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Territory covered by *N* random walkers

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The problem of evaluating the number of distinct sites $S_N(t)$ covered up to time t by N random walkers is revisited. For the nontrivial time regime and for $N \gg 1$ we show how to get the asymptotic behavior of $S_N(t)$ and we calculate the main and first two corrective terms. The mth corrective term decays mildly as $1/\ln^m N$. For d-dimensional ($d=1,2,3$) simple cubic lattices, the main term is the volume of the hypersphere of radius $[(\ln N^2)2Dt/d]^{1/2}$, D being the diffusion constant, and the corrective terms account for the roughening of the surface of the set of visited sites. [S1063-651X(99)50510-2]

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The behavior of a large class of natural and social systems in science (physics, chemistry, ecology, and economy) can be cast into the form of a random walk [1–3]. The properties associated with the wandering of a *single* walker have been the most studied [2,3], but the diffusing properties of a *set* of random walkers (RWs) are much less known, notwithstanding their interest [4]. Our knowledge of so basic a quantity as the number of distinct sites $S_N(t)$ covered by N RWs up to time t is a good example. Its properties when $N=1$ have been thoroughly studied [1–3] since the problem was first suggested [5]. However, its multiparticle counterpart has only been tackled since the recent seminal work of Larralde *et al.* [6,7] in which asymptotic expressions of $S_N(t)$ for large N were found when the set of RWs, initially at the same point, diffuse with steps of finite variance on Euclidean lattices of one, two, and three dimensions. Shortly thereafter this work was extended to fractal substrates by Havlin *et al.* [8]. (Subsequent generalizations and refinements have been appearing since then [9].)

These authors found three distinct time regimes in $S_N(t)$: a very 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 ($t \ll t_\times$) the number of RWs per site is so large that every site that may be visited is effectively visited, so that $S_N(t) \approx A_I t^{d_l}$ when $t \ll t_\times \sim \ln N$, d_l being the chemical dimension [10] ($d_l = d$ for d-dimensional Euclidean lattices) and A_I a constant that depends on the lattice. In regime III ($t \gg t'_\times$), the RWs are so far away from each other that their trails (almost) never overlap so that $S_N(t) \approx N S_1(t)$. This never happens for lattices with spectral dimension $d_s = 2d_f/d_w < 2$, so that $t'_\times = \infty$ (d_w is the anomalous diffusion exponent and d_f is the fractal dimension of the substrate). Also, one has $t'_\times \sim e^N$ for $d=2$ and $t'_\times \sim N^2$ for $d=3$. However, the calculation of $S_N(t)$ for the intermediate regime ($t_\times \ll t \ll t'_\times$) is much more involved and little more is known than that $S_N(t)/t^{d_f/d_w}$ goes asymptotically as $s_0(\ln x)^{d_f/\nu}$ for large N, with $\nu \equiv d_w/(d_w - 1)$ and $x=N$ for $d_s<2$, $x=N/\ln t$ for $d=2$ and $x=N/\sqrt{t}$ for $d=3$ [6–8,11]. However, no prefactors s_0 were given for the Euclidean lattices in [6] nor for the fractals lattices in [8]. (Values of s_0 for Euclidean lattices were given in [7,11], but, except for the two-dimensional case, they do not agree with ours.) Moreover, no corrective term to the main asymptotic term has ever been computed [12] and no direct comparison (value against value) has ever been made between numerical results and theoretical values, apart from testing [6,8] whether

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TABLE I. Parameters appearing in the asymptotic expression of $S_N(t)$, Eq. (6). The symbol dD refers to the d-dimensional simple hypercubic lattice and $S2$ to the two-dimensional Sierpinski lattice. The parameter $\tilde{p}$ is $[2t(2D\pi)^3/3]^{1/2}p(\mathbf{0},1)$, where $p(\mathbf{0},1) \simeq 1.516\,386$ [1,2]. For finitely ramified fractals it can be proved that A is bounded if it is a function of time [16–18]. The values for the Sierpinski lattice are only plausible [see remark following Eq. (4)]; in particular, v_0 is only ''almost'' constant: it is really a function that oscillates slightly around the value 3.

