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Repeated bond traversal probabilities for the simple random walk

T Antal[1], **H J Hilhorst**[2] **and R K P Zia**[3]

[1] Département de Physique Théorique, Université de Genève, CH 1211 Genève 4, Switzerland
[2] Laboratoire de Physique Théorique, Bâtiment 210, Université de Paris-Sud, 91405 Orsay cedex, France
[3] Center for Stochastic Processes in Science and Engineering, Department of Physics, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061, USA

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Abstract

We consider the average number $B_m(t)$ of bonds traversed exactly m times by a t step simple random walk. We determine $B_m(t)$ explicitly in the scaling limit $t \to \infty$ with $m/\sqrt{t}$ fixed in dimension $d = 1$ and $m/\log t$ fixed in dimension $d = 2$. The scaling function is an erfc in $d = 1$ and an exponential in $d = 2$.

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1. Introduction

The simple random walk is a venerable problem, finding its applications in many areas of statistical physics. Despite its long history, novel aspects continue to surface. Motivated by recent experiments on gas transport properties in polycarbonate films, we are led to the following question. Given a simple walk of a certain length on a lattice, how frequently will it traverse a particular bond? Remarkably, distributions of this type are not, to the best of our knowledge, in the literature. This note will be devoted to our findings.

Let us first provide a brief summary of the experiment [1] and a proposed model [2] which gave rise to the question posed here. The experiments explore the effects of cooling rates and physical ageing on polycarbonate films. Specifically, thin films ($\sim$0.1 mm) are prepared by quenching a melt at various rates, so that the polymers are found in a glassy state. Their permeability to various gases, due to a pressure gradient across the film, is measured. In the steady state, a constant flux of gas molecules diffuses through the film. The dependence of this flux on how the samples are prepared and how they are aged is of interest in the context of both fundamental and applied research. A natural paradigm for this process is diffusion through random media. The question is how to account for the effects of ageing on the randomness in the medium. One possibility is to model the voids in the medium by 'cells', with the polymers forming the 'walls'. The gas molecules diffuse from cell to neighbouring cell, via

simple activation over the barriers formed by the walls. If the barriers are of uniform height (i.e. 'walls' of uniform thickness) then finding the flux is a text book exercise. However, nonuniform barrier heights should be expected and a model for the height distribution would be helpful.

In a simplified two-dimensional version, the cells/walls are just squares/bonds on a square lattice. Monomers would occupy a single bond, linking up to form a polymer chain of a fixed length. Given the density of polymers, it is trivial to find the *average* number of monomers on each bond. This number would set the typical scale for the barrier height, while the *distribution* of monomers on each bond will provide a measure of the randomness. Ignoring interactions between monomers (as a modest beginning), this distribution is just an appropriate convolution of the probability that a single polymer covers a bond a given number of times. Thus, we are led to study the frequency of bond-traverses by a random walker.

Let a simple random walk start at the origin of a d-dimensional hypercubic lattice. We wish to know the average number of bonds $B_m(t)$ that it has traversed exactly m times. This quantity satisfies

$$\sum_{m=1}^{\infty} B_m(t) = B(t) \qquad \sum_{m=1}^{\infty} m B_m(t) = t \tag{1}$$

where $B(t)$ is the average total number of distinct bonds traversed by the walk.

If for $t \to \infty$ asymptotically $B(t) \simeq \beta(t)$, then one may reasonably expect that in this limit $B_m(t)$ can be expressed as a scaling function of $m\beta(t)/t$. The sum rules (1) then imply that $B_m(t)$ takes the form

$$B_m(t) \simeq \frac{\beta^2(t)}{t} \mathcal{B}\left(\frac{m\beta(t)}{t}\right) \tag{2}$$

where $\mathcal{B}$ is a scaling function.

In this paper, we will explicitly find $\mathcal{B}$ (and β) in spatial dimensions $d = 1$ and $d = 2$, thereby justifying the scaling form (2). It appears that $\mathcal{B}$ is an error function (erfc) in $d = 1$ and an exponential in $d = 2$. In $d = 2$ we determine, moreover, the leading-order correction to the scaling behaviour (2).

