Path Integral Approach to non-Markovian First-Passage Time Problems

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The computation of the probability of the first-passage time through a given threshold of a stochastic process is a classic problem that appears in many branches of physics. When the stochastic dynamics is Markovian, the probability admits elegant analytic solutions derived from the Fokker-Planck equation with an absorbing boundary condition while, when the underlying dynamics is non-Markovian, the equation for the probability becomes non-local due to the appearance of memory terms, and the problem becomes much harder to solve. We show that the computation of the probability distribution and of the first-passage time for non-Markovian processes can be mapped into the evaluation of a path-integral with boundaries, and we develop a technique for evaluating perturbatively this path integral, order by order in the non-Markovian terms.

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The computation of the statistical distribution of the times at which a stochastic process $\xi(t)$ first reaches a given threshold (the so-called first-passage time problem) is a classic problem that appears in many different contexts in physics, chemistry, and biology. It is relevant for instance to problems appearing in reaction rate theory, nucleation theory or neuron firing, to name just a few, and it is treated in a number of textbooks \cite{1,2,3} and reviews \cite{4}. When the underlying dynamics is Markovian, the function $\Pi(x,t)$ that gives the probability distribution that $\xi(t)$ had a value $x$, in the continuum limit satisfies a Fokker-Planck (FP) equation. The fact that one is interested in the first-passage time problem means that one wants to discard the trajectories once they have reached for the first time a given threshold $x_c$. This is implemented imposing on the FP equation an absorbing boundary condition $\Pi(x_c,t) = 0$. The FP equation with this boundary condition, together with the initial condition $\Pi(x,t=0) = \delta_D(x=0)$, where $\delta_D$ is the Dirac delta, can be elegantly solved using the method of images, and one finds \cite{5}

$$\Pi(x;t) = \frac{1}{\sqrt{2\pi t}} \left[ e^{-x^2/(2t)} - e^{-(2x_c-x)^2/(2t)} \right].$$  \hspace{1cm} (1)

When the underlying dynamics is non-Markovian, however, the problem becomes much more difficult. The system acquires memory properties and the probability $\Pi(x,t)$ no longer satisfy a simple diffusion equation such as the FP equation. Furthermore, the correctness of the “absorbing barrier” boundary condition is now far from obvious \cite{6,7}. For these reasons, first-passage problems for non-Markovian processes are known to be very hard to solve, and have been attacked in various ways, see e.g. \cite{8,9,10,11,12,13} and references therein. Our original interest in the problem arose from a specific question in cosmology, namely the computation of the mass distribution of dark matter halos generated by the evolution of non-Gaussian primordial density fluctuations, which can indeed be formulated as a first-passage time problem with non-Markovian dynamics \cite{14}. We think however that the techniques that we have developed in refs. \cite{15,16,17}, and which allowed us to solve our problem, have a broader interest, and we find it useful to present them here in a more general context.

Let $\xi(t)$ be a variable that evolves stochastically with time $t$, with $\langle \xi(t) \rangle = 0$. We consider an ensemble of trajectories starting at $t_0 = 0$ from an initial position $\xi(0) = x_0$, and we follow them for a time $t$. We discretize the interval $[0,t]$ in steps $\Delta t = \epsilon$, so $t_k = k\epsilon$ with $k = 1,\ldots,n$. A trajectory is then defined by the collection of values $\{x_1,\ldots,x_n\}$, such that $\xi(t_k) = x_k$. There is no absorbing barrier, i.e. $\xi(t)$ is allowed to range freely from $-\infty$ to $+\infty$. The probability density in the space of trajectories is

$$W(x_0; x_1,\ldots,x_n; t_n) = \prod_{i=1}^{n} \delta_D(\xi(t_i) - x_i).$$  \hspace{1cm} (2)

In terms of $W$ we define

$$\Pi_c(x_0; x_1,\ldots,x_n; t_n) \equiv \prod_{i=1}^{n-1} \int_{-\infty}^{x_c} dx_i \, W(x_0; x_1,\ldots,x_n; t_n),$$  \hspace{1cm} (3)

where $t_n = n\epsilon \equiv t$ and we will often write $x_n$ simply as $x$. So, $\Pi_c(x_0; x; t)$ is the probability density of arriving in $x$ at time $t$, starting from $x_0$ at time $t_0 = 0$, through trajectories that never exceeded $x_c$. Observe that the final point $x$ ranges over $-\infty < x < \infty$. For later use, we find useful to write explicitly that $\Pi$ depends also on the temporal discretization step $\epsilon$. We are finally interested in its continuum limit, $\Pi_c \to 0$, and we will see in due course that taking the limit $\epsilon \to 0$ of $\Pi_c$ is non-trivial.

