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A first-passage time problem for many random walkers

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Abstract

The passage of ions through membrane channels plays an important role in many fields of biology. An earlier paper [M. Boguñá, A.M. Berezhkovskii, G.H. Weiss, Phys. Rev. E 62 (2000) 3250] developed a toy model for statistical properties of the occupancy of a single site by different numbers of lattice random walkers chosen from an infinite set. It was assumed there that the residence time in one sojourn at the origin differed from the residence time of points elsewhere. In this paper we derive some properties of the corresponding first-passage time to the occupancy of the special site by $k(>1)$ random walkers in one or two dimensions. Results of our study were obtained from an extensive set of simulations.

Keywords: Membrane channels; Lattice random walks

1. Introduction

Most investigations of random walk properties revolve around those that can be analyzed in terms of a single random walker. Nevertheless, there are many problems in statistical physics relating to ensembles of random walks. As a simple example, the problem of simple diffusion on a line of equispaced sites, in which it is stipulated that no more than a single random walker can occupy a single site at any given time, i.e., single-file diffusion, changes the long-time behavior of the mean-squared displacement from being proportional to t to proportionality to $t^{1/2}$ [1]. A further example of collective behavior involves the calculation of the expected number of distinct sites on a lattice visited in a large time t by N random walkers, rather than by a single one [2]. In this case it has been shown that, depending on the magnitudes of t and N and the initial positions of the random walkers, several asymptotic behaviors can be identified even when similar statistical properties of an individual random walk at long times remain quite simple.

One biophysical problem, in particular, has motivated us to analyze a simplified model formulated in terms of the behavior of an ensemble of independent random walks on a lattice [3], namely the transport of metabolite molecules through membrane channels. A feature of some interest in these systems is that the number of ions that can occupy a given channel at any one time is finite. Further, the pore may consist of

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several types of receptors, which suggests that transport dynamics for an ion inside the channel differs from transport mechanisms in the solvent medium. In the model discussed in Ref. [3] the bulk was represented by a CTRW on a simple cubic lattice while the channel was represented by a single site at the origin with properties differing from those of sites in the bulk. This feature was represented by assigning one probability density for the time between successive steps by a random walk in the bulk, and another for the time taken by a molecule in the channel to return to the bulk. The analysis in Ref. [3] led to expressions for the concentration of molecules at the origin, the occupancy, or expected fraction of time, out of a total observation time t, spent in a state with k molecules in the channel, together with the associated variances. The resulting model can be regarded as an extension of the Smoluchowski model for reaction rates, first proposed and analyzed in 1917 [4], and whose properties have subsequently been studied by a large number of investigators [5].

In this paper we describe the results of an investigation of statistical properties of the first-passage time at which the special point to be occupied by exactly k molecules. This will be done for one- and two-dimensional models. The more interesting question relates to three dimensions, but this required tracking so many diffusing particles that it exceeded the capacity of our computing facility. However, our simulation results do suggest generalizations, which at the present time must remain as conjectures.

2. Problem formulation and results

In all cases we discuss only nearest-neighbor lattice random walks so that steps are allowed to nearest-neighboring sites only. Steps of the random walks were made only at discrete times. Let the random level at step n be denoted by K_n, where by the term "level" we mean the number of particles at the origin at step n, let T_k be the time to reach level k for the first time and let $N_k(n)$ be the number of random walkers for which this first-passage time is equal to n. Because the $N_k(n)$ take values over a wide range it is convenient to present results in terms of $\log_{10}[N_k(n)]$ rather than for the function itself. Notice that when a given channel can accommodate no more than k random walkers T_k can be interpreted as the first-passage time to saturation of the special point.

Consider first the case of diffusion in one dimension. The data generated in our simulations were obtained by following 2.5×10^4 random walkers on a line consisting of 10^5 sites with a single anomalous site at the origin. The initial density of random walkers is denoted by ρ. Periodic boundary conditions were used. The discrepancy between a site in the bulk and the anomalous site is characterized in terms of a probability, p. At each step, if a site in the bulk is occupied by a random walker, a random number, θ, is chosen so that when $\theta > p$ the random walker moves to a new site, and conversely, when $\theta < p$ it remains fixed at the site. Hence large p corresponds to a long waiting time. When the site with the random walker is the special point the critical probability replaces p by $p_0 \neq p$, which accounts for the difference between two types of sites.

Typical sets of simulation results for random walks on the line is shown in Figs. 1a and 1b. All of the one-dimensional data, without exception, were well fit to a function of the form

$$\log_{10}[N_k(n)] \approx a_k + b_k \exp\left[-c_k \ln^2\left(\frac{n}{d_k}\right)^2\right], \tag{2.1}$$

where a_k–d_k are parameters estimated from the data. Because of the somewhat complicated form of this expression it would be quite complicated to derive an expression for the moments. An alternative approach is to examine the behavior of $\max_n[N_k(n)]$. The relative errors in a wide neighborhood of the position of the maximum were mostly 1% or less, with the greatest errors occurring at the smallest and largest values of n. Fig. 1c shows the position of the maximum of $N_k(n)$ as a function of n for different values of k and $p = 0.5$. This set of data, as well as others that we have analyzed strongly suggests that the maximum increases linearly with k as is consistent with the plotted data.