Case	v_0	d_f	d_w	A	c	μ	h_1
1D	2	1	2	$\sqrt{2/\pi}$	1/2	1/2	-1
2D	π	2	2	$1/\ln t$	1	1	-1
3D	$4\pi/3$	3	2	$1/(\tilde{p}\sqrt{t})$	3/2	1	$-1/3$
$S2$	3	ln 3/ln 2	ln 5/ln 2	0.613	0.981	1/2	-0.56

$S_N(t)/t^{d_f/d_w}$ is linear in $(\ln x)^{d_f/\nu}$ [13]. A major objective of this Rapid Communication is to amend these deficiencies. We will see that the solution [cf. Eq. (6)] to the problem of calculating $S_N(t)$ given in this Rapid Communication (i) has a main term that differs from that evaluated by Larralde *et al.* *by a factor* $d_f(d_w-1)/d_w$, *and (ii) contains corrective terms that are not at all negligible when compared with the main term even for very large values of N* because they decay only logarithmically with N. (This fact should be considered when theoretical results are compared with observations, especially when N is not very large [14].) We will connect the main term to the (almost) compact nature of the set of visited sites, and the corrective terms to the roughening of its surface. Finally, our solution is precise enough to disclose the tight relationship between $S_N(t)$ and the escape time, $t_{1,N}(r)$, of the first RW of a set of N diffusing particles from a region of radius r [15,16]. This will lead us to guess an asymptotic expression for $t_{1,N}$ in Euclidean media with $d \geqslant 2$.

Our analysis begins, as in Refs. [6–8], by recognizing that $S_N(t)=\Sigma_{\mathbf{r}}\{1-\Gamma_t^N(\mathbf{r})\}$ for N noninteracting RWs, where the sum is over all the sites in the lattice and $\Gamma_t(\mathbf{r})$ is the probability that site $\mathbf{r}$ has not been visited by a single RW by step t. However, from here on our procedure departs from previous analyses. Since we are interested in the behavior of $S_N(t)$ after a large number of steps (thus outside of the very short time regime I), we replace $\Gamma_t(\mathbf{r})$ and $S_N(t)$ by their continuum approximation,

$$S_N(t)=\int_0^\infty \{1-\Gamma_t^N(r)\}v_0 d_f r^{d_f-1}dr$$

$$=v_0 d_f(2D)^{d_f/2}t^{d_f/d_w}J_N(d_f-1;0,\infty), \qquad (1)$$

where

$$J_N(\alpha;a,b)=\frac{N}{\alpha+1}\int_a^b \Gamma_t^{N-1}(\xi)\frac{d\Gamma}{d\xi}\xi^{\alpha+1}d\xi, \qquad (2)$$

with $\xi^2 \equiv r^2/(2Dt^{2/d_w})$. Here D is the diffusion constant, i.e., $R^2 \approx 2Dt^{2/d_w}$, where R is the root-mean-square displacement of a single RW, and the geometric factor v_0 is a *constant* defined through the relation

$$V(r)=v_0 r^{d_f}, \qquad (3)$$

where $V(r)$ is the volume (number of sites) of the substrate inside a hypersphere of radius r (see Table I) [17,18].

In order to evaluate $J_N(d_f-1;0,\infty)$ for $N \gg 1$ it suffices to know $\Gamma_t(r)$ for large ξ. We will assume that

$$\Gamma_t(r)\approx \tilde{\Gamma}_t(r)=1-A\xi^{-\mu\nu}e^{-c\xi^\nu}\left(1+\sum_{n=1}^\infty h_n\xi^{-n\nu}\right), \qquad (4)$$

