Trapping of Random Walks in Two and Three Dimensions

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We introduce an exact enumeration method for calculating the survival probability $P(n)$ for the n-step random walker on a lattice with randomly distributed high-concentration traps, c. Using it we show that our data scale as $\ln P(n) \simeq a\rho$, where $\rho = [-\ln(1-c)]^{2/(D+2)} n^{D/(D+2)}$, when $\rho \gtrsim 10$ in $D=2$ and $D=3$ dimensions. This value of ρ corresponds to $P(n) \lesssim 10^{-13}$.

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The statistics of the survival of random walks that move in the presence of randomly distributed traps has been studied recently by many investigators.[1-23] The quantity most often analyzed is the survival probability of an n-step random walk, which we here denote by $P(n)$. Donsker and Varadhan[3] have proved that in the limit, $n=\infty$, $P(n)$ satisfies

$$\ln P(n) \approx -a\left[\ln\frac{1}{1-c}\right]^{2/(D+2)} n^{D/(D+2)}, \quad (1)$$

where a is a constant that depends on the lattice, c is the trap concentration, and D is the dimension. In the absence of any correction terms to Eq.(1) (except in one dimension) it is impossible to say how large n must be for the Donsker-Varadhan formula to be a useful approximation. All previous analyses of this question have relied on some form of simulation, but so far there is no information available on the range of validity of Eq. (1). Klafter, Zumofen, and Blumen[6] suggest that Eq. (1) is valid only for $P(n) < 10^{-21}$ for $D=2$ and Fixman[7] sets the limit at $P(n) < 10^{-67}$ in $D=3$ dimensions. In this Letter we present evidence suggesting that (for nearest-neighbor random walks) Eq. (1) is a useful approximation when $\rho > 10$, where ρ is the scaling function

$$\rho = \left[\ln\frac{1}{1-c}\right]^{2/(D+2)} n^{D/(D+2)} \quad (2)$$

appearing in the work of Donsker and Varadhan.[3] This value of ρ corresponds to a survival probability equal to 10^{-13} in both $D=2$ and $D=3$ dimensions. We further argue that pure simulation techniques will always lead to an exponential decay at sufficiently long times, rather than to the correct decay given by the theoretically proven Eq. (1). Our evidence for the new lower value of ρ [or higher value of $P(n)$] is based on two numerical techniques that we have developed. The first of these techniques, to be denoted by ERC (exact enumeration on random configurations), has been described elsewhere[23] and is an exact calculation of survival probabilities on sets of random trap configurations. The second technique, denoted by EEC (exhaustive enumeration of configurations) is an exact calculation of survival probabilities on an exhaustive set of nontrapping regions. We have shown that ERC reproduces the exponent $D/(D+2)=\frac{1}{3}$ to a good approximation in dimension $D=1$.[23] Our second method, EEC, to be described here, is practical for high trap concentrations only ($c \gtrsim 0.9$) and is complimentary to ERC. No method is practical for physically realistic trap concentrations, for example $c \approx 10^{-3}$, so that the extension of any of the present results to these low concentrations must rely on the existence of a scaling function similar to that in Eq. (2). Whether a wider validity exists for Eq. (1) than the limit established by this work is still an open question.

The exhaustive enumeration of configurations method.—In this technique we enumerate all configurations of nontrapping sites and calculate exactly the survival probabilities on these clusters. In practice we have so far been limited to clusters of

twelve or fewer nontrapping sites. A cluster is defined to be a connected group of s nontrap sites surrounded by l traps. The probability that a cluster is characterized by the parameters s and l is $(1-c)^s c^l$. To calculate the survival probability on an (s,l) cluster we must also take into account a connectivity index, which we denote by i, since there may be different survival probabilities depending on the topological configuration of the (s,l) cluster. Let $P_{sli}(n)$ be the probability of survival for at least n steps on an (s,l) cluster characterized by connectivity index i. Let λ_{sli} be the multiplicity of such a cluster. Then the average survival probability is given by

$$P(n)=\frac{\sum_{s,l,i} P_{sli}(n)\lambda_{sli}(1-c)^s c^l}{\sum_{s,l,i}\lambda_{sli}(1-c)^s c^l}. \tag{3}$$

