

Mean first-passage time of continuous non-Markovian processes driven by colored noise

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An equation for mean first-passage times of non-Markovian processes driven by colored noise is derived through an appropriate backward integro-differential equation. The equation is solved in a Bourret-like approximation. In a weak-noise bistable situation, non-Markovian effects are taken into account by an effective diffusion coefficient. In this situation, our results compare satisfactorily with other approaches and experimental data.

The calculation of mean first-passage times (MFPT's) of a stochastic process is a problem of long-standing interest in connection with topics such as activation rates, mean lifetimes of metastable states, decay times of unstable states, exit problems, etc. The problem of calculating the MFPT's for continuous non-Markovian processes has been recently addressed by several authors.¹⁻¹⁰ Some of these works^{1,2,5,9} consider non-Markovian Brownian motion. In this case the stationary solution of the process is known because of the existence of a fluctuation-dissipation relation. Here we consider a non-Markovian process $q(t)$ driven by colored noise $\xi(t)$. The process $q(t)$ is defined by a stochastic differential equation^{4,6,11}

$$\dot{q} = f(q) + g(q)\xi(t). \quad (1)$$

For definiteness we take $\xi(t)$ to be an Ornstein-Uhlenbeck process: Gaussian with zero mean and correlation $\langle \xi(t)\xi(t') \rangle = (D/\tau) \exp(-|t-t'|/\tau)$. The stationary solution of $q(t)$ is at best known approximately.¹¹ The situation described by (1) is of relevance, for example, for systems under the influence of random external perturbations with a finite correlation time. Experimental data obtained from analog simulations of such situations are now often reported.^{10,12,13} In this paper we derive an equation satisfied by a MFPT of the process $q(t)$. This equation contains essential non-Markovian features. Progress in the calculation of MFPT's for Eq. (1) has been hindered by the lack of knowledge of a non-Markovian equation satisfied by the MFPT. For this reason earlier approaches^{6,10} to the problem were based on Markovian approximations of the process $q(t)$. The equation for the MFPT is solved here in an approximation called Bourret's equation in the context of linear stochastic differential equations.¹⁴ In the weak-noise limit for a bistable situation, we obtain from our solution a formula for a MFPT which has the same formal structure as in the white-noise limit, but with an effective diffusion coefficient $\bar{D}(q)$. This coefficient is a decreasing function of τ . As a conse-

quence the MFPT is predicted to be an increasing function of τ . Our results are compared satisfactorily with other approaches^{6,10} and experimental data.¹⁵

In the limit $\tau \rightarrow 0$ in which $\xi(t)$ in Eq. (1) is a Gaussian white noise, $q(t)$ becomes Markovian, and a well-known formula for the MFPT exists. This formula is obtained¹⁶ by integrating a second-order differential equation for the MFPT. The equation for the MFPT is in turn obtained from a time integration of the backward Fokker-Planck equation associated with (1). An obvious possibility to address the non-Markovian problem is to enlarge the number of variables so that (1) can be rewritten as a two-dimensional Markovian problem for the variables (q, ξ) . The MFPT in the two-variable space satisfies a second-order partial differential equation. The MFPT in multidimensional space can be in general calculated by singular perturbation methods.⁹ In practice these methods are only useful if the stationary solution of the problem is known. In our case, the stationary distribution of the two-variable process (q, ξ) is not known, because the detailed-balance condition is not fulfilled by the Fokker-Planck equation (FPE) associated with this process. One can then envisage two other approaches to the problem. The first is to construct a Markovian approximation for the long-time dynamics of the process $q(t)$. A second more radical approach for dealing with the non-Markovian dynamics is to obtain an appropriate backwards equation for the non-Markovian process. The first approach was followed in Refs. 6 and 10. In Ref. 6, $q(t)$ is approximated by a Markovian process defined by a FPE derived for weak noise ($D \ll 1$) in the long-time limit.¹¹ Results of this calculation show discrepancies with a computer simulation.⁶ We note that this Markovian process is known to have a stationary solution which approximates well the main features of the stationary distribution of the non-Markovian process.¹¹ However, dynamical non-Markovian transient effects are not taken into account by the Markovian process because of the long-time

limit implicit in the approximation. These effects might contribute to the MFPT in an uncontrolled way. The Markovian approximation also involves a truncation of a certain Kramers-Moyal expansion. Such a truncation might also contribute to the observed discrepancies. The approximation in Ref. 10 contains a presumably better truncation in which transient effects are still neglected.

