

Number of distinct sites visited by N random walkers on a Euclidean lattice

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The evaluation of the average number $S_N(t)$ of distinct sites visited up to time t by N -independent random walkers all starting from the same origin on an Euclidean lattice is addressed. We find that, for the nontrivial time regime and for large N , $S_N(t) \approx \hat{S}_N(t)(1 - \Delta)$, where $\hat{S}_N(t)$ is the volume of a hypersphere of radius $(4Dt \ln N)^{1/2}$, $\Delta = \frac{1}{2} \sum_{n=1}^{\infty} \ln^{-n} N \sum_{m=0}^n s_m^{(n)} \ln^m \ln N$, d is the dimension of the lattice, and the coefficients $s_m^{(n)}$ depend on the dimension and time. The first three terms of these series are calculated explicitly and the resulting expressions are compared with other approximations and with simulation results for dimensions 1, 2, and 3. Some implications of these results on the geometry of the set of visited sites are discussed.

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I. INTRODUCTION

Usually, the extremely successful theory of random walks is only concerned with problems that involve a *single* ($N = 1$) random walker. A solid reason for this is the understanding that the average properties of the single diffusing walker serve to describe the global properties of systems formed by many walkers. However, there are other interesting diffusion problems that involve many random walkers for which the diffusive behavior of *every* walker of the total of N is relevant, i.e., diffusion process that *cannot* be described by averaging over the properties of a single walker [1]. The problem of evaluating the time spent by the first j particles out of a total of N to escape from a given region is a clear example [2,3]. Another important example, which is the subject of this paper, is the problem of evaluating the average number $S_N(t)$ of distinct sites visited (or territory explored) by a set of N independently diffusing random walkers up to time t [4,5].

The case $N=1$ has been studied in detail since it was posed by Dvoretzky and Erdős [6] and is discussed in many general references [7–9]. However, the multiparticle ($N > 1$) version of this problem has been systematically treated only after the pioneering works of Larralde *et al.* [4,5]. These authors addressed the problem of evaluating the territory covered by a set of N -independent random walkers, all initially placed at the same point, that diffuse with steps of finite variance on Euclidean lattices. They found asymptotic expressions for $S_N(t)$ for $N \gg 1$, and described the existence of three time regimes. Their results can be summarized as follows:

$$S_N(t) \sim \begin{cases} t^d & t < t_{\times} \\ t^{d/2} \ln^{d/2}(x), & t_{\times} \ll t \ll t'_{\times}, \\ NS_1(t), & t'_{\times} \ll t \end{cases} \quad (1)$$

where $x=N$ for $d=1$, $x=N/\ln t$ for $d=2$ and $x=N/\sqrt{t}$ for $d=3$ [4,5]. The properties of $S_1(t)$ are well known; in particular, $S_1(t) \sim t^{1/2}$ for $d=1$, $S_1(t) \sim t/\ln t$ for $d=2$, and $S_1(t) \sim t$ for $d=3$. In the very short-time regime ($t \ll t_{\times}$), or regime I, there are so many particles at every site that all the nearest neighbors of the already visited sites are reached at

the next step, so that the number of distinct sites visited grows as the volume of a hypersphere of radius t , $S_N(t) \sim t^d$. Regime III ($t'_{\times} \ll t$), or long-time regime, corresponds to the final stage in which the walkers move far away from each other so that their trails (almost) never overlap and $S_N(t) \sim NS_1(t)$. The crossover time from regime I to regime II is given by $t_{\times} \sim \ln N$ for every lattice. This can be easily understood if we take into account that the number of particles on the outer visited sites for very short times will decrease as N/z^t , where z is the coordination number of the lattice, so that the overlapping regime will break approximately when $N/z^t \sim 1$ or, equivalently, $t_{\times} \sim \ln N$. Regime III never appears in the one-dimensional case (i.e., $t'_{\times} \sim \infty$), but $t'_{\times} \sim e^N$ for $d=2$ and $t'_{\times} = N^2$ for $d=3$. These crossover times will be obtained readily from the mathematical formalism discussed in the present paper. The most interesting regime is regime II ($t_{\times} \ll t \ll t'_{\times}$), or the intermediate regime. For this time regime, we will obtain explicitly the main term and the first two corrective terms of the asymptotic expression of $S_N(t)$ for $N \gg 1$. Higher corrective terms could be calculated as our method allows them to be obtained in a systematic way. The contribution of these corrective terms cannot be ignored even for very large values of N because they decay logarithmically with N . However, as we will see in Sec. V, the use of two corrective terms leads to a very good agreement with simulation results for relatively small values of N ($N \geq 100$).

The paper is organized as follows. The asymptotic evaluation of $S_N(t)$ for a d -dimensional Euclidean lattice is discussed in detail in Sec. II. Some geometric implications of this result are discussed in Sec. III. In Sec. IV, we compare our zeroth- (i.e., main), first-, and second-order term approximation for $S_N(t)$ with other approximations and with computer simulations for one-, two-, and three-dimensional simple Euclidean cubic lattices. The paper ends with some remarks on the applicability of this method to other diffusion problems and different media. Some technical details are discussed in an Appendix.

II. THE NUMBER OF DISTINCT SITES VISITED

We consider a group of N random walkers starting from an origin site $\mathbf{r}=\mathbf{0}$ at time $t=0$. A survival probability,

TABLE I. Parameters appearing in the asymptotic expression of $S_N(t)$, Eq. (24). The symbol dD refers to the d -dimensional simple hypercubic lattice. The parameter \tilde{p} is $[2t(2D\pi)^3/3]^{1/2}p(\mathbf{0},1)$, where $p(\mathbf{0},1) \approx 1.516386$ [8].

