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On the Survival Probability of a Random Walk in a Finite Lattice with a Single Trap

George H. Weiss,[1] Shlomo Havlin,[1,2] and Armin Bunde[3,4]

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We consider the survival of a random walker in a finite lattice with periodic boundary conditions. The initial position of the random walker is uniformly distributed on the lattice with respect to the trap. We show that the survival of a random walker, $\langle U_n \rangle$, can be exactly related to the expected number of distinct sites visted on a trap-free lattice by

$$\langle U_n \rangle = 1 - \frac{\langle S_n \rangle}{N^D} \qquad (*)$$

where N^D is the number of lattice points in D dimensions. We then analyze the behavior of $\langle S_n \rangle$ in any number of dimensions by using Tauberian methods. We find that at sufficiently long times $\langle S_n \rangle$ decays exponentially with n in all numbers of dimensions. In $D=1$ and 2 dimensions there is an intermediate behavior which can be calculated and is valid for $N^2 \gg n \gg 1$ when $D=1$ and $N \ln N \gg n \gg 1$ when $D=2$. No such crossover exists when $D \geqslant 3$. The form of (*) suggests that the single trap approximation is indeed a valid low-concentration limit for survival on an infinite lattice with a finite concentration of traps.

KEY WORDS: Random walks; trapping; Tauberian theorems.

1. INTRODUCTION

The problem of determining statistical properties of the return of a lattice random walker to its starting point was first discussed by Polya.[1] It can

[1] National Institutes of Health, Bethesda, Maryland 20205.

[2] Department of Physics, Bar-Ilan University, Ramat-Gan, Israel.

[3] Center for Polymer Studies and Department of Physics, Boston University, Boston, Massachusetts 62215.

[4] Permanent address: Fakultät für Physik, Universität Konstanz, D-7750, Konstanz, Federal Republic of Germany.

be framed in terms of properties of a random walk on a lattice containing a single trap. It is well known, for example, that even when return to a starting point is certain, as in $D = 1$ and 2 dimensions, the expected time to trapping of a random walk is infinite provided that the lattice itself is infinite.[2] A number of investigators have analyzed properties of a random walk in the presence of a trap. These have usually focused on properties of the random walk on infinite lattices.[3,4] Detailed results for moments of trapping time on finite lattices were recently presented by Kozak and his collaborators.[5-10] In the present paper we present some results related to the survival probabilities of random walks on finite lattices containing a single trap. We will show that in $D = 1$ and 2 dimensions there is a crossover in the behavior of the asymptotic survival probability that depends on the relation between the step number, n, and the number of sites that comprise the lattice.

2. GENERAL RELATIONS

Let the number of lattice sites in the unit cell be N^D, where D is the number of dimensions and N is the number of lattice sites to an edge. The trapping site will be labeled $\mathbf{s}$ and the starting point is assumed to be at $\mathbf{0}$. Later we will average over all possible trapping sites, leading to a much simplified analysis. Let us first specify some quantities and relations for trap-free random walks that will be needed in our later analysis. If $p(\mathbf{j})$ represents the probability that a single step taken by the random walker is equal to $\mathbf{j}$, then many properties of the random walk can be given in terms of the structure function

$$\lambda(2\pi\mathbf{m}/N) = \sum_{\mathbf{j}} p(\mathbf{j}) \exp(2\pi i\mathbf{m} \cdot \mathbf{j}/N) \tag{1}$$

If $P_n(\mathbf{r})$ is the probability that the random walker is at $\mathbf{r}$ at step n, and $P(\mathbf{r}, z)$ denotes the generating function

$$P(\mathbf{r}, z) = \sum_{n=0}^{\infty} P_n(\mathbf{r})\, z^n \tag{2}$$

then $P(\mathbf{r}, z)$ can be expressed as

$$P(\mathbf{r}, z) = \frac{1}{N^D} \sum_{m_1=0}^{N-1} \cdots \sum_{m_D=0}^{N-1} \exp(2\pi i\mathbf{r} \cdot \mathbf{m}/N)/[1 - z\lambda(2\pi\mathbf{m}/N)] \tag{3}$$

