

# Random Walks on Lattices with Randomly Distributed Traps

## I. The Average Number of Steps Until Trapping

W. Th. F. den Hollander<sup>1</sup>

*Received March 13, 1984*

---

For a random walk on a lattice with a random distribution of traps we derive an asymptotic expansion valid for small  $q$  for the average number of steps until trapping, where  $q$  is the probability that a lattice point is a trap. We study the case of perfect traps (where the walk comes to an end) and the extension obtained by letting the traps be imperfect (i.e., by giving the walker a finite probability to remain free when stepping on a trap). Several classes of random walks of varying dimensionality are considered and special care is taken to show that the expansion derived is exact up to and including the last term calculated. The numerical accuracy of the expansion is discussed.

---

**KEY WORDS:** Random walk; number of distinct lattice points visited; random trap distribution; perfect and imperfect traps; average number of steps until trapping.

### 1. INTRODUCTION

A random walk on a lattice with randomly distributed trapping points can serve as a model for various processes in photosynthetic systems, molecular crystals, ionic crystals, and organic solids. It is, for instance, well suited to describe the transfer and trapping of excitations in a photosynthetic membrane,<sup>(1)</sup> of charge carriers in an anisotropic molecular crystal in an electric field<sup>(2)</sup> and of electrons in an amorphous material.<sup>(3)</sup>

The model is defined as follows. Consider a  $d$ -dimensional lattice  $L$  of which each point can be in either of two different states: with probability  $q$  it is a trap and with probability  $1 - q$  it is a nontrapping point. The states of different lattice points are independent stochastic variables and are "frozen

---

<sup>1</sup> Instituut-Lorentz voor Theoretische Natuurkunde, Nieuwsteeg 18, 2311 SB Leiden, The Netherlands.

in." Next, consider a random walk on  $L$ , starting at the origin  $0$  and proceeding according to a given probability distribution  $p: L \rightarrow \mathbb{R}$  for single steps ( $p(l) \geq 0$ ,  $\sum_{l \in L} p(l) = 1$ ). The walk ends when the walker steps on a trap.

Many authors have studied various properties of this *random trap model*.<sup>(4-24)</sup> Quantities on which interest has centered are: the probability for the walker to survive a given number of steps, the average number of steps made until trapping and the probability of return to the origin. In general these quantities depend on  $L$ ,  $q$  and  $p$ . In this paper we shall be mainly concerned with the second quantity.

The random trap model is obviously akin to other models with a random structure, such as the percolation model and the random Ising model. In this respect it is a member of a class of models that have received much interest in recent years and that by their simple description but complicated nature have become a challenge to the theoretician. So far, only few rigorous results have been obtained for the random trap model<sup>(21,23)</sup> (see also Ref. 25), except in one dimension.<sup>(4,5,7,10,20)</sup> On the other hand, several approximative methods have been developed. With a few exceptions, the results obtained are valid for values of  $q$  that are either small or close to unity.

Rosenstock, who introduced the model in general terms in 1961,<sup>(4)</sup> was the first to find an expression, valid for  $q \rightarrow 0$ , for the average number of steps until trapping  $\langle n \rangle$  for simple random walks.<sup>(14)</sup> He introduced a simple expression for the probability  $f_n$  that the walker is not trapped after  $n$  steps and calculated  $\langle n \rangle$  to leading order in  $q$ , using an approach that has become known as the Rosenstock approximation. Weiss<sup>(15)</sup> investigated  $f_n$  more closely for a class of random walks in  $d = 3$  and showed that the Rosenstock approximation is useful only if  $q \lesssim 0.05$ . Zumofen and Blumen<sup>(17,18)</sup> went on to find better estimates of  $f_n$  for random walks in  $d = 2$  and  $3$ . They also investigated the effect of long-range steps and did Monte Carlo simulations to test their results.

The authors mentioned all make use of some of the results obtained by Montroll and Weiss<sup>(5)</sup> and by Jain *et al.*<sup>(26-31)</sup> for the probability distribution of the number of distinct lattice points visited in an  $n$ -step walk on the lattice without traps. Although the approach followed is essentially correct it is not exact, nor is it complete.

The aim of this paper is twofold. First, in Section 2 we derive an asymptotic expansion for  $\langle n \rangle$  valid for small  $q$ , thus extending Rosenstock's analysis. We consider several classes of random walks of varying dimensionality. We investigate the error that is involved in neglecting certain cumulants and take special care to show that the expansion derived is exact up to and including the last term calculated. Second, in Section 3 we extend

the results to imperfect traps, i.e., to traps where the walker has a finite probability to remain untrapped. We also briefly discuss the extension to several types of imperfect traps, each with a different trapping parameter. Models with two types of imperfect traps are of interest in photosynthesis.<sup>(32)</sup>

Throughout the paper we assume, unless stated otherwise, that the random walk is *aperiodic* (in the sense of Spitzer, Ref. 33, p. 20) and that  $F > 0$ , where  $F$  is the probability of return to the origin in the absence of traps. Aperiodicity means that there is no proper sublattice of  $L$  to which the walk is confined. In terms of the structure function of the random walk defined by  $\hat{p}(\theta) := \sum_{l \in L} e^{i l \cdot \theta} p(l)$ ,  $\theta \in \mathbb{R}^d$ , aperiodicity is equivalent to the property that  $\hat{p}(\theta) = 1$  iff  $\theta = 0 \pmod{2\pi}$  (Ref. 33, p. 67). If the random walk is not aperiodic then there is a smallest sublattice  $L'$  of  $L$  (with dimension  $d' \leq d$ ) to which the walk is confined. Since the distribution of traps in  $L'$  is obviously random and the random walk is aperiodic on  $L'$  the restriction imposed involves no loss of generality. The case  $F = 0$  is trivial: one easily sees that then, e.g., for perfect traps  $f_n = (1 - q)^{n+1}$  and  $\langle n \rangle = (1 - q)/q$ . We further assume that  $L$  is  $d$ -dimensional hypercubic ( $L = \mathbb{Z}^d$ ). This restriction is not serious either, as any random walk on a different type of (Bravais) lattice can be easily translated into a random walk on  $\mathbb{Z}^d$ .

An important classification of random walks is that into *recurrent* and *transient* random walks. In the former case  $G(0; 1) = \infty$  and  $F = 1 - G^{-1}(0; 1) = 1$ ,<sup>(34)</sup> in the latter  $G(0; 1) < \infty$  and  $F < 1$ , where  $G(0; z)$  is the Green's function of the random walk at the origin. All random walks with  $d \geq 3$  or with  $\sum_{l \in L} |l| p(l) < \infty$  and  $\sum_{l \in L} l p(l) \neq 0$  are transient (Ref. 33, pp. 33 and 83). An interesting subclass of transient random walks is that of *strongly transient* random walks for which  $G'(0; 1) < \infty$ . This concept, which was first introduced by Port into the theory of Markov chains,<sup>(35)</sup> plays an important role in the work of Jain *et al.*<sup>(26-31)</sup> All random walks with  $d \geq 5$  or with  $\sum_{l \in L} |l|^2 p(l) < \infty$  and  $\sum_{l \in L} l p(l) \neq 0$  are strongly transient.<sup>(29)</sup>

Our results for  $\langle n \rangle$  depend strongly on  $d$  and on the detailed properties of  $p$ . In the asymptotic expansions obtained coefficients occur that are related to the asymptotic behavior of  $G(0; z)$  for  $z \rightarrow 1$  (and in a few cases also to the value of  $G(l; 1)$  for  $l \neq 0$ ). For most classes of random walks this behavior is known from standard random-walk literature, for others we have extended known results.

A matter of particular convenience in the description of the random trap model is that some of its properties are easily expressed in terms of properties of the random walk in the absence of traps. This is an important simplification.

## 2. PERFECT TRAPS

Consider an infinite  $d$ -dimensional hypercubic lattice  $L$  with a random distribution of traps, and an arbitrary random walk  $p$  on  $L$ . If  $q$  is the probability that a lattice point is a trap, then the probability  $f_n$  that the walker has not been trapped after  $n$  steps is given by<sup>(36)</sup>

$$f_n = \langle (1 - q)^{S_n} \rangle, \quad n \geq 0 \quad (2.1)$$

where  $S_n$  is the number of *distinct* lattice points visited by the walker and the average is over all walks of  $n$  steps on the lattice *without* traps. We assume  $q > 0$ . Clearly,  $f_n$  is a monotone, nonincreasing function of  $n$ . In Ref. 21 it is shown that  $S_n \rightarrow \infty$  with probability 1 as  $n \rightarrow \infty$ , and hence  $f_n \rightarrow 0$ , for all random walks except the *degenerate* random walk with  $p(0) = 1$ . The average number of steps  $\langle n \rangle$  before trapping is found from

$$\langle n \rangle = \sum_{n=1}^{\infty} n(f_{n-1} - f_n) = \sum_{n=0}^{\infty} f_n \quad (2.2)$$

(cf. Ref. 37, p. 213). The higher moments of  $n$  are expressed as similar sums.

