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First-passage time problems for non-Markovian processes

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Subtle difficulties encountered with non-Markovian first-crossing problems are emphasized and illustrated by an exact study of a non-Markovian flow driven by exponentially correlated telegraphic noise. The connection with approximative schemes is made and a general inequality is derived. The relationship with the escape rate at a low noise level is clarified and the Markovian limits to white shot noise and white Gaussian noise are presented.

The study of first-passage time problems has a long history and enjoys great popularity among many engineers, physicists, and chemists.[1] For one-dimensional Fokker-Planck systems the study of first-crossing problems with absorbing (or reflecting) boundary conditions is rather straightforward.[1] For more general processes, however, its broad applicability is marred due to the difficulties with appropriate boundary conditions. In higher dimensions, the problems caused by the boundary conditions in the presence of momentum or velocity degrees of freedom can be substantial. For example, such difficulties already show up very distinctly if one attempts to solve first-crossing problems for a harmonic oscillator.[2-5] Similar arcane difficulties, e.g., boundary jumps, occur in first-passage time problems of systems driven by white shot noise.[6]

Apparently, we might think that we could diminish these problems if we instead first contract the dynamics onto the single variable of interest. For example, we might want to contract the oscillator dynamics onto the amplitude dynamics $|x(t)|$ before investigating first-crossing problems of $|x(t)|$, surpassing a threshold value. This reduction, however, introduces memory into the stochastic one-dimensional flow $|\dot{x}(t)|$—known as non-Markovian dynamics.[7] The formal theory for first-crossing problems in non-Markovian flows has been developed recently by the authors.[8] Given a non-Markovian flow, the problem of obtaining exact results for first-passage time moments is beset with subtle difficulties which we might not have emphasized enough in our previous work.[8] This is further substantiated by recent work by others[9] in which our notions have been adopted erroneously. Thus, a clarification of those concepts together with a pedagogical illustration seems appropriate.

To begin, let $f_t(x|y)$ denote the probability that a trajectory which starts from y at initial time $t_0=0$ within a safe domain I will arrive at x at time t *without ever having left the safe domain.* Then

$$F_t(y)=\int_I f_t(x,y)dx\,;\;\; F_{t_0}(y)=1 \tag{1}$$

is the probability that the system is still in I at time t. With the $w_t(y)dt=-[(\partial/\partial t)F_t(y)]dt$ denoting the probability for the first-crossing variable $\tau(y)$ to lie between t and $t+dt$, the mean first-passage time (MFPT) $t(y)$ is the average

$$t(y)=\int_0^\infty tw_t(y)dt=\int_0^\infty F_t(y)dt\ . \tag{2}$$

Both, the *unrestricted* probability $p_t(x)$ and the *restricted* conditional probability $f_t(x|y)$ obey a generalized master-equation dynamics.[8] Within an operator notation one has

$$\dot{p}_t=\int_0^t K_s p_{t-s}\,ds\ , \tag{3a}$$

$$\dot{f}_t=\int_0^t \bar{K}_s f_{t-s}\,ds\ . \tag{3b}$$

The overbar in $\bar{K}_s$ indicates that the operator must be adjusted so as to prevent transitions back into the interval I (no backflow of probability). In particular, the kernel $\bar{K}_s(x,y)$ is thus restricted not to count the statistical weight induced by the trajectories which start at $y\in I$, but upon evolving time leave the interval I and return at times s at $x\in I$ (see the dotted trajectories in Fig. 1). Most importantly, this implies that the kernel $\bar{K}_s(x,y)$, (x,y) inside I, cannot be identified with the unrestricted kernel $K_s(x,y)$; i.e., $\bar{K}_s(x,y)\neq K_s(x,y)$, $(x,y)\in I$. This is in clear contrast to a Markovian situation, where the kernel $K_s(x,y)$ contains the δ function, $\delta(s)$. Then only the statistical weight of those

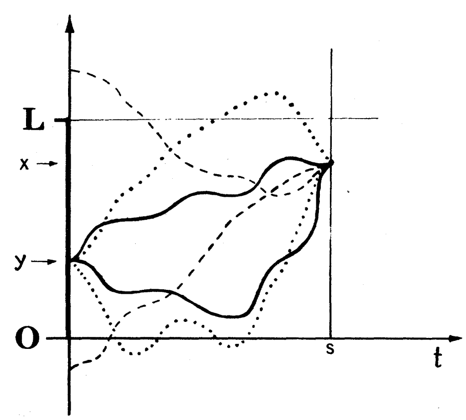

FIG. 1. Typical trajectories which determine the non-Markovian stochastic kernels used in the text. The solid trajectories contribute to the statistical weight of the adjusted kernel $\bar{K}_s(x,y)$, while the dotted trajectories, leaving the safe domain $I=[0,L]$ before time s, must be omitted in the consideration of zero backflow. The statistical weight induced by the dashed trajectories, which initially start outside the safe domain I, is all that is omitted in the construction of the crude approximation $\bar{K}_s^c(x,y)$.

trajectories which start outside I at time s^- and arrive at $x \in I$ at time s must be deleted in operator K_s in order to establish zero backflow.

