First-Passage Times for Random Walks in Bounded Domains

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We present a novel computational method of first-passage times between a starting site and a target site of regular bounded lattices. We derive accurate expressions for all the moments of this first-passage time, validated by numerical simulations. Their range of validity is discussed. We also consider the case of a starting site and two targets. In addition, we present the extension to continuous Brownian motion. These results are of great relevance to any system involving diffusion in confined media.

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How long does it take for a drunkard to go from a given bar to another one? This time is known in the random walk literature as a first-passage time (FPT), and it has generated a considerable amount of work for many years [1,2]. The importance of FPT relies on the fact that many physical properties, including fluorescence quenching [3], neuron dynamics [4] or resonant activation [5] to name a few, are controlled by first-passage events. Unfortunately, explicit determinations of FPT are most of the time limited to very artificial geometries, such as 1D and spherically symmetric problems [2].

The determination of FPT for random walks in realistic geometries is not just a theoretical challenge in its own right. It is actually a very general issue involved as soon as molecules diffuse in confined media as, for example, biomolecules diffusing in the cell and undergoing a series of transformations at precise regions of the cell. An estimation of the time needed to go from one point to another is then an essential step in the understanding of the kinetics of the whole process.

Very recently, two important advances in the calculation of FPT have been performed. First, in the case of discrete random walks, an expression for the mean first-passage time (MFPT) between two nodes of a general network has been found [6]. So far, however, no quantitative estimation of the MFPT has been derived from this formula. Second, the leading behavior of MFPT of a continuous Brownian motion at a small absorbing window of a general reflecting bounded domain has been obtained [7,8]. In the case when this window is a small sphere within the domain, the behavior of MFPT has recently been derived [9]. This result is rigorous but does not give access to the dependence of the MFPT with the starting site.

In this Letter, we present a new computational method that allows us to quantitatively extend all these results in three directions: (i) We obtain an accurate explicit formula for the MFPT, (ii) we also examine all the moments of the FPT, and (iii) we consider the case with two targets. The method is presented in detail in the case of discrete random walks on regular lattices, and then the extension to continuous Brownian motion is outlined.

We first consider a random walker on a bounded lattice, and we address the question of determining the mean time needed to reach one point of the lattice (target site T) from another one (starting site S). The boundaries are assumed to be reflecting. The starting point of the method is a result known in the mathematical literature as Kac's formula [10]. Indeed, after our previous work about first return times (FRTs) for random walks [11], we found out that Kac's formula allows one to extend our results to general finite graphs. Kac's result concerns irreductible graphs (i.e., from any point one can go to any other point), which admit a stationary probability $\pi(\mathbf{r})$ to be at site **r**. Let us consider random walks starting from a random point of a subset Σ of sites of the lattice, with a probability proportional to the stationary probability. Then the mean FRT of the random walk, i.e., the mean number of steps needed to return to any point of Σ , is, according to Kac's formula, $1/\pi(\Sigma)$, where $\pi(\Sigma) = \sum_{\mathbf{r} \in \Sigma} \pi(\mathbf{r})$. This formula gives FRTs and not FPTs. However, we can

This formula gives FRTs and not FPTs. However, we can use it to derive the MFPT $\langle \mathbf{T} \rangle$ by slightly modifying the original lattice (see Fig. 1): We suppress all the original links starting from the target site *T* and add a new one-way link from *T* to the starting point *S*. In this modified lattice,



FIG. 1. Modifications of the original lattice: Arrows denote one-way links.

the FRT to *T* is just the FPT from *S* to *T* in the former lattice, plus one. In what follows, for the sake of simplicity, we consider only regular 2D or 3D lattices, although the argument may be easily extended to any kind of graph. Let \mathbf{r}_T be the position of the target site and \mathbf{r}_S be the position of the starting site. Denoting $\pi(\mathbf{r}_T) = j$, Kac's formula gives $\langle \mathbf{T} \rangle = 1/j - 1$. Thus, all we need to know is the stationary probability for the modified graph. It satisfies the following equation:

$$\pi(\mathbf{r}) = \frac{1}{\sigma} \sum_{\langle \mathbf{r}', \mathbf{r} \rangle} \pi(\mathbf{r}') + j \delta_{\mathbf{r}\mathbf{r}_S} - \sum_{\langle \mathbf{r}', \mathbf{r}_T \rangle} \frac{j}{\sigma} \delta_{\mathbf{r}\mathbf{r}'}, \qquad (1)$$

where $\langle \mathbf{r}, \mathbf{r}' \rangle$ means that these two sites are neighbors and σ is the number of nearest neighbors of a site (by convention, the sites on the boundaries are their own neighbors). The last two terms of the right-hand side of (1) are due to the modifications of the lattice. To solve this equation, we define the auxiliary function π' , equal to π for $\mathbf{r} \neq \mathbf{r}_T$, with $\pi'(\mathbf{r}_T) = 0$. It satisfies:

$$\pi'(\mathbf{r}) = \frac{1}{\sigma} \sum_{\langle \mathbf{r}', \mathbf{r} \rangle} \pi'(\mathbf{r}') + j \delta_{\mathbf{r}\mathbf{r}_{S}} - j \delta_{\mathbf{r}\mathbf{r}_{T}}, \qquad (2)$$

so that π' has the following expression:

$$\pi'(\mathbf{r}) = \frac{1-j}{N} + jH(\mathbf{r}|\mathbf{r}_S) - jH(\mathbf{r}|\mathbf{r}_T), \qquad (3)$$

where N is the total number of sites, and H is the discrete pseudo-Green function [12], which is symmetrical in its arguments and satisfies:

$$H(\mathbf{r}|\mathbf{r}') = \frac{1}{\sigma} \sum_{\langle \mathbf{r}'', \mathbf{r} \rangle} H(\mathbf{r}''|\mathbf{r}') + \delta_{\mathbf{r}\mathbf{r}'} - \frac{1}{N}.$$
 (4)

Indeed, the solution (3) satisfies Eq. (2) and ensures that π is a probability function (of sum unity). The condition $\pi'(\mathbf{r}_T) = 0$ allows us to compute *j* and to deduce the following exact expression:

$$\langle \mathbf{T} \rangle = N[H(\mathbf{r}_T | \mathbf{r}_T) - H(\mathbf{r}_T | \mathbf{r}_S)].$$
(5)

This formula is equivalent to the one found in Ref. [6] but is expressed in terms of pseudo-Green functions. One advantage of our method is that it may be easily extended to more complex situations, as we will show. Another advantage is that, although the pseudo-Green function His not known in general, it is well suited to approximations. The simplest one is to approximate the pseudo-Green function by its infinite-space limit, the "usual" Green function: $H(\mathbf{r}|\mathbf{r}') \simeq G(\mathbf{r} - \mathbf{r}')$, which satisfies:

$$G(\mathbf{r}) = \frac{1}{\sigma} \sum_{\langle \mathbf{r}', \mathbf{r} \rangle} G(\mathbf{r}') + \delta_{0\mathbf{r}}.$$
 (6)

The value of G(0) and the asymptotic behavior of G are well-known [13]. For instance, for the 3D cubic lattice, we have $G(0) = 1.516\,386$ and $G(\mathbf{r}) \simeq 3/(2\pi r)$ for r large. For the 2D square lattice, we have $G(0) - G(\mathbf{r}) \simeq 2/\pi \ln(r) + 3/\pi \ln 2 + 2\gamma/\pi$, where γ is the Euler gamma constant. These estimations of G are used for all the

practical applications in the following. This infinite-space approximation may be improved by two kinds of corrections. First, the constant term 1/N in Eq. (4) may be taken into account:

$$H(\mathbf{r}|\mathbf{r}') \simeq G(\mathbf{r} - \mathbf{r}') + \frac{1}{N}(\mathbf{r} - \mathbf{r}')^2.$$
(7)

In the 3D case, this "uniform correction" is always weak: Its order of magnitude is at most $N^{-1/3}$. However, in the 2D case, it is negligible only if $N \ln(\mathbf{r}_S - \mathbf{r}_T) \gg (\mathbf{r}_S - \mathbf{r}_T)^2$.

