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Universal equivalence of mean first-passage time and Kramers rate

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We prove that for an arbitrary time-homogeneous stochastic process, Kramers's flux-over-population rate is identical to the inverse of the associated mean first-passage time. In this way the mean first-passage time problem can be treated without making use of the adjoint equation in conjunction with cumbersome boundary conditions. [S1063-651X(99)50307-3]

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When does a random process cross the border between two regions of its state space for the first time? This problem of the *mean first-passage time* (MFPT) [1–5] is of central importance in the entire field of random walk theory [6] and noise-assisted surmounting of a potential barrier [4] with many applications in physical, chemical, and biological systems. The proper mathematical formulation of the MFPT problem—the so-called adjoint equation—and especially of the correct boundary conditions is often plagued by considerable difficulties and subtle pitfalls [4,5,7–12]. The main result of our present Rapid Communication is a way to determine the MFPT which is based solely on the master equation that governs the time evolution of the probability density. The cornerstone of this approach is an exact identity between the inverse MFPT and an associated Kramers-like escape rate. This identity has been demonstrated before in Appendix B of Ref. [4] for the special case of a stochastic process driven by Gaussian white noise (multidimensional Fokker-Planck process), and is also well known from activated barrier crossing theories as an asymptotic result in the weak noise limit [4,7,10,13]. It is in this limit that the "reaction rate" defines the macroscopic exponential decay of reactants [4]. Our present proof is *completely general*, including, for instance, colored Gaussian noise [8], dichotomous noise [7,8,10,11,14], pre-Gaussian noise [9], shot noise [7,15,16], and composite noise [12], as well as noisy dynamics in discrete time [13,17,18] without any restriction on the noise strength.

We consider a stochastic process $x(t)$ in arbitrary dimensions. For the moment we restrict ourselves to Markovian processes [the future of $x(t)$ depends only on its present state, not on its past] which are furthermore continuous and homogeneous in time. Generalizations will be discussed later. In a numerical simulation of such a stochastic dynamics, the MFPT is the most straightforward quantity one can think of, one starts at an arbitrary but fixed x_0 and observes, for N independent realizations of the process $x(t)$, the times τ_n, $n=1,2,\dots,N$, it takes to leave some *a priori* prescribed domain G for the first time. Then, $\Sigma_{n=1}^{N}\tau_n/N$ is the best possible estimate for the MFPT that one can obtain from the given samplings τ_n, approaching, by definition, strict equality for $N\to\infty$ (with probability 1), i.e.,

$$T_G(x_0) := \lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} \tau_n . \qquad (1)$$

We remark that the process $x(t)$ need not be continuous in space, i.e., it may typically exit from the domain G without ever actually hitting the boundary δG. We furthermore take for granted that the considered problem is physically meaningful, especially the choice of G should be such that $x_0 \in G$ and $0 < T_G(x_0) < \infty$.

Turning to the definition of the Kramers rate, we imagine an ensemble of independent "particles" $x(t)$ with a constant particle-source q at x_0, that is, in any time interval $[t,t$

$+dt$], a number qdt of new particles are joining the ensemble with seed x_0. Furthermore, particles $x(t)$ are removed from the ensemble as soon as they leave the domain G for the first time. Due to our assumption that the stochastic dynamics is time homogeneous and the MFPT is finite, the particle density $P(x,t)$ approaches a steady state $P(x)$ in the long time limit and the average number of particles leaving G becomes equal to those injected by the source. The rate $k_G(x_0)$ according to Kramers and Farkas [4,19,20] is then *defined* as this resulting constant net flux out of G normalized by the population inside G,

$$k_G(x_0) := q \Big/ \int_G P(x)dx. \tag{2}$$

Since doubling the source strength q will also double the steady state population $\int_G P(x)dx$, this definition is clearly independent of the actual q value.

In contrast to the MFPT, the question of how to determine the Kramers rate (2) from a numerical simulation is slightly less trivial. Due to the time homogeneity, the escape times τ_n contain all the relevant information that one can possibly extract from any type of numerical simulation. Therefore, the Kramers rate can definitely be calculated from the τ_n, but how? A first guess that comes to mind is to take the average over the ''individual rates'' $k_n := 1/\tau_n$. Indeed, each realization of the stochastic process may be considered as representing one possible ''reaction channel'' with a corresponding rate k_n and an *a priori* probability $1/N$. The resulting total rate is thus the sum of the contributions of all channels weighted with their *a priori* probability. A second natural guess of how to obtain the Kramers rate from the simulated escape times τ_n is by taking the inverse of the MFPT from Eq. (1), i.e.,

$$T_G(x_0) = 1/k_G(x_0). \tag{3}$$

The commonly used argument (see, e.g., in [21]) is that each particle injected by the source remains on the average for a time $T_G(x_0)$ in G. The steady state population of G should therefore be equal to $q\,T_G(x_0)$ and the rate equal to the inverse MFPT. The problem with this argument is that the individual particles actually remain in G for a time τ_n and not $T_G(x_0)$, and the net effect of these deviations on the population of G is not so obvious. We also remark that the two guesses are not equivalent unless all of the τ_n are exactly identical. Anticipating that Eq. (3) is indeed correct it follows that the average over $1/\tau_n$ *never* equals the Kramers rate, not even in the weak noise limit of a barrier crossing problem.