The usefulness of $\Pi_c$ is that it allows us to compute the first-crossing rate from first principles, without the need of postulating the existence of an absorbing barrier. Simply, the quantity $\int_{-\infty}^{x_c} dx \, \Pi_c(x_0; x; t)$ gives the probability that at time $t$ a trajectory always stayed in the
region $x < x_c$, for all times smaller than $t$. The rate of change of this quantity is therefore equal to minus the rate at which trajectories cross for the first time the barrier, so the first-crossing rate is

$$F(t) = - \int_{x_0}^{x_c} dx \partial_t \Pi_c(x_0, x; t). \tag{4.1}$$

Observe that no reference to a hypothetical “absorbing barrier” is made in this formalism. We will see below how an effective absorbing barrier emerges from this microscopic approach.

The probability density $W$ can be expressed in terms of the connected correlators $\langle \xi_i \cdots \xi_n \rangle_c$ as

$$W(x_0; x_1, \ldots, x_n; t_n) = \int Dx \sum_{n} \lambda_n \int_{x_n}^{x_c} dx \int_{x_{n-1}}^{x_n} dx \cdots \int_{x_1}^{x_2} dx \langle \xi_i \cdots \xi_n \rangle_c \exp \left\{ \sum_{n=2}^{\infty} \left( \frac{-i}{p!} \sum_{i=1}^{n} \lambda_i \xi_i \right) \right\}. \tag{5}$$

where $\int Dx = \int_{-\infty}^{x_c} dx_1 \cdots dx_n$ and $\xi_i = \xi_i(t_i)$. The problem is therefore reduced to computing the path-integral $\Pi$, over variables $x_i$ bounded by $x_c$, with $W$ given by eq. 5.

We first consider the simple case in which $\xi$ has gaussian statistics (so only the two-point connected function is non-vanishing), and obeys a Langevin equation $\dot{\xi} = \eta(t)$ with a noise $\eta$ whose correlator is a Dirac delta, $\langle \eta(t) \eta(t') \rangle = \delta(t-t')$. In this case the 2-point correlator is easily computed

$$\langle \xi(t_i) \xi(t_j) \rangle_c = \int_0^{t_i} dt_1 \int_0^{t_j} dt_2 \langle \eta(t) \eta(t') \rangle = \min(t_i, t_j), \tag{6}$$

and from this, performing the gaussian integrals in eq. 5, we find

$$W^{\text{gauss}}(x_0; x_1, \ldots, x_n; t_n) = \frac{1}{(2\pi)^n/2} e^{-\frac{1}{2} \sum_{n=1}^{n-1} (x_{i+1} - x_i)^2}. \tag{7}$$

where we denote by $W^{\text{gauss}}$ the value of $W$ when $\xi$ has gaussian statistics and obeys a Langevin equation with Dirac-delta noise. Not surprisingly, in this case we got the Wiener measure. To compute $\Pi^{\text{gauss}}$ by performing directly the integrals over $x_1, \ldots, x_{n-1}$ in eq. 5, and then taking the limit $\epsilon \to 0$ is very difficult, since the integrals in eq. 5 run only up to $x_c$, and already the inner integral gives an error function whose argument involves the next integration variable. In 5, we have then followed a different route. Using the explicit form 7 we proved that

$$\Pi^{\text{gauss}}(x_0; x; \epsilon) = \int_{-\infty}^{\infty} d(\Delta x) \Psi_\epsilon(\Delta x) \Psi^{\text{gauss}}(x_0; x; \Delta x; t), \tag{8}$$