A second correction that may be taken into account is the influence of nearby boundaries. For flat boundaries, it can be computed explicitly. Denoting by $s(\mathbf{r})$ the symmetric point of site \mathbf{r} with respect to the closest flat boundary, *H* becomes

$$H(\mathbf{r}|\mathbf{r}') \simeq G(\mathbf{r} - \mathbf{r}') + G(\mathbf{r} - s(\mathbf{r}')).$$
(8)

If the boundary is not flat, this expression gives only the order of magnitude of the expected correction. These two alternative corrections correspond to two different ways to treat the effect of boundaries: (7) is a mean-field type correction, whereas (8) is a local correction. One should use either (7) or (8) mainly according to the position of the target. A rule of thumb, used in the following, is that as soon as one of the two corrections is negligible, the other one leads to good results. Indeed, the correction (7) is useful for a target far from any boundary, whereas the correction (8) is more appropriate if the target is close to a flat boundary. As for the limitations of these approximations, they are not to be used in two cases: (i) if neither (7) nor (8) are negligible; (ii) if the target is close to an irregular boundary.

We have compared the theoretical predictions with numerical simulations. We first checked (Fig. 2) the behavior of the MFPT when the source-target distance varies (the FPT is averaged over 100 000 random walks). We also studied the influence of the distance between the target and a boundary (Fig. 3), using the correction (8). Finally, we checked that our approximation was also correct for the



FIG. 2 (color online). 3D—Influence of the distance between the source and the target. Simulations (red crosses) vs theory (plain line). The domain is a cube of side 31, the target being in the middle of it. The source takes all the positions in a cube of side 15 centered on the target.



FIG. 3 (color online). 3D—Influence of the distance between the target and a flat boundary. Simulations (red crosses) vs theory (plain line). The domain is a cube of side 41 whose center is at (0, 0, 0); the source is at (0, 0, x - 15), and the target is at (0, 0, x - 20).

2D case (Fig. 4). Since in this case the uniform correction (7) is not negligible, we took it into account.

In all the cases studied, the numerical simulations validate our approximations. Thus, our method provides an efficient way for estimating the MFPT, which up to now was known only formally and for a few specific cases.

Furthermore, it is possible to compute the higher-order moments of the FPT, using an extension of Kac's formula, which gives a relation between the Laplace transform of the FRT to a subset Σ , averaged on Σ , and the Laplace transform of the FPT to this same subset, averaged on the complementary subset $\overline{\Sigma}$.

$$\pi(\Sigma)(\langle e^{-s\mathbf{T}}\rangle_{\Sigma} - e^{-s}) = (1 - \pi(\Sigma))(e^{-s} - 1)\langle e^{-s\mathbf{T}}\rangle_{\bar{\Sigma}}.$$

Both averages are weighted by the stationary probability π . For any starting point M different from T, the behavior of the random walk from M to T is exactly the same on the original and modified lattices until it reaches T. Thus, the FPT from M to T is the same on both lattices. This remark allows one, by applying the above formula to the modified lattice and using the correspondance between the FRT to Tand the FPT from S, to get a relation between the *n*th



FIG. 4 (color online). 2D—Influence of the distance between the source and the target. Simulations (red crosses) vs theory: blue dotted line, without the uniform correction; black plain line (in the middle of the set of points), with this correction. The domain is a square of side 61, the target being in the middle of it, and the source takes all possible positions.

moment of the FPT and the lower-order moments of the FPT:

$$\langle \mathbf{T}^n \rangle_{\mathbf{r}} = \frac{1}{j(\mathbf{r})} \sum_{m=1}^n \sum_{\mathbf{r}' \neq \mathbf{r}_T} (-1)^{m+1} {n \choose m} \pi_{\mathbf{r}}(\mathbf{r}') \langle \mathbf{T}^{n-m} \rangle_{\mathbf{r}'}.$$