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

$\Gamma_N(t, \mathbf{r})$, is defined as the probability that site \mathbf{r} has not been visited by the random walkers before time t . Similarly, we can define a mortality function, $1 - \Gamma_N(t, \mathbf{r})$, as the probability that site \mathbf{r} has been visited by at least one walker in the time interval $(0, t)$. The relationship between the number of distinct sites visited, $S_N(t)$, and the survival probability is [4,5]

$$S_N(t) = \sum_{\mathbf{r}} \{1 - \Gamma_N(t, \mathbf{r})\}. \quad (2)$$

For independent random walkers, we have $\Gamma_N(t, \mathbf{r}) = [\Gamma_t(\mathbf{r})]^N$, where $\Gamma_t(\mathbf{r}) \equiv \Gamma_1(t, \mathbf{r})$ is the one-particle survival probability. Next, the discrete analysis implicit in Eq. (2) is replaced by a continuous one. Thus, we write

$$S_N(t) = \int_0^\infty [1 - \Gamma_t^N(r)] dv_0 r^{d-1} dr, \quad (3)$$

where v_0 is the volume (i.e., the number of lattice sites) of the hypersphere with unit radius. It has been found for Euclidean lattices that [5]

$$\Gamma_t(r) \approx \tilde{\Gamma}_t(\xi) = 1 - A \xi^{-2\mu} e^{-d\xi^2/2} \left(1 + \sum_{n=1}^{\infty} h_n \xi^{-2n} \right), \quad (4)$$

for $\xi \equiv r/\sqrt{2dDt} \gg 1$. Here, D is the diffusion coefficient defined through the Einstein relation $\langle r^2 \rangle \approx 2dDt$, $t \rightarrow \infty$, with $\langle r^2 \rangle$ being the mean-square displacement of a single random walker. The values of A , μ and h_1 for $d=1, 2$, and 3 are shown in Table I. A change to the new variable ξ and integration by parts [taking into account that $\tilde{\Gamma}_t(\infty) = 1$], yields

$$S_N(t) = v_0 (2dDt)^{d/2} J_N(d; 0, \infty), \quad (5)$$

where

$$J_N(d; a, b) = \int_a^b N \Gamma_t^{N-1}(\xi) \frac{d\Gamma_t(\xi)}{d\xi} \xi^d d\xi. \quad (6)$$

In order to evaluate the asymptotic behavior of $J_N(d; 0, \infty)$ it is convenient to make the decomposition

$$J_N(d; 0, \infty) = J_N(d; 0, \xi_\times) + J_N(d; \xi_\times, \infty), \quad (7)$$

where ξ_\times is a value that should satisfy the following two conditions: ξ_\times is (a) large enough that $\Gamma_t(r)$ can be well approximated by its asymptotic approximation $\tilde{\Gamma}_t(\xi)$ for $\xi \gg \xi_\times$, and (b) small enough that

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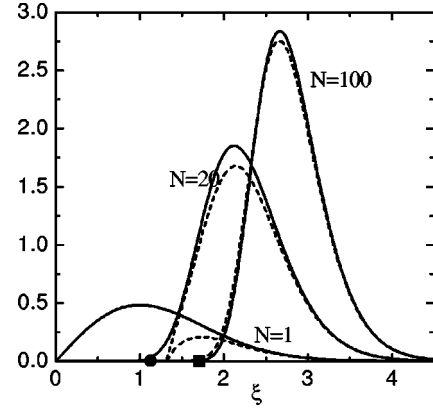


FIG. 1. The integrand $N\xi\Gamma_t^{N-1}(d\Gamma_t/d\xi)$ of $J_N(1; 0, \infty)$ versus ξ for the one-dimensional lattice and $N=1, N=20$ and $N=100$. The solid lines correspond to the integrand when the exact value of $\Gamma_t(\xi)$ is used. The broken lines are obtained by using the first-order asymptotic approximation $\Gamma_t(\xi) \approx 1 - (2/\pi)^{1/2} \xi^{-1} \exp[-\xi^2/2](1 - \xi^{-2})$. The filled circle [square] marks the value of ξ_\times for $N=20$ [$N=100$] using $p=2$ in Eq. (8).

$$\tilde{\Gamma}_t^N(\xi_\times) = 1/N^p, \quad (8)$$

with $p > 1$ (say $p=2$). From Eq. (4) it is straightforward to see that

$$\xi_\times^2 \sim \ln N \quad (9)$$

satisfies both conditions. On the other hand, because at most $d\Gamma/d\xi = \mathcal{O}(1)$, and $\Gamma_t(\xi)$ is a monotonic growing function, $J_N(d; 0, \xi_\times)$ is bounded by a term that goes as $N\tilde{\Gamma}_t^{N-1}(\xi_\times)\xi_\times^d$, or equivalently, from Eq. (8), by a term that goes mainly as N^{1-p} . But shortly we will show that $J_N(d; \xi_\times, \infty)$ goes essentially as $\ln^{d/2} N$; this means that $J_N(d; 0, \xi_\times)$ is asymptotically smaller than any term in the asymptotic expansion for $J_N(d; 0, \infty)$ and thus we can write

$$J_N(d; 0, \infty) \approx J_N(d; \xi_\times, \infty), \quad N \gg 1. \quad (10)$$

