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Some recent variations on the expected number of distinct sites visited by an n-step random walk

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Asymptotic forms for the expected number of distinct sites visited by an n-step random walk, being calculable for many random walks, have been used in a number of analyses of physical models. We describe three recent extensions of the problem, the first replacing the single random walker by $N \rightarrow \infty$ random walkers, the second to the study of a random walk in the presence of a trapping site, and the third to a random walk in the presence of a trapping hyperplane.

1. Introduction

The problem of determining properties of the number of distinct sites visited by an n-step lattice random walk was first suggested in the mathematical literature by Dvoretzky and Erdös [1]. Indeed, the complete characterization of such properties presents a formidable mathematical challenge because the number of distinct sites visited by an n-step random walk, a quantity to be denoted by R_n, is non-Markovian even when the underlying random walk is a Markov process. In practice, only for the one-dimensional nearest-neighbor random walk can one find an exact expression for the probability distribution of R_n.

In spite of the mathematical challenge posed by a calculation of properties of R_n it is nevertheless an important variable in a variety of physical problems. A prime example of this is provided by the trapping problem, in which a trap is assigned to each site on an infinite lattice with a probability c. One then asks for the probability that an arbitrarily placed random walk in the presence of a set of traps will survive for at least n steps. Call this quantity S_n. A formally exact representation of this probability is

$$S_n = \langle (1-c)^{R_n} \rangle , \tag{1}$$

where the brackets indicate an average with respect to the configuration of traps and to the set of all n-step random walks. Eq. (1) indicates that S_n can be regarded a cumulant-generating function of the R_n so that if one knew the form of S_n one would also be able to find the probability distribution of R_n. Even a calculation of an asymptotic form for this distribution requires extremely complicated mathematical machinery [2,3], and little is known about the magnitude of n required to validate the use of asymptotic results. However, it is relatively straightforward to find an asymptotic form of the expected value of $\langle R_n \rangle$ with the aid of Tauberian theorems for power series [4,5]. Even this meager amount of information is sometimes used as a first approximation in the calculation of physically useful properties. Again we refer to the trapping problem in which Rosenstock suggested as an approximation to S_n in eq. (1) [6],

$$S_n \sim (1-c)^{\langle R_n \rangle} . \tag{2}$$

It is now well known that this formula is incorrect at large n, but may nevertheless provide a useful approximation to S_n in the range of relatively small but not physically unrealistic values of n, and at low trap concentration c [7]. Most of the calculations of $\langle R_n \rangle$ to date presume that one is interested in properties of R_n for a single random walker on a completely infinite lattice. In this paper we will review three recent calculations of $\langle R_n \rangle$ which relax one or both of the assumptions mentioned earlier in the paragraph. The first of these deals with the expected number of distinct sites visited by N ($\gg 1$) random walkers, the second with $\langle R_n \rangle$ for a single random walker in the presence of a trapping site, and third to a calculation of $\langle R_n \rangle$ in the presence of a trapping hyperplane.

2. Expected number of distinct sites visited by N random walkers

We have noted the identification of the problem of the distinct number of sites visited by a single random walker with the trapping problem. If we now suppose that there are N independently moving random walkers on a lattice then a knowledge of R_n is equivalent to a knowledge of the survival probability of all N walkers in the presence of a random configuration of traps. A recent analysis of this problem considered the case in which the motion of the N walkers evolves according to symmetric transition probabilities [8]. As is true in the case $N = 1$ the asymptotic results are determined from the generating function for the probability for a single random walker, initially at the origin, to reach a point $\boldsymbol{r}$ for the first time at step n. Call this probability $f_n(\boldsymbol{r})$. Its generating function with respect to n is known in terms of a ratio of integrals [5]. Let the probability that the site $\boldsymbol{r}$ has *not* been visited by step n denoted by $\Gamma_n(\boldsymbol{r})$, which is expressible in terms of the $f_j(\boldsymbol{r})$, $j = 1, 2, \ldots, n$, by