2. Generating function method for repeated bond traversals

In order to determine $B_m(t)$ we need the following notation. Let the vector δ denote any of the d basis vectors of the lattice. Let (x, δ) denote the bond between the sites x and $x + \delta$ (the fact that this bond is identical to $(x + \delta, -\delta)$ is of no importance). Let $B_m(x, \delta; t)$ be the probability that (x, δ) is traversed exactly m times, irrespective of the direction. Then

$$B_m(t) = \sum_{(x,\delta)} B_m(x, \delta; t) \tag{3}$$

where each bond occurs exactly once in the summation. The quantity $B_m(x, \delta; t)$ may be calculated by an adaptation of the analogous method for multiple visits to the same *site* [3]. Let $F(x, \delta; t)$ be the probability that the first traversal of (x, δ) occurs at the tth step, with $t = 1, 2, \ldots$. It is convenient to set $F(x, \delta; 0) \equiv 0$.

For any $X(t)$ defined for $t = 0, 1, 2, \ldots$ we may introduce the generating function $\hat{X}(z) \equiv \sum_{t=0}^{\infty} z^t X(t)$. Let furthermore $R(\tau)$ be the probability that, given a traversal has taken place, the next one occurs exactly τ steps later with $\tau = 1, 2, \ldots$. Then $R(\tau) = F(0, \delta; \tau)$

and hence $\hat{R}(z) = \hat{F}(0, \delta; z)$. Reasoning in a similar way as for the site problem, one finds that

$$\hat{B}_m(z) = \frac{1}{1-z}\left[\sum_{(x,\delta)} \hat{F}(x, \delta; z)\right][1 - \hat{R}(z)]\hat{R}^{m-1}(z) \qquad m = 1, 2, \ldots. \tag{4}$$

Here the function $\hat{F}$, which implies $\hat{R}$, still has to be found.

Let $G(x; t)$ be the probability that after t steps the walk is at lattice site x, for $t = 0, 1, 2, \ldots$. Let $G(x, \delta; t)$ denote the probability that at its tth step it traverses (in either direction) the bond (x, δ), for $t = 1, 2, \ldots$. We set additionally $G(x, \delta; 0) \equiv 0$. Since (x, δ) can be traversed starting either from x or from $x + \delta$, we have

$$G(x, \delta; t) = \frac{1}{2d}[G(x; t-1) + G(x+\delta; t-1)] \qquad t = 1, 2, \ldots. \tag{5}$$

By a slight extension of the standard procedure for calculating first passage probabilities on sites [3–5], we have here

$$G(x, \delta; t) = F(x, \delta; t) + \sum_{\tau=0}^{t} F(x, \delta; \tau)G(0, \delta; t-\tau) \qquad t = 1, 2, \ldots. \tag{6}$$

In terms of generating functions, equations (5) and (6) become, respectively, $\hat{G}(x, \delta; z) = (z/2d)[\hat{G}(x; z) + \hat{G}(x+\delta; z)]$ and $\hat{F}(x, \delta; z) = \hat{G}(x, \delta; z)/[1 + \hat{G}(0, \delta; z)]$. Elimination of $\hat{G}(x, \delta; z)$ from this pair of equations yields

$$\hat{F}(x, \delta; z) = \frac{z}{2d}\frac{\hat{G}(x; z) + \hat{G}(x+\delta; z)}{1 + \frac{z}{2d}[\hat{G}(0; z) + \hat{G}(\delta; z)]}. \tag{7}$$

This achieves the reduction of the desired function $\hat{F}(x, \delta; z)$ to the known function $\hat{G}(x; z)$. Note that expression (7) has the required invariance under the replacement $(x, \delta) \to (x+\delta, -\delta)$. We now exploit the well-known relations $\hat{G}(\delta; z) = [\hat{G}(0; z) - 1]/z$ and $\sum_x \hat{G}(x; z) = 1/(1-z)$. Upon combining these with equations (4) and (7) one gets, writing henceforth $G(z) \equiv \hat{G}(0; z)$, a fully explicit expression for the generating function $\hat{B}_m(z)$ in terms of $G(z)$,

$$\hat{B}_m(z) = \frac{z}{(1-z)^2}\frac{(2d)^2}{[2d + z\tilde{G}(z)]^2}\left[\frac{z\tilde{G}(z)}{2d + z\tilde{G}(z)}\right]^{m-1} \tag{8}$$

where $\tilde{G}(z)$ is defined by

$$\tilde{G} \equiv z^{-1}[(1+z)G(z) - 1].$$

The mth coefficient is extracted as

$$B_m(t) = \frac{1}{2\pi \mathrm{i}}\oint \frac{\mathrm{d}z}{z^{t+1}}\hat{B}_m(z) \tag{9}$$

where the integral runs counterclockwise around the origin. To make $B_m(t)$ more explicit, we have to consider each spatial dimension separately.

