Zero Constant Formula for First-Passage Observables in Bounded Domains

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(Received 17 April 2008; revised manuscript received 22 August 2008; published 24 September 2008)

In this Letter, we develop an analytical approach which provides an explicit determination of mean first-passage times (MFPTs) for random walks in bounded domains for a wide class of transport processes. In particular, we derive for the first time explicit expressions of MFPTs for emblematic models of transport in complex media, such as diffusion on deterministic and random fractals. This approach relies on a scale-invariance hypothesis and a large volume expansion of the MFPT, which actually proves to be very accurate even for small system sizes as shown by numerical simulations. This explicit determination of MFPTs can be straightforwardly generalized to further useful first-passage observables such as occupation times and splitting probabilities.

DOI: 10.1103/PhysRevLett.101.130601 PACS numbers: 05.40.Fb, 87.10.−e

First encounter events constitute limiting factors of a wide range of dynamical processes of practical interest. This is exemplified at the microscopic scale by transport limited chemical [1] and biochemical reactions [2–4], and at larger scales by the behavior of animals searching for food resources [5–7] or even the spread of diseases in human social networks [8]. A first step to quantify these first encounter events consists in evaluating a first-passage time (FPT), namely, the time it takes a random walker to reach a given target site [9].

This highly desirable quantity has motivated a huge number of theoretical works in recent years (see [9,10] for review). However, explicit expressions of mean FPTs (MFPTs) in bounded domains often remain out of reach even for simple random walks, and so far have been obtained only in a few specific situations. An important example of exact result is given by mean return times, for which the target and starting points are one and the same, and which actually turn out to be given by an elegant exact expression first derived by Kac [11]. Other explicit formulas have been obtained for exit times (i.e., the time needed to exit a sphere by any of its points) [12,13] or averages of MFPTs over the starting point [14–16], whose drawback is to lose track of the source or target distance dependence.

Recently, a general formula giving the MFPT in scale invariant confined media has been obtained [17,18]. This formula shows a linear scaling of the MFPT with the volume of the confining domain, and puts forward the importance of its dependence on the source or target distance, in particular, in the case of constrained environments such as percolation clusters or other fractal structures. This effect has strong implications in real situations such as chemical reactions in crowded environments like living cells [18,19]. However, this determination of the MFPT is not fully explicit as it involves two constants which have remained undetermined so far.

Here we provide simple relations verified by these constants, which permit us to determine them explicitly and show that they take one and the same value for a wide class of situations. This allows for an *explicit* solution of long standing problems, namely, a zero constant formula of the MFPT in bounded domains for emblematic models of transport such as diffusion on deterministic and random fractals.

We start by extending the theory developed in [17] to compute the MFPT of a Poissonian continuous time random walk [10,20] to a target $\mathbf{r}_T$, starting from a source point $\mathbf{r}_S$, evolving in a discrete bounded domain of N sites. Let $P(\mathbf{r}, t|\mathbf{r}')$ be the propagator, i.e., the probability density to be at $\mathbf{r}$ at time t, starting from $\mathbf{r}'$ at time 0, which satisfies the master equation [21] $\frac{\partial}{\partial t}P(\mathbf{r}, t|\mathbf{r}') = \Delta_{\mathbf{r}}P(\mathbf{r}, t|\mathbf{r}')$, where $\Delta_{\mathbf{r}}$ denotes the transport operator. We assume that this transport operator has symmetric transition rates and that the stationary probability distribution verifies $P_{\text{stat}} = 1/N$. As shown in [17,22,23], the following exact expression for the MFPT (provided it is finite) can be derived:

$$\langle \mathbf{T} \rangle / N = H(\mathbf{r}_T|\mathbf{r}_T) - H(\mathbf{r}_T|\mathbf{r}_S), \tag{1}$$

where $H(\mathbf{r}|\mathbf{r}') = \int_0^\infty (P(\mathbf{r}, t|\mathbf{r}') - 1/N)dt$ is the pseudo Green function of the problem [24], which satisfies

$$-\Delta_{\mathbf{r}}H(\mathbf{r}|\mathbf{r}') = -1/N + \delta_{\mathbf{r},\mathbf{r}'}. \tag{2}$$