$$\Gamma_n(\boldsymbol{r}) = 1 - \sum_{j=0}^{n} f_j(\boldsymbol{r}) . \tag{3}$$

Let the expected number of distinct sites visited by N random walkers in n steps be denoted by $\langle R_n(N) \rangle$. The probability that the site $\boldsymbol{r}$ has been visited by at least one of the N random walks by step n is equal to $1 - \Gamma_n^N(\boldsymbol{r})$ provided that the random walks are initially at the origin. This allows us to express $\langle R_n(N) \rangle$ as a sum of this function over all lattice sites,

$$\langle R_n(N) \rangle = \sum_{\boldsymbol{r}} [1 - \Gamma_n^N(\boldsymbol{r})] . \tag{4}$$

It is convenient, in considering the dependence on N, to introduce a generating function with respect to this parameter. The generating function will be denoted by $R(u; n)$, which is defined by

$$R(u; n) \equiv \sum_{j=0}^{\infty} \langle R_n(j) \rangle u^j = \frac{u}{1-u} \sum_{\boldsymbol{r}} \frac{1 - \Gamma_n(\boldsymbol{r})}{1 - u\Gamma_n(\boldsymbol{r})} , \tag{5}$$

which is derived by substituting eq. (4) into the definition of the generating function. All of the results obtainable for this problem are based on an analysis of this generating function. The limit $N \to \infty$ can be identified with the limit $u \to 1$, which validates the replacement of the sum in eq. (5) by the integral

$$R(u; n) \sim \frac{1}{1-u} \int \frac{1 - \Gamma_n(\boldsymbol{r})}{1 - u\Gamma_n(\boldsymbol{r})} \, \mathrm{d}^D \boldsymbol{r} , \tag{6}$$

where D is the number of dimensions. Of course, since we have assumed spherical symmetry in D dimensions, eq. (6) is reducible to a single integral with respect to the radial coordinate.

The most striking feature that emerges from the calculations is the existence of a number of different regimes in the dependence of $\langle R_n(N) \rangle$ on n and N. These regimes are determined by the order in which the limits $n, N \to \infty$ are taken. We can observe that when a single random walker can visit at most $\Omega < \infty$ sites on a single step then when n is held fixed and N is taken to infinity, it is certain that all possible accessible sites will be visited. That is to say that for this class of random walks $\lim_{N \to \infty} \langle R_n(N) \rangle = n\Omega$. The corresponding result when the number of permissible steps is infinite has not been investigated.

Let us outline the analysis and the results that follow from it in the case of one-dimensional random walks in which the variance of each individual step is equal to σ^2. Then it has been shown that in the continuum limit in space (this is a reasonable limit to take since we are only interested in the limit of large n) the first passage time density $f_n(x)$ tends towards the form [9]

$$f_n(x) = \frac{|x|}{2\sigma\sqrt{\pi n^2}} \exp\left(-\frac{x^2}{4\sigma^2 n}\right) \tag{7}$$

and the corresponding value of $\Gamma_n(x)$ is

$$\Gamma_n(x) = \operatorname{erf}\left(\frac{|x|}{2\sigma\sqrt{n}}\right). \tag{8}$$

Hence it follows that after a change of the integration variable in eq. (6),

$$R(u; n) \sim \frac{2\sigma\sqrt{n}}{1-u} \int_0^\infty \frac{1-\operatorname{erf}(v)}{1-u\operatorname{erf}(v)}\, \mathrm{d}v = \frac{2\sigma\sqrt{n}}{1-u} I(u), \tag{9}$$