where $\Psi_\epsilon(\Delta x) = (2\pi\epsilon)^{-1/2} \exp(-\Delta x^2/(2\epsilon))$. Equation 8 generalizes the Chapman-Kolmogorov equation, to which it reduces if we send $x_c \to \infty$, i.e. if the integrations in eq. 8 are not bounded, and expresses the fact that the evolution corresponding to a Langevin equation with Dirac-delta noise is a markovian process. Equation 8 allows us to compute the continuum limit of $\Pi^{\text{gauss}}$ as follows. In the limit $\epsilon \to 0$ we have $\Psi_\epsilon(\Delta x) \to \delta_D(\Delta x)$. If $x - x_c < 0$, the integral in eq. 8 includes the support of the Dirac delta, and we just get the trivial identity that $\Pi^{\text{gauss}}(x_0; x; t) = 0$ if $x \geq x_c$. If $x = x_c$ only one half of the support of $\Psi_\epsilon$ is inside the integration region, so we get $\Pi^{\text{gauss}}(x_0; x; t) = (1/2)\Pi^{\text{gauss}}(x_0; x_c; t)$, which again implies $\Pi^{\text{gauss}}(x_0; x; t) = 0$. This is the boundary condition that in the usual treatment is just imposed by hand, while here it follows from the formalism. Consider now eq. 8 when $x < x_c$. In this case the zero-order term in $\epsilon$ gives a trivial identity. Pursuing the expansion to higher orders one finds that, in the limit $(x_c - x)/\sqrt{\epsilon} \to 0^+$, and therefore when $x$ is fixed and strictly smaller than $x_c$ while $\epsilon \to 0^+$, the dependence on the index $\epsilon$ in $\Pi^{\text{gauss}}$ can be expanded in integer powers of $\epsilon$, $\Pi^{\epsilon}(x_0; x; t) = \Pi^{\text{gauss}}(x_0; x; t) + \epsilon \Pi^{\text{gauss}}(x_0; x; t) + \cdots. \tag{9}$

Collecting terms of the same order in $\epsilon$ we then find that, for $x < x_c$, $\Pi^{\epsilon}(x_0; x; t)$ satisfies a FP equation. We therefore end up with a FP equation with the boundary condition $\Pi^{\epsilon}(x_0; x; t) = 0$, so we recover eq. 7. We have therefore succeeded in deriving this standard result from our path integral approach. Observe that the boundary condition $\Pi^{\epsilon}(x_0; x; t) = 0$ emerges only when we take the continuum limit, and does not hold for finite $\epsilon$.

Having computed the path-integral in the markovian case, we can tackle the problem of non-Markovian dynamics treating the non-Markovian terms as perturbations. For illustration, we discuss the case of colored gaussian noise, i.e. again the only non-vanishing connected correlator is the two-point correlator, but now we take it to have the form $\langle \xi(t_i) \xi(t_j) \rangle_c = \min(t_i, t_j) + \Delta(t_i, t_j)$, for some function $\Delta(t_i, t_j) \equiv \Delta_{ij}$. So we want to compute

$$\Pi(x_0; t_n) = \int_{-\infty}^{x_c} dx_1 \cdots dx_{n-1} \int D\lambda \times \exp \left\{ i\lambda_i x_i - \frac{1}{2} \sum_{i=1}^{n} (\min(t_i, t_j) + \Delta(t_i, t_j)) \lambda_i \lambda_j \right\}. \tag{10}$$

where, for simplicity, we set $x_0 = 0$ and we eliminated it from the list of variables on which $\Pi$ depends. We assume that $\Delta_{ij}$ is proportional to a small parameter, and we expand perturbatively in $\Delta_{ij}$. Using $\lambda_i e^{i\lambda x_i} = -i\partial_x e^{i\lambda x}$ and writing $\partial / \partial x_i = \partial_i$, the first-order correction to $\Pi_\epsilon$, that we denote by $\Pi_\epsilon^{\Delta_1}$, is

$$\Pi_\epsilon^{\Delta_1}(x_n; t_n) = \sum_{i,j=1}^{n} \frac{\Delta_{ij}}{2} \int_{-\infty}^{x_c} dx_1 \cdots dx_{n-1} \partial_i \partial_j W^{\text{gauss}}. \tag{11}$$
We rewrite the term $\Delta_{ij}\partial_i\partial_j$ separating explicitly the derivative $\partial_i\equiv \partial/\partial x_i$ from the derivatives $\partial_j$ with $i < n$. Let us at first consider the case in which $\Delta(t_i\text{,} t_j)$ vanishes at least as $t_j-t_i$ as $t_i \rightarrow t_j$. This was indeed the case in the application to the cosmological problem discussed in \[\text{[13]}\]. The more general case will be discussed later. In this case, using also $\Delta_{ij} = \Delta_{ji}$,

$$\frac{1}{2} \sum_{i,j=1}^{n} \Delta_{ij} \partial_i \partial_j = \sum_{i=1}^{n-1} \Delta_{in} \partial_i \partial_n + \sum_{i<j} \Delta_{ij} \partial_i \partial_j,$$