In order to prove Eq. (3) we observe that the relative number of particles $\rho_{t_0}(t)$ that have *not* yet left G at time t, given that they have been launched from x_0 at time t_0, can be calculated from the escape times τ_n as

$$\begin{aligned}\rho_{t_0}(t) &= 1 - \lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} \Theta([t-t_0]-\tau_n)\\ &= \lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} \Theta(\tau_n + t_0 - t),\end{aligned} \tag{4}$$

where the Heaviside function is defined by

$$\Theta(y) := 1 \quad \text{if } y>0, \quad \Theta(y) := 0 \quad \text{if } y \leqslant 0. \tag{5}$$

Due to the assumed time homogeneity of the stochastic dynamics, it follows that

$$\rho_{t_0}(t) = \rho_0(t-t_0). \tag{6}$$

Let us now start at time t_i to constantly inject particles at x_0 at a rate q. Then, the total population inside G at time $t > t_i$ is

$$\int_G P(x,t)dx = \int_{t_i}^{t} dt_0\, q\, \rho_0(t-t_0). \tag{7}$$

By introducing $t' = t - t_0$ and using Eq. (4), this yields

$$\int_G P(x,t)dx = \lim_{N\to\infty} \frac{q}{N}\sum_{n=1}^{N} \int_0^{t-t_i} dt'\,\Theta(\tau_n - t') \tag{8}$$

and thus for $t\to\infty$, i.e., in the steady state,

$$\int_G P(x)dx = q \lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} \tau_n. \tag{9}$$

By comparison with Eqs. (1) and (2) we arrive at the central relation (3) between the Kramers rate and the MFPT.

So far we have restricted ourselves to point sources of particles of the form $S(x) = q\,\delta(x-x_0)$. For more general sources $S(x)$, the net flux of particles across δG in the steady state equals the total source strength $\int_G S(x)dx$ yielding, for the *Kramers-Farkas flux-over-population rate* the generalized definition,

$$k_G[S(x)] := \int_G S(x)dx \Big/ \int_G P(x)dx. \tag{10}$$

The proper definition of the MFPT $T_G[S(x)]$ for a generalized distribution of seeds according to $S(x)$ is still given by the right hand side of Eq. (1), implying

$$T_G[S(x)] = \int_G S(x)T_G(x)dx \Big/ \int_G S(x)dx. \tag{11}$$

Our line of reasoning above can be readily extended to this case with the following result:

$$T_G[S(x)] = 1/k_G[S(x)]. \tag{12}$$

An analogous extension is possible for more general sinks than the so far considered perfect absorption outside G, e.g., for a constant finite absorbtion probability $S(x) \propto -P(x)$ in the region $x \notin G$.

We remark that the same line of reasoning can be adopted also for the case of processes in discrete time. A more serious restriction is the time homogeneity. In the case of a *periodic* time dependence, a generalization of our arguments is still possible via stroboscopic mapping and coarse graining of time but not for a general explicit time dependence. This procedure mimics the averaging of a corresponding time-periodic flux over a full period.

Next we turn to the case of a non-Markovian stochastic dynamics. The time evolution of such a process $x(t)$ and thus the MFPT is not completely specified anymore by the seed x_0 and one has to tacitly take for granted some additional ''preparation conditions'' in order to make the problem well defined. Similarly, in the definition of the Kramers rate, the distribution of the particle sources $S(x)$ has to be supplemented by the same additional ''preparation conditions'' as in the MFPT. Our above line of reasoning can then be carried over without any further modification and the central result (12) still holds true.

The fact that Eq. (12) is an exact identity under such extremely general conditions is certainly of considerable interest in itself. However, its main practical application is the evaluation of the MFPT and, for this, the steady state population $\int_G P(x)dx$ in Eq. (1) has to be determined. In the most general case (Markov and non-Markov), the time evolution of the particle distribution $P(x,t)$ is governed by a master equation of the form

$$\frac{\partial}{\partial t}P(x,t)=\hat{\Gamma}(x,[P(y,s\leq t)])+\hat{Q}(x,[S(y)]), \qquad (13)$$

where the master operator $\hat{\Gamma}$ is a function of x and simultaneously a linear functional of $P(y,s)$, and similarly for the source operator $\hat{Q}$. Due to causality, only time arguments $s \leq t$ can play a role in Eq. (13) and, due to the assumed time homogeneity, both operators involve no explicit time dependence. For a general non-Markovian process those operators take into account memory effects (e.g., memory friction or time correlations of the noise) as well as the above-mentioned additional ''preparation conditions'' in order to make the time evolution unique. To account for the absorption of particles outside G, one has to restrict Eq. (13) to x values inside G with supplementing boundary conditions $P(x,t)=0$ for $x \notin G$. In passing we note that so-called perfect reflecting boundary conditions (i.e., the dynamics is excluded from a subset of G) can always be incorporated into the master operator, e.g., by infinite ''potential walls.''