We denote by $\pi_{\mathbf{r}}$ the stationary distribution of the modified graph whose starting point is \mathbf{r} . The lowercase \mathbf{r} refers to the starting point of the walk. This allows one, by recurrence, to get an estimation of the *n*th order moment, for large enough domains, but in the 3D case only [in fact, $H(\mathbf{r}|\mathbf{r}')$ has to be negligible when \mathbf{r}' is far from \mathbf{r}] After some calculations which will be detailed in a further publication [14], it can be shown that

$$\langle \mathbf{T}^n \rangle = n! N^n [(H_0 - H(\mathbf{r}_S | \mathbf{r}_T))(H_0 - \bar{H})^{n-1} + \mathcal{O}(N^{-2/3})],$$
(9)

where $H_0 = H(\mathbf{r}_T | \mathbf{r}_T)$ and $\bar{H} = 1/N\sum_{\mathbf{r}} H(\mathbf{r} | \mathbf{r}')$. Note that \bar{H} is independent of \mathbf{r}' due to the symmetry property of H and that \bar{H} scales as $N^{-1/3}$, since $G(\mathbf{r}) \sim 1/r$. A good estimation of \bar{H} , to be used for practical applications, is its value for a spherical domain, computed in the continuous limit, $\bar{H} = (18/5)(3/(4\pi))^{2/3}N^{-1/3}$. The estimations (9) are confirmed by numerical simulations (Fig. 5).

It should be pointed out that the moments (9) are close but not equal (see Fig. 5) to the moments of an exponential distribution of the FPT. However, if the particle starts randomly inside the volume, the moments are the same as those of the exponential distribution, with a correction proportional to $N^{-2/3}$. This property sheds a new light on the quasichemical approximation [8], which assumes that, if a particle starts randomly in the volume, it has a constant exit probability at each time step, which leads to an exponential distribution.

We now turn to the situation where the lattice contains several targets, relevant in many chemical applications [3]. For the sake of simplicity, the calculation is driven in the case of two targets but may be easily extended to more absorbing points. We compute here the eventual hitting



FIG. 5 (color online). 3D—Higher-order moments: Theory (black curve) vs simulation (red crosses). The blue dotted curve is the moments of the exponential distribution whose average time is the MFPT. The *n*th moment is normalized by N^n ; the domain is a cube of side 51 centered on the target at (0, 0, 0) and the source at (2, 2, 1).



FIG. 6 (color online). 2D—Two-target simulations. Simulations (red crosses) vs theory (plain line). One target is fixed at (-5, 0); the source is fixed at (5, 0); the other target is at (x, 3). The domain is a square of side 201; the middle is the point (0, 0).

probability to a specified target P_i , the so-called "splitting probability" [2], as well as the mean time until the particle hits either of the two targets $\langle \mathbf{T} \rangle$. We modify the graph in the same way as in Fig. 1: For both absorbing points, denoted by \mathbf{r}_1 and \mathbf{r}_2 , the bonds relating them to their neighbors become one-way bonds, and a link is added from each target to the starting point \mathbf{r}_S . We denote $\pi(\mathbf{r}_1) = j_1$, $\pi(\mathbf{r}_2) = j_2$, and $j = j_1 + j_2$. Again, the relation $\langle \mathbf{T} \rangle = 1/j - 1$ provides the mean absorption time, and the probabilities to hit \mathbf{r}_1 or \mathbf{r}_2 are, respectively, j_1/j and j_2/j . We obtain a relation analogous to (3):

$$\pi'(\mathbf{r}) = \frac{1-j}{N} + jH(\mathbf{r}|\mathbf{r}_S) - j_1H(\mathbf{r}|\mathbf{r}_1) - j_2H(\mathbf{r}|\mathbf{r}_2);$$
(10)

then, writing $\pi'(\mathbf{r}_1) = \pi'(\mathbf{r}_2) = 0$,

$$\begin{cases} \frac{1-j}{N} + (j_1 + j_2)H_{1s} - j_1H_{01} - j_2H_{12} = 0\\ \frac{1-j}{N} + (j_1 + j_2)H_{2s} - j_2H_{02} - j_1H_{12} = 0, \end{cases}$$
(11)

where $H_{12} = H(\mathbf{r}_1|\mathbf{r}_2)$ and, for i = 1 or 2, $H_{is} = H(\mathbf{r}_i|\mathbf{r}_s)$, $H_{0i} = H(\mathbf{r}_i|\mathbf{r}_i)$. These equations yield exact expressions for the mean absorption time and the splitting probabilities, respectively:

$$\begin{cases} \langle \mathbf{T} \rangle = N \frac{[H_{01} - H_{1s}][H_{02} - H_{2s}] - [H_{12} - H_{2s}][H_{12} - H_{1s}]}{H_{01} + H_{02} - 2H_{12}} \\ P_1 = \frac{H_{1s} + H_{02} - H_{2s} - H_{12}}{H_{01} + H_{02} - 2H_{12}} \\ P_2 = \frac{H_{2s} + H_{01} - H_{1s} - H_{12}}{H_{01} + H_{02} - 2H_{12}}. \end{cases}$$

Again, these expressions give excellent results when compared to simulations (Fig. 6).

