Simple relations between mean passage times and Kramers' stationary rate

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The classical problem of the escape time of a metastable potential well in a thermal environment is generally studied by various quantities like Kramers' stationary escape rate, mean first passage time, nonlinear relaxation time, or mean last passage time. In addition, numerical simulations lead to the definition of other quantities as the long-time limit escape rate and the transient time. In this paper, we propose some simple analytical relations between all these quantities. In particular, we point out the hypothesis used to evaluate these various times in order to clarify their comparison and applicability, and show how average times include the transient time and the long-time limit of the escape rate.

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INTRODUCTION

The escape time of a metastable potential well in a thermal environment is a universal problem in physics and chemistry that has been evaluated in various ways. Thermal nuclear fission is a typical example that has motivated this study. The full dissipation-fluctuation dynamics could be solved numerically using either Langevin or Klein-Kramers equations. However, for practical purposes such as the development of deexcitation codes for hot nuclei, analytical formulas are often preferred because of the high computing time required by the latter approaches. Kramers, in his seminal paper [1], evaluated the stationary escape rate for two regimes: in the weak-damping limit, the escape rate is dominated by an energy diffusion process whereas, in the high-friction regime, it is dominated by a spatial diffusion process. We will only consider the latter one here for which a simple approximate formula can be derived when the temperature is lower than the barrier height. Kramers' escape time is then just the inverse quantity. Another possible approach to determine the escape time is the older concept of mean first passage time (MFPT) at an exit point chosen beyond the barrier. In the very-high-friction regime, when the Klein-Kramers equation can be well approximated by the Smoluchowski one, the MFPT can be evaluated analytically [2,3]. In the low-noise limit—i.e., when the temperature is smaller than the potential barrier—the two times are known to be equivalent under the condition that the MFPT's exit point be beyond the barrier, but not too far [3]. Recently, the concept of mean last passage time (MLPT) at the barrier top was introduced as an equivalent escape time [4], in order to cope with the backward currents at the saddle, but no analytical formula is available yet.

Beyond these low-noise approximations, is Kramers' stationary escape rate over the barrier [1] always equivalent to the MFPT at an exit point beyond the barrier [5] or to the MLPT at the barrier [4]? As we shall prove that it is not the case, what is the most-suited quantity to determine for example the fission time of hot nuclei and compare it to other disintegration channels? Several different formulas have been used so far in deexcitation codes. To clarify the situation, we stress the hypothesis underlying each definition. The main task of this paper is to present simple analytical relations inspired by the work of Ref. [6] to ease the comparison between the various escape times. For the sake of completeness, we will also consider the nonlinear relaxation time (NLRT) [7] used to study phase transition phenomena [8] and evaluated analytically for various potentials in the overdamped limit [9].

Numerical simulations give access not only to mean values, but also to the escape rate as a function of time or the passage time distribution that characterizes the dynamics of the escape process. In particular, the transient time needed to reach a quasistationary escape rate can play a crucial role in the context of nuclear fission, because, at high excitation energies, it is long enough to be compared to the time scale of other decay channels such as neutron evaporation. We will also show how these dynamical times are included in the average ones.

UNIVERSAL RELATIONS

Starting from an arbitrary but fixed position x_0, one can calculate the times τ_n^F, $n=1,\ldots,N$, it takes for N realizations of the Brownian process $x(t)$ to leave the prescribed domain G for the *first* time. By definition, the MFPT ($\mathcal{T}_{\mathrm{MFPT}}$) reads

$$\mathcal{T}_{\mathrm{MFPT}}[x_0 \to \partial G] = \lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N}\tau_n^F. \qquad (1)$$

Of course, the problem considered should be physically meaningful: $x_0 \in G$ and the $\mathcal{T}_{\mathrm{MFPT}}[x_0 \to \partial G]$ is finite. To get a stationarity inside G, a constant source q in x_0 is added so that qdt is the number of new particles joining the ensemble during the time dt. In Kramers' approach, the source exactly

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compensates the leak [10], but one can consider a more general situation with an arbitrary value of q. The particle density inside G, $W(x,t)$ approaches a steady state $W(x)$ in the long-time limit and the stationary escape rate from G with an absorbing border is then

$$\Gamma = q \Big/ \int_G W(x)dx. \tag{2}$$

To find a relation between Γ and the MFPT, one needs to define the relative number of particles $P(t-t_0,\partial G;x_0)$ that have not yet left G at time t given that they have been launched from x_0 at time t_0. From the calculated escape times, one has

$$P(t-t_0,\partial G;x_0) = \lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N}\Theta(\tau_n^F + t_0 - t) \tag{3}$$

if the particles never come back in the domain G. This means that a sink at the domain's boundary ∂G is supposed to absorb all the outgoing particles. In the previous equation, Θ is the Heaviside step function. If one starts at time t_i to constantly inject particles at x_0 at a rate q, the total population inside G at time t is

$$\int_G W(x,t)dx = \int_{t_i}^{t} qP(t-t_0,\partial G;x_0)dt_0 \tag{4}$$

$$\to q\lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N}\tau_n^F, \tag{5}$$

in the long-time limit or the steady state. Eventually, one gets

$$\mathcal{T}_{\mathrm{MFPT}}[x_0 \to \partial G] = 1/\Gamma. \tag{6}$$

Such a result, derived in Ref. [6], could easily be extended to more general sources.

