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Diffusion of a set of random walkers in Euclidean media. First passage times

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Abstract. When a large number N of independent random walkers diffuse on a d-dimensional Euclidean substrate, what is the expectation value $\langle t_{1,N}\rangle$ of the time spent by the first random walker to cross a given distance r from the starting place? We here explore the relationship between this quantity and the number of different sites visited by N random walkers all starting from the same origin. This leads us to conjecture that $\langle t_{1,N}\rangle \approx (r^2/4D\ln N)[1+\sum_{n=1}^{\infty}(\ln N)^{-n}\sum_{m=0}^{n} a_m^{(n)}(\ln\ln N)^m]$ for $d \geqslant 2$, large N and $r \gg \ln N$, where $a_m^{(n)}$ are constants (some of which we estimate numerically) and D is the diffusion constant. We find this conjecture to be compatible with computer simulations.

1. Introduction

Problems related to (what is now called) the first passage time of a random walker to reach some place have a long tradition in science: they date back to Huygens' problem 5 in the seventeenth century which was generalized and solved by Jacob Bernoulli in the next century [1]. Usually, the problem considered is the estimate of the time to first reach a given point or a given frontier by a *single* random walker. In this paper, we address a similar question: we want to estimate the mean escape time $\langle t_{1,N}\rangle$ from a given spherical region of the first random walker of a *set* of $N \gg 1$ independent random walkers.

This problem was first considered by Weiss *et al* in 1983 [2]. They found asymptotic expressions for large N of $\langle t_{1,N}\rangle$ and $\langle t_{1,N}^2\rangle$ when the random walkers diffuse in the one-dimensional lattice. Some of these expressions were corrected in [3]. This problem and its extension to some classes of fractal lattices was also studied in [4]. However, there are no similar results for d-dimensional Euclidean lattices (with $d \geqslant 2$), there only being the conjecture, proposed by Weiss *et al* in [2], that $\langle t_{1,N}\rangle \approx Cr^2\ln^{-1}N$, but without a value being stated for C, which, as the authors said, 'may be quite difficult to calculate'. In [4] it was found that, for the one-dimensional lattice and for some fractal substrates, $\langle t_{1,N}\rangle$ goes as $(\ln N)^{1-d_w}$, d_w being the diffusion exponent. Notice that the direct extension of this result to Euclidean substrates is in agreement with the conjecture of Weiss *et al* as $d_w = 2$ for Euclidean lattices.

The aim of this paper is to explore the connection between $\langle t_{1,N}\rangle$ and the territory covered (or number of different sites visited) by N random walkers all starting from the same origin. This connection will lead us to conjecture (taking into consideration an idea proposed previously in [5]) that

$$\langle t_{1,N}\rangle \approx \frac{r^2}{4D\ln N}\left[1+\sum_{n=1}^{\infty}(\ln N)^{-n}\sum_{m=0}^{n} a_m^{(n)}(\ln\ln N)^m\right] \tag{1}$$

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holds for all Euclidean substrates, where D is the diffusion constant defined by the relationship $\langle r^2 \rangle \approx 2dDt$, with $\langle r^2 \rangle$ being the mean-square displacement of a single random walker. Equation (1) has been rigorously derived in [2–4] for the one-dimensional case. Here we will check equation (1) for d-dimensional lattices with $d \geqslant 2$ by resorting to comparison with numerical simulation.

2. Territory explored and first passage time

The territory $S_N(t)$ explored by N independent random walkers as a function of time is a basic and important quantity first studied for Euclidean media by Larralde *et al* [6]. They found that there exist three time regimes in $S_N(t)$: a short-time regime or regime I, an intermediate regime or regime II, and a long-time regime or regime III. The value of $S_N(t)$ in regimes I and III is not difficult to understand: In regime I ($t \ll t_\times \sim \ln N$) the number of random walkers per site is so large that every site that may be visited is effectively visited, so that $S_N(t) \sim t^d$; in regime III ($t \gg t'_\times$), the random walkers are so far away from each other that their trails (almost) never overlap so that $S_N(t) \approx N S_1(t)$. Of course, this never happens for the one-dimensional case (i.e., in this case $t'_\times = \infty$). For $d = 2$ one has $t'_\times \sim \mathrm{e}^N$ whereas $t'_\times \sim N^2$ for $d = 3$. The calculation of $S_N(t)$ for the intermediate regime ($t_\times \ll t \ll t'_\times$) is much more involved (see [5–7]). In this paper $S_N(t)$ is used to estimate $\langle t_{1,N} \rangle$.