In order to calculate  $\langle n \rangle$  from Eqs. (2.1) and (2.2) one has to know the probability distribution of  $S_n$  for all lengths  $n$  of the walk. For general random walks this probability distribution is not known exactly, the difficulty lying in the fact that whether or not a step leads to a new lattice point generally depends on *all* previous steps. The average  $\langle S_n \rangle$ , however, can be found from the simple equation<sup>(5)</sup>

$$\sum_{n=0}^{\infty} z^n \langle S_n \rangle = 1/(1 - z)^2 G(0; z) \quad (2.3)$$

where

$$G(l; z) := \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} d\theta_1 \cdots \int_{-\pi}^{\pi} d\theta_d \frac{e^{-il \cdot \theta}}{1 - z\hat{p}(\theta)}, \quad l \in L, |z| \leq 1 \quad (2.4)$$

is the Green's function of the random walk and  $\hat{p}(\theta) := \sum_{l \in L} e^{il \cdot \theta} p(l)$ .

For large  $n$  the probability distribution of  $S_n$  exhibits a number of simple limiting properties. First of all, as mentioned before, for all nondegenerate random walks  $S_n \rightarrow \infty$  with probability 1 as  $n \rightarrow \infty$ . The asymptotic behavior for large  $n$  of  $\langle S_n \rangle$  can be extracted from Eq. (2.3). Furthermore, for simple random walks with  $d \geq 2$  Dvoretzky and Erdős<sup>(38)</sup> proved that the stochastic variables  $S_n$  satisfy the so-called weak law of large numbers:

$$\lim_{n \rightarrow \infty} P[|S_n - \langle S_n \rangle| / \langle S_n \rangle > \varepsilon] = 0, \quad \text{for } \varepsilon > 0 \quad (2.5)$$

(where  $P$  stands for probability). They achieved this by showing that

$$\text{Var } S_n / \langle S_n \rangle^2 \rightarrow 0, \quad n \rightarrow \infty \tag{2.6}$$

( $\text{Var } S_n := \langle S_n^2 \rangle - \langle S_n \rangle^2$ ) and using the Chebyshev inequality. They further improved Eq. (2.5) by proving that  $S_n / \langle S_n \rangle \rightarrow 1, n \rightarrow \infty$ , with probability 1 (the strong law). Subsequently these results were generalized to arbitrary transient random walks by Spitzer, Kesten, and Whitman (see Ref. 33, p. 38) and to recurrent random walks in  $d = 2$  by Jain and Pruitt.<sup>(29)</sup> For recurrent random walks in  $d = 1$  the asymptotic behavior is in general more complicated<sup>(29)</sup> and Eqs. (2.5) and (2.6) do not hold.

Jain *et al.*<sup>(26-31)</sup> have made a careful study of some further asymptotic properties of the probability distribution of  $S_n$ . For example, they have shown that for random walks with  $d \geq 3$  and for strongly transient random walks in  $d = 1$  and 2,  $(S_n - \langle S_n \rangle) / \text{Var}^{1/2} S_n$  converges to the normal distribution with mean 0 and variance 1 (the central limit theorem) if  $F > 0$ . For a large class of random walks they have calculated  $\text{Var } S_n$  to leading order in  $n$  and in addition obtained a bound for  $\langle (S_n - \langle S_n \rangle)^4 \rangle$ .

We shall use the various asymptotic results obtained for the probability distribution of  $S_n$  to derive an asymptotic expansion for  $\langle n \rangle$  valid for small  $q$ . To this end we first apply the Euler–Maclaurin summation formula to Eq. (2.2):

$$\langle n \rangle = \int_0^\infty dn f(n) + \frac{1}{2}(f_0 + f_\infty) + R \tag{2.7}$$

where  $f(n)$  is a suitably chosen function on  $[0, \infty)$ , to be specified later, which is equal to  $f_n$  for integer  $n$  and has two continuous derivatives,  $f_\infty := \lim_{n \rightarrow \infty} f_n$  and  $R$  is a rest term. To estimate the order of  $R$  we observe that  $f_n$  is positive, monotone and, by Eq. (2.4b) in Ref. 21, convex. Hence it is possible to choose  $f(n)$  also positive, monotone, and convex. It then follows<sup>(39)</sup> that  $R$  is of order  $f'(\infty) - f'(0)$ , where obviously  $f'(\infty) := \lim_{n \rightarrow \infty} f'(n) = 0$ . Since  $f_1 - f_0 = O(q)$  it is also possible to choose  $f(n)$  so that  $f'(0) = O(q)$ , which then ensures that  $R = O(q)$ . We further have  $f_0 = 1 - q$  and  $f_\infty = 0$  (for nondegenerate random walks).

Next, to evaluate the integral in Eq. (2.7), we introduce the variable  $\lambda := -\log(1 - q)$  and make the cumulant expansion

$$f_n = \langle e^{-\lambda S_n} \rangle = e^{-x_n} \tag{2.8a}$$

$$x_n := - \sum_{j=1}^\infty \frac{(-\lambda)^j}{j!} K_{nj} \tag{2.8b}$$

where  $K_{n1} := \langle S_n \rangle$ ,  $K_{n2} := \text{Var } S_n$  and  $K_{nj} (j \geq 3)$  is the  $j$ th cumulant of  $S_n$ . Writing  $f(n) := \exp[-x(n)]$ , where  $x(n) = x_n$  for integer  $n$ , changing the integration variable in Eq. (2.7) from  $n$  to  $x$  and noting that  $x(n)$  is monotone, we get

$$\langle n \rangle = \int_{\lambda}^{\infty} dx e^{-x} \frac{dn}{dx} + \frac{1}{2} + O(q) \quad (2.9)$$

In order to find  $dn/dx$  we construct a systematic expansion in terms of  $\lambda$  (for a given finite  $x$ ) for the inverse function  $n(x)$  of  $x(n)$ , valid for small  $\lambda$ , by substituting into Eq. (2.8b) the asymptotic expressions for the cumulants of  $S_n$ , valid for large  $n$ , and considering  $n$  as a continuous variable. Substitution of this expansion into Eq. (2.9) yields an expansion for  $\langle n \rangle$  in terms of  $\lambda$ , the coefficients of which are standard-type integrals. If  $\sum_n f_n < \infty$  for all  $\lambda > 0$ , the coefficients in this expansion are finite. Finally, by expanding  $\lambda$  in powers of  $q$  we find the desired expansion for  $\langle n \rangle$ .

Observe that we choose for  $f(n)$  the function that is obtained from Eq. (2.8b) by simply considering  $n$  as a continuous variable in the asymptotic expressions for the cumulants. It is not clear that in this way a function is obtained which has the properties required in Eq. (2.7). However, this presents no practical problem. Indeed, as an alternative for  $f(n)$  we may choose the function  $(1 - \Delta)f_{[n]} + \Delta f_{[n]+1}$  with  $\Delta := n - [n]$ . This function *does* satisfy Eq. (2.7) with  $R = 0$  and, what is more important, it turns out that in *each* of the cases to be considered in the sequel this function is identical with  $f(n)$  up to and including the order in  $\lambda$  and  $n$  for which we shall use the cumulant expansion. Therefore  $f(n)$  gives us the correct result.

In the following we shall derive the asymptotic expansion for  $\langle n \rangle$  up to and including the term of lowest order in  $q$  to which the second cumulant  $\text{Var } S_n$  contributes. If Eq. (2.6) holds this term is certainly *not* the leading term in  $q$ . Since only the leading term in  $n$  for  $\text{Var } S_n$  is known thus far we shall have to neglect all subsequent terms in the expansion of  $\langle n \rangle$ . For  $\langle S_n \rangle$ , on the other hand, we can obtain as many terms in the expansion for large  $n$  as are required to carry out the derivation to the order indicated. This is accomplished by expanding  $G(0; z)$  in terms of  $1 - z$ , using Eq. (2.3) and applying a theorem due to Darboux<sup>(40-41)</sup> (cf. Ref. 42, p. 140). In the following we shall need only those terms in the expansion of  $\langle S_n \rangle$  to which the singularity of  $G(0; z)$  at  $z = 1$  contributes. Furthermore, since the asymptotic behavior for large  $n$  of the cumulants  $K_{nj}$  with  $j \geq 3$  is not known we shall also have to neglect contributions arising from these cumulants. However, it can be rigorously shown that if

$$\frac{\langle (S_n - \langle S_n \rangle)^j \rangle}{\langle S_n \rangle^{j-2} \text{Var } S_n} \rightarrow 0, \quad n \rightarrow \infty, \quad \text{for all } j \geq 3 \quad (2.10)$$

such contributions are of higher order in  $q$  than the terms derived. In that case the expansion of  $\langle n \rangle$  thus obtained is exact *up to and including* the last term calculated.

We mention here that Jain and Pruitt<sup>(31)</sup> have proved that for all random walks with  $d \geq 3$  and for a large class of strongly transient random walks in  $d = 1$  and  $2$  (possibly all, but certainly those for which  $G''(0; 1) < \infty$ ; see Ref. 31, p. 117)  $\langle (S_n - \langle S_n \rangle)^4 \rangle = O(\text{Var}^2 S_n)$ . Note that this does *not* follow from the central limit theorem. Together with Eq. (2.6) this establishes Eq. (2.10) for  $j = 4$ . It then follows from the Schwarz inequality that Eq. (2.10) holds also for  $j = 3$ , and from  $1 \leq S_n \leq n + 1$  and  $\langle S_n \rangle \approx (1 - F)n \sim n^{(34)}$  that it holds for  $j > 4$  likewise.