Two types of initial conditions were used in studying the system in two dimensions, the first allowing for multiple occupancy of a given site, as was essentially studied in Ref. [3]. In the second, results were found for the case of excluded volumes, where no more than a single random walker is allowed to occupy a single site. In the case of one dimension we generated results only for multiple occupancy.

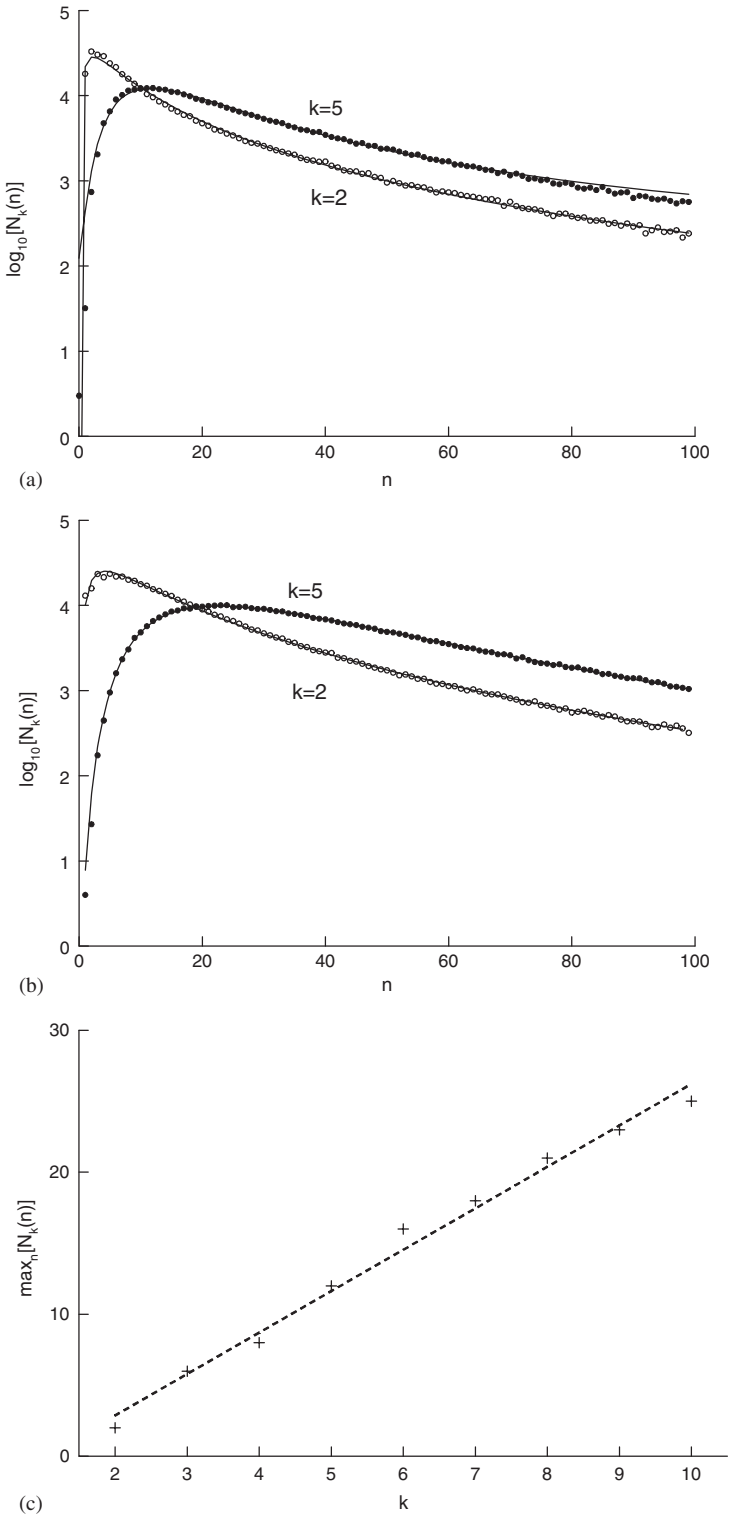

Fig. 1. (a) A plot of $\log_{10}[N_k(n)]$ in one dimension as a function of n for $\rho = 0.25$ and $p = 0.5$ and $k = 2$ and 5. The circles represent simulation data and the solid lines represent the data fit using Eq. (2.1). Both curves are seen to furnish a very good fit in the neighborhood of the maximum. (b) The same comparison made with $p = 0.9$, which is also quite accurate near the maximum. (c) The values of n at which $N_k(n)$ is a maximum as a function of k.