(12)

where $\sum_{i<j} \equiv \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1}$. When inserted into eq. (11) the term $\sum_{i<j} \Delta_{ij} \partial_i \partial_n$ brings a factor $\sum_{i}^{n}$ that, in the continuum limit, produces an integral over an intermediate time $t_i$. Because of this dependence on the past history, we call this the “memory term”. Similarly, the double sum in $\sum_{i<j} \Delta_{ij} \partial_i \partial_j$ gives, in the continuum limit, a double integral over intermediate times $t_i$ and $t_j$, and we call it the “memory-of-memory” term. Thus, $\Pi_{\text{mem}} = \Pi_{\text{mem}} + \Pi_{\text{mem-\mem}}$, where

$$\Pi_{\text{mem}} = \sum_{i=1}^{n-1} \Delta_{in} \partial_i \int_{-\infty}^{x_c} dx_1 \ldots dx_{n-1} \partial_1 W_{\text{gau}},$$

(13)

$$\Pi_{\text{mem-\mem}} = \sum_{i<j} \Delta_{ij} \int_{-\infty}^{x_c} dx_1 \ldots dx_{n-1} \partial_i \partial_j W_{\text{gau}}.$$

(14)

To compute the memory term we integrate $\partial_i$ by parts and we make use of the fact that $W_{\text{gau}}$ satisfies

$$W_{\text{gau}}(x_0; x_1, \ldots, x_i = x_c, \ldots, x_n; t_n) = W_{\text{gau}}(x_0; x_1, \ldots, x_i = x_c; t_i) \times W_{\text{gau}}(x_c; x_{i+1}, \ldots, x_n; t_n - t_i),$$

as can be checked from the explicit expression \[\text{[14]}\], so

$$\int_{-\infty}^{x_c} dx_1 \ldots dx_{n-1} \partial_1 W_{\text{gau}} = \Pi_{\text{gau}}(x_0; x_c; t_i) \Pi_{\text{gau}}(x_c; x_n; t_n - t_i).$$

(15)

(16)

In the continuum limit (if the integral converges, as we will check in a moment), we replace $\sum_{i}^{n-1}$ by $(1/\epsilon) \int_{0}^{t_n} dt_i$ and we get

$$\Pi_{\text{mem}}(x_n; t_n) = \partial_n \int_{0}^{t_n} dt_i \Delta(t_i, t_n) \times \lim_{\epsilon \rightarrow 0+} \frac{1}{\epsilon} \Pi_{\text{gau}}(x_0; x_c; t_i) \Pi_{\text{gau}}(x_c; x_n; t_n - t_i).$$

(17)

Recall that $\Pi_{\text{gau}}(x_0; x_c; t_i)$ represents the probability density for trajectories that start at $x_0$ at the initial time and arrive at $x_c$ at time $t_i$, staying always in the region $x \leq x_c$, for a variable obeying gaussian statistics and driven by a Dirac delta noise. Thus, eq. (17) has a vivid diagrammatic interpretation in terms of a sum over the markovian trajectories that start at $x_0$, touch for the first time the boundary $x_c$ at an intermediate time $t_i$, but rather than crossing the threshold go back into the region $x < x_c$, finally reaching a value $x_c$ at time $t_n$. We see that the probability density $\Pi_{\text{gau}}(x_0; x_c; t_i)$ plays the role that in the perturbative expansion of the path integral in quantum field theory is played by the free propagator, and the whole complexity of non-Markovian dynamics enters through the presence of the boundary at $x = x_c$. The memory-of-memory term can be computed in the same way. Now we integrate by parts the two derivatives $\partial_i\partial_j$ in eq. (11). This leaves us with $W$ evaluated in $x_i = x_c$ and $x_j = x_c$. Using eq. (14) we write it as a product of three terms, and

$$\Pi_{\text{mem-\mem}}(x_0; x_c; t_n) = \sum_{i<j} \Delta_{ij} \Pi_{\text{gau}}(x_0; x_c; t_i)$$