The previous discussion is illustrated in Fig. 1 for the one-dimensional case. In this figure, we have represented the integrand of $J_N(1; 0, \infty)$ for increasing values of N using as survival probability the exact value $\Gamma_t(\xi) = \text{erf}(\xi/\sqrt{2})$ [8,9] and the asymptotic expression of Eq. (4) up to first order ($n=1$). Notice that the area below the solid [broken] curve is just the exact [asymptotic approximate] value of $S_N(t)/(8Dt)^{1/2} = J_N(1; 0, \infty)$. The value of ξ_\times as given by Eq. (8) with $p=2$ is marked with a symbol. It is clear from the figure that, for large N , (a) the integrand of $J_N(1; \xi_\times, \infty)$ is well represented by the asymptotic expression of $\Gamma_t(\xi)$, and (b) that, as stated for the general case in Eq. (10), $J_N(1; 0, \xi_\times) \ll J_N(1; \xi_\times, \infty) \approx J_N(1; 0, \infty)$. From Eq. (4), one easily finds that

$$\frac{d\tilde{\Gamma}_t(\xi)}{d\xi} [1 - \tilde{\Gamma}_t(\xi)]^{-1} = 2\xi \sum_{n=0}^{\infty} j_n \xi^{-2n}, \quad (11)$$

with $j_0 = d/2$, $j_1 = \mu$, $j_2 = h_1, \dots$. By inserting Eq. (11) into Eq. (6) one has the following expansion for $J_N(d; \xi_\times, \infty)$:

$$J_N(d; \xi_\times, \infty) \approx 2N \sum_{n=0}^{\infty} j_n K_{N-1}(d-2n+1), \quad (12)$$

with

$$K_N(\alpha) = \int_{\xi_\times}^{\infty} \xi^\alpha \bar{\Gamma}_t^N(\xi) [1 - \bar{\Gamma}_t(\xi)] d\xi. \quad (13)$$

By means of the substitution

$$\bar{\Gamma}_t(\xi) = e^{-z}, \quad (14)$$

we get a more convenient expression for $K_N(\alpha)$:

$$K_N(\alpha) = \int_0^{z_\times} e^{-Nz} (e^{-z} - 1) \xi^\alpha \frac{d\xi}{dz} dz, \quad (15)$$

where, from Eq. (8), $z_\times \sim \ln N/N$. The integral in Eq. (15) is of Laplace type but it is not possible to use Watson's lemma directly to get its asymptotic behavior because $\xi^\alpha (d\xi/dz)$ has a logarithmic singularity at $z=0$ [10]. The evaluation of $K_N(\alpha)$ requires the inversion of (14) to obtain $\xi(z)$. By using Eqs. (4) and (14) we get

$$\begin{aligned} & -\frac{d}{2} \xi^2 + \ln A + \mu \ln \xi^{-2} + \ln \left(1 + \sum_{n=1}^{\infty} h_n \xi^{-2n} \right) \\ & = \ln(1 - e^{-z}). \end{aligned} \quad (16)$$

The function $\xi(z)$ can be readily obtained from this equation to first approximation: Notice that, as long as

$$\xi^2 \gg |\ln A|, \quad (17)$$

the left hand side of Eq. (16) can be approximated by $-d\xi^2/2$, so that the first-order solution to Eq. (16) is $\xi^2(z) \approx -2 \ln[1 - \exp(-z)]/d$. Equation (16) can be systematically solved in order to get higher-order approximations (see Appendix). The result is

$$\xi = x^{-1/2} \sum_{n=1}^{\infty} \delta_n x^n, \quad (18)$$

where $x = -(d/2)/\ln[1 - \exp(-z)]$. The substitution of Eq. (18) into Eq. (15) [see Eq. (A9) in the Appendix] yields

$$K_N(\alpha) = \sum_{n=0}^{\infty} \sum_{m=0}^n \frac{2^{(\alpha-1)/2}}{d^{(\alpha+1)/2}} k_m^{(n)} I\left(\frac{\alpha}{2} - n - \frac{1}{2}, m; N\right), \quad (19)$$

where

$$I(n, m; N) \equiv \int_0^{z_\times} dz e^{-Nz} (-\ln z)^n \ln^m(-\ln z). \quad (20)$$

The evaluation of $I_N(n, m; N)$ for $N \rightarrow \infty$ has been discussed in Refs. [2] and [10]. For the sake of completeness, we give here explicitly their expressions up to the order required to find $S_N(t)$ to second order in $1/\ln N$:

$$\begin{aligned} I(n, 0; N) & \approx \frac{1}{N} \ln^n N \left[1 + \frac{n\gamma}{\ln N} + \frac{n(n-1)}{2} \right. \\ & \quad \left. \times \frac{\gamma^2 + \pi^2/6}{\ln^2 N} + \dots \right], \end{aligned} \quad (21)$$

$$I(n, 1; N) \approx \frac{1}{N} \ln^n N \left[\ln \ln N \left(1 + \frac{n\gamma}{\ln N} \right) + \frac{\gamma}{\ln N} + \dots \right], \quad (22)$$

$$I(n, 2; N) \approx \frac{1}{N} (\ln^n N) \ln^2 \ln N + \dots, \quad (23)$$

where $\gamma \approx 0.577215$ is the Euler constant. Using these results we get from Eqs. (5), (12), and (19) the following expansion for the average number of distinct sites visited on a Euclidean lattice of dimension d

$$S_N(t) \approx \hat{S}_N(t) (1 - \Delta) \quad (24)$$

with

$$\hat{S}_N(t) = v_0 (4Dt \ln N)^{d/2}, \quad (25)$$

$$\Delta \equiv \Delta(N, t) = \frac{1}{2} \sum_{n=1}^{\infty} \ln^{-n} N \sum_{m=0}^n s_m^{(n)} \ln^m \ln N \quad (26)$$

