chosen in such a way that consists of two smoothly joined harmonic oscillators adding with a post-saddle anharmonic potential as

$$V(q) = \begin{cases} \frac{1}{2}\omega_0^2 q^2, & q \quad \le q_s; \\ V_b - \frac{1}{2}\omega_b^2(q-q_b)^2, & q_s \quad \le q \le q_b; \\ V_b - \frac{1}{2}\omega_b^2(q-q_b)^2 + c_3(q-q_b)^3 + c_4(q-q_b)^4, & q \quad \ge q_b \end{cases}$$

where $c_4 \le 0$. We apply the stochastic Runge-Kutta algorithm to solve numerically Eq. (1) with 1.5×10^6 test particles and use dimensionless data to plot forthcoming each figure.

The distributions of the first passage time and the last passage time across the saddle point are of interest[8] and are plotted in Figs. 1(a) and 1(b) by using the two distributions of initial position via Langevin simulations. In those figures, $\tau_{\text{MFPT}} = 76.7$, $\tau_{\text{MLPT}} = 169.3$, and $\Delta\tau_b = 92.65$ for a δ distribution (δ-D) $W(q_0) = \delta(q_0)$; $\tau_{\text{MFPT}} = 73.1$, $\tau_{\text{MLPT}} = 165.7$, and $\Delta\tau_b = 92.56$ for a Gaussian distribution (G-D) $W(q_0) = (2\pi\sigma^2)^{-1/2}\exp[-q_0^2/(2\sigma^2)]$ with the width $\sigma = 0.8$. It is seen that the distributions of both the first passage time and the last passage time depend on the initial condition, however, the dependence of the oscillating time (i.e., the difference between the two times of leaving and arriving at the saddle point) around the saddle point on the initial position is weakly. Indeed, the distribution of the first passage time starts from a maximum value and that of the last passage time does not. If the initial position of particle obeys a Gaussian distribution, namely, the particle with a probability locates at the potential top, the time needed arriving firstly at the saddle point is short. However, the particle requires still time to leave lastly the barrier, because it could pass over the saddle point multi times.