when $\xi \gg 1$. Although this relation is known to be true for some Euclidean lattices [7] (see Table I), it is only a plausible conjecture for some fractal substrates [19]. Next, we decompose $J_N(\alpha;0,\infty)$ as $J_N(\alpha;0,\xi_\times)+J_N(\alpha;\xi_\times,\infty)$, where $\xi_\times$ is a value that should satisfy two conditions: (i) $\xi_\times$ is large enough for $\Gamma_t(\xi)$ to be approximated by $\tilde{\Gamma}_t(\xi)$ for $\xi \geqslant \xi_\times$, and (ii) small enough so that $\Gamma_t^N(\xi_\times)=1/N^\kappa$, with $\kappa > 1$ (say $\kappa=2$). When these two conditions are fulfilled one finds that $\xi_\times^\nu \sim \ln N$ and that $J_N(\alpha;0,\xi_\times)$ goes, apart from logarithmic terms, as $1/N^{\kappa-1}$. Thus we can neglect $J_N(\alpha;0,\xi_\times)$ and approximate $J_N(\alpha;0,\infty)\approx J_N(\alpha;\xi_\times,\infty)$ for large N because, as we will prove, $J_N(\alpha;\xi_\times,\infty)$ goes essentially as a positive power of $\ln N$. Inserting Eq. (4) into Eq. (2), one finds $J_N(\alpha;\xi_\times,\infty)\approx N\Sigma_{n=0}^\infty j_n K_{N-1}[\alpha-(n-1)\nu)]$, where $K_N(\alpha)=\int_{\xi_\times}^\infty \xi^\alpha \tilde{\Gamma}_t^N(\xi)[1-\tilde{\Gamma}_t(\xi)]d\xi$. By means of the substitution $\tilde{\Gamma}_t(\xi)=\exp(-z)$, $K_N(\alpha)$ becomes a Laplace integral,

$$K_N(\alpha)=\int_0^{z_\times} e^{-Nz}(e^{-z}-1)\xi^\alpha \frac{d\xi}{dz}dz. \qquad (5)$$

However, it is not possible to use here Watson's lemma directly because $\xi^\alpha(d\xi/dz)$ has a logarithmic singularity at $z=0$: From the definition of z and Eq. (4) one gets $-c\xi^\nu+\ln A+\mu\ln\xi^{-\nu}+\ln(1+\Sigma_{n=1}^\infty h_n\xi^{-n\nu})=\ln(1-e^{-z})$, which equation, to a first approximation leads to $\xi=[(-\ln z)/c]^{1/\nu}$ as long as $\xi^\nu \gg |\ln A|$. Taking approximations of higher order (this can be done systematically, although to find definite values of the coefficients becomes increasingly cumbersome) and inserting the result into Eq. (5) one obtains $K_N(\alpha)\approx\Sigma_{n=0}^\infty\Sigma_{m=0}^n k_m^{(n)}\Delta_m(\beta-n-1)$, where $\beta\equiv(\alpha+1)/\nu$ and $\Delta_m(\kappa)=\int_0^{z_\times}\exp(-Nz)(-\ln z)^\kappa \ln^m(-\ln z)dz$. Asymptotic expressions of Δ_m for large N have been used in [15,16] and studied in [20], and will not be quoted here. Uniting all the above relations, Eq. (1) becomes (details will be given elsewhere)

$$S_N(t)\approx\frac{v_0}{c^{d_f/\nu}}(2D)^{d_f/2}t^{d_f/d_w}(\ln N)^{d_f/\nu}F^{d_f/\nu}(N,t), \qquad (6)$$

with

$$F^\beta(N,t)=1+\sum_{n=1}^\infty \ln^{-n}N\sum_{m=0}^n \tilde{s}_m^{(n)}\ln^m \ln N. \qquad (7)$$

We have worked out these expressions up to second order $(n=2)$, obtaining

$$\tilde{s}_0^{(1)}=\beta\omega, \qquad (8)$$

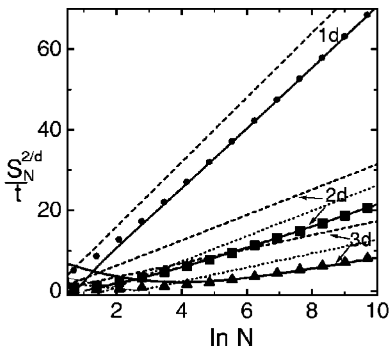

FIG. 1. Dependence on N of the number of distinct sites visited by N independent random walkers, $S_N(t)$, by time $t=200$, for the one-, two-, and three-dimensional simple cubic Euclidean lattices. In our simulations every random walker makes a jump from a site to one of its nearest neighbors placed at one unit distance in each time unit, so that $D=1/2$. For $d=2$ and $d=3$, the symbols correspond to the simulation estimate for $N=2^n$ with $n=1,\ldots,14$. Each simulation point is an average over 10^4 experiments. For the one-dimensional lattice the symbols (circles) correspond to the numerical integration of Eq. (1) with $\Gamma_t(r)=\mathrm{erf}[r/(4Dt)^{1/2}]$. The dashed and solid lines correspond to the approximation of order 0 (main term) and order 2, respectively, of Eq. (6). The dotted lines correspond to the results of Refs. [6,7] but with the amplitude corrected by the factor $2/d$ [21]. This line is absent for $d=1$ because, in this case, the (corrected) results of Larralde *et al. coincide with our approximation of order 0.*

