Exact expressions of mean first-passage times and splitting probabilities for random walks in bounded rectangular domains

S. Condamin[a)] and O. Bénichou
Université Pierre et Marie Curie-Paris6, Laboratoire de Physique Théorique de la Matière Condensée, UMR-CNRS 7600, case courrier 121, 4 Place Jussieu, F-75005 Paris

(Received 24 February 2006; accepted 10 March 2006; published online 31 May 2006)

[DOI: 10.1063/1.2192770]

Recently, we have proposed a novel computation method of first-passage times of a random walker between a starting site and a target site of regular bounded lattices of arbitrary shape.[1] Such first passage time properties are, for example, crucial in describing the kinetics of diffusion limited reactions in confined media.[2,3] The obtained expressions involve pseudo-Green functions,[4] which have been estimated according to different approximation schemes. In this Note, we give the exact expression of these pseudo-Green functions in both cases of a rectangular domain with reflecting boundaries and a rectangular domain with periodic boundary conditions. This allows us to provide exact and explicit expressions of mean first-passage times with one or two target sites.

Consider first a random walker starting at the source S of position $\mathbf{r}_S$ of a rectangular regular lattice with reflecting boundary conditions. The mean time it takes to reach the target T of position $\mathbf{r}_T$ for the first time is given by[1]

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

where H is the pseudo-Green function, which satisfies

$$H(\mathbf{r}_i|\mathbf{r}_j) = \frac{1}{\sigma}\sum_{k \in N_i} H(\mathbf{r}_k|\mathbf{r}_j) + \delta_{ij} - \frac{1}{N}, \tag{2}$$

σ being the coordination number of the lattice, namely, 4 for a two-dimensional (2D) lattice or 6 for a three-dimensional (3D) lattice. In this expression, N_i is the set of neighbors of the site i, considering that a site which is at the boundary of the domain is its own neighbor. N is the total number of sites of the lattice. In the presence of two absorbing targets, the mean time it takes to reach either of the two targets is

$$\langle \mathbf{T} \rangle = N\frac{(H_{01}-H_{1s})(H_{02}-H_{2s})-(H_{12}-H_{2s})(H_{12}-H_{1s})}{H_{01}+H_{02}-2H_{12}}, \tag{3}$$

while the eventual hitting probabilities P_i to reach the target i writes

$$P_1 = \frac{H_{1s}+H_{02}-H_{2s}-H_{12}}{H_{01}+H_{02}-2H_{12}},$$
$$P_2 = \frac{H_{2s}+H_{01}-H_{1s}-H_{12}}{H_{01}+H_{02}-2H_{12}}, \tag{4}$$

where $H_{12}=H(\mathbf{r}_{T_1}|\mathbf{r}_{T_2})$ and, for $i=1$ or 2, $H_{is}=H(\mathbf{r}_{T_i}|\mathbf{r}_S)$ and $H_{0i}=H(\mathbf{r}_{T_i}|\mathbf{r}_{T_i})$.

The exact expression of the pseudo-Green function H involved in previous equations may be computed explicitly with the help of Fourier analysis. For a 2D domain with X sites in the x direction and Y sites in the y direction, H writes

$$H(\mathbf{r}|\mathbf{r}') = \frac{1}{N}\sum_{m=1}^{X-1}\sum_{n=1}^{Y-1}\frac{4\cos(n\pi x'/X)\cos(n\pi y'/Y)\cos(m\pi x/X)\cos(n\pi y/Y)}{1-(1/2)(\cos(m\pi/X)+\cos(n\pi/Y))} + \frac{1}{N}\sum_{m=1}^{X-1}\frac{4\cos(m\pi x'/X)\cos(m\pi x/X)}{1-\cos(m\pi/X)} + \frac{1}{N}\sum_{n=1}^{Y-1}\frac{4\cos(n\pi y'/Y)\cos(n\pi y/Y)}{1-\cos(n\pi/Y)}, \tag{5}$$

where x and y are the coordinates of $\mathbf{r}$ and x' and y' those of $\mathbf{r}'$. Here, the coordinates of the left-bottom corner are taken to be equal to $(1/2,1/2)$, so that all the coordinates are half-integers.

Figure 1 shows the mean absorption time $\langle \mathbf{T} \rangle$ given by Eq. (3) as a function of the target positions together with numerical simulations in the case of a 2D square domain. These simulations have been performed with a method based on the exact enumeration method.[5]

Similar results can be obtained in the case of a rectangular domain with periodic boundary conditions. Here, the pseudo-Green function is

 © 2006 American Institute of Physics

Downloaded 28 Apr 2011 to 134.157.8.33. Redistribution subject to AIP license or copyright; see http://jcp.aip.org/about/rights_and_permissions

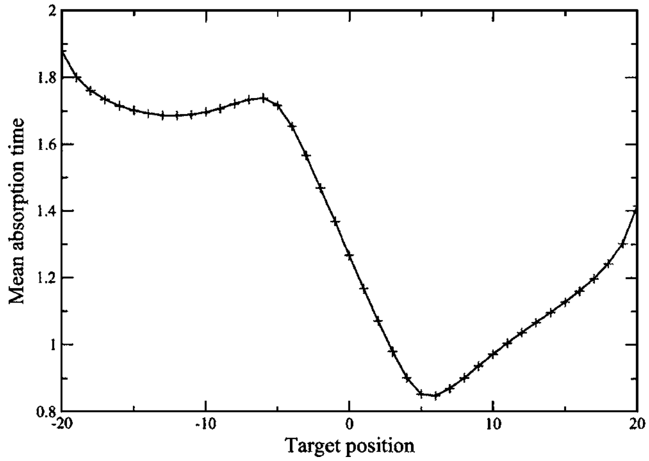

FIG. 1. 2D two-target simulations (red crosses) vs theory (plain line). One target is fixed at $(-5,0)$; the source is fixed at (5,0); the other target is at $(x,3)$. The domain is a square of side 41; the middle is the point (0,0). The absorption time is normalized by the number of sites N.

$$H(\mathbf{r}|\mathbf{r}') = \frac{1}{N}\sum_{m=0}^{X-1}\sum_{n=\delta_{0m}}^{Y-1}\frac{\exp[2im\pi(x-x')/X]\exp[2ni\pi(y-y')/Y]}{1-(1/2)(\cos(2m\pi/X)+\cos(2n\pi/Y))}, \tag{6}$$

where δ_{0m} is the Kronecker delta.

Note that our results can be easily extended to the 3D case.

We gratefully thank S. Redner for suggesting to us the simulation method.

[a]Electronic mail: condamin@lptl.jussieu.fr

[1] S. Condamin, O. Bénichou, and M. Moreau, Phys. Rev. Lett. **95**, 260601 (2005).
[2] S. Rice, *Diffusion-Limited Reactions* (Elsevier, Amsterdam, 1985).
[3] S. Redner, *A guide to First-Passage Processes* (Cambridge University Press, Cambridge, 2001).
[4] G. Barton, *Elements of Green's Functions and Propagation* (Oxford Science, Oxford, 1989).
[5] I. Majid, D. B. Avraham, S. Havlin, and H. E. Stanley, Phys. Rev. B **30**, 1626 (1984).

Downloaded 28 Apr 2011 to 134.157.8.33. Redistribution subject to AIP license or copyright; see http://jcp.aip.org/about/rights_and_permissions