We finally address the case of a continuous Brownian motion. The target *T* is now a sphere of radius *a* centered on \mathbf{r}_T , and the Brownian particle has a diffusion coefficient *D*. It still starts from the point \mathbf{r}_S , at a distance *R* from the center of the target. The results are quite similar to those obtained in the discrete case, and the details of the computation will be published in a future paper [14]. The estimated MFPT within the infinite-space approximation are

$$\langle \mathbf{T}_{3\mathrm{D}} \rangle = \frac{V}{4\pi D} \left(\frac{1}{a} - \frac{1}{R} \right); \qquad \langle \mathbf{T}_{2\mathrm{D}} \rangle = \frac{A}{2\pi D} \ln \frac{R}{a}, \quad (12)$$

where V and A are the volume and area of the domains. If the target is approximately centered, the uniform correction gives a contribution to $\langle \mathbf{T} \rangle$ of $-R^2/(6D)$ in 3D and $-R^2/(4D)$ in 2D. The correction due to a flat reflecting boundary is the following:

$$\begin{cases} \langle \mathbf{T}_{3\mathrm{D}} \rangle = \frac{V}{4\pi D} \left(\frac{1}{a} + \frac{1}{2d} - \frac{1}{R} - \frac{1}{R'} \right) \\ \langle \mathbf{T}_{2\mathrm{D}} \rangle = \frac{A}{2\pi D} \left(\ln \frac{R}{a} + \ln \frac{R'}{2d} \right), \end{cases}$$
(13)

with d the distance between the center of the sphere T and the boundary, and R' the distance between this same center and the reflexion of the starting point by the boundary. Note that these results significantly extend the (exact) formula of Pinsky [9], which gives only the leading term in a.

In summary, we have presented here a new method of computation that yields very accurate expressions of mean first-passage times for discrete random walks and continuous Brownian motion. These approximations have proven to be especially useful when the target is roughly in the middle of the bounded domain or near to a flat boundary. This approach also gives access to more complex quantities such as higher-order moments. These results may be of the greatest interest for systems involving diffusion in confined media.

- [1] N. V. Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1992).
- [2] S. Redner, A Guide to First-Passage Processes (Cambridge University Press, Cambridge, England, 2001).
- [3] S. A. Rice, *Diffusion-Limited Reactions*, Comprehensive Chemical Kinetics Vol. 25 (Elsevier, Amsterdam, 1985).
- [4] H. Tuckwell, Introduction to Theoretical Neurobiology (Cambridge University Press, Cambridge, England, 1988).
- [5] C. Doering and J. Gadoua, Phys. Rev. Lett. 69, 2318 (1992).
- [6] J.D. Noh and H. Rieger, Phys. Rev. Lett. **92**, 118701 (2004).
- [7] A. Singer, Z. Schuss, D. Holcman, and R.S. Eisenberg, math-ph/0412048.
- [8] I. Grigoriev, Y. Makhnovskii, A. Berezhkovskii, and V. Zitserman, J. Chem. Phys. 116, 9574 (2002).
- [9] R. Pinsky, J. Funct. Anal. 200, 177 (2003).
- [10] D. Aldous and J. Fill, *Reversible Markov Chains and Random Walks on Graphs*, monograph (1999), http://www.stat.berkeley.edu/users/aldous/RWG/book.html.
- [11] S. Condamin, O. Bénichou, and M. Moreau, Phys. Rev. E 72, 016127 (2005).
- [12] G. Barton, Elements of Green's Functions and Propagation: Potentials, Diffusion and Waves (Oxford University Press, New York, 1989).
- [13] B. Hughes, *Random Walks and Random Environments* (Oxford University Press, New York, 1995), Vol. 1.
- [14] S. Condamin, O. Bénichou, and M. Moreau (unpublished).