In the following we shall first consider the class of *unbiased* random walks with *finite single-step variance*, i.e., random walks for which  $\mu := \sum_{l \in L} lp(l) = 0$  and  $m_2 := \sum_{l \in L} |l|^2 p(l) < \infty$  (finite mean-squared displacement per step). This includes, e.g., all random walks with  $p(l) = p(-l)$  and with  $p(l) > 0$  on a finite subset of  $L$ . For this class  $\hat{p}(\theta) = 1 - \frac{1}{2} \sum_{i,j} C_{ij} \theta_i \theta_j + o(|\theta|^2)$ ,  $\theta \rightarrow 0$ , with  $C_{ij} := \sum_{l \in L} l_i l_j p(l)$ ,  $i, j = 1, \dots, d$ . The constants  $C_{ij}$  are finite, the matrix  $\{C_{ij}\}$  is positive definite (Ref. 33, p. 74) and we define  $C^2 := \det\{C_{ij}\}$ . Random walks in this class are recurrent for  $d = 1$  and  $2$ , transient for  $d = 3$  and  $4$  and strongly transient for  $d \geq 5$ . The case  $d = 1$  will have to be treated in a special way since neither Eq. (2.6) nor Eq. (2.10) holds in this case, so that the procedure sketched above cannot be followed. Furthermore, for  $d = 2, 3$ , and  $4$  we shall have to distinguish between the two subclasses with  $m_3 := \sum_{l \in L} |l|^3 p(l) < \infty$  and with  $m_3 = \infty$ .

Subsequently we shall discuss other classes of random walks.

**(i)  $d = 1$ .** For this special case we start from the *exact* result for the simple random walk

$$\langle n \rangle = (1 - q)/q^2 \tag{2.11}$$

derived by Montroll<sup>(7)</sup> (apart from the factor  $1 - q$ , which is due to the fact that we allow the origin to be a trap). Equation (2.11) is one of the few exact results known thus far for  $\langle n \rangle$ . Crucial in the derivation of this result is the argument that the simple random walk starting in an interval between two traps is confined to this interval. If steps of two or more lattice spacings are allowed this argument is no longer valid and no exact result is known. We can, however, in this case determine the behavior of  $\langle n \rangle$  for  $q \rightarrow 0$  as follows. Jain and Pruitt<sup>(29)</sup> have proved that the probability distribution of  $S_n/\langle S_n \rangle$  converges for  $n \rightarrow \infty$  to a limit distribution of which we merely note that it is *independent* of the random walk. They have also proved that  $\langle S_n^k \rangle / \langle S_n \rangle^k$ ,  $k \geq 2$ , converges to the  $k$ th moment of this limit distribution. Using this

result, together with the fact that  $\langle S_n \rangle \simeq C(8n/\pi)^{1/2}$ ,<sup>(34)</sup> we readily find from Eqs. (2.1) and (2.2) that to leading order in  $q$ ,  $\langle n \rangle$  is a function of the product  $Cq$ . A comparison with Eq. (2.11) then yields

$$\langle n \rangle \simeq 1/C^2q^2 \tag{2.12}$$

(ii)  $d = 2$ . First we assume  $m_3 < \infty$ . Then it is easily shown that for  $z \rightarrow 1$

$$G(0; z) = -u_1 \log(1 - z) + u_1u_2 + o((1 - z)^{1/2}) \tag{2.13}$$

where  $u_1 = 1/2\pi C$  and  $u_2$  is a constant that depends on further details of  $p$  and can take any value in  $(-\infty, \infty)$  depending on  $p$ . For a few random walks  $u_2$  has been calculated exactly<sup>(34,43)</sup>; e.g., for the simple random walk  $u_2 = \log 8$ . From Eqs. (2.3) and (2.13) it follows, as Henyey and Seshadri<sup>(43)</sup> have shown, that

$$\langle S_n \rangle = \frac{n}{u_1 \log un} \sum_{k=0}^{\infty} \frac{c_k}{\log^k un} + o(n^{1/2}/\log^2 n) \tag{2.14}$$

with  $c_k := (-d/dx)^k \Gamma^{-1}(x)|_{x=2}$  ( $\Gamma$  is the gamma function) and  $\log u := u_2$ . We shall need only the following terms:

$$\langle S_n \rangle = \frac{n}{u_1 \log un} \left( 1 + \frac{c_1}{\log un} + \frac{c_2}{\log^2 un} \right) + O(n/\log^4 n) \tag{2.15}$$

with  $c_1 = 1 - \gamma$  and  $c_2 = (1 - \gamma)^2 + 1 - \frac{1}{6}\pi^2$  ( $\gamma$  is Euler's constant).

Jain and Pruitt<sup>(29)</sup> have proved that  $\text{Var } S_n \simeq 8\pi^2 K^* C^2 n^2 / \log^4 n$  with  $K^* := K + \frac{1}{2}(1 - \frac{1}{6}\pi^2)$  and  $K := -\int_0^1 dx(1 - x + x^2)^{-1} \log x = 1.171953\dots$  Using this together with Eq. (2.15) and following the procedure sketched earlier, we find after some algebra for  $\langle n \rangle$  the expansion

$$\begin{aligned} \langle n \rangle = \frac{u_1}{q} & \left[ \log \left( \frac{u_1 u}{q} \right) + \log \log \left( \frac{u_1 u}{q} \right) + \frac{\log \log(u_1 u/q)}{\log(u_1 u/q)} \right. \\ & \left. + \frac{2K}{\log(u_1 u/q)} + \dots \right] + \dots \end{aligned} \tag{2.16}$$

where the brackets are understood to contain only so-called slowly varying functions of  $q$ .

Thus far there are no results known for this case that establish Eq. (2.10) and thereby ensure that the higher cumulants of  $S_n$ , i.e., the  $K_{nj}$  with  $j \geq 3$  in Eq. (2.8b), cannot contribute to the order of the terms in Eq. (2.16). However, since Eq. (2.6) holds it is surely sufficient that



$\langle (S_n - \langle S_n \rangle)^j \rangle = O(\langle S_n \rangle^{j-3} \text{Var}^{3/2} S_n)$  for  $j \geq 3$ . As this relation holds for all random walks with  $\mu = 0$  and  $m_2 < \infty$  both for  $d = 1$  and for  $d \geq 3$ , which are strongly differing cases, it is not unreasonable to expect that it also holds for  $d = 2$ . This, however, needs further investigation.

It is interesting to note that in the calculation of  $\langle n \rangle$  the constants  $c_1$  and  $c_2$  cancel and that only the constant  $K$  appears in the expansion. Moreover, the final result seems to suggest that for all random walks in this class the (slowly varying) function between the square brackets in Eq. (2.16) depends on  $q$  and  $p$  only through the combination  $\log(u_1 u/q)$ . The product  $u_1 u$  can take any value in  $(0, \infty)$  depending on  $p$ . Equation (2.16) makes sense only if  $q < u_1 u$ ; however, for most random walks  $u_1 u$  is not a small number. For example, if  $C_{ij} = C\delta_{ij}$  it follows from Eq. (2.4) and the inequality  $1 - \text{Re } \hat{p}(\theta) \leq \frac{1}{2} \sum_{i,j} C_{ij} \theta_i \theta_j$  that  $u_1 u > \pi/4$ .

If  $m_3 = \infty$  the expansion of  $\langle n \rangle$  may differ from that given in Eq. (2.16), though not to leading order in  $q$ . In this case the term  $o((1-z)^{1/2})$  in Eq. (2.13) is to be replaced by one of lower order in  $1-z$ , which in turn affects Eq. (2.14). If, however,  $\hat{p}(\theta) - 1 + \frac{1}{2} \sum_{i,j} C_{ij} \theta_i \theta_j = o(|\theta|^2 / \log^2 |\theta|)$ ,  $\theta \rightarrow 0$ , it follows that this term is  $o(1/\log(1-z))$  and hence that the first three terms in Eq. (2.15) are unaffected and so is Eq. (2.16).

**(iii)  $d = 3$ .** For  $z \rightarrow 1$  we have, if  $m_3 < \infty$ ,

$$G(0; z) = u_0 - u_1(1-z)^{1/2} + o((1-z) \log(1-z)) \tag{2.17}$$

where  $u_0 = G(0; 1) = 1/(1-F) < \infty$  and  $u_1 = 1/2^{1/2} \pi C$  (see also Refs. 5 and 34). For a few random walks  $u_0$  has been calculated exactly<sup>(34,44-48)</sup>; e.g., for the simple random walk  $u_0 = 1.516386\dots$ . Insertion of Eq. (2.17) into (2.3) leads to

$$\langle S_n \rangle = u_0^{-1} n + 2\pi^{-1/2} u_1 u_0^{-2} n^{1/2} + o(\log n) \tag{2.18}$$

For this case Jain and Pruitt<sup>(28)</sup> have found that  $\text{Var } S_n \simeq \{(1-F)^4 / 2\pi^2 C^2\} n \log n$ . Using this together with Eq. (2.18) we find

$$\langle n \rangle = \frac{u_0}{q} - u_1 u_0^{-1} \left( \frac{u_0}{q} \right)^{1/2} + \frac{1}{2} u_1^2 u_0^{-2} \log \left( \frac{u_0}{q} \right) + \dots \tag{2.19}$$

Since  $\langle (S_n - \langle S_n \rangle)^4 \rangle = O(\text{Var}^2 S_n)$ ,<sup>(28)</sup> Eq. (2.10) holds and the terms occurring in Eq. (2.19) represent the correct expansion.