In this paper we follow the second more fundamental approach. An approximate backwards equation for the probability density of (1) has already been derived¹⁷ in the same weak-noise approximation as the FPE in Ref. 11, but keeping transient dynamical effects. This equation has time-dependent coefficients. As a consequence, it does not lead to a closed equation for the MFPT. At best, it could lead to a hierarchy of equations for the different moments of the distribution of passage times. This issue is intimately connected with the use of equations for the probability distribution which are local in time. Here we circumvent the problem by deriving an integro-differential backwards equation with a memory kernel, from which a closed equation for the MFPT can be derived.

Before considering the backwards equation we recall that the forward equations¹⁸ for the probability density of the process $q(t)$ have been derived by many procedures. Generally speaking these equations can be divided in two groups: memory-free equations and integro-differential equations. The first are ordinarily associated with cumulant expansions;^{14,19} they can also be obtained using functional techniques.¹¹ These equations contain time-dependent coefficients if a long-time limit is not taken.¹¹ The second group of equations is associated with

projector-operator techniques.²⁰ However, memory-free equations are also obtained using projector-operator techniques²⁰ and integro-differential equations also follow from cumulant expansions.^{21,22} Of course, all these equations are equivalent²³ when considering an infinite expansion but a low-order truncation may be better in one or the other scheme, depending on the questions addressed or on the statistical properties of the system. For the calculation of a MFPT we use here an integro-differential equation that can be obtained following the cumulant expansion scheme of Terwiel.²¹ The stochastic Liouville equation associated with (1) is

$$\partial_t \rho(q, t) = -\partial_q [f(q) + g(q)\xi(t)] \rho(q, t) \quad (2)$$

and the probability density $P(q, t)$ is

$$P(q, t) = \langle \rho(q, t) \rangle \equiv \mathcal{P} \rho(q, t), \quad (3)$$

where the operator \mathcal{P} averages over the realizations of ξ . Equation (2) is a linear equation for ρ . For this equation, we can follow the same scheme used in Ref. 21 in which the mean value of a variable satisfying a linear stochastic differential equation was obtained. The interaction representation is here introduced as

$$\rho^{(1)}(q, t) = e^{-\partial_q f(q)t} \rho(q, t). \quad (4)$$

Following the steps in Ref. 21 we finally obtain

$$\partial_t P(q, t) = -\partial_q f(q) P(q, t) + \int_0^t dt' K(t | t') P(q, t'), \quad (5)$$

where

$$K(t | t') = \sum_{n=2}^{\infty} K_n(t | t'), \quad (6)$$

$$\begin{aligned} K_n(t | t') &= \int_{t'}^t dt_1 \int_{t'}^{t_1} dt_2 \cdots \int_{t'}^{t_{n-3}} dt_{n-2} (-1)^n (\partial_q g(q)\xi(t) e^{-(t-t_1)\partial_q f(q)} \partial_q g(q)\xi(t_1) e^{-(t_1-t_2)\partial_q f(q)} \\ &\quad \times (1 - \mathcal{P}) \partial_q g(q)\xi(t_2) \cdots (1 - \mathcal{P}) \partial_q g(q)\xi(t_{n-2}) \\ &\quad \times e^{-(t_{n-2}-t')\partial_q f(q)} \partial_q g(q)\xi(t')) \rangle. \end{aligned} \quad (7)$$