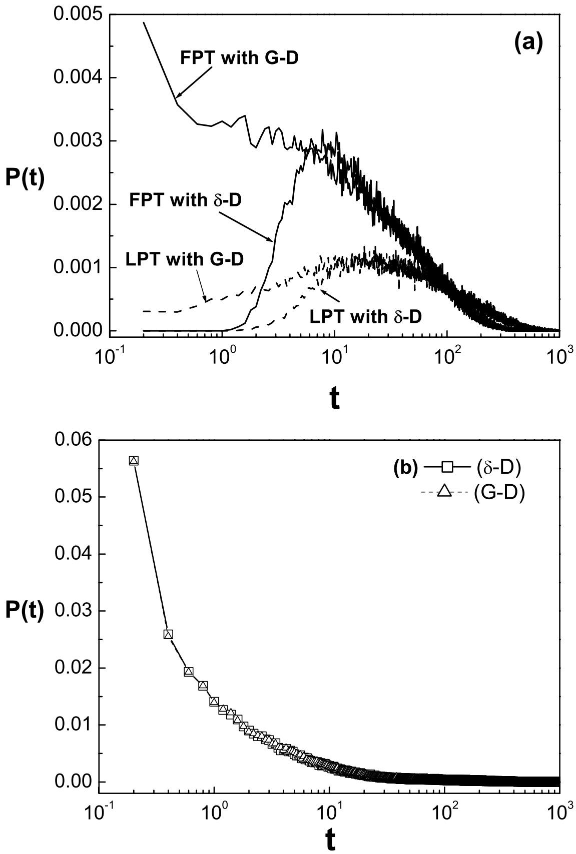


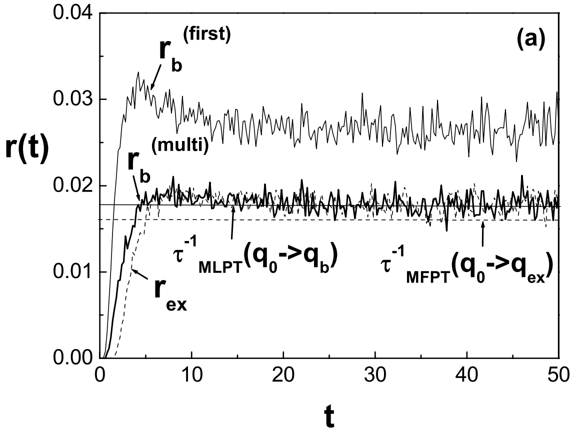
Fig. 1. (a) The distributions of the first passage time (FPT) and last passage time (LPT). (b) The distribution of the oscillating time ($\tau_{\mathrm{LPT}} - \tau_{\mathrm{FPT}}$) around the saddle point. The parameters used are $\gamma = 10.0$, $\omega_0 = \omega_b = 1.0$, $c_3 = c_4 = 0.0$, $T = V_b = 1.0$, $q_b = 2.0$, and $\sigma = 0.8$.

3. ESCAPE RATE CONNECTED WITH MLPT

In contrast to the MFPT and MLPT, the question of how to calculate the escape rate is slightly less trivial. Who do two time scales of the MFPT and MLPT contain all the relevant information that one can possibly extract from numerical simulation? To this end, we determine numerically time-dependent escape rate by

$$r(t) = -\frac{1}{N(t)}\frac{\Delta N(t)}{\Delta t} \tag{4}$$

where $N(t)$ denotes the number of test particles that have not undergone escape at time t, $\Delta N(t)$ is the number of test particles that have undergone escape from



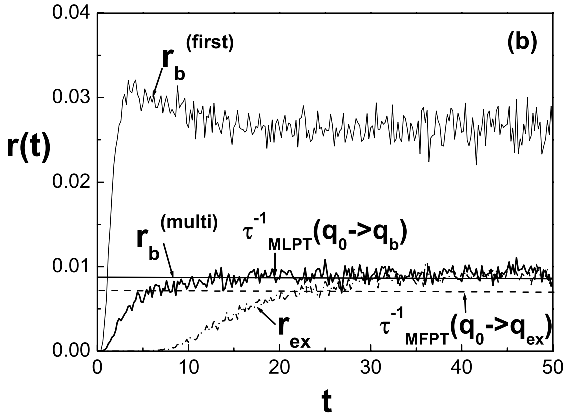


Fig. 2. Time-dependent escape rate at $T = 1.0$ for different postsaddle anhanmonic potentials and numerical results for the inverses of MFPT and MLPT at the saddle point are also plotted. The parameters used are $\gamma = 5.0$, $V_b = 1.0$, $\omega_0 = \omega_b = 1.0$, and the exit position $q_{\rm ex} = 10.0$. (a) $c_3 = -3$ and $c_4 = 0$, the potential is steep; (b) $c_3 = 0.23$ and $c_4 = -0.04$, the potential is gentle.

the barrier during a time interval $t \to t + \Delta t$. Here we would like to point out a fact that $\Delta N(t)$ is the recorded number of test particles crossing over the saddle point for the last time after the test particles perform passing back and forth over the saddle point multi times. This treatment differs from the previous method in which only those particles passing over the saddle point for the first time are taken into account.

Figures 2(a) and 2(b) show time-dependent escape rate calculated by test particles starting from the metastable potential minimum with a $\delta(q_0)$ distribution and for different post-saddle potentials. It is seen that the stationary escape rate

$r_b^{(\mathrm{multi})}$ determined at the saddle point by means of test particles passing over the saddle point multi times approaches the calculated result r_{ex} by means of test particles finally arriving at an exit, because in each of these cases a positive average current is built up in the stationary state. The *backstreaming* ($r_b^{(\mathrm{frist})} - r_{\mathrm{ex}}$) is quite large when the post-saddle potential is gentle, where $r_b^{(\mathrm{first})}$ is the steady escape rate calculated by test particles passing over the saddle point first time. This is clear as it should be because in the mean first passage process the test particles cannot recross back over the boundary if the saddle point is chosen to be an absorbing boundary.[2]