If  $m_3 = \infty$  this may affect Eq. (2.19), but only after the second term as a closer analysis shows.

**(iv)  $d = 4$  and  $d \geq 5$ .** For  $z \rightarrow 1$  we have

$$G(0; z) = u_0 + u_1(1-z) \log(1-z) + u_2(1-z) + o((1-z)^{3/2}), \quad d = 4 \tag{2.20a}$$

$$G(0; z) = u_0 - u_2(1-z) + O((1-z)^{3/2}), \quad d \geq 5 \tag{2.20b}$$

where  $u_0 = G(0; 1) = 1/(1 - F) < \infty$  as before, but  $u_1 = 1/4\pi^2 C$ ;  $u_2$  is for  $d = 4$  a constant that depends on further details of  $p$ , whereas  $u_2 = G'(0; 1) < \infty$  for  $d \geq 5$ . For  $d = 4$ , but not for  $d \geq 5$ , we have assumed  $m_3 < \infty$ .

From Eqs. (2.3) and (2.20a,b) we deduce

$$\langle S_n \rangle = u_0^{-1}n + u_1 u_0^{-2} \log n + \{u_0^{-1} + (\gamma u_1 - u_2)u_0^{-2}\} + o(1/n^{1/2}), \quad d = 4 \quad (2.21a)$$

$$\langle S_n \rangle = u_0^{-1}n + \{u_0^{-1} + u_2 u_0^{-2}\} + O(1/n^{1/2}), \quad d \geq 5 \quad (2.21b)$$

In Refs. 26 and 28 it is proved that both for  $d = 4$  and for  $d \geq 5$   $\text{Var } S_n \simeq \{F(1 - F) + 2a\}n$  with  $0 < a < \infty$ . From a closer inspection of the derivation of this result it readily appears that

$$a = \sum_{l \neq 0} \frac{G^2(l; 1) G(-l; 1) [G(0; 1) - G(-l; 1)]}{G^3(0; 1) [G^2(0; 1) - G(l; 1) G(-l; 1)]} \quad (2.22)$$

This is shown in Appendix A. Using Eqs. (2.21a, b) and the asymptotic expression for  $\text{Var } S_n$ , we then find

$$\langle n \rangle = \frac{u_0}{q} - u_1 u_0^{-1} \log \left( \frac{u_0}{q} \right) - \{1 + (u_1 - u_2)u_0^{-1} - u_0^2 a\} + \dots, \quad d = 4 \quad (2.23a)$$

$$\langle n \rangle = \frac{u_0}{q} - \{1 + u_2 u_0^{-1} - u_0^2 a\} + \dots, \quad d \geq 5 \quad (2.23b)$$

Since again  $\langle (S_n - \langle S_n \rangle)^4 \rangle = O(\text{Var}^2 S_n)$ ,<sup>(31)</sup> Eq. (2.10) holds and the corrections to Eqs. (2.23a, b) are  $o(1)$ .

For the simple random walk Montroll<sup>(34)</sup> has derived the following asymptotic series for  $u_0$  in powers of  $1/2d$ :

$$u_0 = 1 + \frac{1}{2d} + \frac{3}{(2d)^2} + \frac{12}{(2d)^3} + \frac{60}{(2d)^4} + \frac{355}{(2d)^5} + \dots \quad (2.24)$$

In Appendix A we derive a similar series for  $u_2$  for  $d \geq 5$ :

$$u_2 = \frac{2}{2d} + \frac{12}{(2d)^2} + \frac{78}{(2d)^3} + \frac{570}{(2d)^4} + \frac{4650}{(2d)^5} + \dots \quad (2.25)$$

and one for  $a$  for  $d \geq 4$ :

$$a = \frac{1}{(2d)^2} + \frac{4}{(2d)^3} + \frac{23}{(2d)^4} + \frac{160}{(2d)^5} + \frac{1294}{(2d)^6} + \dots \quad (2.26)$$

From a numerical analysis of Eq. (2.4) for the simple random walk in  $d = 4$  we estimate that  $u_0 = 1.239 \pm 0.001$  and  $u_2 = 0.139 \pm 0.001$ .

If, for  $d = 4$ ,  $m_3 = \infty$  this may have its effect on Eq. (2.23a), but only after the second term. If  $\hat{p}(\theta) - 1 + \frac{1}{2} \sum_{i,j} C_{ij} \theta_i \theta_j = o(|\theta|^2 / \log |\theta|)$ ,  $\theta \rightarrow 0$ , Eq. (2.23a) is unaffected up to and including the term of order 1.

Equations (2.12), (2.16), (2.19), and (2.23a, b) are the results for  $\langle n \rangle$  for small values of  $q$  for the class of unbiased random walks with finite single-step variance. We next consider random walks with  $m_2 < \infty$  and  $\mu \neq 0$  (biased).<sup>2</sup> Jain and Pruitt<sup>(29)</sup> have shown that *all* random walks in this class are strongly transient, regardless of the dimensionality. This property means that  $G'(0; 1) < \infty$  and implies that  $G(0; z)$  has the asymptotic form given by Eq. (2.20b). In addition, Jain and Orey<sup>(26)</sup> have proved that for all strongly transient random walks  $\text{Var } S_n \simeq \{F(1 - F) + 2a\}n$ . As mentioned earlier,  $\langle (S_n - \langle S_n \rangle)^4 \rangle = O(\text{Var}^2 S_n)$  for random walks with  $d \geq 3$  and for a large class of strongly transient random walks in  $d = 1$  and 2, including those for which  $G''(0; 1) < \infty$ . By a straightforward generalization of the proof for  $G'(0; 1) < \infty$  given in Ref. 29 it can be shown, using  $G(l; 1) \leq G(0; 1)$  for  $l \neq 0$ , that if  $\mu \neq 0$  and  $m_2 < \infty$  *all* the derivatives of  $G(0; z)$  at  $z = 1$  are finite. It then follows that  $\langle n \rangle$  is given by Eq. (2.23b) with  $u_0, u_2$ , and  $a$  related to the Green's function through Eqs. (2.20b) and (2.22).

It remains to consider the class of random walks with  $m_2 = \infty$ . This is the hardest class (obs.: if  $m_1 = \infty$ ,  $\mu$  is not defined and the terms "biased" and "unbiased" lose their meaning). If the random walk is strongly transient, which is always the case when  $d \geq 5$ ,  $\langle n \rangle$  is, of course, given by Eq. (2.23b) (with the proviso mentioned before for  $d = 1$  and 2). If not, a variety of asymptotic behavior may be expected depending on  $p$  (see Refs. 49 and 50 for some interesting properties of random walks in this class). If the random walk is transient, which is the case when  $m_1 < \infty$  and  $\mu \neq 0$ <sup>(33)</sup> or when  $d \geq 3$ , it is clear that  $\langle S_n \rangle \simeq (1 - F)n$  and that, by Eq. (2.6),  $\langle n \rangle \simeq u_0/q$ . In Ref. 31 it is shown that when  $d \geq 3$   $\text{Var } S_n \simeq \{F(1 - F) + 2a\}n$ , except when  $d = 3$  and  $\sum_{l \in L} G^2(l; 1) G(-l; 1) = \infty$  in which case  $a = \infty$  and  $\text{Var } S_n = O(n \log n)$ .<sup>(28)</sup> Using Eq. (2.3) one then easily shows that  $\langle n \rangle = u_0/q + o(q^{1/2})$  for  $d = 3$  and  $\langle n \rangle = u_0/q + o(\log q)$  for  $d = 4$ . Higher-order terms in  $q$  can be obtained in both cases if the behavior of  $G(0; z)$  is known for  $z \rightarrow 1$ . For recurrent random walks in  $d = 1$  and 2 with  $m_2 = \infty$  very little is known thus far about the probability distribution of  $S_n$ . This lack of knowledge bars a statement about the asymptotic behavior of  $\langle n \rangle$ .

Before concluding this section we remark the following. Consider a random walk  $p$  with  $p(0) = 0$  and the "scaled" random walk  $p'$  with  $p'(0) = p_0$  and  $p'(l) = (1 - p_0) p(l)$ ,  $l \neq 0$ , for some  $0 < p_0 < 1$ , i.e., the random walk obtained from  $p$  by giving the walker at each step a probability

<sup>2</sup> Part of the results in this section were presented in Ref. 23 (without a derivation). There are two misprints in that paper: on pp. 370 and 371 the word "asymmetric" should be replaced by "biased."

$p_0$  to pause instead of proceeding. A simple argument shows that the averages  $\langle n \rangle$  and  $\langle n \rangle'$  for these random walks satisfy the relation  $\langle n \rangle' = \langle n \rangle / (1 - p_0)$ . Since this is an exact relation and independent of  $q$  it should be reflected to *each* order of  $q$  in the asymptotic expressions derived in this section. The reader may find it instructive to see how this comes about in each of the cases considered.

### 3. EXTENSION TO IMPERFECT TRAPS

Up to now we have been concerned with perfect traps. We shall now extend the results of the previous section to *imperfect* traps. Let the traps be such that the walker, when stepping on any one of them, has a probability  $\eta$  to remain free (i.e., to continue his random walk) and a probability  $1 - \eta$  to be trapped. Let again  $f_n$  denote the probability that the walker has not been trapped after  $n$  steps. It is clear that with this extension  $f_n$  can no longer be expressed in terms of the stochastic variable  $S_n$  alone. In the course of his walk the walker may return not only to nontrapping points but also to traps. In the latter case one or more "escapes" take place and to fit these into the description the multiplicity of the visits to traps must be taken into account.