3. One dimension

In dimension $d = 1$ we have to evaluate equation (9) with [3, 4] $G(z) = (1 - z^2)^{-1/2}$. It turns out to be advantageous to consider the differences $B_{m+1}(t) - B_m(t)$. After slight rewriting, this yields

$$B_{m+1}(t) - B_m(t) = -\frac{1}{\pi \mathrm{i}}\oint \frac{\mathrm{d}z}{z^{t+m+2}}\left[\sqrt{\frac{1+z}{1-z}} - 1\right]\left[1 - \sqrt{1-z^2}\right]^m. \tag{10}$$

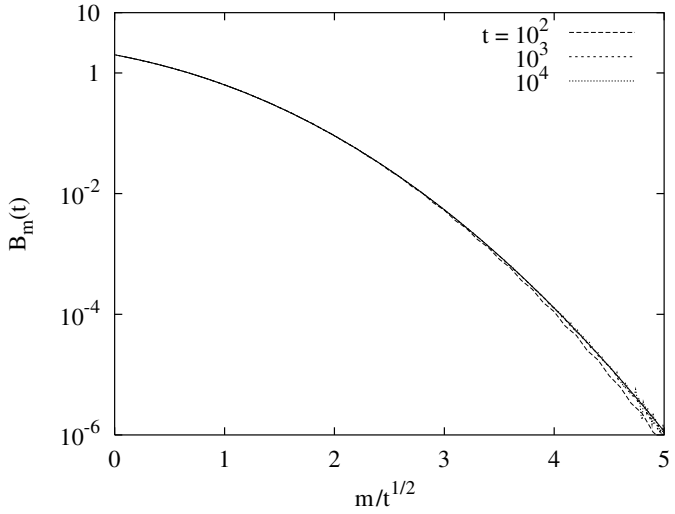

Figure 1. Simulation results for $B_m(t)$ in one dimension at different finite values of time and its scaling form in the $t \to \infty$ limit (solid line).

We will now fold the integration path around the branch cut that runs from $z = 1$ to $z = \infty$ along the positive real axis. In the limit $t \to \infty$ we expect a meaningful result only if also $m \to \infty$ at fixed ratio $m/\sqrt{t}$. We anticipate that in this limit the integral on z draws its main contribution from a region at a distance of order $t^{-1/2}$ from the branch point at $z = 1$. We therefore introduce the scaling variable

$$\mu_1 = m/\sqrt{2t} \tag{11}$$

and the scaled variable of integration $y = (z - 1)t$. The integrand of equation (10) may now be expanded in powers of $t^{-1/2}$ at fixed μ and y. This leads to

$$B_{m+1}(t) - B_m(t) = -\sqrt{\frac{2}{\pi^2 t}} \int_0^\infty \frac{\mathrm{d}y}{\sqrt{y}} (\mathrm{e}^{2\mathrm{i}\mu_1\sqrt{y}} + \mathrm{e}^{-2\mathrm{i}\mu_1\sqrt{y}})\, \mathrm{e}^{-y} \tag{12}$$

where the two terms on the right-hand side come from above and below the branch cut, respectively. The integral is easily found to be equal to $-2^{3/2}(\pi t)^{-1/2}\, \mathrm{e}^{-\mu_1^2}$. With the boundary condition $B_\infty(t) = 0$ we therefore find upon integrating

$$B_m(t) = 2\,\mathrm{erfc}(\mu_1) + \mathcal{O}(t^{-1/2}) \tag{13}$$

which is the final result, valid for $t \to \infty$ at fixed μ_1. When summing equation (13) on m (or alternatively when evaluating the integral obtained by summing equation (9) on m), one obtains $B(t) \simeq \sqrt{8t/\pi}$. Together with equation (13) this confirms the validity of the hypothesized scaling form (2).