A simple relation between MFPT, MLPT and the Kramers escape rate was proposed by Reimann *et al.*[17] and modified by Boilley *et al.*[18] The escape rate is as the ratio of the probability flux j over the saddle point and the population of a well (i.e., $q \le q_b$) in the quasi-stationary state. An equality for the population reads

$$\int_{-\infty}^{q_b} W(q)dq = \int_G W(q)dq - \int_{q_b}^{q_{\mathrm{ex}}} W(q)dq \tag{5}$$

where the domain G is determined as the fact that particles are removed from the ensemble as soon as they leave the domain G for the first time. The Kramers escape rate is then defined as the constant net flux out of G normalized by the population inside barrier,

$$r_k := j / \int_{-\infty}^{q_b} W(q)dq \tag{6}$$

The steady state populations at other regions are $\int_G W(q)dq = j\tau_{\mathrm{MFPT}}(q_0 \to q_{\mathrm{ex}})$ and $\int_{q_b}^{q_{\mathrm{ex}}} W(q)dq = j\tau_{b\to\mathrm{ex}}$, respectively. This finally yields

$$\tau_{\mathrm{MFPT}}(q_0 \to q_{\mathrm{ex}}) = r_k^{-1} + \tau_{b\to\mathrm{ex}} \tag{7}$$

where $\tau_{b\to\mathrm{ex}}$ is the mean saddle-to-exit diffusive time, which differs from $\tau^*_{b\to\mathrm{ex}}$ determined in Eq. (2), because $\tau_{b\to\mathrm{ex}}$ still includes some times oscillating around the saddle point. Here, $\tau_{\mathrm{MFPT}}(q_0 \to q_{\mathrm{ex}}) - \tau_{b\to\mathrm{ex}}$ can be regarded as an approximate expression of the mean last passage time at the saddle point. In order to calculate the escape rate, we propose to use the MLPT at the saddle point instead of the MFPT at the exit point. It is found in Figs. 2(a) and 2(b) that a relation of theirinverses and the Kramers rate is given by $r_k \gtrsim \tau^{-1}_{\mathrm{MLPT}}(q_0 \to q_b) > \tau^{-1}_{\mathrm{MFPT}}(q_0 \to q_{\mathrm{ex}})$.

The MFPT has an exact expression for arbitrary barrier height in the overdamped case,[2,7,14] and the mean saddle-to-exit diffusive time $\tau_{b\to\mathrm{ex}}$ can be obtained analytically from the particle with an average velocity of the Kramers' distribution at the saddle point travelling from the saddle point to the exit point in an inverted harmonic potential [$c_3 = c_4 = 0$ in $V(q)$] for moderate-to-large

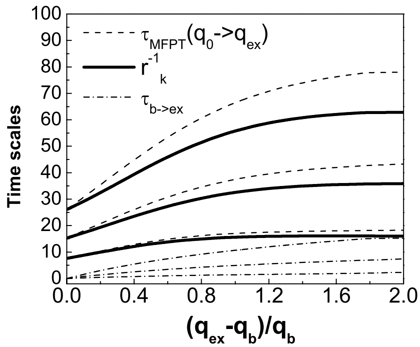


Fig. 3. Various time scales in the unit of γ^{-1} vs exit positions. The parameters used are $T/V_b = 0.5$, $c_3 = c_4 = 0$, $\omega_b/\omega_0 = \frac{1}{3}, \frac{1}{2}$, and 1.0 from top to bottom in each group lines.

damping.[20–22] They can be expressed, respectively, as

$$\tau_{\mathrm{MFPT}}(q_0 \to q_{\mathrm{ex}}) = \frac{\gamma}{T}\int_{q_0}^{q_{\mathrm{ex}}} dy \exp\left[\frac{V(y)}{T}\right]\int_{-\infty}^{y} dz \exp\left[-\frac{V(z)}{T}\right] \tag{8}$$

and

$$\tau_{b\to\mathrm{ex}} = \frac{2}{\omega_b}\left[\sqrt{1+\eta^2}+\eta\right]R(\sqrt{\Delta V/T}) \tag{9}$$

where ΔV denotes the potential difference between the saddle point and the exit point, and $\eta = \gamma/(2\omega_b)$. The expression (9) reduces to $2\gamma/\omega_b^2 R(\sqrt{\Delta V/T})$ in the overdamped case.[22] The function R is $R(q) = \int_0^q dy \exp(y^2)\int_y^\infty dz \exp(-z^2)$.