$$\tilde{s}_1^{(1)}=-\beta\mu, \tag{9}$$

$$\tilde{s}_0^{(2)}=\beta(\beta-1)\left(\frac{\pi^2}{12}+\frac{\omega^2}{2}\right)+\beta(ch_1-\mu\omega), \tag{10}$$

$$\tilde{s}_1^{(2)}=\beta\mu^2-\beta(\beta-1)\mu\omega, \tag{11}$$

$$\tilde{s}_2^{(2)}=\frac{1}{2}\beta(\beta-1)\mu^2, \tag{12}$$

where $\omega=\gamma+\ln A+\mu\ln c$ and $\gamma\simeq 0.577\,215$ is Euler's constant. In Fig. 1 we compare Eq. (6) with numerical results. The importance of the corrective terms is evident, as is the good performance of the second-order asymptotic expression from relatively small values of N, i.e., from $N\gtrsim 2^5$.

We must compare Eq. (6) with the expressions obtained in Refs. [6–8] (see Fig. 1). To start with, the main term given in Ref. [7] is $d_f(d_w-1)/d_w$ times the main term reported in this Rapid Communication, and thus they only agree for the two-dimensional lattice in which $d_f=d_w=2$ [21]. With respect to the corrective terms to the main term, it was found in Ref. [6] that $[S_N(t)/(s_0t^{d_f/d_w})]^{\nu/d_f}/\ln N\approx F$ with $F=1$ for $d=1$, $F=1-(\ln\ln t)/\ln N$ for $d=2$ and $F=1-\ln\sqrt{t}/\ln N$ for $d=3$. However, from Eq. (7) and up to first order ($n=1$), one easily finds that $F=1+(\omega-\mu\ln\ln N)/\ln N$, so that from Table I one sees that the values for $F(t,N)$ reported in this Rapid Communication and in Ref. [6] agree to order zero for $d=1$ and only *partially* [because the term $\mu\ln(\ln N)/\ln N$ is absent in Ref. [6]] up to first order for $d=2$ and $d=3$. For the two-dimensional lattice this absent first-order term could be comparable to or even larger than the first-order term $\ln(\ln t)/\ln N$ given by Larralde *et al.* [6].

Equation (6) is precise enough to allow us to discover some of the properties of $S_N(t)$. For example, for d-dimensional simple cubic lattices with $d\geqslant 2$ we can draw from this equation, i.e., from $S_N(t)\approx v_0[2D(t/d)\ln N^2]^{d/2}F^{d/2}(N,t)$, some interesting conclusions concerning the geometry of the set of visited sites. Let $R_+(N,t;d)$ be the average maximum distance reached by any of the N walkers by time t in the d-dimensional lattice. It is clear that, to order zero in $1/\ln N$, $R_+(N,t;1)=S_N(t)/2\approx[2Dt\ln N^2]^{1/2}$. As the d-dimensional walk of a RW over the simple cubic lattice can be seen as the (orthogonal) composition of d one-dimensional random walks, then $R_+(N,t;d)\approx R_+(N,t/d;1)\approx[2D(t/d)\ln N^2]^{1/2}$ because each RW travels in each direction only a dth part of the total time t. But the main asymptotic term of $S_N(t)$ is just $v_0[R_+(N,t;d)]^d$, i.e., $S_N(t)$ is (to order zero in $1/\ln N$) approximately given by the volume of the hypersphere of radius $R_+(N,t;d)$. Notice that this statement is equivalent to saying that the exploration performed by the N RWs is (almost) compact in the sense of de Gennes [10,22] (most sites inside a compact region are visited before a new site outside this region is reached). But we know from two independent arguments that the above two (equivalent) statements are only very roughly correct: first, because the corrective terms of Eq. (6) are non-negligible and, second, because the set of visited sites has a ring of dendritic nature, i.e., the set has a rough surface [23]. Therefore, it is natural to assume that the asymptotic corrective terms to $S_N(t)$ account for the number of visited sites that are inside this dendritic ring. This suggests that we could estimate the thickness of this layer through the corrective terms as follows: Defining the half-thickness of the layer as $h_N(t;d)/2=R_+(N,t;d)-R_0(N,t;d)$, with $R_0(N,t;d)=[S_N(t)/v_0]^{1/d}$ being an estimate of the average or typical distance that separates the visited sites of the ring from the center, one easily finds from Eq. (6) that $h_N(t;d)/R_+(N,t;d)\sim-\ln A(t)/\ln N$. Thus, we have discovered that the size of this dendritic region grows with respect to the size of the full set as $\ln\ln t$ for $d=2$ and $\ln\sqrt{t}$ for $d=3$. For the crossover time $t'_\times$, $h_N(t'_\times;d)$ and $R_+(N,t'_\times;d)$ are comparable; beyond this time, the dendritic ring outruns the inner compact core and one enters the time regime III.