where $I(u)$ is the integral in this equation. As mentioned, we are interested in the limit $N \to \infty$ or, since Tauberian methods will be used to derive the behavior in this limit, we need the singular behavior of $R(u; n)$ in the limit $u \to 1$. One singularity comes from the multiplicative factor $(1-u)^{-1}$ and the second is a result of the singularity of the integral when u is set equal to 1. The second of these two contributions to the singular behavior of $R(u; n)$ is due to the fact that the integrand is equal to 1 when $u = 1$, hence the singularity originates in the behavior of the integrand at very large values of v. This implies that in finding the form of the singularity we need only retain the asymptotic form for $\operatorname{erf}(v)$ in the calculation,

$$1 - \operatorname{erf}(v) \sim \frac{\mathrm{e}^{-v^2}}{v\sqrt{\pi}}, \tag{10}$$

from which one finds

$$I(u) \sim \int_0^\infty \frac{\mathrm{d}v}{1 + \sqrt{\pi}\, v\, \mathrm{e}^{v^2}(1-u)}. \tag{11}$$

An analysis of the behavior of $I(u)$ for u close to 1 has been carried out in ref. [8], and the final result for $R(u; n)$ in this regime is

$$R(u; n) \sim \frac{\sigma\sqrt{n}}{1-u} \sqrt{\ln\left(\frac{1}{1-u}\right)}. \tag{12}$$

This is equivalent to the estimate

$$\langle R_n(N) \rangle \sim \sigma\sqrt{n \ln(N)} \tag{13}$$

valid when N is large. This calculation establishes the fact that the functional form of the large n behavior of $\langle R_n(N) \rangle$ has the square-root dependence that appears in the corresponding result for $n = 1$. However, in addition, we can assert that the overlap effect due to there being N rather than a single random walker is proportional to $\ln^{1/2}(N)$.

A striking feature that emerges from the one-dimensional model is the existence of two regimes in the time-dependent behavior, the first occurring when n is fixed and N tends towards ∞ in which case $\langle R_n(N) \rangle$ is proportional to n, and the second occurring when N is large but fixed and $n \to \infty$ which in which $\langle R_n(N) \rangle$ is proportional to $n^{1/2}$. A crossover between these two regimes occurs at a time n that is of the order of $\ln(N)$. An additional feature of interest in one dimension is that it is possible to find an asymptotically exact representation of the complete distribution of $R_n(N)$. Our result indicates that the distribution tends towards a delta function when the limit $N \to \infty$ is taken.

The analogous problems in higher dimensions are also amenable to analysis based on the fundamental formula in eq. (6). No details will be given here but we cite the results for $D = 2$ and 3 [8]. In two dimensions a first regime, in which $\langle R_n(N) \rangle$ is proportional to n^2 also occurs according to the same argument as for $D = 1$. However, there is a second region in which $\langle R_n(N) \rangle$ is also proportional to n. For the completely isotropic two-dimensional walk

$$\langle R_n(N) \rangle \sim 4\pi\sigma^2 n \ln\left(\frac{N}{\ln(n)}\right). \tag{14}$$

The crossover between these two regimes occurs for n of the order of $\ln(N)$. The final regime in two dimensions is characterized by the result

$$\langle R_n(N) \rangle \sim \frac{Nn}{\ln(n)}, \tag{15}$$

the crossover to this behavior occurring at $n = \mathcal{O}(e^N)$. This third regime gives essentially the two-dimensional result multiplied by the number of random walkers unlike the one-dimensional result, which exhibits a more pronounced screening effect. This behavior reflects the increased space available to the set of random walkers in two dimensions. Finally, in three dimensions there are again three regimes; in the first $\langle R_n(N) \rangle$ is proportional to n^3, in the second

$$\langle R_n(N) \rangle \sim 2\pi\sigma^3 (2n)^{3/2} \ln^{3/2}(N/\sqrt{n}), \tag{16}$$

the crossover time being of the order of $\ln(N)$, and in the final regime, the transition occurring at a time proportional to N^2, $\langle R_n(N)\rangle$ becomes proportional to Nn as might be expected based on our remarks for the two-dimensional case. It is furthermore possible to demonstrate a scaling form for $\langle R_n(N)\rangle$, which is

$$\langle R_n(N)\rangle \sim Cn^{3/2} f(N/\sqrt{n}) , \tag{17}$$

where the function $f(x)$ has the properties

$$f(x) = \begin{cases} x , & x \ll 1 , \\ \ln^{3/2}(x) , & x \gg 1 . \end{cases} \tag{18}$$

These properties all agree with the results of numerical calculations based on the method of exact enumeration [8,11].