Our first step is the statement that Eq. (2.1) generalizes to

$$f_n = \left\langle \prod_{k=1}^{n+1} (1 - q + \eta^k q)^{V_n^{(k)}} \right\rangle, \quad n \geq 0 \quad (3.1)$$

where  $V_n^{(k)}$ ,  $k = 1, \dots, n + 1$ , is the number of distinct lattice points visited by the walker *exactly*  $k$  times ( $V_n^{(k)} = 0$  for  $k > n + 1$ ) and the average is over all walks of  $n$  steps on the lattice without traps. To see this, observe that if the walker visits a certain point  $k$  times, then if this point *is not* a trap he remains free at each of his visits, whereas if it *is* a trap he can only remain free by escaping  $k$  times. These two contingencies have probability  $1 - q$  and  $\eta^k q$ , respectively. To be still free after  $n$  steps the walker has to survive all visits made to traps. Since the trap distribution is random this implies Eq. (3.1).

We assume  $\eta < 1$ . Just as in the case of perfect traps  $f_n$  is monotone, nonincreasing in  $n$  and, by Eq. (3.3) in Ref. 21, convex. Since  $\sum_k V_n^{(k)} = S_n$  it follows from Eq. (3.1) that  $f_n(q, \eta) \leq f_n((1 - \eta)q, 0)$ , so that  $f_n \rightarrow 0$  as  $n \rightarrow \infty$  for all nondegenerate random walks. The average number of steps until trapping  $\langle n \rangle$  is again given by Eq. (2.2).

To find  $\langle n \rangle$  we require the knowledge of the *joint* probability distribution of the set of variables  $\{V_n^{(k)}\}_{k=1}^{n+1}$  for all lengths  $n$  of the walk. The variables  $V_n^{(k)}$  are mutually correlated stochastic variables, the joint probability distribution of which is difficult to study in detail, except in some

trivial cases, and about which so far not much is known. The averages  $\langle V_n^{(k)} \rangle$ , however, can be found from the simple equation

$$\sum_{n=0}^{\infty} z^n \langle V_n^{(k)} \rangle = \left\{ 1 - \frac{1}{G(0; z)} \right\}^{k-1} \left/ (1-z)^2 G^2(0; z) \right. \quad (3.2)$$

which was derived by Montroll and Weiss.<sup>(5)</sup>

To obtain an asymptotic expansion for  $\langle n \rangle$  valid for small  $q$  we shall follow the approach developed in the previous section. We write

$$f_n = \langle e^{-U_n} \rangle \quad (3.3)$$

with

$$U_n := \sum_{k=1}^{n+1} \lambda_k V_n^{(k)} \quad (3.3a)$$

$$\lambda_k := -\log(1 - q + \eta^k q) \quad (3.3b)$$

and make the cumulant expansion of  $\log f_n$ . Note that

$$0 < \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_{n+1} \leq \lambda < \infty \quad (3.4)$$

(Note also that in the symbol  $U_n$  we suppress the dependence on  $q$  and  $\eta$ .) We are interested in the asymptotic behavior of  $\langle U_n \rangle$  and the cumulants of  $U_n$  for small  $q$  and large  $n$ .

Using an ergodic theorem due to Kingman,<sup>(51)</sup> together with Eq. (3.4), we prove in Appendix B that for an arbitrary random walk  $\lim_{n \rightarrow \infty} n^{-1} \langle U_n \rangle =: \zeta$  exists and

$$\lim_{n \rightarrow \infty} n^{-1} U_n = \zeta, \quad \text{with probability 1} \quad (3.5)$$

This is the strong law for the stochastic variables  $U_n$ . For recurrent random walks, since  $G(0; 1) = \infty$ , we deduce from Eq. (3.2) that  $\lim_{n \rightarrow \infty} n^{-1} \langle V_n^{(k)} \rangle = 0$  for all  $k$ . Since  $0 < U_n \leq \lambda S_n$ , by Eqs. (3.3a) and (3.4), it follows from Eq. (2.4) that in this case  $\zeta = 0$ . For transient random walks, on the other hand, we have  $\langle V_n^{(k)} \rangle \simeq F^{k-1} (1-F)^2 n$  for fixed  $k$  and hence

$$\zeta = (1-F)^2 \sum_{k=1}^{\infty} \lambda_k F^{k-1} \quad (3.6)$$

where we use Eq. (3.4) and  $\langle S_n \rangle \simeq (1-F)n$  to show that  $\lim_{n \rightarrow \infty} n^{-1} \sum_{l>k} \lambda_l \langle V_n^{(l)} \rangle \rightarrow 0$  as  $k \rightarrow \infty$ . In the latter case  $0 < \zeta < \infty$ .

Equation (3.5) implies the weak law:  $\lim_{n \rightarrow \infty} P[|n^{-1}U_n - \zeta| > \varepsilon] = 0$ , for  $\varepsilon > 0$ . Since  $0 < U_n \leq \lambda(n+1)$  we have, for any  $\varepsilon > 0$ , the bound  $\text{Var } U_n \leq \lambda^2(n+1)^2 P[|U_n - \langle U_n \rangle| > \varepsilon n] + \varepsilon^2 n^2$  and with the weak law this leads to

$$\lim_{n \rightarrow \infty} n^{-2} \text{Var } U_n = 0 \tag{3.7}$$

For recurrent random walks this result, as we shall see later, is not strong enough for our purpose. For *transient* random walks, however, it follows from Eq. (3.7) that

$$\lim_{n \rightarrow \infty} \frac{\langle (U_n - \langle U_n \rangle)^j \rangle}{\langle U_n \rangle^j} = 0, \quad \text{for all } j \geq 2 \tag{3.8}$$

where it is crucial that  $\zeta > 0$  in Eq. (3.6). Observe that Eqs. (3.5), (3.7), and (3.8) hold for all  $0 < q \leq 1$  and  $0 \leq \eta < 1$ .

We need Eq. (3.8) to calculate  $\langle n \rangle$  for  $q \rightarrow 0$ . By Eqs. (3.3a, b)  $\langle (U_n - \langle U_n \rangle)^j \rangle$  is a power series in  $q$  that begins with  $q^j$  and has coefficients that are functions of  $n$  and  $\eta$ . Equation (3.8) implies, by a well-known theorem (cf. Ref. 37, p. 232), that for transient random walks these coefficients are all  $o(n^j)$  and therefore that the term of leading order in  $q$  in the asymptotic expansion of  $\langle n \rangle$  is determined by the asymptotic behavior for  $q \rightarrow 0$  and  $n \rightarrow \infty$  of  $\langle U_n \rangle$  alone and that the cumulants of  $U_n$  contribute only in higher order. Noting that  $\lambda_k \simeq (1 - \eta^k) q [1 + O(q)]$  uniformly in  $k$  and using Eq. (3.6), we find that  $\langle U_n \rangle = \{(1 - \eta)(1 - F)/(1 - \eta F)\} nq [1 + O(q)]$  uniformly in  $n$ , and hence

$$\langle n \rangle \simeq \left( (1 - F)^{-1} + \frac{\eta}{1 - \eta} \right) \frac{1}{q} \tag{3.9}$$

Thus we have calculated the leading term of  $\langle n \rangle$  for transient random walks. To go further we need to know more about the joint probability distribution of  $\{V_n^{(k)}\}_{k \geq 1}$ . To begin with, we need to know  $\text{Var } U_n$  to leading order in  $q$  and  $n$ . This requires a calculation of the leading term in  $n$  of  $\text{Cov}(V_n^{(k)}, V_n^{(k')}) := \langle V_n^{(k)} V_n^{(k')} \rangle - \langle V_n^{(k)} \rangle \langle V_n^{(k')} \rangle$  for all  $k, k' \geq 1$ . To evaluate  $\langle n \rangle$  we must also extend the expansion of  $\langle U_n \rangle$  beyond the term of leading order in  $q$  and  $n$ . If we combine the first two terms in the cumulant expansion of  $\log f_n$  we have, using Eqs. (3.3a, b),

$$\langle U_n \rangle - \frac{1}{2} \text{Var } U_n \simeq \phi(n)q - \frac{1}{2} \psi(n)q^2, \quad q \rightarrow 0 \tag{3.10}$$

with

$$\phi(n) := \sum_k (1 - \eta^k) \langle V_n^{(k)} \rangle \tag{3.10a}$$

$$\psi(n) := - \sum_k (1 - \eta^k)^2 \langle V_n^{(k)} \rangle + \sum_{k, k'} (1 - \eta^k)(1 - \eta^{k'}) \text{Cov}(V_n^{(k)}, V_n^{(k')}) \tag{3.10b}$$

From Eq. (3.2) it follows that

$$\sum_{n=0}^{\infty} z^n \phi(n) = 1/(1-z)^2 \left[ G(0; z) + \frac{\eta}{1-\eta} \right] \tag{3.11}$$

and with Darboux’s theorem we can easily deduce from this equation an expansion for  $\phi(n)$ . It is much harder to find  $\psi(n)$ . In Appendix C we calculate  $\psi(n)$  to leading order in  $n$  for random walks with  $d \geq 3$  and for strongly transient random walks in  $d = 1$  and 2. It is the work of Jain *et al.*<sup>(26–31)</sup> that has inspired this calculation.