In order to compare the large time scaling behaviour of $B_m(t)$ with its finite time forms, we have performed Monte Carlo simulations. For $t = 10^2, 10^3, 10^4$ the bond distribution was averaged over several independent runs. Figure 1 shows that for increasing values of t the simulation data rapidly converge to the scaling function, and they are practically indistinguishable on this figure for $t \geqslant 10^3$.

4. Two dimensions

For a two-dimensional square lattice, the expansion [3, 4] $G(z) = \frac{1}{\pi}\log\frac{8}{1-z} + \mathcal{O}((1-z)\log(1-z))$ enables one to evaluate equation (9) for t asymptotically large. The only integral whose asymptotic behaviour we need is [5, 6]

$$\frac{1}{2\pi\mathrm{i}}\oint\frac{\mathrm{d}z}{z^{t+1}}\frac{1}{(1-z)^2}\frac{\pi^n}{\log^n\frac{8}{1-z}} = \frac{\pi^n t}{\log^n 8t}\left[1+\frac{n(1-C)}{\log 8t}+\mathcal{O}(\log^{-2}8t)\right] \tag{14}$$

where $C = 0.577\,215\ldots$ is Euler's constant. We anticipate a meaningful result for $t\to\infty$ if also $m\to\infty$ in such a way that the ratio $m/\log t$ remains fixed. We expect that in this scaling limit the z integral will draw its main contribution from a region in the complex plane near the branch point $z = 1$ where the ratio $m/G(z)$ is finite. Keeping this in mind, we expand the integral (9) for $B_m(t)$ as

$$B_m(t) = \frac{1}{2\pi\mathrm{i}}\oint\frac{\mathrm{d}z}{z^{t+1}}\frac{1}{(1-z)^2G^2(z)}\,\mathrm{e}^{-2m/G(z)}\left[1+\left(\frac{m}{G(z)}-1\right)\frac{1}{G(z)}+\mathcal{O}(G^{-2}(z))\right]. \tag{15}$$

We may now insert in (15) the explicit expression $G(z)\simeq\frac{1}{\pi}\log\frac{8}{1-z}$, knowing that the $\mathcal{O}((1-z)\log(1-z))$ terms in the expansion of $G(z)$ will contribute only terms with higher powers of t^{-1} to the final asymptotic series. The exponential in equation (15) may then be expanded, the resulting series integrated term by term with the aid of equation (14), and summed again. Upon introducing the scaling variable

$$\mu_2 = \frac{2\pi m}{\log 8t} \tag{16}$$

one finds the final result

$$B_m(t) = \frac{4\pi^2 t}{\log^2 8t}\,\mathrm{e}^{-\mu_2}\left[1+(\mu_2-2)\frac{\frac{\pi}{2}+1-C}{\log 8t}+\mathcal{O}(\log^{-2}8t)\right] \tag{17}$$

valid for $t\to\infty$ at fixed μ_2. As expected, the correction terms decay only as powers of the inverse logarithm of the number of steps. The next few higher order terms in the asymptotic series (17) may be calculated without great effort. Since the kth order correction term is multiplied by a kth degree polynomial in μ_2, this is actually an expansion in powers of $\mu_2/\log 8t$. One may verify that equation (17) satisfies the sum rules (1) up to and including the first-order correction term. The scaling function $\mathcal{B}$ introduced in equation (2) here appears to be a simple exponential. One finds that the average total number of bonds traversed increases as $\beta(t) = 2\pi t/\log 8t + \mathcal{O}(t\log^{-2}8t)$.

Figure 2 compares simulation data for $t = 10^2, 10^3, \ldots, 10^8$ with the theoretical scaling law (the first term of equation (17)). The $t = 10^2$ data are also compared with the exact curve, which we obtained by Taylor expanding equation (8) through the one-hundredth term with the aid of a symbol manipulation program. For $t = 10^8$ the scaling law plus leading correction (the first two terms of equation (17)) is also displayed. Upon collapsing the data of figure 2 one finds figure 3, which shows that in $d = 2$ the convergence to the asymptotic scaling law is very slow.