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

$$s_0^{(1)} = -d\omega, \quad (27)$$

$$s_1^{(1)} = d\mu, \quad (28)$$

$$s_0^{(2)} = d \left(1 - \frac{d}{2} \right) \left(\frac{\pi^2}{12} + \frac{\omega^2}{2} \right) - d \left(\frac{dh_1}{2} - \mu\omega \right), \quad (29)$$

$$s_1^{(2)} = -d \left(1 - \frac{d}{2} \right) \mu\omega - d\mu^2, \quad (30)$$

$$s_2^{(2)} = \frac{d}{2} \left(1 - \frac{d}{2} \right) \mu^2. \quad (31)$$

Here, $\omega = \gamma + \ln A + \mu \ln(d/2)$, and A , μ and h_1 are given in Table I for $d=1, 2$ and 3 . Notice that the time dependence of $\Delta(N, t)$ comes from the term ω through the function $A(t)$. However, this function does not depend on time for the one-dimensional case and thus Δ only depends on N .

Recently, Sastry and Agmon [11] found an approximate formula for $S_N(t)$ for the one-dimensional case. The straightforward method used by these authors is based on the fact that the function $\Gamma_t^N(r)$ that appears in the integrand of Eq. (2) approaches a step function when $N \rightarrow \infty$. In this way, they found

$$S_N(t) \approx 4 \sqrt{Dt} \sqrt{\ln N - \ln \sqrt{\alpha \ln N}} \quad (32)$$

$$\approx 4\sqrt{Dt \ln N} \left[1 - \frac{1}{4} \frac{\ln \ln N - \ln \alpha}{\ln N} + \mathcal{O}\left(\frac{\ln^2 \ln N}{\ln^2 N}\right) \right], \quad (33)$$

where α is given by $\alpha = \pi \exp(-2/\pi) \approx 1.66$. It is instructive to compare this formula with the first-order approximation of Eq. (24) for the one-dimensional case

$$S_N(t) \approx 4\sqrt{Dt \ln N} \left[1 - \frac{1}{4} \frac{\ln \ln N - 2\omega}{\ln N} + \mathcal{O}\left(\frac{\ln^2 \ln N}{\ln^2 N}\right) \right]. \quad (34)$$

Note that the prefactor $4(Dt \ln N)^{1/2}$ of the formula of Sastry and Agmon is in agreement with that of Eq. (34). In Ref. [11], they found it ‘‘amusing’’ that the value $\alpha = 1$ produces very good agreement between the approximation of Eq. (32) and the exact numerical integration. Our Eq. (34) enlightens this point: Comparing Eqs. (33) and (34) one sees that $\ln \alpha$ is playing the role of 2ω . But $\omega = \gamma - \frac{1}{2} \ln \pi = 0.0048507 \dots$ for the one-dimensional lattice, so that $\ln \alpha$ when $\alpha = 1$ leads to a good approximation to the rigorous coefficient 2ω . The equation of Sastry and Agmon for $\alpha = 1$ and our first-order approximation should thus be very close. This is clearly confirmed in Fig. 4.

A question to be answered is why Eq. (24) is valid for time regime II only, i.e., why it is not always valid for arbitrarily large values of time. The reason is that our formulas have been obtained by assuming that the condition (17) holds for those values of ξ , which are inside the integration interval $[\xi_\times, \infty]$ of the relevant integral $J_N(d; \xi_\times, \infty)$ that is responsible for the asymptotic behavior of $S_N(t)$. This implies that for our procedure to work, it is necessary that $\xi_\times^2 \gg \ln A$ or, from Eq. (9), that

$$\ln N \gg |\ln A|. \quad (35)$$

Thus we can estimate the time τ_\times for which our method breaks down by solving $|\ln A(\tau_\times)| \sim \ln N$. From the expressions for A quoted in Table I one finds that $\tau_\times \sim e^N$ for $d = 2$ and $\tau_\times \sim N^2$ for $d = 3$. For $d = 1$ and large N , the condition (35) always holds because $A = (2/\pi)^{1/2}$ is a constant and then $\tau_\times = \infty$. We see that the upper times τ_\times beyond which Eq. (24) is no longer valid coincide with the crossover times t'_\times defined in Sec. I, so we can say that the expressions for $S_N(t)$ given in this paper are valid only in time regime II. This means that our procedure marks its own limit of validity as that of regime II, thus predicting the existence of a crossover time in a natural way, i.e., as a consequence of the mathematical formalism.