A backwards equation is now obtained from (5) as follows: we first Laplace-transform Eq. (5) and formally solve it with the initial condition $P(q, 0) = \delta(q - q_0)$,

$$\hat{P}(q, s) = [s + \partial_q f(q) - \hat{K}(s)]^{-1} \delta(q - q_0). \quad (8)$$

We next transform (8) to a backwards representation. To this end we introduce backwards operators acting on the initial conditions. A backwards operator $O^\dagger(q_0, \partial_{q_0})$ is defined by¹⁷

$$O(q, \partial_q) \delta(q - q_0) \equiv O^\dagger(q_0, \partial_{q_0}) \delta(q - q_0). \quad (9)$$

This is to be satisfied in the usual integral sense. The backwards operator O^\dagger has the same functional form as the ordinary adjoint operator but with q, ∂_q replaced by $q_0, -\partial_{q_0}$. In particular we have $[\partial_q f(q)]^\dagger = -f(q_0) \partial_{q_0}$. Equation (8) can then be rewritten as

$$\hat{P}(q, s) = [s - f(q_0) \partial_{q_0} - \hat{K}_0^\dagger(s)]^{-1} \delta(q - q_0) \quad (10)$$

and using the inverse Laplace transformation

$$\begin{aligned} \partial_t P(q, t) &= f(q_0) \partial_{q_0} P(q, t) \\ &\quad + \int_0^t dt' K_{q_0}^\dagger(t | t') P(q, t'). \end{aligned} \quad (11)$$

This is the desired integro-differential backwards equation in which $K_{q_0}^\dagger(t | t')$ is the inverse Laplace transform of the backwards operator $\hat{K}_{q_0}^\dagger(s)$. It acts on the initial condition of $P(q, t')$. We note that the derivation of (11) requires the time translational invariance of $K(t | t')$. In particular, $\xi(t)$ must be stationary.

The equation for the mean first passage time $T(q_0)$ for the process $q(t)$ to leave the interval (q_a, q_b) with initial condition q_0 ($q_a < q_0 < q_b$) can now be easily obtained from (11).³ The distribution of passage times is $-\partial_t w(t)$ where $w(t) = \int_{q_a}^{q_b} dq P(q, t)$ and $T(q_0) = \int_0^\infty w(t) dt$.¹⁶ With these definitions it immediately follows that

$$f(q_0)\partial_{q_0}T(q_0)+\Omega^\dagger(q_0)T(q_0)=-1, \quad (12)$$

where

$$\Omega^\dagger(q_0)\equiv\int_0^\infty dt K_{q_0}^\dagger(t). \quad (13)$$

Equation (12) is the final closed equation for the MFPT.

Equations (12) and (13) contain the non-Markovian dynamic evolution from $t=0$ onwards. We have been able to obtain a closed equation for $T(q_0)$ due to the convolution form of Eq. (5). We remark that in general $\Omega^\dagger(q_0)$ involves derivatives of all orders with respect to q_0 . Finally we point out that (12) and (13) can be used for any stationary nonwhite process $\xi(t)$ and not only for the Ornstein-Uhlenbeck noise.

A first natural approximation to Eq. (12) which we consider here is to truncate the expansion (6) in the first nontrivial term $n=2$. The character of this approximation is more easily discussed in the equation for the probability density (5). Explicitly, setting $K_n=0$ for $n>2$, this equation becomes

$$\begin{aligned} \partial_t P(q,t) &= -\partial_q f(q)P(q,t) \\ &+ \partial_q g(q) \int_0^t dt' \langle \xi(t)\xi(t') \rangle e^{-(t-t')\partial_q f(q)} \\ &\times \partial_q g(q)P(q,t'). \end{aligned} \quad (14)$$