5. Concluding remarks

We conclude this paper with a series of comments and remarks.

An alternative route to $B_m(t)$ is to consider a complementary process, by focusing on a *particular* bond in, say, a finite periodic L^d lattice. Now, we can ask how often this bond is traversed by a t step random walk which starts at x_0 and ends at x. By summing over

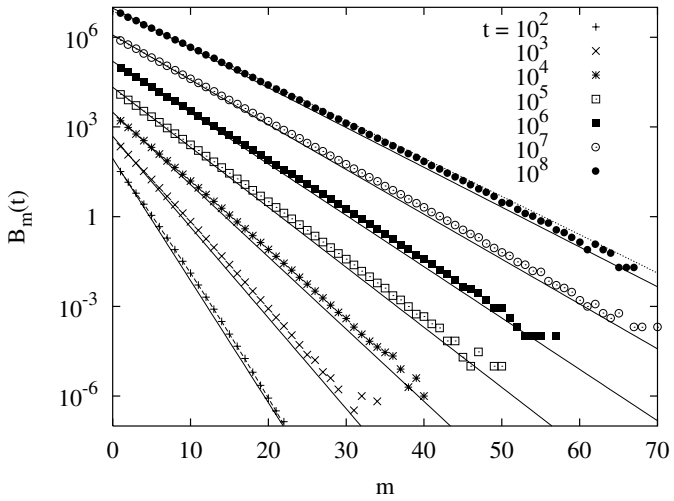

Figure 2. Simulation data for $B_m(t)$ in two dimensions at different values of time (symbols) compared with the theoretical scaling form (solid lines). The exact result for $t = 10^2$ (dashed line) and the scaling law plus leading correction for $t = 10^8$ (dotted line) are also displayed.

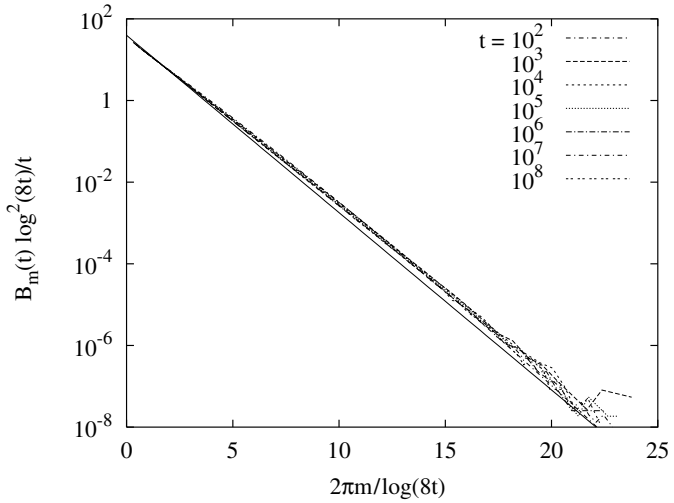

Figure 3. Data collapse of two-dimensional simulation results for $B_m(t)$. The $t \to \infty$ scaling limit is shown as a solid line.

(x, x_0) and invoking translational invariance, we obviously access $B_m(t)$. In this approach, we can easily generalize the problem to a study of the frequency of traversing in only *one direction*. To solve both problems, consider a modified random walker for which the rate of traversing our chosen bond is $p/2d$ instead of $1/2d$. Solving the master equation for $P(x, t|x_0, 0; p)$ (the usual probability) by standard generating function techniques and defining $\tilde{B}(p, z) \equiv \sum_{x,x_0} \sum_{t=0}^{\infty} z^t P(x, t|x_0, 0; p)$, we obtain

$$\tilde{B}(p, z) = \frac{L^d}{1 - z} - \frac{2z(1 - p)}{(1 - z)^2[2d + (1 - p)z\tilde{G}(z)]}. \tag{18}$$