In this work we define Kramers' escape rate Γ_K as the normalized stationary flux over the potential barrier. In contrast to the escape rate of Eq. (2), the domain G considered when evaluating Γ_K encloses the metastable well and is limited to the saddle. Therefore, Kramers' stationary rate includes backward currents and in this case Eq. (3) cannot be applied. But after the *last* passage time τ_n^L, the particle will not enter the domain anymore. Assuming that for each realization the time spent out of the domain within τ_n^L is small in comparison to the time spent inside, one rather has, instead of Eq. (3),

$$P(t-t_0,x_b;x_0) \lesssim \lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N}\Theta(\tau_n^L + t_0 - t) \tag{7}$$

and then, similarly,

$$\Gamma_K \gtrsim 1/\mathcal{T}_{\mathrm{MLPT}}[x_0 \to x_b], \tag{8}$$

where x_b defines the position of the barrier. In the low-noise limit, the time spent inside the domain is very large and the previous equation is almost an equality. Such a result is confirmed by the numerical simulations done in Ref. [4].

To exactly get Kramers' stationary rate at the barrier, one should only count the periods of time when the test particle is in the domain G bounded by the saddle. Time periods during which the test particle is out of G that are included in the MLPT should not be taken into account:

$$P(t-t_0,x_b;x_0) = \lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N}p_n(t-t_0), \tag{9}$$

with $p_n(t-t_0)=1$ when the nth particle is in G and $p_n(t-t_0)=0$ else. The p_n's could easily be written in term of Heaviside step functions. Then, the exact equivalent of Kramers' stationary rate is the mean time spent in the domain G.

To make the MFPT physically meaningful, one should keep the domain G up to a point x_e beyond the saddle where one can safely neglect the backward currents due to the potential slope. In the steady-state limit, the flux q is the same in any point, but to get the usual Kramers' stationary rate, one needs to evaluate the population inside the well up to the saddle only:

$$\int_{-\infty}^{x_b} W(x)dx = \int_G W(x)dx - \int_{x_b}^{x_e} W(x)dx. \tag{10}$$

The second term of the right-hand side of the previous equation can be evaluated easily by the well-known concept of average saddle-to-scission time in nuclear physics, $\tau_{b\to e}$:

$$\int_{x_b}^{x_e} W(x)dx = q\tau_{b\to e}. \tag{11}$$

Taking this into consideration, Eq. (5) finally yields

$$\mathcal{T}_{\mathrm{MFPT}}[x_0 \to x_e] = \frac{1}{\Gamma_K} + \tau_{b\to e}. \tag{12}$$

$\tau_{b\to e}$ can be evaluated analytically within Kramers' approximations if the potential is locally an inverted parabola [11]. Again, in the low-noise limit, if x_e is not too far, the time spent inside the well is far longer than the saddle-to-scission time and one recovers the well-known equivalence between Kramers' rate at the saddle and the MFPT beyond. But this is not correct in general.

In Ref. [4] another saddle-to-scission time was introduced:

$$\tau_{b\to e}^L = \mathcal{T}_{\mathrm{MFPT}}[x_0 \to x_e] - \mathcal{T}_{\mathrm{MLPT}}[x_0 \to x_b]. \tag{13}$$

From Eqs. (8) and (12), one immediately has that $\tau_{b\to e}^L \lesssim \tau_{b\to e}$, which can be easily understood because $\tau_{b\to e}^L$ is the direct time from saddle to scission. In the low-noise limit, these two times are close.

DYNAMICAL TIMES

An important point concerns numerical simulations done with test particles that generally do not include any source term in the well and are closer to reality in the escape problem. Even if the escape rate tends to a constant value, the population in the domain and the escape current are not stationary anymore. Naturally, both MFPT and MLPT do not depend on the existence of the source. Thus, instead of Kramers' stationary rate which needs a source, we will rather use the mean time spent in the domain bounded by x_b as an equivalent quantity and show that this mean time is also equal to the mean passage time at the top of the barrier. The escape current, defined as

$$j(t-t_0,x_b;x_0) = -\frac{\partial P(t-t_0,x_b;x_0)}{\partial t}, \tag{14}$$

gives the distribution of the escape time. Equation (14) is a consequence of the continuity equation. Then, the mean passage time (MPT) could simply be evaluated:

$$\mathcal{T}_{\mathrm{MPT}}[x_0 \to x_b] = \int_{t_0}^{+\infty} tj(t-t_0,x_b;x_0)dt \tag{15}$$

$$= \int_{t_0}^{+\infty} P(t-t_0,x_b;x_0)dt. \tag{16}$$

The second line was obtained by a trivial integration by parts using the fact that $P(t-t_0,x_b;x_0)$ vanishes for large time. We would like to stress here that the mean passage time coincides with the nonlinear relaxation time. The latter was compared analyticaly to the MFPT in Ref. [12] in some particular situations.

