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Number of distinct sites visited by N particles diffusing on a fractal

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We study the mean number of distinct sites, $S_N(t)$, visited up to time t by $N \gg 1$ noninteracting random walkers all starting from the same origin on a fractal substrate of dimension d_f. Using analytic arguments and numerical simulations, we find $S_N(t) \sim (\ln N)^{d_f/\delta}\, t^{d_s/2}$ for fractals with spectral dimension $d_s \equiv 2d_f/d_w < 2$, where $\delta \equiv d_w/(d_w-1)$ and d_w is the fractal dimension of a random walk.

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The number of distinct sites visited by a single random walker $S_1(t)$ has been studied extensively for square and cubic lattices and for fractals [1–4]. This quantity is useful for the analysis of problems of trapping and kinetic reactions and is related to the vibrational density of states [5]. In the simple diffusion reaction [6,7], $A+B \to B$, where A are static particles and B is a particle diffusing randomly, $S_1(t)$ is proportional to the total number of reactions. In the analogous case $A+B \to A$ where B is static (the target problem [2]) the survival probability of a B particle is given by $\exp[-a\langle S_1(t)\rangle]$. For the reaction $A+B\to B$ where the A's are moving and the B's are static and distributed randomly with concentration c, the survival probability of an A particle is given by [1,8] $\langle (1-c)^{S_1(t)}\rangle$.

The generalization of this problem to the number of distinct sites visited by N random walkers, $S_N(t)$, has recently been studied for d-dimensional Euclidean lattices [9]. The number of distinct sites visited by N walkers is not related to the the number of distinct sites visited by *each* walker. It is found that there are distinct time regimes, separated by two crossover times $t_\times$ and $t'_\times$, where $t_\times \sim \ln N$ (for all d) while $t'_\times$ is different for different dimensions: $t'_\times = \infty$ ($d=1$), e^N ($d=2$), and N^2 ($d=3$).

• *Regime I*: The extremely short-time regime $[t \ll t_\times]$, for which $S_N(t) \sim t^d$.

• *Regime II*: An intermediate-time regime $[t_\times \ll t \ll t'_\times]$, for which $S_N(t) \sim t^{d/2}(\ln u)^{d/2}$ with $u \equiv NS_1(t)/t^{d/2}$.

• *Regime III*: A long-time regime $[t \gg t'_\times]$, for which $S_N(t) \sim NS_1(t)$ when $d \geq 2$.

In this work we study what happens to these growth laws when the diffusion takes place on a fractal substrate of dimension d_f. We use exact enumeration, Monte Carlo and analytic arguments. We find that for spectral dimension [5] $d_s = 2d_f/d_w < 2$, $S_N(t)$ has *only* two time regimes (here d_w is the fractal dimension of a random walk), separated by the crossover time $t \ll t_\times \sim \ln N$.

• *Regime I:* An extremely short-time regime in which

$$S_N(t) \sim t^{d_\ell}, \qquad t \ll t_\times \tag{1}$$

where d_ℓ is the chemical distance exponent [8].

• *Regime II*: A long-time regime, where

$$S_N(t) \sim (\ln N)^{d_f/\delta}\, t^{d_s/2}, \qquad t \gg t_\times \tag{2}$$

where $\delta \equiv d_w/(d_w-1)$.

Thus, in the fractal case with $d_s < 2$, we find that "screening" occurs at all times (screening refers to the overlap of the contributions of different walkers), and the "unscreened" regime III is never reached. For this reason only the first two regimes exist ($t'_\times = \infty$); we expect that the third regime will appear only for fractals with $d_s \geq 2$.

We use here a formalism similar to that used for homogeneous lattice systems [9]. Let $f_t(\mathbf{r})$ be the probability that a single random walker is at site $\mathbf{r}$ of the fractal *for the first time* at step t, and let $\Gamma_t(\mathbf{r})$ be the probability that site $\mathbf{r}$ has *not* been visited by this walker by step t, then $\Gamma_t(\mathbf{r}) = 1 - \sum_{t'=0}^{t} f_{t'}(\mathbf{r})$. Since the N walkers are independent, the probability that site $\mathbf{r}$ on the fractal has *not* been visited by any of the N random walkers is $\Gamma_t^N(\mathbf{r})$, so the probability that site $\mathbf{r}$ has been visited by at least one walker by step t is $1 - \Gamma_t^N(\mathbf{r})$. Thus the expected number of distinct sites visited by any of the N random walkers by step t is

$$S_N(t) = \sum_{\mathbf{r}} \{1 - \Gamma_t^N(\mathbf{r})\}. \tag{3}$$

The sum in (3) is over all the sites in the fractal lattice.