The analytic arguments used to derive the results just cited are calculated on the assumption that the random walkers are all initially at the same site. It is reasonable to expect that these asymptotic results will also be valid for initially dispersed random walkers provided that the initial sites all lie within a region whose linear dimension (say the radius of a hypersphere) is approximately of the order of $(t_{\mathrm{cross}})^{1/2}$, where t_{cross} is the crossover times between the earliest and the immediately following regimes. Conversely, when the random walkers are initially very widely dispersed one expects to see only the final regime.

We have seen that there are generally three identifiable regimes in the behaviour of the parameter $\langle R_n(N)\rangle$ as a function of the step number n when the random walk is made on the sites of a translationally invariant lattice. The analogous problem has been investigated when the random walk is made on a fractal lattice having a fractal dimension d_{f} (i.e., the "mass" of the lattice scales as $m \sim L^{d_{\mathrm{f}}}$, where L is a length characterizing the size of the fractal) using both a heuristic argument and by an exact enumeration calculation for a random walk on a two-dimensional infinite percolation cluster [10]. The major finding of that investigation is that when the spectral dimension d_{s} is less than 2, $\langle R_n(N)\rangle$ is characterized by two rather than three regimes. The behavior of $\langle R_n(N)\rangle$ at short times is derived by reasoning based on the representation of this quantity in eq. (4). If the limit $N \to \infty$ is taken in that equation the function $\Gamma_n^N(\boldsymbol{r})$ tends to zero provided that $\boldsymbol{r}$ is accessible to the random walker by step n. Hence when n is fixed the expression for $\langle R_n(N)\rangle$ reduces to the sum of all sites accessible to the random walker at that step. If we restrict ourselves to random walks allowed to make steps to nearest-neighbors only, and on defining d_ℓ to be the chemical distance exponent, we find the asymptotic relationship

$$\langle R_n(N)\rangle \sim n^{d_\ell}, \tag{19}$$

which is independent of the number of random walkers. A simple argument shows that the crossover time from this to the second regime occurs at a time of the order of $\ln(N)$.

The behavior of $\langle R_n(N)\rangle$ in the second regime is found through the assumption that $\Gamma_n(r)$ has a scaling form

$$\Gamma_n(r) \sim g(r/n^{d_w}), \tag{20}$$

where d_w is defined by the asymptotic relation $\langle r^2\rangle \sim n^{2/d_w}$. Motivated by the scaling form of the probability density for the location of a random walker at step n we have assumed that the function $g(v)$ in eq. (20) can be expressed as

$$g(v) \sim 1 - v^{-d_f}\exp(-v^\delta) \tag{21}$$

for large values of v, where $\delta = d_w/(d_w - 1)$. If we let d_s be the fracton dimension, and make use of eq. (6) suitably modified for a fractal structure, we find

$$R(u;n) \sim \frac{n^{d_s/2}}{1-u}\int_0^\infty \frac{1-g(v)}{1-ug(v)}\, v^{d_f-1}\,dv \sim \frac{n^{d_s/2}}{1-u}\int_0^\infty \frac{v^{d_f-1}}{1+v^{d_f}e^{v^\delta}(1-u)}\,dv\,. \tag{22}$$

The behavior of this expression as a function of u is derivable by Tauberian methods, leading to the asymptotic behavior

$$\langle R_n(N)\rangle \sim [\ln(N)]^{d_f/\delta} n^{d_s/2}\,. \tag{23}$$

Numerical results obtained by the method of exact enumeration on a percolation cluster have been found to agree with this result [10].

