Journal of Statistical Physics, Vol. 15, No. 5, 1976

A Simple Calculation for the Average Number of Steps to Trapping in Lattice Random Walks

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Received April 28, 1976

We show that the asymptotic results for the average number of steps to trapping at an irreversible trapping site on a D-dimensional finite lattice can be obtained from the generating function for random walks on an *infinite perfect lattice*. This introduces a significant simplification into such calculations. An interesting corollary of these calculations is the conclusion that a random walker traverses, on the average, all the distinct nontrapping lattice sites before arriving on the trapping site.

KEY WORDS: Random walk; steps to trapping; lattice walk.

1. INTRODUCTION

An important property of random walks which has been calculated for a variety of model lattices is the average number of steps $\langle n \rangle_N$ that a walker takes on a finite lattice with one trapping site per N lattice sites before arriving at the trapping site where he is irreversibly removed from the system.[1–3] These calculated values have been compared with experimental measurements on various systems modeled by random walks. For example, there are measurements of trap-limited lifetimes of excitons in networks of chlorophyll molecules,[4] in organic crystals,[5] and in polymers[6] which are at least qualitatively well described by random walk models.[1,3]

The average number of steps to trapping $\langle n \rangle_N$ has been evaluated for nearest-neighbor random walks on hypercubic and nonsimple lattices[1] and for one-dimensional walks with next-nearest-neighbor[2] and with exponentially distributed steps.[2] For symmetric nearest-neighbor random walks on

This work was supported in part by NSF Grants MPS72-04363-A03 and CHE75-20624.

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hypercubic lattices the asymptotic (large N) results in D dimensions are[1]

$$\begin{aligned} \langle n \rangle_N &\sim \tfrac{1}{6} N^2, && D = 1 \\ &\sim (1/\pi) N \ln N, && D = 2 \\ &\sim uN, && D \geqslant 3 \end{aligned} \tag{1}$$

Here $u \geqslant 1$ is a numerical factor of order unity which depends on dimensionality.

These and other such results for different lattices are obtained from the generating function for walks on *finite* lattices. Such generating functions are generally more difficult to calculate than those for *infinite perfect* lattices. We will show that the asymptotic expressions for the average number of steps to trapping as given in Eq. (1) can be obtained from the infinite perfect lattice generating function and specifically from the generating function for walks that return to the origin.

2. CALCULATION OF $\langle n \rangle_N$

Heuristically we argue (and later justify more formally for various cases) that if $N \gg 1$, a walker on a finite defective lattice will on the average visit essentially all $N - 1$ nontrapping lattice sites before being trapped. This assumption becomes more accurate with increasing dimensionality D. We therefore assume that we can obtain $\langle n \rangle_N$ from calculating the average number of distinct sites $S_{\langle n \rangle_N}$ visited in a walk of $\langle n \rangle_N$ steps on an infinite perfect lattice. The distinct number of sites S_n visited in an n-step walk can be obtained from the perfect infinite lattice generating function for walks that return to the origin.[7] In all the cases we have investigated we find, for large N,

$$S_{\langle n \rangle_N} \sim \alpha N \tag{2}$$

where $0 < \alpha \leqslant 1$ and where α may depend weakly on dimensionality, structure, and type of walk. The asymptotic (large n) results for S_n for nearest-neighbor walks on hypercubic lattices obtained by Montroll and Weiss[7] are

$$S_n = \begin{cases} (8/\pi)^{1/2} n^{1/2}, & D = 1 \\ \pi n / \ln n, & D = 2 \\ (1/u) n, & D \geqslant 3 \end{cases} \tag{3}$$

where u here is the same numerical factor as in Eq. (1). Combining Eqs. (2) and (3) leads to

$$\begin{aligned} \langle n \rangle_N &\sim \alpha^2 (\pi/8) N^2, && D = 1 \\ &\sim (\alpha/\pi) N \ln N, && D = 2 \\ &\sim \alpha u N, && D \geqslant 3 \end{aligned} \tag{4}$$

If we set $\alpha = 1$, which implies [see Eq. (2)] that the random walker visits all the $N - 1$ distinct nontrapping sites before stepping on the trap, we find complete agreement between the results of Eq. (4) and the exact asymptotic results of Eq. (1) for $D \geqslant 2$. For $D = 1$, our result agrees with the exact one if we set $\alpha = 2/(3\pi)^{1/2} < 1$. This is not surprising since in a one-dimensional random walk it is impossible for the random walker to visit, on the average, *all* the $N - 1$ distinct nontrapping sites prior to his arrival at the trapping site.

We believe that $\langle n \rangle_N$ can be evaluated in this manner for other types of walks, for instance, for non-nearest-neighbor walks on nonsimple lattices. Equation (2) thus provides a simple algorithm for asymptotic evaluation of $\langle n \rangle_N$, given the asymptotic form of S_n.