A naive (Markovian-like) method of accounting for no return transitions in a non-Markovian situation consists in the "crude" approximation $\overline{K}_s^c$, which neglects only backflow into the domain I from points which initially lie outside the domain I (see the dashed trajectories in Fig. 1). Thus, we set equal to zero all transition probabilities $K_s(y \to x)ds = K_s(x,y)ds$, with x in I and y not in I. This crude approximation then implies

$$\overline{K}_s^c(x,y) \geq \overline{K}_s(x,y) \ . \tag{4}$$

This is so because the statistical weight coming from the dotted runaway trajectories overestimates the operator $\overline{K}_s$. Following Ref. 8, the exact mean first-passage time $t(y)$, $y \in I$, obeys

$$\overline{\Omega}^+ t = -1, \quad \overline{\Omega}^+(x,y) = \int_0^\infty \overline{K}_s(y,x)ds \ . \tag{5}$$

With the crude approximation, we have

$$\overline{\Omega}_c^+ t_c = -1, \quad \overline{\Omega}_c^+(x,y) = \int_0^\infty \overline{K}_s^c(y,x)ds \ . \tag{6}$$

In view of (4), we therefore obtain the general lower bound

$$t_c(y) \leq t^{\text{exact}}(y) \ , \tag{7}$$

i.e., the crude approximation will *underestimate* the exact result. The differences between (5) and (6) vanish in the Markovian (zero memory) limit in which both $\overline{K}_s$ and $\overline{K}_s^c \to \overline{\Gamma}^{\text{Markov}}\delta(s)$.

All of that shows that extreme care must be taken if one attempts to obtain exact results for the MFPT of non-Markovian processes.[10] Some of those difficulties will be washed out in situations where the MFPT takes on exponentially large values. For example, if we consider the weak noise activated escape rates in bistable non-Markovian flows,[11] the mean escape time T is given by the inverse of the rate. This average escape time can also be estimated in terms of a mean first-passage time. In that case, the complex details such as the dependence on initial preparation (see also below) between monitored variable and residual environmental background[7] do not enter the result for the exponentially large value of the MFPT, being determined by an Arrhenius factor and a prefactor.[11,12] Incorrect absorbing boundary conditions, however, do generally impact the exact result for the prefactor.

In the remainder of this Rapid Communication we now illustrate the above difficulties by an example of a non-Markovian, diffusivelike flow

$$\dot{x}(t) = \xi(t) \ , \tag{8}$$

wherein $\xi(t)$ is telegraphic noise;[11] i.e., it jumps between positive velocity a' with rate μ', and negative velocity $a < 0$ with rate μ. Moreover, we assume a vanishing mean $\langle \xi(t) \rangle = 0$, i.e., $l = |a|/\mu = a'/\mu'$.[11] For the correlation function of the noises we find an exponential decay

$$\langle \xi(t)\xi(s) \rangle = \frac{D}{\tau}\exp(-|t-s|/\tau) \ , \tag{9}$$

where $D = a'|a|\tau$, $\tau = (\mu+\mu')^{-1}$. The flow in (8) and (9) is equivalent with the two-dimensional Markovian dynamics[11]

$$\dot{p}_t(x,a) = \left\{ |a|\frac{\partial}{\partial x} - \mu \right\} p_t(x,a) + \mu' p_t(x,a') \ ,$$
$$\dot{p}_t(x,a') = \mu p_t(x,a) - \left\{ a'\frac{\partial}{\partial x} + \mu' \right\} p_t(x,a') \ . \tag{10}$$

By virtue of (10), the MFPT's, $t(y,a)$ and $t(y,a')$, $y \in I$, obey, on the interval $I = [0,L]$, the equations

$$-\left\{ |a|\frac{\partial}{\partial y} + \mu \right\} t(y,a) + \mu t(y,a') = -1 \ ,$$
$$\mu' t(y,a) + \left\{ a'\frac{\partial}{\partial y} - \mu' \right\} t(y,a') = -1 \ . \tag{11}$$

The absorbing boundary conditions outside $(0,L)$ are given by

$$t(y,\Delta) = 0, \quad \Delta = a,a', \quad y \notin [0,L] \ , \tag{12a}$$

$$t(0^+,a) = 0, \quad t(L^-,a') = 0, \quad L > 0 \ . \tag{12b}$$

The conditions (12b) account for the fact that with certainty the process escapes from the domain $[0,L]$ at $y = 0^+$ with initial negative velocity a and, likewise, certain escape occurs at $y = L^-$ with initial positive velocity a'.