To start with, it is clear from the very definition of time regime I that the radius of the frontier of the set of visited sites grows ballistically in this regime so that $\langle t_{1,N}(r) \rangle \sim r$ for $r \ll r_\times \sim \ln N$. Let us now study what happens for larger values of r ($r \gg r_\times$). In figure 1 we show a typical snapshot of the region of visited sites for the two-dimensional case in regime II. It is clear that if the N random walkers had performed a compact exploration in the sense of de Gennes (most sites inside a compact region are visited before a new site outside this region is reached) then almost every site of the hypersphere of radius r would have been visited when the distance r is first reached by a random walker at time $t_{1,N}(r)$; this implies that $S_N[t_{1,N}(r)]$ would be (roughly) given by $v_0 r^d$, v_0 being the volume of a hypersphere of unit radius: $v_0 = \pi^{d/2}/\Gamma(1 + d/2)$. Certainly, as figure 1 shows, the exploration is not truly compact as there exists a significant dendritic ring. This implies that there will be some worsening of the estimate of $\langle t_{1,N}(r) \rangle$ obtained by solving

$$S_N[\langle t_{1,N}(r) \rangle] = v_0 r^d. \tag{2}$$

This procedure for obtaining $\langle t_{1,N}(r) \rangle$ was proposed previously in [5], and in this paper we will study to what extent it is accurate.

In order to solve the above equation we need to know $S_N(t)$ for regime II. Fortunately this expression has been obtained in [5] through the asymptotic expansion for large N of the exact (for non-interacting random walkers) relation $S_N(t) = \sum_{\boldsymbol{r}} \{1 - \Gamma_t^N(\boldsymbol{r})\}$, where the sum is over all the sites in the lattice and $\Gamma_t(\boldsymbol{r})$ is the probability that site $\boldsymbol{r}$ has not been visited by a single random walker by step t. The final result is

$$S_N(t) \approx v_0 (4Dt \ln N)^{d/2} (1 - \Delta) \tag{3}$$

with

$$\Delta = \tfrac{1}{2} \sum_{n=1}^{\infty} (\ln N)^{-n} \sum_{m=0}^{n} s_m^{(n)} (\ln \ln N)^m \tag{4}$$

and where, up to second-order corrective terms ($n = 2$),

$$s_0^{(1)} = -d\omega \tag{5}$$

$$s_1^{(1)} = d\mu \tag{6}$$

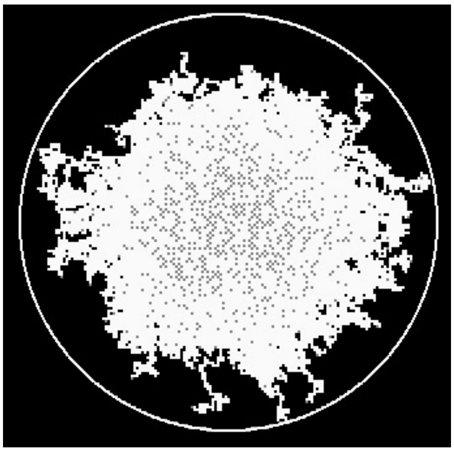

Figure 1. A snapshot of the set of visited sites by $N = 1000$ random walkers on the two-dimensional lattice. The visited sites are in white, the unvisited ones are in black, and the internal grey points are the random walkers. We have taken the snapshot at just the instant $t_{1,1000}(r)$ at which the circular frontier placed at distance r from the starting point is reached for the first time by one of the $N = 1000$ random walkers.

Table 1. Parameters appearing in the asymptotic expression of $S_N(t)$, equation (3), for d-dimensional cubic lattices. The symbol dD refers to the d-dimensional lattice. The parameter $\widetilde{p}$ is $[2t(2D\pi)^3/3]^{1/2}p(\mathbf{0},1)$, where $p(\mathbf{0},1) \simeq 1.516\,386$ is the expected number of returns of a single random walker to the starting site [8].

Case	A	μ	h_1
1D	$\sqrt{2/\pi}$	$\frac{1}{2}$	-1
2D	$1/\ln t$	1	-1
3D	$1/(\widetilde{p}\sqrt{t})$	1	$-\frac{1}{3}$

$$s_0^{(2)} = d\left(1-\frac{d}{2}\right)\left(\frac{\pi^2}{12}+\frac{\omega^2}{2}\right) - d\left(\frac{dh_1}{2}-\mu\omega\right) \tag{7}$$

$$s_1^{(2)} = -d\left(1-\frac{d}{2}\right)\mu\omega - d\mu^2 \tag{8}$$

$$s_2^{(2)} = \frac{d}{2}\left(1-\frac{d}{2}\right)\mu^2. \tag{9}$$

Here $\omega = \gamma + \ln A + \mu\ln(d/2)$, where $\gamma \simeq 0.577\,215$ is Euler's constant, and A, μ and h_1 are given in table 1.