For *strongly transient* random walks we find

$$\phi(n) = v_0^{-1}n + (v_0^{-1} + u_2v_0^{-2}) + o(1) \tag{3.12a}$$

$$\psi(n) \simeq \left[ -v_0^{-2} \left( \frac{1 + \eta F}{1 - \eta F} \right) + 2a \right] n \tag{3.12b}$$

with

$$v_0 := u_0 + \eta/(1 - \eta) \tag{3.13a}$$

$$a := \sum_{l \neq 0} \frac{G^2(l; 1) G(-l; 1) \left\{ \left[ G(0; 1) + \frac{\eta}{1-\eta} \right] - G(-l; 1) \right\}}{\left[ G(0; 1) + \frac{\eta}{1-\eta} \right]^3 \left\{ \left[ G(0; 1) + \frac{\eta}{1-\eta} \right]^2 - G(l; 1)G(-l; 1) \right\}} \tag{3.13b}$$

This leads to the expansion

$$\langle n \rangle = \frac{v_0}{q} - \left\{ 1 + u_2v_0^{-1} - v_0^2a + \frac{\eta F}{1 - \eta F} \right\} + \dots \tag{3.14}$$

which generalizes Eq. (2.23b). For random walks with  $\mu = 0$  and  $m_3 < \infty$  in  $d = 3$  and 4 we find

$$\phi(n) = \begin{cases} v_0^{-1}n + 2\pi^{-1/2}u_1v_0^{-2}n^{1/2} + o(\log n), & d = 3 \\ v_0^{-1}n + u_1v_0^{-2} \log n + \{v_0^{-1} + (\gamma u_1 - u_2)v_0^{-2}\} + o(1/n^{1/2}), & d = 4 \end{cases} \tag{3.15a}$$

$$\tag{3.15b}$$

$$\psi(n) \simeq \begin{cases} (1/2\pi^2v_0^4C^2)n \log n, & d = 3 \\ \left[ -v_0^{-2} \left( \frac{1 + \eta F}{1 - \eta F} \right) + 2a \right] n, & d = 4 \end{cases} \tag{3.16a}$$

$$\tag{3.16b}$$

and we arrive at

$$\langle n \rangle = \frac{v_0}{q} - u_1 v_0^{-1} \left( \frac{v_0}{q} \right)^{1/2} + \frac{1}{2} u_1^2 v_0^{-2} \log \left( \frac{v_0}{q} \right) + \dots, \quad d = 3 \quad (3.17a)$$

$$\langle n \rangle = \frac{v_0}{q} - u_1 v_0^{-1} \log \left( \frac{v_0}{q} \right) - \left\{ 1 + (u_1 - u_2) v_0^{-1} - v_0^2 a + \frac{\eta F}{1 - \eta F} \right\} + \dots, \quad d = 4 \quad (3.17b)$$

thus generalizing Eqs. (2.19) and (2.23a). For random walks in  $d = 3$  and 4 with  $m_3 = \infty$  similar expansions can be obtained if the behavior of  $G(0; z)$  for  $z \rightarrow 1$  is known.

In Appendix C we further show that in *all* the cases considered above  $\text{Var } U_n \sim \text{Var } S_n$  for all  $0 < q < 1$  and  $0 \leq \eta < 1$ . This implies that the higher powers of  $q$  in  $\langle U_n \rangle - \frac{1}{2} \text{Var } U_n$  each carry a coefficient that is  $O(\text{Var } S_n)$ , so that their contribution to  $\langle n \rangle$  is  $o(1)$ . Finally, in Appendix D we prove that in all these cases  $\langle (U_n - \langle U_n \rangle)^4 \rangle = O(\text{Var}^2 U_n)$  (with a proviso for strongly transient random walks in  $d = 1$  and 2 with  $G''(0; 1) = \infty$ ). This in turn implies that  $U_n$  satisfies an equation similar to Eq. (2.10) and ensures that the higher cumulants of  $U_n$  also contribute only in higher order. Thus Eqs. (3.14) and (3.17a, b) are exact.

The generalization of Section 2 is now nearly complete and it remains to consider *recurrent* random walks. When  $d = 2$ ,  $\mu = 0$  and  $m_2 < \infty$  it follows from Eqs. (2.13) and (3.2) that for *fixed*  $k$

$$\langle V_n^{(k)} \rangle = n/u_1^2 \log^2 un + O(n/\log^3 n) \quad (3.18)$$

with the leading term independent (!) of  $k$ . By Eqs. (3.3a, b)  $\langle U_n \rangle = \phi(n) q [1 + O(q)]$  uniformly in  $n$ , with  $\phi(n)$  given by Eq. (3.10a), and it follows from Eqs. (2.13) (provided  $m_3 < \infty$ ) and (3.11) that

$$\phi(n) = \frac{n}{u_1 \log un} + \left( 1 - \gamma - \frac{1}{u_1} \frac{\eta}{1 - \eta} \right) \frac{n}{u_1 \log^2 un} + O(n/\log^3 n) \quad (3.19)$$

[see also Eq. (2.15)]. After some algebra we find

$$\begin{aligned} \langle n \rangle &= \frac{u_1}{q} \left[ \log \left( \frac{u_1 u}{q} \right) + \log \log \left( \frac{u_1 u}{q} \right) + \frac{\log \log (u_1 u/q)}{\log (u_1 u/q)} + \dots \right] \\ &+ \frac{\eta}{1 - \eta} \frac{1}{q} + \dots \end{aligned} \quad (3.20)$$

which generalizes Eq. (2.16). If also in this case  $\text{Var } U_n \sim \text{Var } S_n$  for all  $0 < q < 1$  and  $0 \leq \eta < 1$ , then it is clear that the contribution to  $\langle n \rangle$  coming



from  $\text{Var } U_n$  is  $O(1/q \log q)$  because  $\text{Var } S_n \sim n^2/\log^4 n$ . We expect that it is possible to prove  $\text{Var } U_n \sim \text{Var } S_n$  along the lines of Ref. 29 with the use of the analysis given in Appendix C. Unfortunately, even if this were known to hold still more information would be needed to exclude a contribution from the higher cumulants of  $U_n$  of the order of the terms calculated. Thus, whether or not Eq. (3.20) is exact is an open question. Observe that  $\langle n \rangle - \langle n \rangle_{\eta=0} \simeq \eta/(1-\eta)q$ , as for transient random walks [Eq. (3.9)].

For all other recurrent random walks with  $d = 2$  the above argument carries through. The average  $\phi(n)$  behaves differently from Eq. (3.19) and  $\langle n \rangle$  has a leading term of higher order in  $q$  than  $q^{-1} \log q$ , but to leading order in  $n$ ,  $\langle V_n^{(k)} \rangle$  is independent of  $k$  [because in Eq. (3.2)  $G(0; z) \rightarrow \infty$  as  $z \rightarrow 1$ ] and one finds that  $\langle n \rangle - \langle n \rangle_{\eta=0} \simeq \eta/(1-\eta)q$  in all cases.

For recurrent random walks in  $d = 1$  very little can be said in general. Examples are easily found for which  $\langle n \rangle - \langle n \rangle_{\eta=0} \simeq \eta/(1-\eta)q$  does not hold. For example, for the simple random walk the average length of the first "run," starting with the first and ending with the second visit to a trap, is  $\frac{3}{2}q^{-1} - \frac{1}{2} \simeq \frac{3}{2}q^{-1}$  and not  $q^{-1}$ .

Before we conclude this section we briefly discuss a further extension of our model, viz. to the case of *different* types of imperfect traps. Suppose that each lattice point can be in either of  $t + 1$  different states. With probability  $1 - q$  it is a nontrapping point and with probability  $p_i q$ ,  $i = 1, \dots, t$ , it is a trap with "escape" parameter  $0 \leq \eta_i < 1$ . The states of different lattice points are again independent. The set  $\{p_i\}_{i=1}^t$  may be any set of probabilities with  $\sum_i p_i = 1$ . This defines a random distribution of  $t$  different types of imperfect traps.

A little reflection shows that Eq. (3.1) generalizes to

$$f_n = \left\langle \prod_{k=1}^{n+1} \left[ 1 - q + \left( \sum_{i=1}^t p_i \eta_i^k \right) q \right]^{V_n^{(k)}} \right\rangle, \quad n \geq 0 \tag{3.21}$$

It is clear that this extension introduces no additional complications as it involves only a change in parameters. Therefore we can follow the same lines of reasoning as in the case of a single type of imperfect trap. The stochastic variable of interest is now

$$U_n := \sum_{k=1}^{n+1} \lambda_k V_n^{(k)} \tag{3.22a}$$

with

$$\lambda_k := -\log \left[ 1 - q + \left( \sum_{i=1}^t p_i \eta_i^k \right) q \right] \tag{3.22b}$$

It is important to note that the inequalities (3.4) hold in this general case as well. They played an important role in the derivation of Eqs. (3.5) and (3.9). We list the main results without derivation.