A point which will prove to be important in the following is that averaging Eq. (1) for $\mathbf{r}_S$ covering the nearest neighbors of $\mathbf{r}_T$ can be shown using Eq. (2) to give back the expression of the averaged MFPT $\overline{\langle \mathbf{T} \rangle}$ expected from Kac formula [11]:

$$\overline{\langle \mathbf{T} \rangle} = 1/P_{\text{stat}} - 1 = N - 1, \tag{3}$$

where the mean step duration is set to 1. An explicit derivation of this useful formula, which elegantly expresses mean return times of random walks (see [25,26] for recent applications) can be found for instance in [27]. Following [17], we consider the leading order of H for large N, which is precisely the usual Green function G_0:

$$H(\mathbf{r}|\mathbf{r}') \sim G_0(\mathbf{r}|\mathbf{r}') = \int_0^\infty P_0(\mathbf{r}, t|\mathbf{r}')dt, \tag{4}$$

where P_0 is the infinite space propagator and $\sim$ denotes mathematical equivalence for large N. When introduced in the exact Eq. (1), this expansion gives the leading term of the MFPT for large N, with the prescription that all points of the domain boundary go to infinity:

$$\langle \mathbf{T} \rangle / N \sim G_0(\mathbf{r}_T|\mathbf{r}_T) - G_0(\mathbf{r}_T|\mathbf{r}_S). \tag{5}$$

It is useful to notice that this leading term of the MFPT still satisfies the Kac formula.

We now suppose that the transport process and the medium have length scale invariant properties, and therefore assume that the infinite space propagator satisfies the standard scaling:

$$P_0(\mathbf{r}, t|\mathbf{r}') \propto t^{-d_f/d_w} \Pi\left(\frac{|\mathbf{r} - \mathbf{r}'|}{t^{1/d_w}}\right), \tag{6}$$

where the fractal dimension d_f characterizes the accessible volume $V_r \propto r^{d_f}$ within a sphere of radius r, and the walk dimension d_w characterizes the distance $r \propto t^{1/d_w}$ covered by a random walker in a given time t. This formalism, in particular, covers the cases of random walks on fractals [28]. Injecting the scaling (6) in Eq. (5) then yields the large N equivalence of the MFPT first derived in [17]:

$$\langle \mathbf{T} \rangle / N \sim \begin{cases} A - B r^{d_w - d_f} & \text{for } d_w < d_f, \\ A + B \ln r & \text{for } d_w = d_f, \\ A + B r^{d_w - d_f} & \text{for } d_w > d_f, \end{cases} \tag{7}$$

where $r = |\mathbf{r}_T - \mathbf{r}_S|$. In these expressions the constants A and B can be explicitly written in terms of the infinite space propagator [17]. Equation (7) puts forward two distinct regimes. When the exploration is not compact ($d_w < d_f$), as in the case of a Brownian particle in the 3-dimensional space, the dependence on the starting point disappears at large r. On the other hand, in the case of compact exploration ($d_w \geq d_f$), as for subdiffusion on fractals, the mean FPT diverges at large r and the starting point position is crucial.

We now go further and derive new relations involving the unknown constants A and B, making use of the Kac formula (3). Taking $r = 1$ in (7) and comparing with (3) gives

$$1 \approx \begin{cases} A - B & \text{for } d_w < d_f, \\ A & \text{for } d_w = d_f, \\ A + B & \text{for } d_w > d_f. \end{cases} \tag{8}$$

In the case of noncompact exploration, one can check on the example of a nearest neighbors random walk on the square lattice (case where the infinite space Green function is exactly known [10]) that the relation (8) is satisfied numerically with a good approximation [27].