In many cases of practical interest, a non-Markovian process can be made exactly or approximately Markovian by including some auxiliary state variables into $x(t)$. In this way, the problem is typically much easier to handle. As a matter of fact, we do not know of any example for which such a transformation is *not* known but the explicit forms of the operators $\hat{\Gamma}$ and $\hat{Q}$ in Eq. (13) *are* known. For all practical purposes we can therefore restrict ourselves to the Markovian case. The source operator $\hat{Q}(x,[S(y)])$ then becomes equal to $S(x)$ and the steady state density is governed by

$$\begin{aligned} \hat{\Gamma}(x,[P(y)])&=-S(x), \qquad && x\in G \\ P(x)&=0, && x\notin G. \end{aligned} \qquad (14)$$

In other words, to determine the MFPT via Eqs. (10) and (12) one has to know the master operator $\hat{\Gamma}$ and solve the *time-independent* problem (14). (The calculation of the MFPT from an equivalent, but *time-dependent* problem is well known [5] but its actual evaluation is much more difficult.)

We close with a few remarks with special emphasis on the escape over a potential barrier in the presence of a small amount of noise. It was in this context that Kramers [19] introduced the flux-over-population definition of the rate (10), based on an earlier work by Farkas [20]. Their original strategy was to start with an ingenious ansatz for the steady state solution $P(x)$ on the entire state space and then to determine the corresponding sinks and sources *a posteriori* by inserting that solution back into Eq. (14) [4]. While, in principle, any $P(x)$ satisfies Eq. (14) with properly adapted $S(x)$, the art of arriving at the physically relevant solution is by concocting a $P(x)$ with a negligible $S(x)$ in the barrier region. In our slightly modified formulation of the problem (14), sinks do not explicitly appear but could of course be determined *a posteriori* as well.

Our second remark is that the usual choice of x_0 is at or close to the metastable potential well. To calculate the Kramers rate (for weak noise), G is typically assumed to be sufficiently much *larger* than the *basin of attraction* of this metastable state, such that it is very unlikely that a particle $x(t)$, had it not been taken out of the game after having left G, would return into this basin of x_0 in the near future. On the other hand, the MFPT is often meant with respect to a domain G which coincides with the basin of attraction of the metastable state. This type of MFPT is known to approach in the weak noise limit *twice* the inverse Kramers rate in many cases, yet this fact does not always hold true for discontinuous stochastic processes [18]. While for any finite noise strength this equality is generically not verified exactly, our result (12) is always exact. Moreover, in our present approach, the domain G has to always be chosen identical for the MFPT and the Kramers rate, but need not agree with any of the above-mentioned standard choices.

Besides the MFPT and the Kramers flux-over-population rate, the smallest positive eigenvalue of the master operator $\hat{\Gamma}$ is another frequently used quantity to characterize the lifetime of a metastable state [4]. Again, this quantity is known to become equal to the Kramers rate (in a bistable potential, to the sum of forward and backward Kramers rates) in the *weak noise limit*. It is interesting to note that the MFPT from Eq. (11) can also be identified with an eigenvalue of the master operator $\hat{\Gamma}$ in the very special case that the source $S(x)$ is required to be proportional to the steady state population $P(x)$. This condition singles out the smallest, relvalued eigenvalue of the eigenvalue problem with absorting boundary condition, cf. Eq. (14).

It has been known previously that for moderate-to-strong noise the decay of a metastable state depends on many details of the system and thus the various possibilities to quantify the decay do no longer agree. Whereas the MFPT and the Kramers flux-over-population rate both have an immediate physical (or chemical) meaning, and on top of that are equivalent, the physical relevance of the third above-mentioned concept—the smallest nonvanishing eigenvalue—and the closely connected exponential decay of the metastable state are questionable *when* the noise is no longer weak.

In this context it is also worth noting that the so-called *resonant activation effect* [22] has been mainly discussed so far in terms of the MFPT; see [23] for a review. The first reason for this is again the clear-cut physical meaning of the MFPT even when the escape no longer follows an exponential decay in time. Nevertheless, the concept of the flux-over-population still applies for any noise strength. The second reason is that, in terms of the smallest nonvanishing eigenvalue of the master operator, the effect typically no longer occurs [23,24]. The conclusion of our present work is that all of the previous literature on resonant activation in terms of the MFPT can be immediately translated into statements about the associated Kramers-Farkas flux-over-population rates.

To summarize, we have shown that the MFPT is exactly equal to the inverse of the associated Kramers escape rate. Our proof is both completely general and surprisingly simple. As a consequence, all of the explorations of ‘‘resonant activation’’ [22,23], which have been mainly conducted in terms of the MFPT, especially in the regime where an exponential decay is no longer observed, can be immediately translated into conclusions in terms of the Kramers rate. It is well known, especially for colored noise processes [7–11], but also, e.g., for white shot noise [7,11,15,16,25], that the derivation of the adjoint equation governing the MFPT and especially of the correct boundary conditions is not straightforward at all. In such cases, the calculation of the exactly equivalent Kramers rate [(10) and (12)] by solving Eq. (14) may amount to a considerable technical simplification of the task.

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