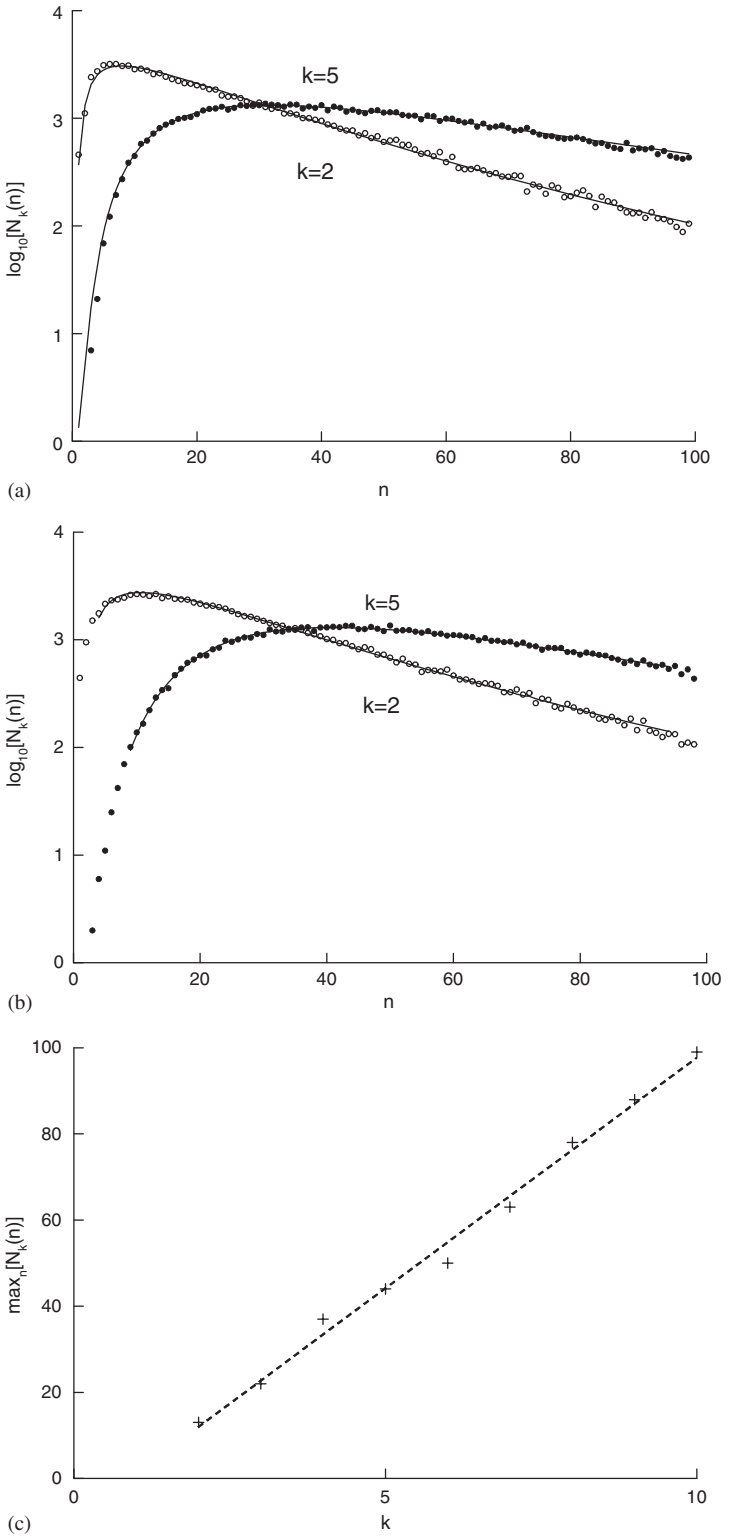

Fig. 2. (a) A plot of $\log_{10}[N_k(n)]$ in two dimensions as a function of n for $\rho = 0.1$ and $p = 0.9$ and $k = 2$ and 5. As in the case of one dimension, similarly good curve fits were found for all values of k from 1 to 10. (b) The values of n at which $N_k(n)$ is a maximum as a function of k for the parameters in (a). (c) The values of n at which $N_k(n)$ is a maximum as a function of k in two dimensions.

The results in two dimensions take a slightly simpler form than those for one dimension. Again, the same form of mathematical function provides an excellent fit for all of the data that we analyzed. In this case Eq. (2.1) is replaced by a formula whose specification requires only three parameters:

$$\log_{10}[N_k(n)] \approx a_k \exp\left(-b_k n - \frac{c_k}{n}\right). \tag{2.2}$$

This function, considered as a function of n, proved to be independent of the choice of the initial condition. Some typical results of our simulation results and Eq. (2.2) are shown in Fig. 2. Our data lead us to conjecture that in three dimensions the dependence on n will also be uniform over a wide range. That is, the expression for the distribution will take the same form as a function of n and that the position of the maximum increases approximately linearly with k. One further extension of some interest would be to divide the space into two parts separated by a reflecting line or plane, with different concentrations of random walkers in each half space. Since, in this case the statistical properties of the arrival rate of random walkers at the special site differ depending on which side of the separating barrier is the source, we might expect that the mathematical fitting functions for $\log[N_k(n)]$ as a function of n might change. However, we might also expect that the position of the maximum with respect to k would remain an approximately linearly dependent function of k.

There are a number of other recent studies, both theoretical and experimental, of properties of materials with a single trap, either perfect or partial, in the presence of a diffusing liquid [6,7]. These, however, focus on properties of the solute in a neighborhood of the trapping site, which enters only peripherally into the present set of simulations.

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