When dealing with the mean value of a variable satisfying a linear stochastic differential equation, the equation corresponding to (14) is known as the Bourret equation.¹⁴ It is known to be reliable for weak and rapid fluctuations. To be more precise, we note that the second cumulant approximation of Van Kampen¹⁴ (or small- D approximation of Ref. 11) is obtained from (14) when substituting $P(q,t')$ according to a nonstochastic dynamics: $P(q,t') \simeq e^{(t-t')\partial_q f(q)}P(q,t)$ and replacing the upper limit of integration t by ∞ . In this sense (14) contains the second Van Kampen cumulant approximation and additional contributions. Equation (14) is known to be equivalent to the second Van Kampen cumulant approximation after transients have died out and to lowest order in the noise strength.¹⁴ Beyond this limit (14) is not the result of a low-order truncation in an expansion in the noise parameters. It rather corresponds to some resummation of terms in such expansions and it contains contributions from high-order coefficients in a Kramers-Moyal expansion. This view is supported by the fact that Bourret's equation is equivalent to the first truncation of continued-fraction expansions which are of nonperturbative nature.²⁴ An important mathematical difference between (14) and the small- D approximation is that (14) contains derivatives of $P(q,t)$ with respect to q to all orders while the small- D approximation leads to a FPE for $P(q,t)$. One might expect that (14) would be a reasonable approximation to calculate a MFPT. A different suggestive interpretation can be given to the approximation in (14). Indeed, Eq. (14) coincides with the exact equation satisfied by the probability density of the process defined by (1) when $\xi(t)$ is a dichotomous Markov process with the same correlation function as the Ornstein-Uhlenbeck noise considered here.²⁵ Equation (14) corresponds then to an approximation of Ornstein-Uhlenbeck noise (Gaussian) by a dichotomous

Markov process (non-Gaussian).²⁶ This reinterpretation of (14) sets a bound to the validity of (14): the approximation introduces artificial boundaries in the process. These boundaries are those of a process $q(t)$ defined by (1) with $\xi(t)$ in (1) being a dichotomous Markov process. Such boundaries are given by $\bar{D}(q)=0$ where

$$\bar{D}(q)\equiv Dg^2(q)-\tau f^2(q). \quad (15)$$

A criterion of validity of the approximation is that the interval (q_a, q_b) lies within these boundaries. This implies that for a given q_a and q_b , D/τ has to be larger than the value for which q_a or q_b first makes $\bar{D}(q)=0$.

In the approximation (14) discussed above the operator $\Omega^\dagger(q_0)$ is given by

$$\Omega^\dagger(q_0)=Dg(q_0)\partial_{q_0}[1-\tau f(q_0)\partial_{q_0}]^{-1}g(q_0)\partial_{q_0}. \quad (16)$$

Equation (12) with (16) is here solved with the standard boundary conditions^{16,27}

$$\partial_{q_0}T(q_0)|_{q_a}=0, \quad T(q_b)=0. \quad (17)$$

With the introduction of the quantity

$$R(q_0)=[1-\tau f(q_0)\partial_{q_0}]^{-1}g(q_0)\partial_{q_0}T(q_0) \quad (18)$$

Eq. (16) becomes a linear first-order differential equation for $R(q_0)$,

$$\partial_{q_0}R(q_0)=-\frac{f(q_0)}{\bar{D}(q_0)}R(q_0)-\frac{g(q_0)}{\bar{D}(q_0)}, \quad (19)$$

where the effective diffusion coefficient $\bar{D}(q)$ is defined in (15). The boundary condition for $R(q_0)$ associated with (17) is

$$R(q_a)=\tau f(q_0)\partial_{q_0}R(q_0)|_{q_0=q_a}=-\frac{g(q_a)}{f(q_a)}. \quad (20)$$

The solution of (19) with (20) is

$$R(q_0)=-\int_{q_a}^{q_0} dq \frac{g(q)}{\bar{D}(q)} e^{-\hat{U}(q_0,q)} - R(q_a) e^{-\hat{U}(q_0,q_a)}, \quad (21)$$

where

$$\hat{U}(q,q')=\int_q^{q'} dq'' \frac{f(q'')}{\bar{D}(q'')}. \quad (22)$$

The MFPT $T(q_0)$ is finally obtained from (17), (18), and (21) by a simple quadrature

$$\begin{aligned} T(q_0) &= \int_{q_0}^{q_b} dq \frac{Dg(q)}{\bar{D}(q)} \int_{q_a}^q dq' \frac{g(q')}{\bar{D}(q')} e^{-\hat{U}(q,q')} \\ &- R(q_a) \int_{q_0}^{q_b} dq e^{-\hat{U}(q,q_a)} \frac{Dg(q)}{\bar{D}(q)} \\ &- \tau \hat{U}(q_b, q_0). \end{aligned} \quad (23)$$

This equation gives an explicit result for the MFPT obtained as a solution of (12) with well-defined approximations.