The results described in this section suggest a host of further problems that remain as yet unexplored. These include a generalization to the calculation of the asymptotic forms of moments of higher order as well as finding the forms of the actual distribution of the random variable $R_n(N)$. Since these basic problems are extremely difficult to solve even for $N = 1$ it is to be expected that the level of difficulty will increase considerably when N exceeds 1. From a physical point of view our initial motivation for seeking to find properties of $R_n(N)$ was based on a possible extension of the Smoluchowski model to take many-body effects into account. This suggests that a direct solution of the

N-random walker extension of the trapping model [12], would be desirable in the context of the Smoluchowski model. Another problem possibly amenable to analysis by an extension of present methods is that of the occupancy of a given set of points [5,13], which is the number of times that set has been visited by the N n-set random walks. This quantity, too, has found application in a physical setting [14].

3. $\langle R_n \rangle$ in the presence of a trap

Returning now to the case of a single random walk, we consider a second problem of recent interest in which one seeks an expression for the asymptotic behavior of $\langle R_n \rangle$ in the presence of either a single trap or a trapping boundary [15,16]. In this version of the problem the behavior of $\langle R_n \rangle$ is determined by a balance between two types of contributions, those due to trapped and untrapped random walks, respectively. The initial analysis of this problem, by Dayan and Havlin, which dealt with a one-dimensional random walk in the presence of a single trapping point [15], essentially gives an exact solution for the case of one dimension provided that the variance of a single step, $\langle r^2 \rangle$, is finite. The solution in that paper is based on the identification of R_n with the span of the random walk [17,18]. In dimensions greater than one this is no longer a viable approach and it is only possible to calculate the first moment of this random variable by rather more elementary means.

Consider first the problem of a random walk in the presence of a single trapping site. Let the initial position of the random walker be at $\boldsymbol{r} = \boldsymbol{0}$ and the trap be at $\boldsymbol{r} = \boldsymbol{s}$. The contribution of untrapped random walkers is equal to $S_n(\boldsymbol{s})\langle R_n(\boldsymbol{s})\rangle$ where $S_n(\boldsymbol{s})$ is the probability that the random walker remains untrapped by step n and $\langle R_n(\boldsymbol{s})\rangle$ is the expected number of sites visited by an n-step random walk forbidden to visit the site $\boldsymbol{s}$ during that time. The expected number of distinct sites visited by an n-step random walk, averaged over all walks including both walks that have been trapped before step n, and those which have not yet been trapped will be denoted by $\langle \mathcal{R}_n(\boldsymbol{s})\rangle$ to distinguish it from $\langle R_n(\boldsymbol{s})\rangle$.

When correlations are neglected, a step which can be justified in some detail, the function $\langle R_n(\boldsymbol{s})\rangle$ can be represented in terms of the $f_j(\boldsymbol{r})$ as

$$\langle R_n(\boldsymbol{s})\rangle = \sum_{j=0}^{n} \left(\sum_{\boldsymbol{r}} f_j(\boldsymbol{r}) - f_j(\boldsymbol{s}) \right), \tag{24}$$

whose generating function with respect to the parameter n is

$$\bar{R}(\boldsymbol{s}; z) = \frac{1}{(1-z)p(\boldsymbol{0}; z)} \left(\frac{1}{(1-z)} - p(\boldsymbol{s}; z) \right). \tag{25}$$