Next we introduce the initial preparation function $w_0(\Delta|y)$; i.e.,

$$p_0^{(2)}(y,\Delta) = w_0(\Delta|y)p_0(y) \ ,$$

and in what follows we use the correlation-free initial preparation

$$w_0(a|y) = 1, \quad w_0(a'|y) = 0 \ . \tag{13}$$

In other words, we initially prepare the system in state y with certain negative velocity a. The exact mean first-passage time $t^{\text{exact}}(y)$ of the reduced non-Markovian dynamics is then given by

$$t^{\text{exact}}(y) \equiv t(y) = t(y,a)w_0(a|y) + t(y,a')w_0(a'|y) \ , \tag{14a}$$

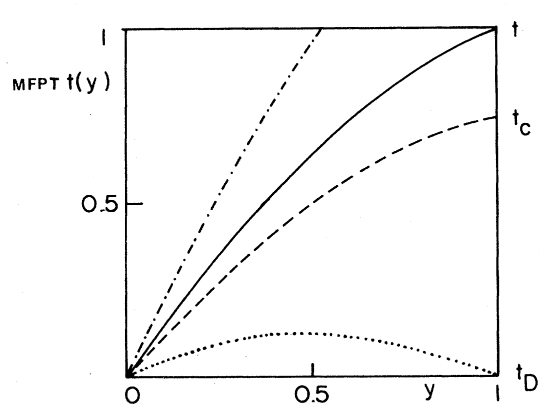

FIG. 2. Values of the mean first-passage time $t(y)$, $y \in [0,1]$, for the parameters: $L=1$, $|a| = a' = 1$, $\mu = \mu' = \frac{1}{2}$ (i.e., $l=2$), and diffusion $D=1$. ——, exact non-Markovian result (15); – – –, crude approximation (22); – · – ·, white shot-noise limit (24a); · · · ·, simple diffusion limit (23).

which for our preparation in (13) simplifies to

$$t(y) = t(y,a) \ . \tag{14b}$$

From (11), this exact MFPT is evaluated to be[13]

$$t(y) = -\frac{y^2}{2D} + \left[\frac{L(L+2l)}{2D} + \frac{1}{\mu}\right]\frac{y}{(L+l)} \ , \tag{15}$$

expressed in terms of the length scale $l = |a|/\mu = a'/\mu'$. In particular, note that the exact non-Markovian MFPT has a jump at $y = L$:

$$t(L) = \frac{L^2 l}{2D(L+l)} + \frac{L}{\mu(l+L)} \ . \tag{16}$$

Next we illustrate the crude approximation scheme in (6). With the initial preparation (13), the non-Markovian retarded master equation is given by [see Ref. 11(b), Eq. (2.9) with $f(x) = 0$ and $g(x) = 1$]

$$\dot{p}_t(x) = |a|\frac{\partial}{\partial x}p_t(x) - (|a| + a')\mu\frac{\partial}{\partial x}\int_0^t \left[\exp - \left[(\mu+\mu') + a'\frac{\partial}{\partial x}\right]s\right]p_{t-s}(x)ds \ . \tag{17}$$

The adjusted operator $\overline{\Omega}_c^{+}$, Eq. (6), is nonseparable, and explicitly reads (θ denotes the step function)

$$\overline{\Omega}_c^{+} h(y) = -|a|\frac{\partial}{\partial y}h(y) + \mu\left[\frac{|a|}{a'} + 1\right]\int_{-\infty}^{\infty} \theta(y)\theta(z-y)\exp\left[-\frac{\mu+\mu'}{a'}(z-y)\right]\frac{\partial}{\partial z}h(z)dz, \quad y \in I \ . \tag{18}$$