It will also be convenient, in what follows, to decompose $P(\mathbf{r}, z)$ as

$$P(\mathbf{r}, z) = \frac{1}{N^D(1-z)} + \varphi(\mathbf{r}, z) \tag{4}$$

where the first term contains the singularity at $z=1$ and $\varphi(\mathbf{r}, z)$ remains finite as $z \to 1$. Let $F_n(\mathbf{r})$ be the probability that the first passage time to $\mathbf{r}$ is equal to n, and let $F(\mathbf{r}, z)$ be the corresponding generating function with respect to n. The function $F(\mathbf{r}, z)$ can be expressed in terms of the $P(\mathbf{r}, z)$ as[11]

$$\begin{aligned} F(\mathbf{r}, z) &= [1 - P(\mathbf{0}, z)]/P(\mathbf{0}, z), \qquad & \mathbf{r} \neq \mathbf{0} \\ &= P(\mathbf{r}, z)/P(\mathbf{0}, z), \qquad & \mathbf{r} \neq \mathbf{0} \end{aligned} \tag{5}$$

Having defined these functions for the trap-free lattice random walk let us define $g_n(\mathbf{r})$ be the probability that the random walker is at $\mathbf{r}$ at step n in the presence of a trap at $\mathbf{s}$, and let $g(\mathbf{r}, z)$ be the generating function with respect to step number. This function can easily be found in terms of the functions defined in the last paragraph by noting that random walks that reach $\mathbf{r}$ at step n can be represented as all walks that do so in the absence of traps less those that reach $\mathbf{s}$ before n and then reach $\mathbf{r}$ at n, again on the trap-free unit cell. Thus we can immediately write

$$\begin{aligned} g(\mathbf{r}, z) &= P(\mathbf{r}, z) - F(\mathbf{s}, z)\, P(\mathbf{r} - \mathbf{s}, z) \\ &= P(\mathbf{r}, z) - P(\mathbf{s}, z)\, P(\mathbf{r} - \mathbf{s}, z)/P(\mathbf{0}, z) \end{aligned} \tag{6}$$

If the probability that a random walk survives until step n with a trap at $\mathbf{s}$ is denoted by $U_n(\mathbf{s})$, then we can write

$$U_n(\mathbf{s}) = \sum_{\mathbf{r}(\neq \mathbf{s})} g_n(\mathbf{r}) \qquad \text{or} \qquad U(\mathbf{s}, z) = \sum_{\mathbf{r}(\neq \mathbf{s})} g(\mathbf{r}, z) \tag{7}$$

in terms of the generating functions. Taking account of the identity $\sum_{\mathbf{r}} P(\mathbf{r}, z) = (1-z)^{-1}$ we can perform the indicated sum over $\mathbf{r}$ in Eq. (6), finding

$$U(\mathbf{s}, z) = \frac{1}{1-z}\left[1 - \frac{P(\mathbf{s}, z)}{P(\mathbf{0}, z)}\right] \tag{8}$$

This expression has the obviously necessary properties that when $\mathbf{s} = \mathbf{0}$, $U(\mathbf{s}, z) = 0$ or $U_n(\mathbf{0}) = 0$, and when $|s| \gg 1$, $|P(\mathbf{s}, z)/P(\mathbf{0}, z)|$ is very small by the Riemann–Lebesgue lemma, so that $U_n(\mathbf{s}) \to 1$. Equation (8) is completely general and independent of whether the lattice is finite or infinite.