The idea that knowledge of the asymptotic form of S_n is sufficient to determine the large-N behavior of the number of steps to trapping has been discussed previously by Rosenstock.[8] His reasoning led him to the following approximate expression for $\langle n \rangle_N$:

$$\langle n \rangle_N \simeq \sum_{n=1}^{\infty} n(1 - 1/N)^{S_{n-1}} \frac{1}{N} \tag{5}$$

The factor $(1 - 1/N)^{S_{n-1}}$ is approximately the probability that the walker is not trapped in the first $n - 1$ steps; $1/N$ is the approximate probability for trapping on the nth step. Rosenstock was able to perform the sum indicated in Eq. (5) for $D \geqslant 3$ and obtained agreement with the exact asymptotic results of Eq. (1). He was unable to carry out the summation for $D = 2$.

3. COMPARISON OF THE GENERATING FUNCTIONS

We now give a more formal justification for our heuristically developed results. Let $p(\mathbf{l})$ be the probability that the walker takes a step of length $\mathbf{l}$. For simplicity we consider only symmetric walks, i.e., $p(-\mathbf{l}) = p(\mathbf{l})$, of finite variance, i.e., $\langle \mathbf{l}^2 \rangle \equiv \sum_{\mathbf{l}} \mathbf{l}^2 p(\mathbf{l}) < \infty$. The structure factor $\lambda(\boldsymbol{\theta})$ is defined by

$$\lambda(\boldsymbol{\theta}) \equiv \sum_{\mathbf{l}} p(\mathbf{l}) \exp(i\mathbf{l}\cdot\boldsymbol{\theta}) \tag{6}$$

We will now show that the small-$\boldsymbol{\theta}$ behavior of $\lambda(\boldsymbol{\theta})$ and the dimensionality effectively determine the asymptotic forms of both $\langle n \rangle_N$ and S_n. It is therefore not surprising that these two properties are related to each other.

For translationally invariant walks on D-dimensional finite hypercubic lattices of $N = m^D$ sites it has been shown that[1]

$$\langle n \rangle_N \sim N\phi_N(1), \qquad N \to \infty \tag{7}$$

where

$$\phi_N(z) = \frac{1}{N} \sum_{j_1=0}^{m-1} \cdots \sum_{j_D=0}^{m-1} \frac{1}{1 - z\lambda(2\pi\mathbf{j}/m)}, \qquad \mathbf{j} \neq (0, 0, \ldots, 0) \tag{8}$$

After using the periodicity of the summand to restrict the upper limit of the j_i to $[(m - 1)/2]$, we note that the main contribution to $\phi_N(1)$ for large N comes from those terms in the sum with all the j_i less than $[\epsilon(m - 1)/2]$, where ϵ is an arbitrarily small, positive number. For these terms we can expand the structure factor of Eq. (6) as

$$\lambda(\boldsymbol{\theta}) \simeq 1 - \tfrac{1}{2}\langle l^2\rangle\|\boldsymbol{\theta}\|^2 \tag{9}$$

and then use (9) to evaluate the sums in Eq. (8) to leading order for large N. In one dimension this yields

$$\begin{aligned}\phi_N(1) &\sim \frac{2}{N}\sum_{j=1}^{[\epsilon(m-1)/2]} \frac{1}{\frac{1}{2}\langle l^2\rangle(2\pi j/N)^2} \\ &\sim \frac{N}{\langle l^2\rangle\pi^2}\sum_{j=1}^{\infty}\frac{1}{j^2} = \frac{N}{6\langle l^2\rangle}\end{aligned} \tag{10}$$

For $D = 2$ we find

$$\phi_N(1) \sim (1/\pi\langle l^2\rangle)\ln N \tag{11}$$

and for $D \geqslant 3$,

$$\phi_N(1) \sim P(0, 1) = u \tag{12}$$

where $P(0, z)$ is defined below. These results are in agreement with the expressions in Eq. (1).

Now let us consider the generating function $S(z)$ for the distinct number of sites visited in n steps on an infinite lattice. The average number S_n of distinct sites visited is the coefficient of z^n in this generating function, which is given by[7]

$$S(z) = (1 - z)^{-2}P(0, z)^{-1} \tag{13}$$

where

$$P(0, z)\frac{1}{(2\pi)^D}\int_{-\pi}^{\pi}\cdots\int_{-\pi}^{\pi}\frac{d^D\theta}{1 - z\lambda(\boldsymbol{\theta})} \tag{14}$$

is the infinite perfect lattice generating function for walks that return to the origin. $S(z)$ is a regular function of z inside the unit circle and has branch point singularities at $z = \pm 1$. Expansion about these points is performed after substitution of Eq. (9) into Eq. (14). The leading asymptotic term of S_n from Eq. (13) is then obtained through the application of a Tauberian theorem.[7] This procedure leads to the result given in Eq. (2).

Hence we have shown that, for all dimensions D, the asymptotic behavior of both $\langle n\rangle_N$ and S_n is determined by the small-$\boldsymbol{\theta}$ behavior of $\lambda(\boldsymbol{\theta})$. On the basis of this analysis it is not surprising that the average number of steps to trapping $\langle n\rangle_N$ is closely related to S_n, the average number of distinct sites visited in an n-step random walk.

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