III. GEOMETRIC PROPERTIES OF THE EXPLORED REGION

In this section we will give a geometric interpretation of the main result of this paper, namely, Eq. (24). The quantity $S_N(t)$ is by definition the volume of the region Ω explored by N random walkers after a time t from their initial deposition on a given site of the lattice (if the length of the lattice bonds is taken as the unit). For very short times (regime I or $t \ll \ln N$) the exploration is performed in a compact way because all the neighbor sites of any visited site are always

visited at the next time step. Therefore, the explored region Ω is a hypersphere whose radius grows ballistically and its volume is proportional to t^d . After regime II is reached, the development of two qualitatively different zones in the explored volume is observed: (i) a hyperspherical compact core of visited sites, and (ii) a corona of dendritic nature characterized by filaments created by those relatively few walkers that are wandering in the outer regions, i.e., wandering at distances significantly larger than the root-mean-square displacement $\langle r^2 \rangle^{1/2} = \sqrt{2dDt}$ of a single walker. Figure 2 shows a snapshot of the set of sites visited by $N = 1000$ random walkers at time $t = 900$ (every walker makes a jump at each time unit) for dimension two. The visited sites are in white and the inner black and outer white circles delimit the corona. The radius R_+ of the outer circle is equal to the maximum displacement from the origin reached by any of the walkers at time t . It has been argued in Ref. [12] that the volume of this outer circle is on average given by the main term of Eq. (24), i.e., by $\hat{S}_N(t) = v_0(4Dt \ln N)^{d/2}$. From this statement we can draw two conclusions: First, that the average radius of this outer circle is

$$R_+ \approx (4Dt \ln N)^{1/2}, \quad (36)$$

and second, that the asymptotic corrective terms (given by Δ) to $S_N(t)$ account for the number of *unvisited* sites that are inside the corona. In other words, Δ is the fraction of the volume inside the external circumference that has not been visited by any of the N random walkers. This result can be used [12] to easily estimate that the thickness of the dendritic corona is approximately given by $R_+ \Delta$.

It is also noteworthy that $\Delta(N, t)$ depends on t very smoothly in the time regime II as this dependence is due to terms proportional to powers of $\ln A(t)$ [and $A(t)$ does not change exponentially; see Table I]. For the two-dimensional case, this statement is especially valid because $A(t) \sim 1/\ln t$.

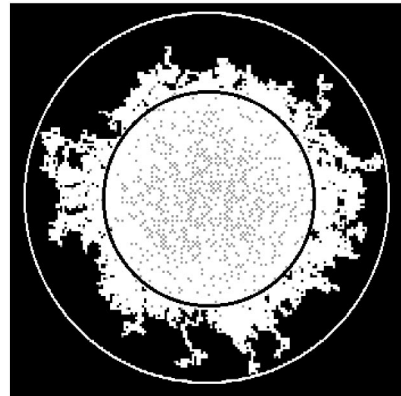


FIG. 2. A snapshot of the set of sites visited by $N = 1000$ random walkers on the two-dimensional lattice. The visited sites are in white, the unvisited ones are in black and the internal gray points are the random walkers. The outer white circle is centered on the starting point of the random walkers and its radius is the maximum distance from that point reached by any walker at the time the snapshot was taken. The internal black circle is concentric with the former but its radius is the distance between the origin and the nearest unvisited site.

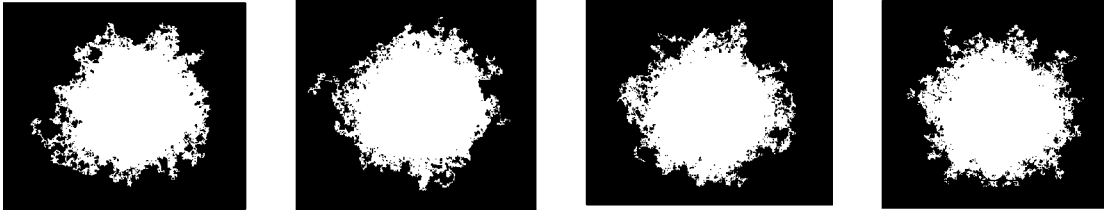


FIG. 3. Four successive scaled snapshots of the set of sites visited by $N=700$ random walkers on the two-dimensional lattice for times (from left to right) $t=2000$, $t=4000$, $t=6000$, and $t=8000$. The second snapshot has been shrunk by the factor $1/\sqrt{2}$, the third by the factor $1/\sqrt{3}$, and the last by the factor $1/2$.

Therefore, the ratio (given by Δ) between the radial size of the corona of Ω and the radial size of Ω itself remains almost constant throughout time regime II. This implies that a conveniently scaled sequence of snapshots of the set of visited sites should be very similar (in a statistical sense), i.e., we find that Ω grows, to a large extent, in a self-similar way inside time regime II. This property is illustrated in Fig. 3. As Eq. (36) shows, the appropriate scale factor must be proportional to \sqrt{t} . This ‘‘almost’’ self-similar behavior disappears as the regime III is approached because the correction to the main term of $S_N(t)$ becomes as large as this main term, i.e., because $\Delta(N, t)$ approaches the value 1. This transition takes place when $t \approx \tau_\times$ as follows from Eq. (26), i.e., this value coincides with the threshold for regime III deduced in the previous section. From the geometric point of view this transition corresponds to the breaking of the self-similar growing behavior by the appearance of a corona of filaments as large as the compact core, which finally gives rise to a set of separated trails that (almost) never more overlap. For the two-dimensional case the transition time from regime II to regime III is so great for any significant number of walkers that it cannot be studied by numerical simulation.

IV. NUMERICAL RESULTS

We carried out numerical simulations for the number of distinct sites visited by $N=2^m$, with $m=0, 1, \dots, 14$ in two and three dimensions. For the one-dimensional case it is not necessary to carry out simulations because the survival probability is exactly known on this lattice, $\Gamma_r(\mathbf{r}) = \text{erf}(\xi/\sqrt{2})$, and therefore the integral for $S_N(t)$ as given by Eq. (3) can be computed numerically.