For the relatively small clusters that we have dealt with it is easy to enumerate the λ_{sli}. To find the values of $P_{sli}(n)$ one can use either a matrix approach or the exact enumeration approach described in Ref. 23. The matrix method requires knowledge of the incidence matrix A whose jkth element is 1 if sites j and k are nearest neighbors, and 0 otherwise. Letting $P_{sli}(j;n)$ be the joint probability of surviving till step n and being at site j at that step, we have the recursion relation

$$P(j;n+1)=\sum_k A_{jk}P(k;n), \tag{4}$$

where we have suppressed the subscripts sli. Thus, $P(j;n)$ can be expanded in a series of eigenfunctions of the $s\times s$ matrix A. Since the coefficients in such a series depend on the site j, which itself is of no intrinsic interest, we effectively can sum over j by using the relation

$$P_{sli}(n)=\sum_{j=1}^{s} a_j\beta_j^n, \tag{5}$$

and can calculate the $2s$ parameters $\{a_j,\beta_j\}$ from $2s$ consecutive values of P_{sli} found by the exact enumeration approach. The use of Eq. (3) also allows us to perform an accurate check on the number of configurations required for the calculations, since it is possible to check the convergence as a function of this number. The value of $P(n)$ has converged when adding larger nontrap configurations to the sum in Eq. (3) does not change its value.

Results and discussion.—Figure 1 shows our results for $P(n)$ for $D=2$ dimensions and different trap concentrations. The results for $c>0.9$ were generated by the EEC method described above, while the data for lower concentrations were generated by the ERC method, described in Ref. 23. The results for $c=0.9$ were generated by both methods. It is evident from Fig. 1 that there is a regime $(n>10)$ for $c\geq 0.9$ in which the slope of $-\ln P(n)$ is $\frac{1}{2}$ as predicted by Donsker and Varadhan.[3] In this regime Eq. (3) was found to converge. However, for the larger step numbers the slope must necessarily tend to 1 (see points D in Fig. 1) as a result of the finite number of configurations taken into account. The larger number of steps require that more configurations are to be taken into account to make Eq. (3) converge. This is due to the necessity of using in Eq. (3) a finite, rather than an infinite, number of configurations. When the data for $D=2$ are plotted as a function of the parameter $\rho=\{[-\ln(1-c)]n\}^{1/2}$, they scale nicely for $\rho\gtrsim 10$ or $P(n)\lesssim 10^{-13}$. This is shown in Fig. 2, where the indicated slope is equal to its theoretically predicted value of 1. Similar results are obtained for $\rho\gtrsim 10$ and $P(n)\lesssim 10^{-13}$ in $D=3$, as shown in Fig. 3. Our results cannot yet be used to say that for $P(n)>10^{-13}$ $(\rho<10)$ the Donsker-Varadhan result is not useful, since for high concentrations, where we have exact results, the lowest number of steps used, $n=10$, corre-

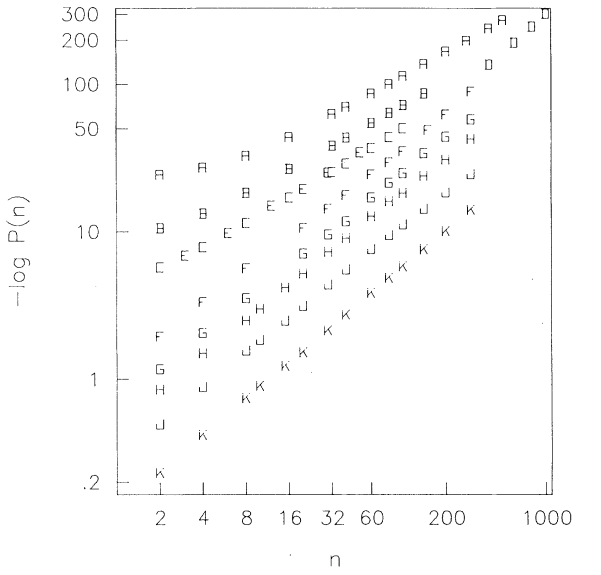

FIG. 1. Results for $\ln P(n)$ for different values of trap concentrations c in $D=2$ represented by different letters: A for $1-c=10^{-5}$; B for $1-c=10^{-2}$; C, D, and E for $1-c=10^{-1}$; F for $c=0.7$; G for $c=0.5$; H for $c=0.4$; J for $c=0.25$; K for $c=0.125$. Points C represent results obtained by the EEC and points E by the ERC method. Points D represent results obtained by the EEC for large numbers of steps, where Eq. (1) yields an exponential decay.