A glance at the terms in large parentheses shows that the most singular of the two terms as $z \to 1$ is the first, hence to lowest order in n we can write $\langle R_n(s)\rangle \sim \langle R_n \rangle$, which is logical since the single excluded point is unlikely to affect the leading term in the limit of a large number of steps. Thus, the contribution of the untrapped walkers to $\langle \mathcal{R}_n(s)\rangle$ is, to a good approximation, equal to the simpler expression $S_n(s)\langle R_n\rangle$. In order to calculate the lowest order term in the remaining contribution we note that the probability of being trapped at exactly step k is equal to $S_{k-1}(s) - S_k(s)$ so that the contribution of the trapped random walkers is

$$\sum_{k=1}^{n} \langle R_k \rangle [S_{k-1}(s) - S_k(s)] \sim -\int^{n} \langle R_k \rangle \frac{\mathrm{d}S_k(s)}{\mathrm{d}k}\, \mathrm{d}k\,, \tag{26}$$

where the smallest value of k can be set equal to any number that is $\mathcal{O}(1)$. If we add the two types of contribution and integrate the result by parts we find that

$$\langle \mathcal{R}_n(s)\rangle \sim \int^{n} S_k(s) \frac{\mathrm{d}\langle R_k\rangle}{\mathrm{d}k}\, \mathrm{d}k\,. \tag{27}$$

For example, in $D = 1$ the contribution to $\langle \mathcal{R}_n(s)\rangle$ due to the untrapped walks is found to equal $4|s|/\pi$, which is a constant, while the corresponding contribution from the trapped random walkers is asymptotically given by $(2\sigma|s|/\pi)\ln(n)$, which is therefore the principal contribution for large n, as originally given by Dayan and Havlin [15]. We may describe this result by the statement that trapping is extremely efficient in one dimension because of the restricted geometry. In two dimensions, in contrast, the asymptotic behavior is predominantly due to the untrapped random walks and $\langle \mathcal{R}_n(s)\rangle$ is asymptotically proportional to $n/\ln^2(n)$, in place of the trap-free asymptotically proportionality to $n/\ln(n)$.

The same type of analysis can be applied to calculate $\langle \mathcal{R}_n(s)\rangle$ for random walks on fractal structures. Let d_s be the fracton dimension. Then, combining the results [19]

$$\langle R_n \rangle \sim n^{d_s/2} \tag{28}$$

and

$$S_n(s) \sim n^{-1+d_s/2}\,, \tag{29}$$

one readily finds

$$\langle \mathcal{R}_n(s)\rangle \sim n^{d_s-1}\,, \qquad d_s \leqslant 2\,. \tag{30}$$

The intermediate steps of the calculation suffice to show that the contributions from both the trapped and untrapped random walkers have the same dependence on step number.

As a final point in our discussion of the calculation of $\langle \mathcal{R}_n(s) \rangle$ in the presence of a single trap, we mention that if we have a random walk in one dimension with $p(j)$ of stable-law type, i.e., the probability of a step of j lattice sites having the asymptotic form $p(j) \sim 1/|j|^{1+\alpha}$, with $0 < \alpha \leq 2$, the balance of contributions from trapped and untrapped random walks can shift, depending on the value of α. For sufficiently small α (<1) the untrapped random walks give the dominant contribution, while for $1 < \alpha < 2$ both trapped and untrapped random walks give the same contribution to $\langle \mathcal{R}_n(s) \rangle$.

Finally, much more intriguing problems are posed by the case in which single trapping points are replaced by trapping surfaces. We have been led to consider such problems by a random walk model of photon migration in a turbid material which has been quite successfully applied to laser measurements of properties of biological tissues [20]. The original formulation of this model consisted of a planar surface separating the tissue from the exterior. A laser beam is generally used to inject photons into the tissue, and measurements of the light retransmitted through the surface are made by a collecting optode. The path of a single photon is modelled in terms of a lattice random walk (the corresponding diffusion model, rather surprisingly, does not give results in as good agreement with experimental data as the far less believable lattice picture!). There are a number of ways to characterize the path taken by the photons, which is information that is useful to the biologist. One of these relates to how much of the tissue has been traversed by photons which ultimately reach the interface between the tissue and exterior. An obviously useful parameter than can be used to provide this information is the expected number of distinct sites visited by such photons in the (model) of the tissue interior.