In the case of compact exploration, a second equation can be obtained. In this case, explicit expressions of A and B can be derived from Eq. (5) by extracting the r dependence of G_0 in (4) [17]:

$$A = \lim_{R \to \infty} \left[\int_0^\infty (P_0(0, t) - P_0(R, t))dt - B R^{d_w - d_f} \right] \tag{9}$$

and

$$B = \int_0^\infty \frac{du}{u^{d_f/d_w}} \Pi^*(u^{-1/d_w}). \tag{10}$$

Here the scaling function is regularized according to $\Pi^*(x) \equiv \Pi(0) - \Pi(x)$. Assuming now that the scaling form (6) is valid for any distance r (including $r = 0$), we find from Eq. (9) that $A = 0$. Note that this prediction for A can be also understood by taking the continuous limit of the problem where the step length of the network tends to zero with fixed r and fixed domain volume. As the exploration is compact, the MFPT to a single point remains well defined even in this limit, as opposed to the case of noncompact exploration: in this continuous limit, the limit $r \to 0$ can be safely taken and yields by definition a limit MFPT equal to 0 [19]. Equation (7) gives in turn $\langle \mathbf{T} \rangle (r \to 0) \propto A$ and therefore $A = 0$. Using Eq. (8), our results can then be summarized as follows:

$$\langle \mathbf{T} \rangle / N \sim \begin{cases} 1 + B(1 - r^{d_w - d_f}) & \text{for } d_w < d_f, \\ 1 + B \ln r & \text{for } d_w = d_f, \\ r^{d_w - d_f} & \text{for } d_w > d_f. \end{cases} \tag{11}$$

In the case of compact exploration, the MFPT is therefore *explicitly determined* under the scaling hypothesis (6).

We add that the order of magnitude of the subleading term of this large volume expansion can be evaluated. We start from the exact expression (1) of the MFPT and define the correction ϵ by $H(\mathbf{r}|\mathbf{r}') = G_0(\mathbf{r}|\mathbf{r}') + \epsilon(\mathbf{r}|\mathbf{r}')$. It then follows from (2) and from the equation $-\Delta_{\mathbf{r}} G_0(\mathbf{r}|\mathbf{r}') = \delta_{\mathbf{r},\mathbf{r}'}$ satisfied by the Green function that $\Delta_{\mathbf{r}} \epsilon(\mathbf{r}|\mathbf{r}') = 1/N$. Following [29], we assume further that the diffusion current of ϵ can be approximated by the generalized Ficks's law $J(\epsilon) = K r^{2-d_w} d_r \epsilon(r)$, where ϵ depends only on $r = |\mathbf{r} - \mathbf{r}'|$ in the large volume limit and d_r is the derivative with respect to r. Taking the divergence of this current then gives the transport operator $\Delta_r \epsilon(r) = (K/r^{d_f - 1}) d_r (r^{d_f - d_w + 1} d_r \epsilon(r))$, which finally yields $\epsilon(r) = r^{d_w}/(d_f d_w K N)$. This equation indicates that the subleading term $\epsilon(r)$ of the large N expansion (7) of $\langle \mathbf{T} \rangle / N$ is of order r^{d_w}/N.

We now validate numerically the zero constant prediction (11) on representative examples of compact exploration using exact enumeration methods [28].

Sierpinsky gasket.—The Sierpinsky gasket is a standard example of deterministic fractal (see Fig. 1). We consider triangular gaskets of finite order, and make use of the chemical distance, that is the step length of the shortest path between two points. The fractal dimension of a triangular gasket is then given by $d_f = \ln 3 / \ln 2$ [28], and we are interested in a nearest neighbors random walker on this