The short-time behavior of $S_N(t)$ (regime I) can be derived from Eq. (3). When N tends to infinity, $\Gamma_t^N(\mathbf{r})$ tends to zero if it is possible that a walker may arrive at site $\mathbf{r}$ by step t. In this limit, $S_N(t)$ consists of all the sites which have nonzero probability of being visited by step t. Since we are dealing with nearest-neighbor steps, t is equal to the chemical distance ℓ and

$$S_N(t) \sim t^{d_\ell}. \tag{4}$$

Thus we find that in regime I $S_N(t)$ is independent of N. This behavior is valid as long as $NP_{\min}(t) \gg 1$, where $P_{\min}$ is the smallest nonzero occupation probability on the lattice at time t. If z is the mean lattice coordination number, then $P_{\min}(t) = z^{-t}$. Therefore, we expect this short-time regime to end at a crossover time

$$t_\times \sim \ln N. \tag{5}$$

To find the other regimes, we define the generating function $\hat{S}_u(t) \equiv \sum_{N=0}^{\infty} S_N(t) u^N$. From Eq. (3), we have

$$\hat{S}_u(t) = \frac{u}{1-u} \sum_{\mathbf{r}} \frac{1 - \Gamma_t(\mathbf{r})}{1 - u\Gamma_t(\mathbf{r})}. \tag{6}$$

Since we are interested in the behavior of $S_N(t)$ after a large number of steps, $t \gg 1$, we can use the continuum approximation to calculate $\Gamma_t(\mathbf{r})$. In analogy with Euclidean lattices, we expect the following scaling relation to hold for fractal substrates:

$$\Gamma_t(\mathbf{r}) \sim g(v), \quad [v \equiv r/t^{1/d_w}]. \tag{7}$$

Replacing the sum over the lattice in Eq. (6) by an integral over space we obtain

$$\hat{S}_u(t) \sim \frac{2\sigma u t^{d_s/2}}{1-u} \int_0^\infty \frac{1 - g(v)}{1 - ug(v)} v^{d_f - 1} dv. \tag{8}$$

Using standard Tauberian methods, we relate the behavior of $\hat{S}_u(t)$ near $u = 1$ to the large N limit of $S_N(t)$. The integral in Eq. (8) diverges as $u \to 1$ because of the behavior of the integrand at large v. Hence, in determining the behavior of $\hat{S}_u(t)$ as $u \to 1$, we can replace the function $g(v)$ by its asymptotic expression.

To study the form of $g(v)$ we analyzed $1 - g(v) \sim v^{-d_f} f(v)$, which is the probability of reaching site r on the fractal for the first time within t steps. One might expect that the form of $f(v)$ is the exponential part of the free particle probability density on a fractal, $p(r,t) \sim t^{-d_s/2} \exp[-a(r/t^{1/d_w})^\delta]$, i.e. [8],

$$f_t(r) \equiv f(v) \sim \exp(-v^\delta). \tag{9}$$

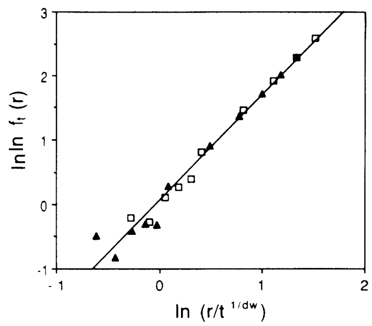

FIG. 1. Numerical simulations based on exact enumeration for the probability of a random walker on a fractal to reach a site $\mathbf{r}$ for the first time at time t. The simulations were performed on the $d = 2$ incipient infinite percolation cluster at criticality. For a given configuration the results were calculated exactly and averages were taken over 200 configurations. Results are for $t = 200$ (□) and $t = 500$ (▲) and the slope of 1.6 ± 0.1 is in good agreement with the theoretical prediction, $\delta = d_w/(d_w - 1) \approx 1.54$ from Eq. (9).

Figure 1 shows numerical data from simulations for the first passage time, $f_t(\mathbf{r})$, calculated on a $d = 2$ percolation cluster at criticality. The slope, 1.6 ± 0.1, is in good agreement with $d_w = 2.87$ and $\delta = d_w/(d_w - 1) \simeq 1.54$, supporting Eq. (9). Substitution of Eq. (9) into Eq. (8) yields

$$\hat{S}_u(t) \sim \frac{u t^{d_s/2}}{1-u} \int_0^\infty \frac{v^{d_f - 1} dv}{1 + v^{d_f} e^{v^\delta}(1-u)}. \tag{10}$$

A Tauberian theorem applied to the above expressions leads to an asymptotic expression for regime II $[t \gg t_\times]$,

$$S_N(t) \sim (\ln N)^{d_f/\delta}\, t^{d_s/2}, \quad d_s \leqslant 2. \tag{11}$$

The logarithmic dependence in the number of walkers can be understood to be a consequence of a "screening" effect due to the relatively small number of distinct sites available to the walkers on a fractal.

The results obtained for $S_N(t)$ were compared with simulations generated by the method of exact enumeration based on Eq. (3). The results of these simulations support Eq. (11) and are shown in Figs. 2 and 3.