We will derive the analytic form of the asymptotic results both in two and three dimensions, the two-dimensional version of the problem being phrased in terms of a trapping line in place of the plane. The basic idea behind the derivation starts by noting that if a $(D-1)$-dimensional hyperplane consisting only of trapping sites is inserted into a D-dimensional space, the random walk projected along the coordinate perpendicular to the plane is one-dimensional. But it is known that in one dimension

$$S_n(s) \sim n^{-1/2}, \tag{31}$$

which is therefore also the survival probability in D dimensions for a random walk in the presence of a trapping plane. In two dimensions the expected number of distinct sites visited in a half-plane has the same functional dependence on n as that of a random walker in an unbounded plane, which means that $\langle R_n \rangle \sim n/\ln(n)$. Eq. (27) then suggests that

$$\langle \mathcal{R}_n(s) \rangle \sim \int^n \frac{\mathrm{d}k}{\sqrt{k}\,\ln(k)} \sim \frac{\sqrt{n}}{\ln(n)} . \tag{32}$$

This is in agreement with results obtained by an essentially exact solution of the evolution equations that describe the random walk, as indicated in fig. 1. Similarly, in $D \geqslant 3$ the same argument predicts that

$$\langle \mathcal{R}_n(s) \rangle \sim \sqrt{n} . \tag{33}$$

This prediction is compared to numerically exact results in fig. 2, with good agreement. A more intriguing set of problems is posed by the situation in which the trapping surfaces are not necessarily planar. In this formulation it might well be the case that the results in the last two equations still remain valid for large classes of the geometric form of the trapping surfaces, but this extension is so far unexplored. It is obvious that a calculation of properties of higher order moments of R_n would pose much more difficult mathematical problems.

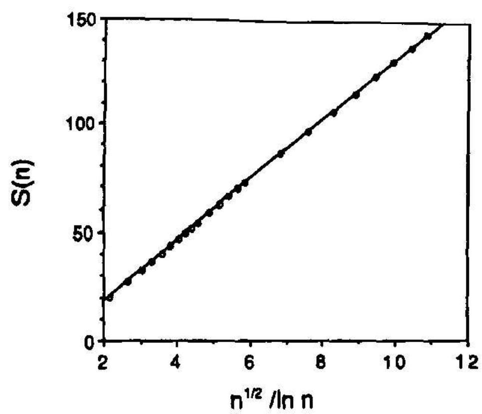

Fig. 1.

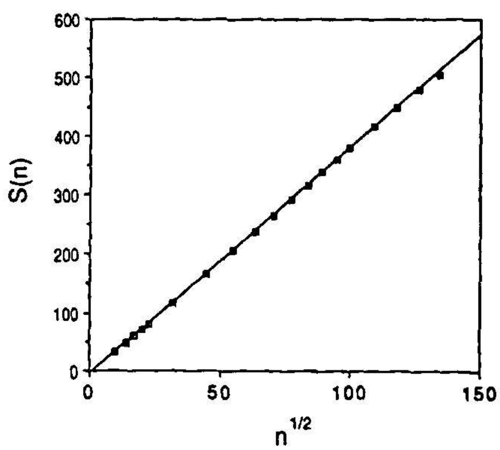

Fig. 2.

Fig. 1. A plot of the expected number of distinct sites visited in the presence of a line of traps in two dimensions, as a function of $n^{1/2}/\ln(n)$. These data were obtained using Monte Carlo simulations based on 10 000 random walkers each of which started 2 lattice sites away from the absorbing line. The straight line plot suggests the validity of eq. (32).

Fig. 2. A plot of the expected number of distinct sites visited in the presence of a line of traps in three dimensions, as a function of $n^{1/2}$, showing good agreement with eq. (33). Again, 10 000 random walkers were used in the simulation and the starting point was two lattice units from the absorbing plane.

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