From here on, the sailing is smooth though there are still irksome details related to the possible jump of $t_c(y)$ at $y = L^-$. With (6) and (18) we have (prime denotes differentiation with respect to y)

$$-|a|t_c'(y) + \mu\left[\frac{|a|}{a'} + 1\right]\int_y^{\infty} t_c'(z)\exp\left[-\frac{(\mu+\mu')}{a'}(z-y)\right]dz = -\chi(y) \ , \tag{19}$$

where χ is the characteristic function $\chi(y) = 1$, $y \in [0,L]$, $\chi(y) = 0$, $y \notin [0,L]$, and $t_c(y) = 0$ for y not in I. The boundary condition at $y = 0^+$ reads [see (12)]

$$t_c(0^+) = 0 \ . \tag{20a}$$

With a possible jump at $y = L^-$; i.e., $\lim_{y\downarrow L} t_c(y) = 0$, $\lim_{y\uparrow L} t_c(y) = t_c(L) \neq 0$, we must set

$$\frac{\partial}{\partial y}t_c(y) = t_c'(y) - t_c(L)\delta(y-L) \ .$$

Settting $y = L - \epsilon$, $\epsilon \to 0^+$, one obtains from the integral equation (19) the jump condition

$$|a|t_c'(L^-) + \mu\left[\frac{|a|}{a'} + 1\right]t_c(L^-) = 1 \ . \tag{20b}$$

Upon differentiating (19) once more, whereupon one is destroying any information about the boundary conditions, one obtains in the open interval $(0,L)$

$$D\frac{d^2}{dy^2}t_c(y) = -1 \ . \tag{21}$$

This is of the form of the MFPT equation of a Fokker-Planck process describing simple diffusion. Just as with Ref. 6, the absorbing boundary condition in (20b), however, is clearly different from that for simple diffusion, yielding $t_c(L^-) = 0$. Combining (21) with (20), the crude approximation is calculated to be

$$t^{\text{exact}}(y) \geq t_c(y) = -\frac{y^2}{2D} + dy \ , \tag{22}$$

with

$$d = (D/\mu + Ll + \tfrac{1}{2}l^2L^2\mu/D)/[l(D + lL\mu)] \ .$$

A somewhat cumbersome calculation shows that the inequality (7), follows from the inequality $1/\mu' \geq 1/(\mu+\mu')$.[14] On the other hand, without further justification in (21), simply using the absorbing boundary condition $t_c(0) = t_c(L) = 0$ for diffusion [see, e.g., Ref. 9], the resulting MFPT $t_D(y)$ reads

$$t_D(y) = -\frac{y^2}{2D} + \frac{L}{2D}y \ , \tag{23}$$

which disagrees with both the crude approximation in (22) and the exact result in (15) (see Fig. 2).

Moreover, we mention that in the Markovian shot-noise limit, $a' \to \infty$, $\mu' \to \infty$, $D = a^2/\mu$;[11] both (15) and (22) yield the exact result t^{WSN},

$$t^{\text{WSN}}(y) = -\frac{y^2}{2D} + \frac{1}{2D}\left[\frac{2l^2 + 2lL + L^2}{l+L}\right]y \ , \tag{24a}$$

with the jump

$$t^{\text{WSN}}(L) = Ll(L+2l)/[2D(l+L)] \ . \tag{24b}$$

In the white Gaussian limit, $l \to 0$, all our results (15), (22), and (24) coincide, of course, with (23). Finally, the results of this example can also be extended to more general non-Markovian flows, $\dot{x} = f(x) + g(x)\xi(t)$.[15]

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[2]For example, see the very illustrative approach by M. Kac [John von Neumann Lecture, Summer Meeting of Society for Industrial and Applied Mathematics, Stillwater, Oklahoma, 1961 (unpublished)], wherein he succeeds to recast the problem of the MFPT $t(x,p)$ of a harmonic oscillator with the absorbing boundary condition, $t(x,p)=0$, $p \leq 0$, and $x \leq 0$, into a problem of potential theory.

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[10]Those same difficulties occur if one does not use a retarded master-equation dynamics, (3a) and (3b), but uses instead a time-convolutionless formulation [P. Hanggi, H. Thomas, H. Grabert, and P. Talkner, J. Stat. Phys. **18**, 155 (1978); R. F. Fox, J. Math. Phys. **18**, 2331 (1977)].

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[12]Note also that the results in Ref. 9, which are not exact and, additionally, do not possess the correct absorbing boundary condition, nevertheless possess the same Arrhenius factor as the rate calculated earlier in Refs. 11(a) and 11(b).

[13]P. Talkner and I. Jermann, University of Basel (unpublished).

[14]Interestingly enough, the slopes, $t'_{\text{exact}}(0^+)$, $t_c'(0^+)$, and $t_D'(0^+)$ also do not agree with each other.

[15]This work has been presented at the International Conference on Rate Processes and First Passage Times in Chemical Physics, National Institutes of Health, Bethesda, May 6–8, 1985 (unpublished).