To find a simple expression for the generating function of survival probability let us average Eq. (8) over all possible trap sites, assigning the probability $1/N^D$ to each site. If the survival probability averaged over all sites is denoted by $\langle U_n \rangle$, we find that

$$U(z) = \sum_{n=0}^{\infty} \langle U_n \rangle z^n = \frac{1}{1-z}\left[1 - \frac{1}{N^D (1-z)\, P(\mathbf{0}, z)}\right] \tag{9}$$

This can be written in an interesting way if we recall that the generating function for the expected number of distinct points visited by an n step random walk is[11]

$$S(z) = \sum_{n=0}^{\infty} \langle S_n \rangle z^n = [(1-z)^2 P(\mathbf{0}, z)]^{-1} \tag{10}$$

On substituting this result into Eq. (9), we find that $\langle U_n \rangle$ can be written in terms of $\langle S_n \rangle$ as

$$\langle U_n \rangle = 1 - \frac{\langle S_n \rangle}{N^D} \tag{11}$$

so that we need only study the properties of $\langle S_n \rangle$ to elucidate those of the survival probabilities.

3. ASYMPTOTIC PROPERTIES

The asymptotic behavior of $\langle S_n \rangle$ on an infinite lattice has been known and rederived in many ways since the original investigation by Dvoretzky and Erdös,[12] but the comparable results have not yet appeared for random walks on finite lattices. To derive such results let us substitute Eq. (4) into the expression for $S(z)$ given in Eq. (10) which leads to

$$S(z) = \frac{1}{(1-z)} \cdot \frac{1}{(1-z)\,\varphi(\mathbf{0}, z) + 1/N^D} = f(z)/(1-z) \tag{12}$$

where the function $f(z)$ is a rational function of z and can therefore be expressed as

$$f(z) = \sum_{n=0}^{\infty} f_n z^n \tag{13}$$

The behavior of f_n for large n can be determined by examining the behavior of $f(z)$ near its radius of convergence. To find this behavior we must find the root with the smallest magnitude of the equation

$$(1-z)\,\varphi(\mathbf{0}, z) = -1/N^D \tag{14}$$

We consider only the case of $N^{-D} \ll 1$ so that both sides of this equation are approximately equal to 0. Since $\varphi(\mathbf{0}, z)$ is just a finite sum of terms of the form $[1 - z\lambda(2\pi m/N)]^{-1}$ where $|\lambda| \leqslant 1$ it can have no zeros inside of $|z| = 1$ so that the smallest root of Eq. (14) must have the property $|z| > 1$.

Because the right-hand side of Eq. (14) is small in the limit of large N this root must be close to 1. For $z \sim 1$, $\varphi(\mathbf{0}, 1)$ remains finite, and has been shown by Montroll and Weiss[11] to have the form, for symmetric random walks,

$$\begin{aligned} \varphi(\mathbf{0}, 1) &\sim N/(6\sigma^2), && D=1 \\ &\sim \ln N/(\pi\sigma_1\sigma_2), && D=2 \\ &\sim \text{const}, && D \geqslant 3 \end{aligned} \tag{15}$$

Hence, in the neighborhood of $z=1$, $f(z)$ has the singular behavior

$$f(z) \sim \frac{1}{(1-z)\,\varphi(\mathbf{0}, 1) + 1/N^D} \tag{16}$$

which implies that asymptotically

$$f_n \sim \frac{1}{\varphi(\mathbf{0}, 1)} \cdot \frac{1}{[1 + 1/(N^D \varphi(\mathbf{0}, 1))]^{n+1}} \tag{17}$$

But since $S(z)$ is related to $f(z)$ through Eq. (12) it follows that

$$\frac{\langle S_n \rangle}{N^D} \sim \frac{1}{N^D} \sum_{j=0}^{n} f_j = 1 - \left[1 + \frac{1}{N^D \varphi(\mathbf{0}, 1)}\right]^{-(n+1)} \sim 1 - \exp\left[-\frac{n}{N^D \varphi(\mathbf{0}, 1)}\right] \tag{18}$$