A simplified form of (23) is obtained in a symmetric bistable situation in which $f(q)$ has three zeros at

$q_1 < \tilde{q} < q_2$ with q_1, q_2 representing stable states and \tilde{q} an unstable state. If q_a is identified with the left boundary introduced in the approximation $q_0 = q_1$ and $q_0 = q_2$, the two last terms on the right-hand side (rhs) of (23) vanish, and the escape time out of the stable state q_1 is given by the first term on the rhs of (23). If we further assume that D is a small quantity the integrals in (23) can be performed by a steepest-descent approximation. We finally obtain

$$T(q_1) \simeq \frac{2\pi}{|f'(q_1)f'(\tilde{q})|^{1/2}} e^{\hat{U}(q_1, \tilde{q})}. \quad (24)$$

We observe that $T(q_1)$ in (24) has the same functional form as the standard weak noise formula for a Markovian process. The difference is the substitution of a diffusion coefficient [$Dg^2(q)$ in the white-noise limit of $\xi(t)$] by an effective coefficient $\bar{D}(q)$. Since $\bar{D}(q)$ is a decreasing function of τ , $\hat{U}(q_1, q)$ is a positive quantity which grows with τ . As a consequence $T(q_1)$ grows with τ through the exponential factor $\exp[\hat{U}(q_1, \tilde{q})]$.²⁸ To test the validity of the results obtained in the formal presentation given so far we have calculated explicitly $T(q_0)$ for a prototype bistable model in which

$$f(q) = q - q^3 = -\frac{\partial U}{\partial q}, \quad g(q) = 1. \quad (25)$$

The results obtained for $T(q_0)$ from (23) are shown in Figs. 1 and 2 for different values of the noise parameters D and τ . We consider two different definitions of $T(q_0)$. The first corresponds to placing q_0 and q_b at the minima of the potential U , i.e., $q_0 = 1$, $q_b = -1$. In this case we denote $T(q_0)$ as $T_{1,-1}$. As discussed above, the evaluation of $T_{1,-1}$ admits several simplifications in the general expression (23). In the second definition of $T(q_0)$ we take the same initial condition $q_0 = 1$ but q_b is now identified with the maximum of U , $q_b = 0$. In this second case we denote $T(q_0)$ as $T_{1,0}$. The MFPT $T_{1,0}$ is closely related to the mean sojourn time introduced in Ref. 10. Our results for $T_{1,-1}$ and $T_{1,0}$ are compared in Figs. 1 and 2 with the results obtained from the approximations in

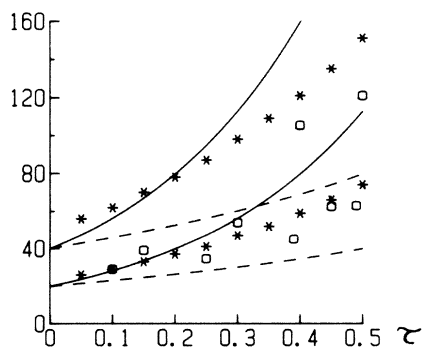


FIG. 1. $T_{1,-1}$ (above) and $T_{1,0}$ (below) vs τ for $D=0.114$. The solid and dashed lines correspond, respectively, to the approximations in Refs. 10 and 6. The asterisks correspond to our result (23). The open circles are experimental data (Ref. 10).