The first term represents, since $\sum_x P(x,t|x_0,0;\ p=1)=1$, the L^d points of origination of the walks we considered. Due to this difference in normalization, the bivariate generating function for $B_m(t)$, i.e. $\sum_{m=1}^{\infty}\sum_{t=0}^{\infty} p^m z^t B_m(t)$, is precisely $d[\tilde{B}(p,z)-\tilde{B}(0,z)]$. With the extra factor d, the quantity $d\tilde{B}(1,z)$ represents nothing but the total number of bonds in the lattice. Interestingly, this $\tilde{B}(p,z)$ contains an extra term $(\tilde{B}(0,z))$ which carries the information on the bonds *never* traversed. So, $d[L^d/(1-z)-\tilde{B}(0,z)]$ is just $\sum_{t=0}^{\infty} z^t B(t)$. For completeness, we report the result for unidirectional traverses:

$$\tilde{B}(p,z)=\frac{L^d}{1-z}-\frac{z(1-p)}{(1-z)^2[2d+(1-p)zG(z)]}.$$

Finally, note that finite size effects are fully incorporated in this approach, although they are implicitly 'buried' in $G(z)=L^{-d}\sum_{\{k_i\}}\left[1-(z/d)\sum_{i=1}^{d}\cos k_i\right]^{-1}$ (where the sum is over the set $\{k_i\}$ of allowed L^d wave vectors). Needless to say, generalizations to strip- or slab-like samples ($L_1\leqslant L_2\leqslant\cdots$) are straightforward. Thus, it is possible to study the crossover of our distributions, at least in principle, when the polymer length exceeds the shortest dimension significantly ($t\gg L_1$). Physically, ultra-thin membranes made from extra-long polymers can be manufactured. Until they become reality, however, it may not be worthwhile to extend our analysis to this class of crossover behaviour.

A second remark concerns the statistics of multiple *visits to sites*, as opposed to traversals of bonds. Visits have been of considerable interest in the literature (see Hughes [3] and references therein). The average $V_m(t)$ of the number of sites visited exactly m times by a t step random walk was studied by Montroll and Weiss [7] and by Barber and Ninham [8]. Hamana [9] very recently studied the variance and the full distribution of this random variable. The $t\to\infty$ limit of $V_m(t)$ at fixed m was considered by Hughes [3] (see also [10]) in $d=1$ and by Montroll and Weiss [7] (see also [11]) in $d=2$; however, the scaling limit expression of $V_m(t)$ has not to our knowledge appeared in the literature. Since the analysis of $V_m(t)$ runs exactly parallel to that of $B_m(t)$, we content ourselves to state the results here.

In dimension $d=1$ the average number of sites visited m times is, to leading order in the scaling limit, equal to the average number of bonds visited m times: $V_m(t)=2\,\mathrm{erfc}(\mu_1)$ for $t\to\infty$ at fixed μ_1. In dimension $d=2$ one has in terms of the scaling variable $\mu_2'=\pi m/\log 8t$

$$V_m(t)=\frac{\pi^2 t}{\log^2 8t}\,\mathrm{e}^{-\mu_2'}\left[1+(\mu_2'-2)\frac{\frac{\pi}{2}-1+C}{\log 8t}+\mathcal{O}(\log^{-2}8t)\right] \tag{19}$$

valid for $t\to\infty$ at fixed μ_2'. Comparison of equations (19) and (17) shows that to leading order $V_m(t)$ and $B_m(t)$ are identical up to a coefficient and a scale factor; however, the coefficients of the first correction terms are different. The leading-order relation between $V_m(t)$ and $B_m(t)$ in $d=1,2$ is heuristically clear as follows. Given a large number m of visits to an arbitrary site x, there will be typically $m/(2d)$ traversals, starting from x, of a specific bond $(x,x+\delta)$. Now the same bond will be traversed, typically, the same number of times in the opposite direction. So for each site visited m times, there are d bonds traversed m/d times.

Although we have not shown so explicitly, the scaling function in $d=2$ is expected to be universal, i.e. lattice structure independent. In dimensions $d>2$ the random walk is transient and it is easy to show that as a consequence in the large t limit $B_m(t)\simeq b_m t$ and $V_m(t)\simeq v_m t$, where b_m and v_m are nonuniversal. For random walks that are not simple (i.e. have a step size distribution not limited to nearest neighbour steps), bond traversals are not unambiguously defined; however, visits to sites still are, and for such walks $V_m(t)$ is readily calculated by the present method. One case of interest is the scaling limit of $V_m(t)$ for lattice Lévy flights

(also called Riemann walks) [12, 13], for which the distribution of step sizes decreases as a power law.

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