so that at sufficiently large n $\langle U_n \rangle$ decays exponentially with n, independent of dimension. This is verified in detail for $D=1$ in the Appendix to this paper and has been verified for higher dimensions in a simulation study. Notice that although we have inserted the specific decay constant $[N^D \varphi(\mathbf{0}, 1)]^{-1}$ in Eq. (18) this is only approximate and the more accurate constant depends on the solution to Eq. (14) Although the exponential form in Eq. (18) appears to be valid for all n in fact it is only good for $n > N^D \varphi(\mathbf{0}, 1)$. Thus, when $D=1$ it is useful when $n > N^2$ for symmetric random walks and for $n > 0(1)$ for asymmetric random walks. In $D=2$ dimensions it is valid when $n > N^2 \ln N$ for the symmetric random walk, and for $D=3$ we must have $n > N^3$ for the exponential to be a useful approximation. Den Hollander[13] has also obtained the long-time exponential limit for symmetric random walks using a completely different argument. His treatment is also valid for several traps.

Next, let us consider the regime $N \gg n \gg 1$ so that the random walk has sampled relatively few of the lattice points. In that case for $D=1$ and a symmetric walk, the function $\varphi(\mathbf{0}, z)$ behaves like

$$\varphi(\mathbf{0}, z) \sim [\sigma(1-z)^{1/2}]^{-1} \tag{19}$$

in the neighborhood of $z=1$. This implies, by Eq. (12), that

$$\begin{aligned} S(z) &\sim \frac{1}{(1-z)} \cdot \frac{1}{(1/\sigma)[(1-z)/2]^{1/2} + 1/N} \\ &\sim 2^{1/2}\sigma \cdot \frac{1}{(1-z)^{3/2}} \left[1 - \frac{\sigma\sqrt{2}}{N(1-z)^{1/2}} + \cdots\right] \end{aligned} \tag{20}$$

By using a Tauberian theorem common in random walk analyses[14] we see that the lowest-order term in this last equation leads to the estimate

$$\frac{\langle S_n \rangle}{N} \sim \frac{\sigma}{N} \left(\frac{8n}{\pi}\right)^{1/2} \tag{21}$$

which is just the result obtained on the infinite lattice. Higher-order terms can also be obtained provided that correction terms to Eq. (19) are evaluated. There is a crossover in the behavior of $\langle U_n \rangle$ from the behavior in Eq. (21) to the exponential form that occurs when $n = O(N^2)$. This can be demonstrated in detail for the one-dimensional case, as shown in the Appendix, but not in higher dimensions since there is no comparable solution in closed form. In $D=2$ dimensions one finds the analog of Eq. (21),

$$\frac{\langle S_n \rangle}{N^2} \sim \frac{\pi\sigma_1\sigma_2 n}{N^2 \ln n} \tag{22}$$

where σ_1^2 and σ_2^2 are the variances in x and y directions. A crossover to the exponential form occurs when $n = O(N^2 \ln N)$. In three or more dimensions, since $\varphi(\mathbf{0}, 1)$ is a constant as $N \to \infty$ we expect there to be no change in the asymptotic behavior of $\langle U_n \rangle$ over the whole range $n \gg 1$.

4. DISCUSSION

While the present theory has been developed for the case of a single trap it is readily extended to the analysis of k traps on a finite lattice by using the theory originally developed by Montroll.[15] We do not expect this generalization to lead to qualitatively different conclusions from those of the present analysis, nor do we expect any qualitative differences to occur when different boundaries are used as is confirmed by the analysis of den Hollander[13]. The exponential limit for sufficiently large n does show up in simulations of trapping problems because one necessarily deals with finite lattices. It can sometimes obscure other behavior, such as the Donsker–Varadhan[15,17] form for asymptotic survival probability in a field of traps.