For *transient* random walks

$$\langle n \rangle \simeq v_0/q, \quad q \rightarrow 0 \tag{3.23}$$

with

$$v_0^{-1} := \sum_i p_i [u_0 + n_i/(1 - \eta_i)]^{-1} \tag{3.24a}$$

The correction terms follow again from Eq. (3.10). The generalization of  $\phi(n)$  is easy. Writing  $\phi(n; \eta)$ , to display the dependence on  $\eta$  in Eq. (3.10a), we see from Eqs. (3.22a, b) that  $\phi(n; \eta)$  generalizes to  $\sum_i p_i \phi(n; \eta_i)$ . Thus, in Eqs. (3.12a) and (3.15a, b)  $v_0^{-1}$  is replaced by that given in Eq. (3.24a) and  $v_0^{-2}$  by

$$w_0^{-2} := \sum_i p_i [u_0 + n_i/(1 - \eta_i)]^{-2} \tag{3.24b}$$

leading to a replacement of  $u_1 v_0^{-1}$  by  $u_1 v_0 w_0^{-2}$  in the two second terms in Eqs. (3.17a, b). Furthermore, in Eq. (3.20)  $\eta/(1 - \eta)$  is replaced by  $\sum_i p_i \eta_i/(1 - \eta_i)$  and the first three terms are unaffected. The generalization of  $\psi(n)$  in Eq. (3.10) is not so easy. To find it one has to repeat a large part of the calculation given in Appendix C starting from Eqs. (3.22a, b). In particular, the generalization of Eq. (3.13b) is somewhat complicated.

#### 4. DISCUSSION

First we discuss Section 2 which treated the case of perfect traps. In the cumulant expansion of  $\log f_n$  [Eqs. (2.8a, b)] we have neglected the higher cumulants of  $S_n$  as well as certain higher-order terms in the expansion of  $\langle S_n \rangle$  and  $\text{Var } S_n$ . To the sum  $\langle n \rangle = \sum_n f_n$ , however, these neglected terms turn out to give additive corrections that are of higher order in  $q$  than the terms calculated. It is for this reason that Eqs. (2.8a, b) are well suited to find  $\langle n \rangle$  for small  $q$ . On the other hand, to the individual  $f_n$  the neglected terms give multiplicative corrections and therefore Eqs. (2.8a, b) are *not* suited to find  $f_n$  for large  $n$ . What is worse, for any  $q > 0$ , no matter how small, the terms in Eq. (2.8b) blow up as  $n \rightarrow \infty$ .

In this connection it is worth mentioning a strong result on the asymptotic behavior of  $f_n$  for  $n \rightarrow \infty$  found by Donsker and Varadhan<sup>(25)</sup> (see also Refs. 52–55). They proved that for aperiodic random walks, either with the property that  $1 - \hat{p}(\theta) \simeq A(e_\theta) |\theta|^\alpha$ ,  $\theta \rightarrow 0$ , where  $e_\theta := \theta/|\theta|$ ,  $A$  is a strictly positive, bounded function,  $A(e_\theta) = A(-e_\theta)$  and  $0 < \alpha < 2$ , or with the property  $\mu = 0$  and  $m_2 < \infty$  (in which case  $\alpha = 2$ ), the following holds for all  $\lambda > 0$ :

$$\lim_{n \rightarrow \infty} n^{-d/(d+\alpha)} \log f_n = -\lambda^{\alpha/(d+\alpha)} \left( \frac{d+\alpha}{\alpha} \right) \left( \frac{\alpha\beta}{d} \right)^{d/(d+\alpha)} \tag{4.1}$$

where  $\beta > 0$  is a specified function of  $p$ . The derivation of this result is truly impressive and rather complex. There is no obvious connection between Eqs. (2.8a, b) and (4.1). These relate to two different regimes, one with  $n$  fixed and  $q \rightarrow 0$ , the other with  $n \rightarrow \infty$  and  $q$  fixed, in which the behavior of  $f_n$  as a function of  $n$  is very different. From Eqs. (2.8a, b) one finds the behavior of  $f_n$  for small  $n$  and  $q$  fixed. Since this determines  $\sum_n f_n$  for small  $q$ , Eqs. (2.8a, b) served well as a starting point. Equation (4.1) gives only the tail of  $f_n$ . Thus it should be clear that one learns little from Eq. (4.1) about the asymptotic behavior of  $\langle n \rangle$  for  $q \rightarrow 0$ . Equation (4.1) does, however, imply that  $\langle n \rangle$  and all the higher moments of  $n$  are finite for all  $q > 0$ , a fact which we did not establish independently. It seems rather hard to find a suitable upper bound for  $f_n$  to prove that  $\langle n \rangle < \infty$  for an *arbitrary* nondegenerate random walk. This in contrast to the lower bound  $f_n \geq (1 - q)^{\langle S_n \rangle}$ , which follows from Eq. (2.1) and Jensen's inequality and which is the approximation to  $f_n$  originally used by Rosenstock.<sup>(14)</sup>

The asymptotic expansions found for  $\langle n \rangle$  are valid for small  $q$ . How large the domain of  $q$ -values is for which our results give a reasonable approximation to  $\langle n \rangle$  depends, of course, on the coefficients in the expansion. For the class of random walks with  $\mu = 0$  and  $m_2 < \infty$  the results are very accurate in most practical cases when  $d \geq 3$  and  $q \lesssim 0.05$ , the more so as  $d$  increases. For example, for the simple random walk and for  $q = 0.05$  the relative contributions to  $\langle n \rangle$  from the successive terms in the expansion are 1:0.14:0.03 for  $d = 3$ , 1:0.04:0.04 for  $d = 4$  and 1:0.06 for  $d = 5$ . For  $d = 2$  the situation is less favorable and the corresponding ratios are 1:0.35:0.09:0.15. In most cases the expansion for  $d = 2$  is useful only if  $q \lesssim 10^{-3}$ .

It is interesting to compare Eq. (2.16) with the corresponding asymptotic expansion, derived by Montroll [see Ref. 56, Eq. (31)], for a *strictly periodic* distribution of traps (with  $N$ , the number of lattice points per trap, replaced by  $q^{-1}$ ), e.g., for the simple random walk. Except for the identical leading terms, the two expansions are different in structure. Moreover, even for values of  $q$  as small as  $q = 10^{-20}$  the  $\langle n \rangle$  is in the random case 10% larger than in the strictly periodic case, which is somewhat surprising.

For random walks with  $\mu \neq 0$  and  $m_2 < \infty$  Eq. (2.23b) holds regardless of the dimensionality and in most cases it is accurate when  $q \lesssim 0.05$ . For example, for the Bernoulli random walk in  $d = 1$  with  $p(1) = \gamma$ ,  $p(-1) = 1 - \gamma$  ( $\frac{1}{2} < \gamma \leq 1$ ) we have  $G(0; z) = 1/[1 - 4\gamma(1 - \gamma)z^2]^{1/2}$ ,  $G(l; 1) = G(0; 1)$  for  $l > 0$  and  $G(l; 1) = [(1 - \gamma)/\gamma]^{-l} G(0; 1)$  for  $l < 0$  (see Ref. 33, p. 8), so that  $u_0 = 1/(2\gamma - 1)$ ,  $u_2 = 4\gamma(1 - \gamma)/(2\gamma - 1)^3$  and  $a = 1 - \gamma$  and the ratio of the first two terms in Eq. (2.23b) is  $\gamma q/(2\gamma - 1)$ .

If we ask, not for  $\langle n \rangle$ , but for the average number  $\langle S \rangle$  of *distinct* lattice points visited by the walker before he is trapped, then the answer is very

simple. Indeed, consider a given infinite walk on the lattice without traps with the property that there is an *infinite* sequence of step numbers  $m_0 < m_1 < m_2 < \dots$  at which a new point is visited (such that visits to old points occur at intermediate steps). Let  $R_n = 1$  for  $n = m_0, m_1, m_2, \dots$ , and  $R_n = 0$  otherwise. Now, if this walk takes place on the lattice *with* traps, then the average under the random distribution of the number of *distinct* lattice points that it visits before running into a trap is  $S = 1 + \sum_{n=1}^{\infty} R_n (1-q)^{R_0 + R_1 + \dots + R_{n-1}}$ , where the 1 counts the origin. Obviously,  $m_0 = 0$  and  $S = 1 + R_{m_1}(1-q) + R_{m_2}(1-q)^{1+R_{m_1}} + \dots = 1 + (1-q) + (1-q)^2 + \dots = q^{-1}$ . This is true for any walk with the required property. But any nondegenerate random walk has this property with probability 1 (as  $S_n \rightarrow \infty$  with probability 1) and hence we have the simple result

$$\langle S \rangle = q^{-1} \quad (4.2)$$

Equation (4.2) can be shown to be related to the following asymptotic property, valid for all random walks except for recurrent random walks in  $d = 1$ :

$$\langle S_{\langle n \rangle} \rangle \simeq q^{-1} \quad (4.3)$$

Equation (4.3) follows from a combination of the asymptotic expansions for  $\langle S_n \rangle$  and  $\langle n \rangle$  given in Section 2. The connection with Eq. (4.2) comes essentially from Eqs. (2.5) and (2.6), although it is somewhat involved. Equation (4.3) is identical with a property first noted by Shuler, Silver, and Lindenberg<sup>(57)</sup> for a *strictly periodic* distribution of traps (with  $q = N^{-1}$ ). In the latter case, however, Eq. (4.2) does *not* hold and an explanation of Eq. (4.3) is far from obvious. Moreover, in this case Eq. (4.3) is less general in that it does not hold for all transient random walks in  $d = 1$ .