It is quite interesting to observe that the memory term is determined by the finite-$\epsilon$ corrections to the markovian term. We found above that $\Pi_{\text{gau}}(x_0; x_n; t)$ vanishes for $x_n = x_c$. However, we see from eq. (17) that it is not enough to know that $\Pi_{\text{gau}}(x_0; x_c; t_i) = 0$ for $\epsilon \rightarrow 0$, but we also need to know how fast it goes to zero with $\epsilon$. For $x - x_c$ fixed and strictly negative, in the limit $\epsilon \rightarrow 0$ we have seen above that the correction to $\Pi_{\text{gau}}^{\text{gau}}(x_0; 0)$ are $O(\epsilon)$. However, in eq. (17) we need $\Pi_{\text{gau}}^{\text{gau}}$ for $x = x_c$. In this case the form of the correction changes qualitatively. Technically this comes from the fact that, after changing the integration variables from $x_i$ to $y_i = x_i/\sqrt{2\epsilon}$, which makes the exponential factors in eq. (17) independent of $\epsilon$, the lower integration limit in eq. (18) becomes $(x - x_c)/\sqrt{2\epsilon}$. For $x$ fixed and strictly smaller that $x_c$, with $x_c - x$ finite, it approaches eq. (17), plus corrections $O(\epsilon)$. For $x > x_c$ and $x - x_c$ finite it is equal to zero, plus corrections which can be shown to be exponentially small in $\epsilon$, $O(\exp(- (x - x_c)^2/(2\epsilon)))$. These two regimes are connected by an infinitesimal boundary layer, of thickness $|x - x_c| = O(\sqrt{\epsilon})$, where the corrections to the continuum solution are themselves $O(\sqrt{\epsilon})$. In particular, when $x = x_c$, we find in \[\text{[15]}\] that, for $x_0 < x_c$,

$$\Pi_{\text{gau}}^{\text{gau}}(x_0; x_c; t) = \sqrt{\frac{x_c - x_0}{\sqrt{\pi} t^{3/2}}},$$

which is equal to

$$\Pi_{\epsilon=0}(x_n; t_n) = \frac{1}{\pi} \partial_n \int_{0}^{t_n} dt_i \Delta(t_i, t_n) \times \exp\left\{ \frac{x_c - x_n}{\sqrt{2(2\epsilon)}(t_n - t_i)^{3/2}} \right\}.$$
As an application, we illustrate our results setting \( \Delta_{ij} = \kappa t_i (t_j - t_i) / t_j \) for \( t_i \leq t_j \). (The value for \( t_i > t_j \) is obtained by symmetry, \( \Delta_{ij} = \Delta_{ji} \)). This was indeed the form of \( \Delta_{ij} \) in the problem studied in [15], where \( \kappa \approx 0.44 \) played the role of the expansion parameter. All integrals can then be computed analytically, and for the first-crossing rate we find

\[
\mathcal{F}(t) = \frac{1 - \kappa}{\sqrt{2 \pi} t^{3/2}} e^{-x_c^2/(2t)} + \frac{\kappa}{2 \sqrt{2 \pi} t^{3/2}} \Gamma\left(0, \frac{x_c^2}{2t}\right),
\]

where \( \Gamma(0, z) \) is the incomplete Gamma function. The result is shown in Fig. 1 together with the markovian case, which is obtained setting \( \kappa = 0 \).

In the above example, \( \Delta(t_i, t_j) \) goes to zero linearly as \( t_j - t_i \to 0 \). If however \( \Delta(t_i, t_j) \) goes to a non-zero constant at \( t_i = t_j \), we see that the integral over \( dt_j \) in eq. (21) diverges at the lower limit \( t_j = t_i \). At the same time, in eq. (12) we must also include a term proportional to \( \Delta_{ii} \), since \( \Delta_{ii} \) is non-zero, and this term also leads to a divergent integral. After regularizing the sums over \( i, j \) one can extract the divergent part of both integrals, which are both proportional to \( 1/ \sqrt{\epsilon} \), plus the finite part. The divergent parts of these two terms cancel among them, and we remain with a finite result. We refer the reader to appendix B of ref. [15] for details.

The same strategy can be applied to all higher-order correlators. In ref. [17] we performed the computation expending eqs. (3) and (5) to linear order in the three-point correlator \( \langle \xi_i \xi_j \xi_k \rangle \). The result fits quite well the outcome of cosmological N-body simulations with non-Gaussian initial conditions [15], giving further confidence in our technique.

In conclusion, we have developed a very general method for computing systematically the non-Markovian contributions to the first-crossing rate, whenever they can be treated as perturbations of the markovian dynamics.

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