From equations (2) and (3) one easily finds for the one-dimensional case that

$$\langle t_{1,N}\rangle \approx \frac{r^2}{4D\ln N}\left[1+\frac{\frac{1}{2}\ln\ln N-\omega}{\ln N}+\frac{\frac{1}{4}(\ln\ln N)^2-(\omega+1/4)\ln\ln N+a_0^{(2)}}{\ln^2 N}\right.$$
$$\left. + \mathcal{O}\left(\frac{\ln^3\ln N}{\ln^3 N}\right)\right] \tag{10}$$

where $\omega = \gamma - \frac{1}{2}\ln\pi = 0.004\,8507\ldots$ and $a_0^{(2)} = \omega(\omega+\frac{1}{2}) + \pi^2/24 + \frac{1}{2} = 0.913\,68\ldots$. Comparing this expression with that derived rigorously in [4] we discover that they only differ in the value of $a_0^{(2)}$ as the rigorous value is $\omega(\omega+\frac{1}{2})+\pi^2/6+\frac{1}{2} = 2.147\,38\ldots$. So we find that the procedure for estimating $\langle t_{1,N}(r)\rangle$ via $S_n(t)$ is exact up to the first-order corrective terms for the one-dimensional lattice. In fact, it is 'nearly' exact up to the second-order corrective terms as the main term and the coefficients $a_0^{(1)} = -\omega$, $a_1^{(1)} = \frac{1}{2}$, $a_1^{(2)} = -\omega-\frac{1}{4}$ and $a_2^{(2)} = \frac{1}{4}$ are the exact values, with only the coefficient $a_0^{(2)}$ being inexact.

Now we consider d-dimensional media with $d \geqslant 2$. It should be noted that the procedure used so successfully for the one-dimensional case cannot be implemented as easily as before because the parameter A now depends on time (see table 1). Therefore equation (2) becomes a transcendental equation:

$$\langle t_{1,N}\rangle \approx \frac{r^2}{4D\ln N}\left[1+\frac{\mu\ln\ln N-\omega(\langle t_{1,N}\rangle)}{\ln N}\right.$$
$$\left.+\frac{\mu^2\ln^2\ln N-\mu[2\omega(\langle t_{1,N}\rangle)+\mu]\ln\ln N+a_0^{(2)}}{\ln^2 N}+\mathcal{O}\left(\frac{\ln^3\ln N}{\ln^3 N}\right)\right] \tag{11}$$

with $a_0^{(2)} = [\omega(\langle t_{1,N}\rangle)+\mu/2]^2-\mu^2/4+\pi^2(2-d)/24-dh_1/2$. However, neglecting the corrective terms in equation (11), one has the asymptotic approximation

$$\langle t_{1,N}(r)\rangle \approx \frac{r^2}{4D\ln N} \tag{12}$$

for large N. It would be futile to strive to find a better estimate of the solution of equation (11) because even the numerical solution of equation (11) is a worse estimate of $\langle t_{1,N}(r)\rangle$ than that of equation (12). At first sight this might seem strange. The reason, however, is not difficult to understand: as was argued in [5], the main term of the asymptotic expansion of $S_N(t)$ accounts for the number of explored sites if the exploration were fully compact and the corrective terms account for the necessary correction to this number due to the fact that the exploration is *not* fully compact, i.e. because there exists a non-negligible outer dendritic region (see figure 1). As equation (11) comes from equation (2) and this latter equation is valid as long as the exploration performed by the N random walkers is compact, one deduces that the inclusion of the asymptotic corrective terms (i.e. the 'dendritic' terms) of $S_N(t)$ will *worsen* the approximation†.

In sum, one expects that only equation (12) should yield a reasonable estimate of $\langle t_{1,N}(r)\rangle$ for $d \geqslant 2$. As a check, we carried out simulations for two- and three-dimensional simple cubic lattices for $N = 2^0, \ldots, 2^{15}$. Figure 2 is a plot of the simulation results for the quantity $T \equiv \langle t_{1,N}\rangle(4D/r^2)\ln N$ with $r = 100$ for $d = 2$ and $r = 50$ for $d = 3$. We see that the simulation results seem to point to the value 1, i.e. to the asymptotic value predicted by equation (12). We can give some further support to this guess by assuming that the corrective terms to the main term (which is given by equation (12)) have the same functional form as those of the one-dimensional case, i.e. we assume that $\langle t_{1,N}(r)\rangle$ is given by equation (1) for large N, $a_m^{(n)}$ being unknown coefficients. A way of checking this conjecture is by studying to what extent the simulation results for T are compatible with the functional form $1+\sum_{n=1}^{\infty}(\ln N)^{-n}\sum_{m=0}^{n}a_m^{(n)}(\ln\ln N)^m$. To this end we fitted the simulation results for T to the above functional form keeping only the main term and the first-order corrective terms (those corresponding to $n = 1$), i.e. we fitted the simulation results to the expression $A+(a_0^{(1)}+a_1^{(1)}\ln\ln N)/\ln N$ (notice that it would not be reasonable to use the functional form corresponding to $n \geqslant 2$ given the relatively small number of simulation points). Neglecting the values corresponding to N smaller than $N = 16$ (recall that our formulae are asymptotic expressions valid for large N) the fit leads to $A = 1.00 \pm 0.02$ ($a_0^{(1)} = -0.45$, $a_1^{(1)} = -0.22$) for the two-dimensional lattice and $A = 1.00 \pm 0.02$ ($a_0^{(1)} = -0.42$, $a_1^{(1)} = -0.68$) for the three-dimensional lattice. These results are in excellent agreement with our theoretically predicted value of $A = 1$, which supports the validity of equation (12) and, given the way in which these results were obtained, the plausibility of the conjecture of equation (1).