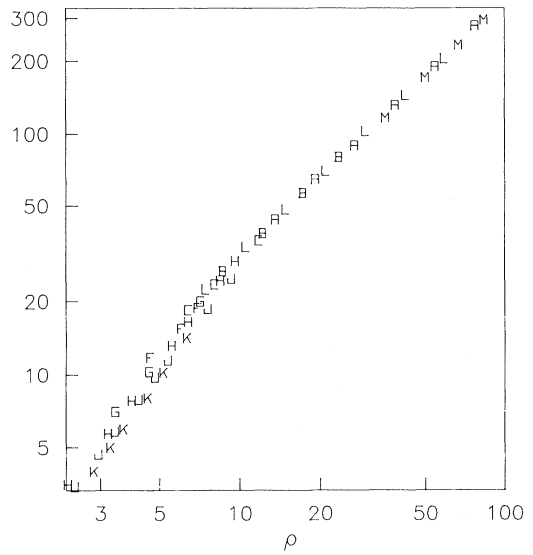

FIG. 2. Results for $\ln P(n)$ for different values of trap concentrations c in $D=2$ dimensions (the points are denoted as in Fig. 1 and also points M for $1-c=10^{-6}$, N for $1-c=10^{-4}$, and L for $1-c=10^{-3}$) and step sizes n plotted as a function of $\rho=[-\ln(1-c)]^{1/2}n^{1/2}$.

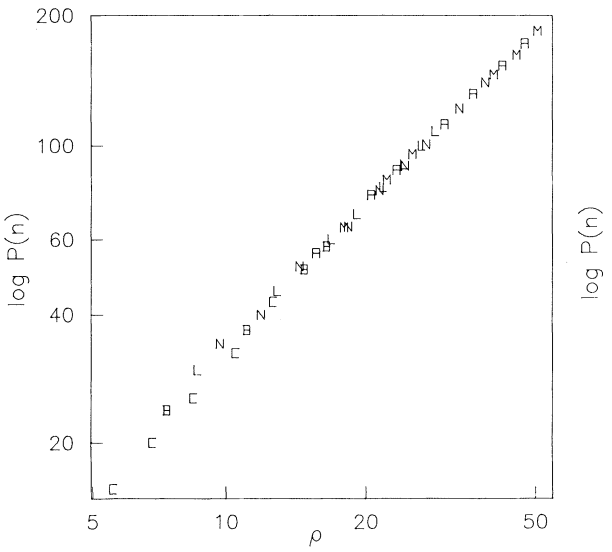

FIG. 3. Results for $\ln P(n)$ for different values of trap concentrations c in $D=3$ dimensions (denoted as in Figs. 1 and 2) and step sizes n plotted as a function of $\rho=[-\ln(1-c)]^{2/5}n^{3/5}$. The results plotted here have been obtained by the EEC method.

sponds to $\rho \gtrsim 10$. The scattering of the data for $\rho < 10$ that was found in $D=1$, 2, and 3 dimensions seems to be due to corrections to the scaling form of Eq. (1).

Limitation of lattice size is critical for recognizing the Donsker-Varadhan regime in simulations. When the maximum cluster size is fixed, Eq. (3) indicates that the $n \to \infty$ decay regime will be exponential in n, the largest eigenvalue β giving the rate of approach of $P(n)$ to 0. It has long been appreciated that the fractional powers of n appearing in the expression for $\ln P(n)$ are due to the rare large nontrapping clusters.[4] Our numerical techniques allow us to estimate the minimum size of a lattice needed to see the behavior of Eq. (1). For example, in $D=2$ dimensions all clusters of at least $s=10$ sites are needed for convergence for $c=0.9$ at step numbers $n<20$. The probability of occurrence of such a cluster is $\approx 10^{-11}$. For $n>20$ steps one needs larger size clusters for convergence, otherwise one sees a crossover to exponential decay. Hence, in order to obtain good statistical ensembles in simulation, one would need a system of $\approx 10^{13}$ sites which cannot be achieved by present-day computers.

Indeed, careful study of the data in Fig. 1 shows that for our ERC method ($c<0.9$) we do not obtain the asymptotic values of Eq. (1). We are able to obtain only an effective expression $\exp(-an^{\alpha})$, where $\alpha \simeq 0.7$–0.8, instead of $\alpha=0.5$ in $D=2$. It seems that we see a crossover value for the exponent in agreement with Klafter, Zumofen, and Blumen.[6] A larger number of steps leads to higher values for α (indeed, $\alpha \to 1$) as clearly found in our enumerations. The reason for this behavior is the absence of rare configurations in these small systems used in simulations as discussed above. However, since we expect all data to scale with ρ, we argue that for $\rho>10$, or $P(n)<10^{-13}$, the low-concentration data in Fig. 1 should also behave as in Eq. (1). Moreover, since for high concentrations $P(n)$ behaves as $\exp(-an^{D/D+2})$ it cannot be that the low-concentration survival probability will decay faster than the high-concentration results. Thus, we conclude that all concentrations results should behave as Eq. (1) for $\rho \gtrsim 10$.

Macroscopic systems are large enough to contain the rare configurations that would produce the behavior of Eq. (1). However, since at present $P(n)$ can be experimentally measured only to the order of 10^{-4}, it is unclear whether Donsker-Varadhan scaling can be seen in physical systems.

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