In our simulations, the random walkers are placed initially at the center of a hypercubic box of side L . Regime II is reached almost immediately with the number of random walkers we have used ($t_\times \approx 10$ for $N=2^{14}$). The simulations were carried out only to a maximum time $t=200$ which is sufficient for the stabilization of regime II conditions. The square box side for $d=2$ was taken to be $L=400$ to avoid any random walker reaching the edge of the box before the maximum time $t=200$. Memory limitations forced us to reduce the box side to $L=200$ for the three-dimensional case. While this implies a possible appearance of finite-size effects, we can consider them to be negligible because the average displacement of the random walkers at the maximum time is small compared with $L/2$. Each experiment was repeated 10^4 times in order to achieve reasonable statistics.

Results are plotted in Fig. 4 for one, two, and three dimensions. The dots are the simulation results (numerical in-

tegration results in one dimension) and the broken and solid lines are the prediction of Eq. (24) to first and second order, respectively. The crosses are the results of Sastry and Agmon [11] given by Eq. (32) with $\alpha=1$. The dotted lines correspond to the result of Larralde *et al.* given by Eq. (1) using the correct amplitude of the main term (see Ref. [12]). The quantity plotted is

$$\mathcal{S} \equiv \frac{1}{d} \left[\frac{S_N}{\hat{S}_N} \right]^{2/d}, \quad (37)$$

versus $1/\ln N$. From Eq. (24) one sees that the theoretical prediction for this quantity is $\mathcal{S} \approx (1/d)(1-\Delta)^{2/d}$. The agreement between the second-order approximation and the simulations is found to be excellent for $N \geq 100$. Good agreement for lower values of N would be expected if higher-order terms in the series were included. The importance of the corrective terms is evident. For example, for the one-

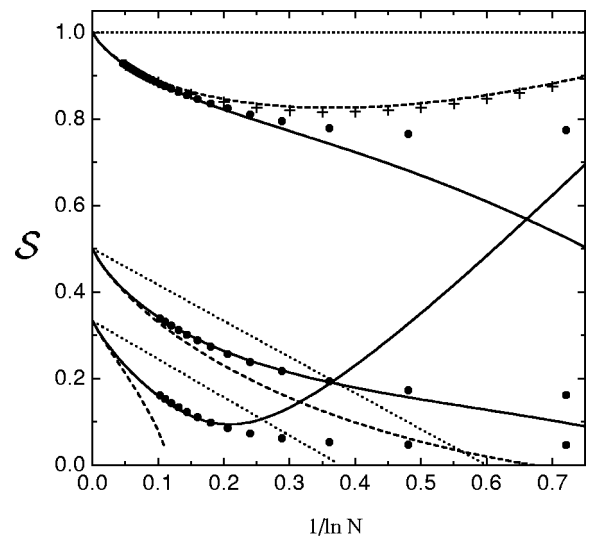


FIG. 4. $\mathcal{S} = [S_N(t)/v_0]^{2/d}/(4dDt \ln N)$ versus $1/\ln N$ for, from top to bottom, dimension 1, 2, and 3 and $t=200$ (inside time regime II). We have used $N=2^m$ with $m=3, \dots, 14$ for $d=2, 3$, and $m=3, \dots, 30$ for $d=1$. The numerical results are plotted as filled circles and the broken [solid] lines correspond to the theoretical predictions for $S_N(t)$ to first [second] order as given by Eq. (24). Notice that the approximation of order 0 would be a horizontal line (not shown here) passing through $1/d$. The crosses correspond to the Sastry and Agmon result of Eq. (32) with $\alpha=1$. The dotted lines correspond to the result of Larralde *et al.* given by Eq. (1) in which the corrected amplitude of the main term has been used (see Ref. [12]).

dimensional case, we would need to use values of N as large as 10^{25} in order to obtain the same precision with the main term as we get with the main and two corrective terms for values of N as small as 2^6 . Similar statements can be made for the other lattices, as Fig. 4 shows.

V. REMARKS

In this paper, we have developed a method for calculating the mean number of distinct sites visited by N independent random walkers on Euclidean lattices. The method allows the systematic calculation of the main and corrective asymptotic terms to any order for large N . These corrective terms are generally non-negligible as they (essentially) decay as powers of $1/\ln N$. However, we found that the main and first two corrective terms lead to reasonably good results when relatively small values of N are used (say, for $N \gtrsim 2^7$). In Sec. III, we proposed a geometric meaning for the main and corrective terms: the main term would account for the volume of the set of visited sites if the exploration of the random walkers were compact, and the corrective terms just improve this rough estimate because, in the outer regions, the exploration performed by the (relatively few) random walkers that move there is really not compact, thus leading to the formation of a noncompact (a dendritic) external ring in the set of visited sites. We hope the above results and ideas could serve as a basis to gain insight into problems with interacting random walkers.