† The fact that keeping more corrective terms in $S_N(t)$ does not lead to a better estimate of $\langle t_{1,N}\rangle$ through equation (2) reinforces the interpretation (first proposed in [5]) that there is a connection, on the one hand, between the main

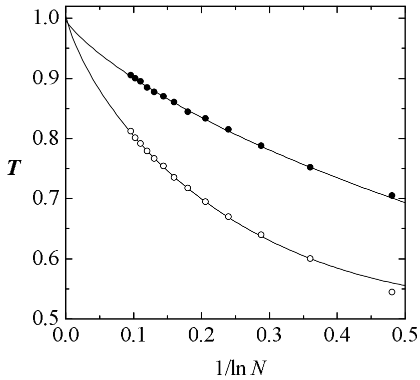

Figure 2. The dependence on N of the average time $\langle t_{1,N}\rangle$ to first reach the distance r of the first random walker of a set of N independent diffusing random walkers all starting from the same origin on a two- and three-dimensional simple cubic lattice. We have plotted $T = \langle t_{1,N}(r)\rangle(4D/r^2)\ln N$ versus $1/\ln N$ for $N = 2^3, \dots, 2^{15}$, where $r = 100$ for $d = 2$ (solid circles) and $r = 50$ for $d = 3$ (open circles). The lines are curves of the form $A + (a_0^{(1)} + a_1^{(1)} \ln\ln N)/\ln N$ fitted to the simulation points corresponding to $N \geqslant 16$. The fitting parameters are $A = 0.997$, $a_0^{(1)} = -0.453$, $a_1^{(1)} = -0.222$ for $d = 2$, and $A = 1.004$, $a_0^{(1)} = -0.423$, $a_1^{(1)} = -0.682$ for $d = 3$. In our simulations after each time unit every random walker makes a jump from a site to one of its nearest neighbours placed at one unit distance. Each simulation point is an average of 10^4 experiments.

Finally, the reader may wonder why no expression for $S_N(t)$ in the time regime III has been considered in our discussion. The reason is that our approximation rests on the validity of equation (2) and this equation is reasonable as long as the exploration of the N random walkers is (mainly) compact. As regime III is precisely characterized by an essentially non-compact exploration, our procedure based on equation (2) cannot use the expression for $S_N(t)$ corresponding to time regime III. However, this does not imply that our results are limited to regime II. The reason is that the difference between time regime II and time regime III stems only from the degree of overlap of the trails of the N random walkers. This is due to the fact that this property is essential for computing the number $S_N(t)$ of *distinct* sites visited by these walkers. But this feature is irrelevant with regard to the quantity $\langle t_{1,N}(r)\rangle$, so that the expressions for $\langle t_{1,N}(r)\rangle$ considered previously must hold for all $r \gg r_\times$.

3. Conclusions

In this paper we have explored the relationship between $\langle t_{1,N}(r)\rangle$ (the mean escape time from a spherical region of radius r of the first random walker of a set of N all starting at site $r = 0$ at time $t = 0$) and $S_N(t)$ (territory covered by these same N random walkers up to time t). We have learnt that, from $S_N(t)$ and through equation (2), we can get $\langle t_{1,N}\rangle$ up to first-order corrective terms in $\ln^{-1} N$ for $d = 1$ (see equation (10)) and up to the zeroth-order term only (main term) for $d \geqslant 2$ (see equation (12)). We conjectured that $\langle t_{1,N}\rangle$ has the same asymptotic form for $d \geqslant 2$ as for $d = 1$ and we showed this conjecture to be plausible by comparison with simulation results. Of course, in order to get a full rigorous asymptotic expression for large N of $\langle t_{1,N}(r)\rangle$ when $d \geqslant 2$ one should resort to other approximations or techniques such as that employed in [2–4]. Work is in progress along this line.

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asymptotic term of $S_N(t)$ and the compactness of the set of visited sites, and, on the other, between the asymptotic corrective terms of $S_N(t)$ and the dendritic nature of the outer ring of the set of visited sites.

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