We conclude our Rapid Communication by exploring the relation between $S_N(t)$ and the order statistic quantity $t_{1,N}(r)$ [15,16] defined as the time to first reach a given distance r by the first RW of a set of N independent RWs all starting from the same origin. Reference [16] discussed how to connect the two quantities. However, at that time, it was only possible to relate the dominant behavior of the two quantities, but not their amplitudes or corrective terms because, as noted above, those of $S_N(t)$ were either incorrect or unknown. Equation (6) has emended this situation, and it now turns out that it is possible to make a good estimate of $t_{1,N}$ from $S_N(t)$, and vice versa, by means of the relation $S_N[t_{1,N}(r)]\approx v_0r^{d_f}$. The meaning of this equation is clear: as the exploration performed by the N RWs is (roughly) compact (as was discussed above), then almost every site of the hypersphere of radius r has been visited when the distance r is first reached by a RW at time $t_{1,N}(r)$; this implies that $S_N[t_{1,N}(r)]$ is (roughly) given by $v_0r^{d_f}$. Then, from this relation and from Eq. (6), one deduces

$$t_{1,N}(r) \approx \left[\frac{r}{\sqrt{2D}} \right]^{d_w} \left[\frac{\ln N}{c} \right]^{1-d_w} F^{1-d_w}(N, t_{1,N}). \qquad (13)$$

It is remarkable that Eq. (13) is a good approximation to $t_{1,N}(r)$ for the one-dimensional and (some) fractal substrates, differing from that obtained rigorously in Ref. [16] by terms of *second* order only. At this point, it seems natural to conjecture that Eq. (13) could also lead to a good approximation to $t_{1,N}(r)$ for Euclidean substrates with $d \geqslant 2$. This would be notable indeed because for these media there only exists the conjecture that $t_{1,N}(r)$ goes as $1/\ln N$ [15]. [Equation (13) supports this conjecture because $d_w = 2$ for Euclidean substrates.] Equation (13) should be a better approximation for the one-dimensional and fractal substrates than for Euclidean lattices with $d \geqslant 2$ because the exploration of a *single* RW is not compact for these latter media. However, as the exploration is made by *many* particles, this effect should be weakened.

In summary, we have addressed the problem of finding a full and rigorous solution to the problem of calculating, for the nontrivial time regime, the number of different sites $S_N(t)$ explored by $N \gg 1$ random walkers. Our solution is Eq. (6), which is valid for any diffusive problem for which Eq. (3) and Eq. (4) hold. We have learned that, except for enormously large values of N, it is necessary to include corrective terms to the main term of $S_N(t)$ as such terms decay very mildly as powers of $1/\ln N$. For d-dimensional simple cubic lattices the value of the main term can be understood as the manifestation of the (almost) compact character of the exploration performed by the N walkers. This property was used to conjecture the relation (13) for the escape time of the first random walker of a set of N from a hyperspherical region. We related the fact that the main term is only a rough approximation to the fact that the set of visited sites is not truly compact as it has a rough surface: a dendritic ring. The number of sites of this ring was then related to the corrective asymptotic terms, thus allowing us to estimate the thickness of the roughening.

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