The method developed here for calculating $S_N(t)$ is also useful for evaluating other statistical quantities related to the diffusion of a set of independent random walkers. An example is the number $S_{N+}(t)$ of sites visited by N random walkers on a one-dimensional lattice along a given direction [11]. It turns out that the moments (of arbitrary order) of $S_{N+}(t)$ can be readily obtained through a slight modification of Eq. (24). Another example is the first passage time $t_{1,N}(r)$ to a distance r of the first random walker of a set of N . First passage times are relevant statistical quantities in the study of diffusion processes where the arrival of the first particles at a given site produces a significant effect (a ‘‘trigger’’ effect). These quantities have been calculated for one dimension [3,13] (and for some classes of fractals [3]) but little is known for dimensions greater than one [2]. The approximate compact form of the set of visited sites allows one to estimate the first passage time via the relation $S_N(t_{1,N}(r)) \approx v_0 r^d$ [12], which means geometrically that we consider the region inside the hypersphere of radius r where a random walker has arrived by time $t_{1,N}(r)$ as completely visited (a compact exploration in the sense of de Gennes [14]). Results on $S_{N+}(t)$ and $t_{1,N}(r)$ obtained using the above ideas will be reported elsewhere.

The function $S_N(t)$ we have studied is indeed an important quantity concerning the diffusion of N independent random walkers but there are still many open questions in this problem. One can think, for example, of the absorption probability of the set of N random walkers on a lattice with a random distribution of pointlike traps. This problem can be formulated in terms of the moments of the number of distinct sites visited by the set of N walkers. A prediction for the variance of the number of visited sites is a necessary requisite to tackle this interesting problem as the first-order ap-

proximation based only on its first moment, i.e., on $S_N(t)$, seems to be very imprecise [8]. As no relationship is known for moments of order higher than one, the absorption problem remains unsolved.

Finally, it should be pointed out that the expression for $S_N(t)$ given in this paper can be extended to fractal media with some slight changes. We are currently running simulations for deterministic (Sierpinski gasket) and stochastic (percolation aggregate) fractals. Results for these substrates will be published elsewhere.

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APPENDIX

We will show in this Appendix how to get Eq. (19) from Eq. (15). Let us start by showing that the solution $\xi(z)$ of Eq. (16) for $z \rightarrow 0$ has the form given in Eq. (18). For simplicity of notation, we will write $u = \xi^{-2}$, $\phi = 1 - \exp(-z)$ and $c = d/2$. Hence, Eq. (16) takes the form

$$-\frac{c}{u} + \mu \ln u + \ln A + \ln \left(1 + \sum_{n=1}^{\infty} h_n u^n \right) = \ln \phi. \quad (\text{A1})$$

In the limit $z \rightarrow 0$, it is clear that $u \rightarrow 0$ and $\phi \rightarrow 0$. This means that as long as $1/u \gg |\ln(A)|$, the first term on the right-hand side of (A1) is the most divergent one so that, as a first approximation, we have

$$u \approx -\frac{c}{\ln \phi} \equiv x. \quad (\text{A2})$$

This first-order approximation was already obtained in Sec. II [see below Eq. (17)]. A better approximation is achieved by writing $u = x(1 + \epsilon)$, with ϵ a small quantity. The substitution of this expression in Eq. (A1) yields

$$\begin{aligned} \epsilon - \epsilon^2 + \frac{\mu x}{c} \ln x + \frac{x}{c} \ln A + \frac{\mu x}{c} \epsilon - \frac{\mu x}{2c} \epsilon^2 + \frac{h_1 x^2}{c} + \frac{h_1 x^2 \epsilon}{c} \\ + \dots = 0, \end{aligned} \quad (\text{A3})$$

where Eq. (A2) has been taken into account. This equation can be solved by writing ϵ as

$$\epsilon = \sum_{n=1}^{\infty} \epsilon_n x^n, \quad (\text{A4})$$

and inserting it in Eq. (A3). We thus find the following values for ϵ_n up to $n=2$:

$$\epsilon_1 = -\frac{1}{c} \ln(Ax^\mu), \quad (\text{A5})$$

$$\epsilon_2 = \frac{1}{c^2} \ln^2(Ax^\mu) + \frac{\mu}{c^2} \ln(Ax^\mu) - \frac{h_1}{c}. \quad (\text{A6})$$

Therefore,

$$\xi(z) = u^{-1/2} = x^{-1/2}(1 + \epsilon)^{-1/2} = x^{-1/2} \sum_{n=0}^{\infty} \delta_n x^n, \quad (\text{A7})$$

where $\delta_0 = 1$ and

$$\delta_1 = \frac{\ln(Ax^\mu)}{2c},$$

$$\delta_2 = -\frac{1}{8c^2} [\ln^2(Ax^\mu) + 4\mu \ln(Ax^\mu) - 4ch_1]. \quad (\text{A8})$$

The evaluation of the integral for $K_N(\alpha)$ in Eq. (15) requires the expression of $\xi^\alpha d\xi/dz$ as a function of z . From Eq. (A7) and taking into account that $d\xi/dz = (d\xi/dx)(dx/dz)$ and $dx/dz = [x^2/(c\phi)]d\phi/dz$, we find that

$$\xi^\alpha \frac{d\xi}{dz} = -\frac{1}{2c\phi} \frac{d\phi}{dz} x^{(1-\alpha)/2} \left[1 + \sum_{n=1}^{\infty} x^n \sum_{m=1}^n \hat{k}_m^{(n)} \ln^m(Ax^\mu) \right], \quad (\text{A9})$$

where the coefficients $\hat{k}_m^{(n)}$, $m=0, \dots, n$ for $n=1, 2$ are

$$\begin{aligned} \hat{k}_0^{(1)} &= -\frac{\mu}{c}, \\ \hat{k}_1^{(1)} &= \frac{\alpha-1}{2c}, \\ \hat{k}_0^{(2)} &= \frac{(\alpha-3)h_1}{2c} + \frac{\mu^2}{c^2}, \\ \hat{k}_1^{(2)} &= \frac{\mu(2-\alpha)}{2c^2}, \\ \hat{k}_2^{(2)} &= \frac{\alpha(\alpha-4)+3}{8c^2}. \end{aligned} \quad (\text{A10})$$