The logarithmic dependence on N can be understood using a heuristic argument. The probability of finding a random walker outside a radius R is given by

$$\int_R^\infty p(r,t) r^{d_f - 1} dr \sim t^{-d_s/2} \int_R^\infty \exp\left[-a\left(\frac{r}{t^{1/d_w}}\right)^\delta\right] r^{d_f - 1} dr \sim \exp\left[-a\left(\frac{R}{t^{1/d_w}}\right)^\delta\right]. \tag{12}$$

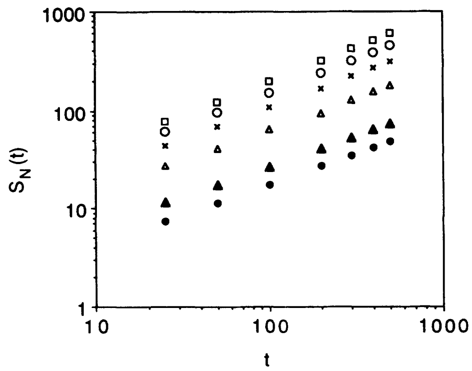

FIG. 2. Number of distinct sites $S_N(t)$ visited by N random walkers on the $d=2$ incipient infinite percolation cluster at criticality. Shown are exact enumeration results for $N=1$ (•), $N=2$ (▲), $N=16$ (△), $N=128$ (×), $N=1024$ (○), and $N=8192$ (□).

Let us assume that this probability is of the order of $1/N$, i.e., only a few particles (of the order of 1) are outside R. By comparing Eq. (12) to $1/N$ it follows that $R \sim (\ln N)^{1/\delta} t^{1/d_w}$. By assuming that up to a radius R a site is visited with a finite probability we obtain $S_N(t) \sim R^{d_f}$ which implies the scaling relation in Eq. (11).

Our results may be useful for studying the problem of the survival probability of N diffusing particles which start from the same origin in the presence of a random distribution of trapping centers. The short-time probability that *all* N particles survive after time t will be given by

$$F_N(t) \sim \exp[-cS_N(t)] \sim \exp\{-c(\ln N)^{d_f/\delta}\, t^{d_s/2}\}, \tag{13}$$

where c is a constant depending on the concentration of traps c_T. The asymptotic time result can be derived by using analogous considerations to those used for the single particle result [10,11]. The probability $P(V,t)$ that a given particle survives for time t in a trap-free region of volume V, which is enclosed by a trapping boundary is

$$P(V,t) \sim \exp\left[-\text{const} \times \frac{t}{V^{2/d_s}}\right]. \tag{14}$$

The probability of finding a trap-free region of fractal

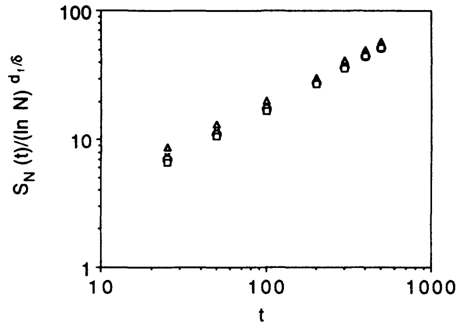

FIG. 3. Same data as in Fig. 2 for $N \geq 16$ are presented by plotting $S_N(t)/(\ln N)^{d_f/\delta}$ vs t on a double-logarithmic scale. The data collapse and the slope ~ 0.66 support Eq. (11), since $d_s \approx 1.32$ for $d=2$ percolation clusters at criticality.

volume V in the system follows a Poisson distribution, $P_0(V) \sim \exp(-c_T V)$. For randomly distributed traps, the survival probability of N walkers, $F_N(t)$, is dominated by the large but rare trap-free regimes. Hence, for $t \to \infty$

$$F_N(t) \sim \max_{\{V\}}[P_0(V)P^N(V,t)] \tag{15}$$

which yields

$$F_N(t) \sim \exp[-\text{const} \times c_T^{2/(d_s+2)}(Nt)^{d_s/(d_s+2)}]. \tag{16}$$

Equation (16) is the analog of the single particle Donsker and Varadhan result [12] when generalized to N particles and a fractal substrate.

The different time regimes are a consequence of the initial condition that all the walkers start at the same origin. Our result may change as the degree of initial localization varies, which can be seen as follows. Let ℓ be the linear size of the region in which the walkers are initially distributed, and let $\xi(t)$ be the characteristic distance traveled by a random walker in t steps, $\xi(t) \sim t^{1/d_w}$. Then, if $\ell \ll \xi(t_\times) \sim [\ln(N)]^{1/d_w}$, we expect to have a growth regime similar to regime I. On the other hand if $\xi(t_\times) \ll \ell$, we will not have regime I but we still expect to see the screening effects which characterize regime II.

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