In Fig. 3, we plot the theoretical results for various time scales of the particle in the metastable potential by using Eqs. (8) and (9). It is seen that both the mean saddle-to-exit diffusive time and the Kramers time r_k^{-1} increase as the post-saddle potential becomes gentle. In this case the barrier backstreaming should be large and thus the dynamical effect between the saddle point and the exit point cannot be neglected.

Figure 4 shows numerical results for the three typical time scales, such as the mean first passage time $\tau_{\mathrm{MFPT}}(q_0 \to q_b)$, the mean saddle-point oscillating time $\Delta\tau_b$, and the mean saddle-to-exit descent time $\tau^*_{b\to\mathrm{ex}}$. It is clearly seen that $\Delta\tau_b$ is the longest time scale. At low temperatures, the time spent inside the well is very large, the particle has only a small positive velocity when it arrives at the saddle point and then descents to the exit point, so that the MFPT at the saddle point and the mean saddle-point oscillating time around the saddle point are equivalent. Nevertheless, with the increase of temperature, the difference between these two time scales is observably. This is due to that the Kramers time decreases and the oscillation of particle around the saddle point becomes strongly.

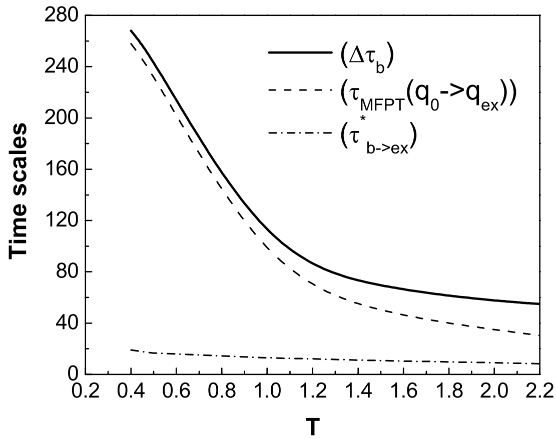


Fig. 4. Dependence of three time scales on the temperature. The parameters used are $\gamma = 10.0$, $V_b = 1.0$, $\omega_0 = \omega_b = 1.0$, $q_{\text{ex}} = 6.0$, $c_3 = 0$, $c_4 = 0$, and $q_b = 2.0$.

4. SUMMARY

We have proposed the mean last passage time at the saddle point and discussed the dependence of several time scales in the metastable potential on the temperature. The distributions of the first passage time (arriving at the saddle point) and the last passage time (leaving the saddle point) depend on the initial condition, but the dependence of the mean saddle-point oscillating time on the initial condition is weakly. We have also performed Langevin simulation for time-dependent escape rate by considering test particles passing back and forth over the saddle point and evaluated the mean last passage time at the saddle point, where the back-streaming across the saddle point has to be taken into account. If the temperature is close to the barrier height, the Kramers time (the inverse of the Kramers rate) required for a particle stating from the metastable potential minimum arriving at the potential top is shorter than the mean oscillating time of particle across over the saddle point. Therefore, the dynamics of unstable system is dominated by the mean last passage time scale for the escape out of the barrier of a metastable potential. It should believe that the concept of the mean last passage time proposed in this work has a very practical application for various problems.

ACKNOWLEDGMENTS

This work was supported by the Special Research Fund for Doctoral Program of Higher Education of China under Grant No. 20050027001 and the National Natural Science Foundation of China under Grant No. 10235020.

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