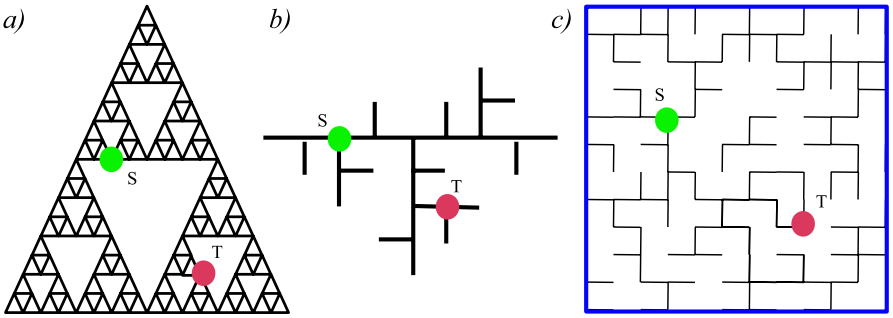

FIG. 1 (color online). Examples of bounded fractal domains. The random walker starts from S and reaches T. (a) Sierpinsky gasket (here of order 5). (b) T graph (here of order 3). (c) 2-dimensional critical percolation cluster (case of bond percolation on a square lattice) in a bounded domain.

structure. The determination of first-passage quantities on Sierpinsky gaskets has motivated a considerable amount of works, which have been mostly limited to either exit times [12,13] or averages of MFPTs over the starting point [15]. Our approach actually allows for an explicit determination of the MFPT to a given target point keeping track of the source or target distance r.

The propagator of the random walk on a Sierpinsky gasket is known to be self-similar after averaging over all pairs of points [30] separated by a distance r, leading to a walk dimension $d_w = \ln 5/\ln 2$ (the exploration is therefore compact). Our approach is hence applicable in this case and following (11) we expect:

$$\langle \mathbf{T} \rangle \sim N r^{\ln(5/3)/\ln 2}. \tag{12}$$

This zero constant prediction has been validated by numerical simulations (see Fig. 2) for gaskets of various sizes, and proves to be very accurate even for small system sizes.

T graph.—Along the same line, our approach applies to the T graph which is another example of deterministic fractal (see Fig. 1 and [9,16] for definition) where exploration is compact ($d_f = \ln 3/\ln 2$ and $d_w = \ln 6/\ln 2$). Figure 2 shows an excellent agreement between the zero constant prediction and numerical simulations.

Critical percolation cluster.—Critical percolation clusters constitute a representative example of random fractals [28,31,32]. Here we consider the case of bond percolation, where the bonds connecting the sites of a regular lattice of the d-dimensional space are present with probability p (see Fig. 1). When $p = p_c$, an infinite cluster of bonds, characterized by its fractal dimension d_f, appears.

We use here the chemical distance as above and consider a nearest neighbor random walk on such critical percolation cluster, with the so-called "blind ant" dynamics [10]: on arrival at a given site $\mathbf{s}$, the walker attempts to move to one of the adjacent sites on the original lattice with equal probability, and remains at site $\mathbf{s}$ if the corresponding link does not exist. As opposed to the previous case, the mean step duration is therefore $2d\langle 1/k \rangle$, where $\langle 1/k \rangle$ is the average of the inverse of the connectivity over all points of the cluster.

In chemical space, the propagator is known to be self-averaging and to verify the scaling (6) [32]. Our approach is therefore applicable and expression (11) can be safely averaged over the disorder, leading to the following zero constant prediction for the disordered average MFPT:

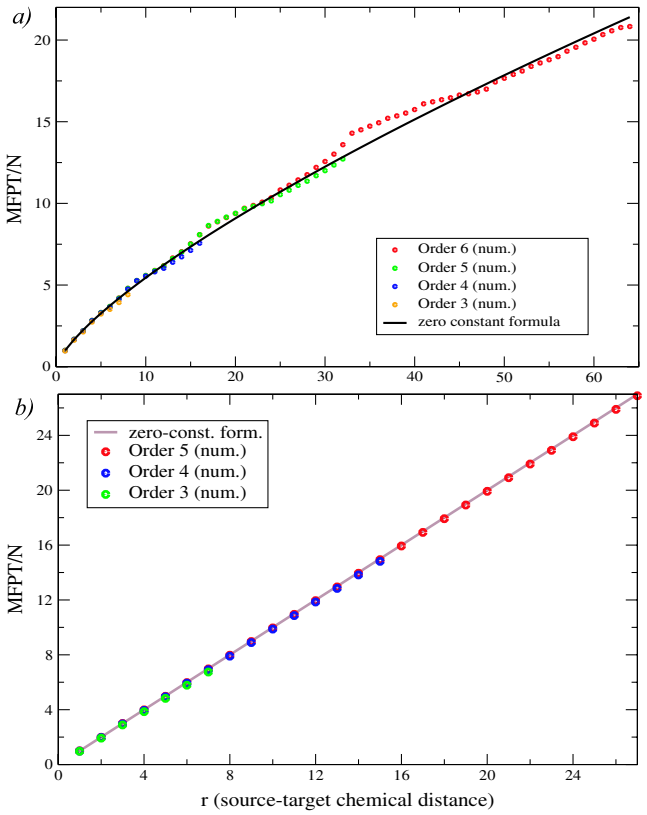

FIG. 2 (color online). Random walks on deterministic fractals of various orders: (a) Sierpinsky gasket and (b) T graph. Numerical simulations (symbols) of the MFPT rescaled by the system size N and averaged over all source or target pairs separated by a given distance r are plotted as functions of r. The zero constant prediction (12) is given by the plain line.

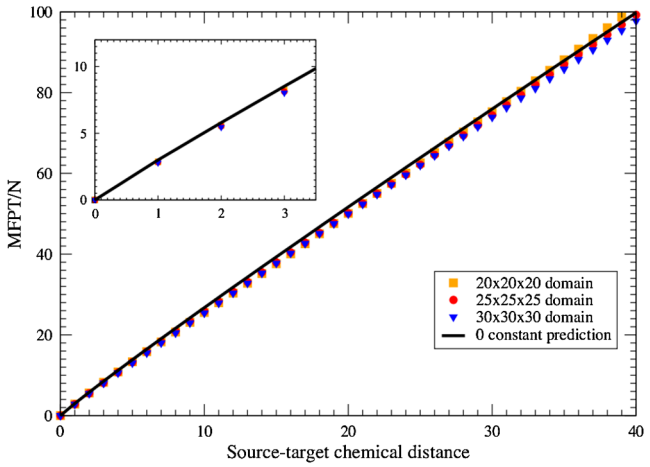

FIG. 3 (color online). Numerical simulation of MFPTs for random walks on 3-dimensional critical percolation clusters embedded in domains with reflecting boundary. For each size of the confining domain, the MFPT, normalized by the number of sites N, is averaged both over the different target and starting points separated by the corresponding chemical distance, and over percolation clusters. The black plain curve corresponds to the zero constant prediction (13) with $d_w - d_f \simeq 0.98$. The zoom (inset) shows that the Kac formula $\langle \mathbf{T} \rangle / N \sim 2d\langle 1/k \rangle \approx 3.1$ is verified for $r = 1$.

$$\langle \mathbf{T} \rangle \sim 2d\langle 1/k \rangle N r^{d_w - d_f}, \tag{13}$$

where $d_f \approx 1.94$, and $d_w \approx 2.93$ [32] and the mean step duration is $2d\langle 1/k \rangle \approx 3.1$ (numerical value) on the example of the 3-dimensional cubic lattice. Figure 3 shows that the simulations fit very well this explicit formula even for systems of small sizes.

To conclude, we have proposed a general theoretical framework which provides a zero constant determination of MFPTs for random walks in bounded domains in the case of compact exploration. This approach leads to an explicit solution of long standing problems, namely, the determination of the MFPT for emblematic models of transport, such as diffusion on deterministic and random fractals. Following [18], this explicit determination of MFPTs can be generalized to obtain zero constant expressions of other relevant first-passage observables, such as occupation times and splitting probabilities.

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