Defining $P(t-t_0,x_b;x_0)$ as in Eq. (9) from the time spent by test particles in the domain G bounded by the saddle, this last equation could be integrated and yields

$$\int_{t_0}^{+\infty} P(t-t_0,x_b;x_0)dt = 1/\Gamma_K, \tag{17}$$

where Kramers' stationary rate is defined as the mean time spent in the domain G limited to the saddle. Equation (17) is then a convenient way to evaluate Kramers' stationary rate in a nonstationary context without any source term.

For systems initially in the well, but far from thermal quasiequilibrium, numerical simulations also show that a relaxation regime appears before reaching a quasistationary flux [13]. The corresponding additional transient time is linked to the thermalization process of the system in the metastable well and naturally depends on the initial conditions. It generally takes a finite time to the variable x to be thermally distributed in the potential well, especially if one starts with a fixed initial position, whereas the momenta thermalize faster in the high-viscosity case. Unfortunately, a general analytic formula is so far not available for this transient regime and simple phenomenological functions are generally used to match the numerical results. In the overdamped regime, a realistic approximate transient function was derived in Ref. [14], based on the exact solution of the Langevin or Klein-Kramers equations in a parabolic potential well [15].

Let us denote $\Gamma(t)$ the escape rate at saddle from a metastable well without any source and Γ_∞ its long time-limit. By definition, one has

$$-\frac{\partial P(t,x_b;x_0)}{\partial t} = \Gamma(t)P(t,x_b;x_0). \tag{18}$$

In the absence of a relaxation regime, assuming that the escape rate is constant, this last equation could easily be integrated into

$$P(t,x_b;x_0) = e^{-\Gamma_\infty t}, \tag{19}$$

and then, Eq. (17) yields $\Gamma_K = \Gamma_\infty$. In order to express simply the effect of the transient regime on the escape rate, we will assume a crude description of the transient function. Considering a step function up to the transient time τ_r,

$$\Gamma(t) = \Theta(t-\tau_r)\Gamma_\infty, \tag{20}$$

Eqs. (18) and (17) yield

$$1/\Gamma_K = \mathcal{T}_{\mathrm{MPT}}[x_0 \to x_b] = \tau_r + 1/\Gamma_\infty. \tag{21}$$

Then, Kramers' rate depends on the transient time, but should also depend on the nature of the relaxation process. Consequently, the MFPT to a point beyond the saddle includes all these dynamical times as well. Such a result contradicts the claim of Ref. [5] that "in the very concept of MFPT there is no room for a transient effect." It may look surprising that Kramers' stationary rate corresponding to a long-time limit includes a relaxation process. But the stationarity is due to a source and each injected particle has to first experience a thermalization process. Then, one should also be cautious with numerical tests, not assimilating Γ_K and Γ_∞. At low temperature, $1/\Gamma_\infty$ becomes very large and the transient time τ_r can be neglected in Eq. (21). Thus, one has $\Gamma_K \simeq \Gamma_\infty$.

Finally, we would like to stress that Kramers' formula [1] corresponds to a very specific case of Kramers' escape rate over the saddle since several assumptions were made to get it. Besides the low-temperature limit, a specific source term is implicitly supposed [10] that is close to a thermalized distribution. With such an initial distribution, the relaxation time vanishes and thus, Kramers' formula is close to Γ_∞.

CONCLUSION

As a conclusion, we have shown that the stationary escape rate from a thermally unstable potential well is equal to the mean time spent in the domain or the MPT at the border. When the domain is limited by a sink on the boundaries, MPT, MFPT, and MLPT are exactly the same quantities since the particle crosses the border only once. On the contrary, when the domain is limited to the barrier top, backward currents change the situation. Kramers' stationary escape time is then equivalent to the NLRT. It is close to the MLPT and an additional saddle-to-scission time should be added to get the MFPT to a point beyond the barrier. These relationships make Kramers' theory useful, even for problems without a source assuring stationarity. The choice of the most suitable concept to evaluate the escape time depends on the physical situation. As for the nuclear fission problem, this will be discussed in another paper. Finally, we have also shown that Kramers' stationary rate and, consequently, the

MFPT include both the relaxation time and the long-time limit escape rate of the realistic problem without any source. In the case of Kramers' formula derived with very specific assumptions, the initial condition is such that the relaxation time vanishes and the formula rather corresponds to the long time limit rate Γ_∞.

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