We also point out that Montroll's[18] suggestion that the single-trap problem can be regarded as an approximation to the multiple randomly scattered trapping problem at low trap densities receives some confirmation from our result in Eq. (11). The survival probability in any field of traps can be expressed as

$$\langle T(n) \rangle = \langle (1-c)^{S_n} \rangle \tag{23}$$

where the brackets indicate an average over all configurations and all random walks. In the low trap concentration limit one can expand Eq. (27) as

$$\langle T(n) \rangle \sim 1 - c\langle S_n \rangle + \langle S_n(S_n - 1) \rangle \frac{c^2}{2} - \cdots \tag{24}$$

If one sets $c = N^{-D}$ and truncates this series at the linear term one finds Eq. (11). Equation (24) indicates that higher-order terms require calculation of $\langle S_n^2 \rangle$ which requires a much more sophisticated approach than that taken here.[19–22] It is unclear whether the approximation obtained by decomposing an infinite lattice into unit cells with a small number of traps, will advance our understanding of how the survival probability behaves as a function of trap concentration. An analysis of the survival probability that is at best valid at low trap concentrations has been given by Weiss,[23] by using the asymptotic distribution developed by Jain and his collaborators.[19–22] Whether that theory is more accurate than the simple theory developed here remains to be tested by a simulation study.

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APPENDIX: ANALYSIS OF THE CROSSOVER IN ONE DIMENSION

Since the geometry of a one-dimensional random walk is necessarily a simple one we can identify the number of distinct sites visited by the random walk with the span, i.e., the maximum displacement minus the minimum displacement.[24,25] This allows us to derive an expression for $\langle S_n \rangle$ that will be valid for all values of n. We start from a representation for the span, S, at step n, that is due to Weiss and Rubin[25]:

$$\begin{aligned} p_n(S) &\sim \frac{8}{S^3} \sum_{l=0}^{\infty} \frac{d^2}{d\theta^2} [\lambda^n(\theta)]_{\theta=\pi(2l+1)/S} \\ &= \frac{8}{S^3} \sum_{l=0}^{\infty} g_n\left(\frac{\pi(2l+1)}{S}\right) \end{aligned} \tag{A1}$$

where $g_n(x)$ is defined by the equation. Equation (A1) is valid for $n \gg 1$. In this approximation we can, with small error, replace the discrete lattice by a continuous circle since the trap can be regarded as a point both for the lattice and for the circle.

Let the circumference of the circle be L. It then follows that $\langle S_n \rangle$ is given by

$$\langle S_n \rangle = L \int_L^{\infty} p_n(S)\, dS + \int_0^L S p_n(S)\, dS \tag{A2}$$

since once the span reaches the value L it remains there. By making a change of variables to $v = \pi(2l+1)/S$ we find

$$\begin{aligned} \langle S_n \rangle = &\frac{8L}{\pi^2} \sum_{l=0}^{\infty} \frac{1}{(2l+1)^2} \int_0^{\pi(2l+1)/L} v g(v)\, dv \\ &+ \frac{8}{\pi} \sum_{l=0}^{\infty} \frac{1}{(2l+1)} \int_{\pi(2l+1)/L}^{\infty} g(v)\, dv \end{aligned} \tag{A3}$$

In $D = 1$ dimension we can make the approximation

$$h(\theta) = \lambda^n(\theta) \sim \exp(-n^2\sigma^2\theta^2/2) \tag{A4}$$

where σ^2 is the variance for a single step. In Eq. (A3) we can write $g(v) = h''(v)$ and integrate by parts in the first set of integrals. In this way we find

$$\langle S_n \rangle \sim \frac{8L}{\pi^2} \sum_{l=0}^{\infty} \frac{1}{(2l+1)^2} \left\{1 - \exp\left[-\frac{\pi^2(2l+1)^2\,\sigma^2 n}{2L^2}\right]\right\} \tag{A5}$$

But this sum has been discussed by Weiss and Havlin,[26] who found a result that implies

$$\langle S_n \rangle \sim \sigma \left(\frac{8n}{\pi}\right)^{1/2} \tag{A6}$$

which is known to be the result for the infinite lattice.[12] On the other hand, when $n\sigma^2 \gg L^2$, $\langle S_n \rangle$ is approximately given by the $l=0$ term in Eq. (A5) which is an exponential dependence on n. Hence Eq. (A5) gives a formula that interpolates between the square root and exponential behavior of $\langle S_n \rangle$.

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