Let us use $\hat{K}_N(\alpha, z)$ to denote the integrand of Eq. (15), i.e.,

$$K_N(\alpha) = \int_0^{z \times} \hat{K}_N(\alpha, z) dz. \quad (\text{A11})$$

Then, from Eq. (A9),

$$\begin{aligned} \hat{K}_N(\alpha, z) &= \frac{1}{2c} e^{-Nz} e^{-z} x^{(1-\alpha)/2} \\ &\times \left[1 + \sum_{n=1}^{\infty} x^n \sum_{m=1}^n \hat{k}_m^{(n)} \ln^m(Ax^\mu) \right]. \end{aligned} \quad (\text{A12})$$

Writing $e^{-z} = 1 + \mathcal{O}(z)$, $x = -(c/\ln z)[1 + \mathcal{O}(z/\ln z)]$ and $\ln(Ax^\mu) = \ln A - \mu \ln(-\ln z) + \mu \ln c + \mathcal{O}(z/\ln z)$, Eq. (A12) becomes

$$\begin{aligned} \hat{K}_N(\alpha, z) &= [1 + \mathcal{O}(z)] \frac{1}{2c^{(\alpha+1)/2}} e^{-Nz} (-\ln z)^{(\alpha-1)/2} \\ &\times \sum_{n=0}^{\infty} \sum_{m=0}^n k_m^{(n)} (-\ln z)^n \ln^m(\ln z), \end{aligned} \quad (\text{A13})$$

where the coefficients $k_m^{(n)}$ up to second order ($n=2$) are

$$\begin{aligned} k_0^{(1)} &= (\alpha-1) \frac{\omega}{2} - \mu, \\ k_1^{(1)} &= (1-\alpha) \frac{\mu}{2}, \\ k_0^{(2)} &= (3-\alpha)(1-\alpha) \frac{\omega^2}{8} + \mu(2-\alpha)\omega + \mu^2 + \frac{h_1 c}{2}(\alpha-3), \\ k_1^{(2)} &= \mu \left[(\alpha-2)\mu + (\alpha-3)(1-\alpha) \frac{\omega}{4} \right], \\ k_2^{(2)} &= \frac{\mu^2}{8} (\alpha-3)(\alpha-1), \end{aligned}$$

and $\omega = \gamma + \ln A + \mu \ln c$. Finally, inserting Eq. (A13) into Eq. (A11) we get Eq. (19). It should be noted that we have approximated the factor $1 + \mathcal{O}(z)$ of Eq. (A13) by 1. This can be done safely because the contribution of the neglected terms to the asymptotic behavior of $K_N(\alpha)$ decays as least as $(\ln N)^{(\alpha-1)/2}/N^2$, i.e., decays to zero faster than the contribution of the retained terms by (roughly) a factor N [see Eqs. (19)–(23)].

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- [1] M.F. Shlesinger, *Nature (London)* **355**, 396 (1992).
 [2] G.H. Weiss, K.E. Shuler, and K. Lindenberg, *J. Stat. Phys.* **31**, 255 (1983); S.B. Yuste and K. Lindenberg, *ibid.* **85**, 501 (1996).
 [3] S.B. Yuste, *Phys. Rev. Lett.* **79**, 3565 (1997); *Phys. Rev. E* **57**, 6237 (1998).
 [4] H.E. Larralde, P. Trunfio, S. Havlin, H.E. Stanley, and G.H. Weiss, *Nature (London)* **355**, 423 (1992).
 [5] H.E. Larralde, P. Trunfio, S. Havlin, H.E. Stanley, and G.H. Weiss, *Phys. Rev. A* **45**, 7128 (1992).
 [6] A. Dvoretzky and P. Erdős, *Proceedings of the Second Berkeley Symposium on Mathematical Statistics and Probability*

- (University of California Press, Berkeley, 1951).
 [7] E.W. Montroll and M.F. Shlesinger, in *Nonequilibrium Phenomena II: From Stochastics to Hydrodynamics*, edited by E.W. Montroll and J.L. Lebowitz (North-Holland, Amsterdam, 1984).
 [8] B. H. Hughes, *Random Walks and Random Environments, Volume 1: Random Walks* (Clarendon Press, Oxford, 1995); *Random Walks and Random Environments, Volume 2: Random Environments* (Clarendon Press, Oxford, 1996).
 [9] G.H. Weiss, *Aspects and Applications of the Random Walk* (North-Holland, Amsterdam, 1994).
 [10] R. Wong, *Asymptotic Approximations of Integrals* (Academic

- Press, San Diego, 1989).
- [11] G.M. Sastry and N. Agmon, J. Chem. Phys. **104**, 3022 (1996).
- [12] S.B. Yuste and L. Acedo, Phys. Rev. E **60**, R3459 (1999).
- [13] G.H. Weiss, K.E. Shuler, and K. Lindenberg, J. Stat. Phys. **31**, 255 (1983); S.B. Yuste and K. Lindenberg, *ibid.* **85**, 501 (1996).
- [14] P.G. de Gennes, C. R. Acad. Sci., Ser. I: Math. **296**, 881 (1983); J. Chem. Phys. **76**, 3316 (1982).