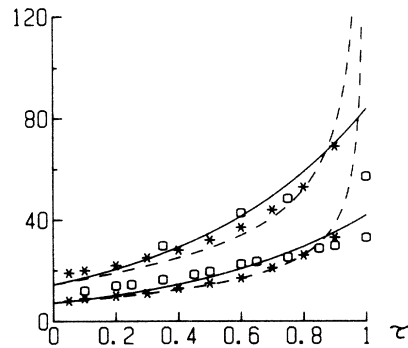


FIG. 2. Same as in Fig. 1 for $D=0.212$.

Refs. 6 and 10,²⁹ and with experimental data from an electronic circuit.¹⁵ The results that follow from the approximation scheme presented in this paper seem to give the best fit to the experimental data (with no adjustable parameters) for the two values of D considered. The fit is better for the smallest value of D .³⁰ Our results predict that the relation $T_{1,-1} = 2T_{1,0}$ is not satisfied. This relation is fulfilled in other approaches.^{6,10} The results obtained for the MFPT (including prefactors) with the approximation used in Ref. 6 are not unreasonable, especially for τ small and the largest value of D studied. The long-time Markovian approximation of Ref. 10 leads, when using no free parameters, to good results for the value $D=0.212$ but the agreement is worse for the other value of D when τ increases. Another point to be noted in Figs. 1 and 2 is that our results for $\tau \rightarrow 0$ do not coincide with those of Refs. 6 and 10. This is due to the fact that our results are not obtained by a steepest-descent approximation. Of course, the limit $\tau \rightarrow 0$ of (24) does coincide with the same limit in Refs. 6 and 10. We finally note that the experimental data for large T might underestimate the true value of the MFPT since realizations of the process with FPT larger than the time of experimental observation are not considered in taking the average.

In summary, we have derived a non-Markovian equation for the MFPT through a backwards equation for the process.³¹ This equation has been solved in a well-defined approximations. For a bistable situation our explicit results are in good agreement with experiments and compare favorably with other previous theoretical approaches based on Markovian approximations.

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- ²⁶This shows how low-order truncations are better suited in different situations: the first truncation in (6) gives the exact result for a nonlinear process driven by dichotomous noise while the first truncation in Van Kampen's cumulant expansion (without neglecting transients) gives the exact results for linear processes driven by Gaussian noise.
- ²⁷These boundary conditions are known to be the appropriate ones for a Markovian process. The proper boundary conditions for a non-Markovian process are a rather delicate matter [P. Hanggi and P. Talkner, *Phys. Rev. A* **32**, 1934 (1985)], which is also bypassed in Markovian approximations to this problem (Refs. 6–8 and 10). We feel that the boundary conditions (17) are physically reasonable for the model presented below in which $T(q_0) \gg \tau$ and q_0 is largely different from q_b .
- ²⁸The growth of the escape time with τ was also obtained in Refs. 4 and 8 in an approximate calculation of an escape rate when $\xi(t)$ is a dichotomous Markov process. The concept of an effective diffusion coefficient also appears there.
- ²⁹The numerical data in Figs. 1 and 2 corresponding to the theory presented in Ref. 10 have been evaluated using the exact values $\langle x^2 \rangle_{st} = 0.83$ ($D=0.212$) and $\langle x^2 \rangle_{st} = 0.86$ ($D=0.114$) instead of using $\langle x^2 \rangle_{st}$ as an adjustable parameter as done in Ref. 10. We also take $T_{1,-1} = 2T_{1,0}$, which follows from the approximation in Ref. 10.
- ³⁰Our results for $D=0.114$ have been obtained here with a minor modification of the effective diffusion coefficient $[\bar{D}(q)]^{-1} \simeq D^{-1}[1 + (\tau/D)f^2(q)]$. We avoid in this way the boundaries introduced in this case by the dichotomouslike approximation (14).
- ³¹The extension of the derivation of Eq. (12) to obtain the equation satisfied by higher-order moments of the first-passage time distribution is not straightforward. It requires a detailed analysis of the implications of the non-Markovian nature of the process in the boundary conditions [L. Pesquera and M. A. Rodriguez (private communication)].