Next we discuss Section 3, where we considered the extension that is obtained by introducing a finite probability for the walker to remain untrapped when stepping on a trap. With this extension the model was found to be significantly harder, but we were able to generalize the results in nearly all the cases considered in Section 2. We further extended the analysis to different types of imperfect traps. In this connection it is noteworthy that Eq. (3.23) can also be derived starting from a simple approximation. The average number of steps that the walker makes between his  $i$ th and  $(i+1)$ th visit to a trap (given that these take place) is  $\simeq 1/q$ ,  $q \rightarrow 0$ , for all  $i \geq 1$ ; this follows from Eq. (3.9). If the walker "escapes" from a trap there is a probability  $\leq F$  that he returns to that trap before hitting another one. As  $q \rightarrow 0$  the probability of such a return tends to  $F$  and the approximation consists in assuming that the walker can never return to a trap other than through a sequence of such returns. By this approximation every new trap visited is with probability  $p_i$  one with escape parameter  $\eta_i$ , independent of

previous visits. This then enables one to derive Eq. (3.23) along the lines sketched in Section 4 of Ref. 58.

The approach followed in this paper to obtain the asymptotic expansion for  $\langle n \rangle$  is systematic and exact. More work would be needed to estimate the error involved in approximating  $\langle n \rangle$  by the terms derived, let alone to establish a possible convergence of the expansion. For this we do not yet have the means. For the case  $d = 2$  with  $\mu = 0$  and  $m_2 < \infty$  the product  $u_1 u$  in Eqs. (2.16) and (3.20) is a very small number when the random walk is highly anisotropic [see, e.g., Ref. 34, Eq. (II.22)] and for  $q \geq u_1 u$  the expansion does not make sense, indicating that convergence is not a trivial matter.

We conclude this paper with the following reflection. If one compares the results of Section 2 and 3 one is struck by a remarkable similarity. It appears that *nearly all* the terms in the expansions for  $\langle n \rangle$  found for imperfect traps can be obtained from the corresponding terms found for the perfect-trap case through a simple “recipe”: replace  $G(0; z)$  by  $G(0; z) + \eta/(1 - \eta)$  in the analysis of Section 2 and leave  $G(l; z)$  for  $l \neq 0$  untouched. In view of the way in which the parameter  $\eta$  comes into play in the analysis of Section 3, it is truly amazing that such a simple recipe exists [see in particular Eq. (3.13b)]. There are only two exceptions: in Eqs. (3.14) and (3.17b) an extra term  $-\eta F/(1 - \eta F)$  occurs that does not fit into this picture, indicating that the recipe is *not exact*. We checked Eq. (3.14) for the Bernoulli random walk in  $d = 1$ . Following the approach of Ref. 7 we calculated the exact average length of the first “run” (i.e., the subwalk between the first and the second visit to a trap) and found that  $\langle n_1 \rangle = q^{-1} + O(q)$ . This is correctly predicted by Eq. (3.14), where the term between braces has an expansion in powers of  $\eta$  in which for the Bernoulli random walk the power  $\eta$  happens to drop out.

If one tries to understand why the recipe nearly works but not quite, one runs into a somewhat unexpected problem. Not only is the recipe not exact, as it is formulated above it is *not even unambiguous*. The reason for this is simply that the functions  $G(l; z)$  for different values of  $l$  are related. As an example take the simple random walk. If, instead of  $u_0 = G(0; 1)$ , we would have used the equivalent expression  $u_0 = 1 + (2d)^{-1} \sum_{|l|=1} G(l; 1)$ , then our recipe obviously would have led to totally wrong answers. At first this objection may seem a bit pedantic, but a closer inspection reveals that it is a serious one and that until one manages to remove it there is little or no sense in trying to explain the situation. Still, the observed similarity is striking and there is no harm in trying to develop some feeling for it.

To that end consider once again the infinite lattice  $L$ . Suppose that we divide  $L$  into identical finite unit cells  $\tilde{L}$  and place identical imperfect traps at identical position  $l_i \in \tilde{L}$ ,  $i = 1, 2, \dots$ . This gives us a periodic trap

configuration on  $L$ . For the trapping problem it suffices to consider a single unit cell with periodic boundary conditions. Let the walker start from  $l_0 \in \tilde{L}$ , let  $T_{i;n}$  denote the probability that he is trapped by trap  $i$  at step  $n$  and let  $f_i(z) := \sum_{n=0}^{\infty} z^n T_{i;n}$ . A simple argument shows that

$$\sum_i \left[ G(l_j - l_i; z) + \frac{n}{1-\eta} \delta_{ji} \right] f_i(z) = G(l_j - l_0; z), \quad j = 1, 2, \dots \quad (4.4)$$

[see Ref. 58, Eq. (4.2)], where now  $G(l; z)$  is the Green's function for  $\tilde{L}$ . If we are not interested in the label of the trap at which the walk ends, we may sum  $f_i(z)$  over  $i$  to obtain  $\sum_i f_i(z) =: f(z)$  and the average number of steps until trapping, given that trapping occurs, then follows from

$$\langle n \rangle = f'(1)/f(1) \quad (4.5)$$

Equations (4.4) and (4.5) express the fact that for *any* arrangement of traps in  $\tilde{L}$  that does *not* include the starting point the recipe works in principle, at least in the form in which the equations appear here. If, however, the starting point is a trap it does *not* work. Yet, if we average over all possible starting points and use that  $\sum_{l \in \tilde{L}} G(l; z) = 1/(1-z)$ , then we may replace the right-hand side of Eq. (4.4) by  $1/N(1-z)$ , where  $N$  is the number of lattice points in  $\tilde{L}$ , and the recipe works again.

This example indicates a possible origin of the observed similarity and at the same time illustrates the limitations of the recipe. In the random trap model the unit cell is infinite and we have to average over all possible trap configurations, which makes the situation only more complicated. Apparently the recipe fails in this case (a failure which, incidentally, is not repaired if we exclude the origin from being a trap).

All in all, it appears that interesting, and possibly useful, connections lay hidden behind the relations derived.

## ACKNOWLEDGMENT

I am grateful to Professor P. W. Kasteleyn for his stimulating influence. Through discussions with him I have developed a deeper understanding of the problems dealt with in this paper.

## APPENDIX A

For strongly transient random walks  $G(0; z)$  behaves for  $z \rightarrow 1$  as given by Eq. (2.20b) with

$$u_0 = (2\pi)^{-d} \int_{-\pi}^{\pi} d\theta_1 \cdots \int_{-\pi}^{\pi} d\theta_d [1 - \hat{p}(\theta)]^{-1} \tag{A1}$$

$$u_0 + u_2 = (2\pi)^{-d} \int_{-\pi}^{\pi} d\theta_1 \cdots \int_{-\pi}^{\pi} d\theta_d [1 - \hat{p}(\theta)]^{-2} \tag{A2}$$

[see Eq. (2.4)]. For the simple random walk Montroll<sup>(34)</sup> has derived the asymptotic series (2.24) for  $u_0$ . We follow his approach and derive a similar series for  $u_0 + u_2$ . For the simple random walk  $\hat{p}(\theta) = d^{-1} \sum_{i=1}^d \cos \theta_i$ . Using the identity  $s^{-2} = \int_0^\infty dt te^{-st}$ , we can write Eq. (A2) as

$$u_0 + u_2 = \int_0^\infty dt te^{-t} [I_0(t/d)]^d \tag{A3}$$

where  $I_0(x) := \pi^{-1} \int_0^\pi d\theta \exp(x \cos \theta)$  is the modified Bessel function of order 0.<sup>(59)</sup> Substituting the expansion  $I_0(x) = \sum_{k=0}^\infty (\frac{1}{2}x)^k / (k!)^2$  we find

$$u_0 + u_2 = 1 + \frac{3}{2d} + \frac{15}{(2d)^2} + \frac{90}{(2d)^3} + \frac{630}{(2d)^4} + \frac{5005}{(2d)^5} + \dots \tag{A4}$$

Subtraction of Eq. (2.24) leads to Eq. (2.25).

As mentioned in the text, for all strongly transient random walks and for a large class of random walks with  $d \geq 3$   $\text{Var } S_n \simeq [F(1 - F) + 2a]n$ . From the expressions given in Refs. 26 (p. 375), 28 (p. 374), and 31 (p. 99) it appears that

$$a = \sum_{l \neq 0} \frac{(1 - F) F_l F_{-l} (1 - F_{-l})}{1 - F_l F_{-l}} F_l \tag{A5}$$

where  $F_l$  stands for the total probability that the walker reaches  $l$  from 0. The generating function for first passage in  $l$  is  $F(l; z) = [G(l; z) - \delta_{l0}] / G(0; z)$ .<sup>(34)</sup> Noting that  $F_l = F(l; 1)$  we get for  $a$  the expression given in Eq. (2.22).

For the simple random walk it is easy to find for  $a$  an asymptotic expression similar to Eq. (A4). Indeed, using Eq. (2.4) we may write

$$G(l; 1) = \int_0^\infty dt e^{-t} \prod_{i=1}^d I_{l_i}(t/d) \tag{A6}$$

where  $I_m(x) := \pi^{-1} \int_0^\pi d\theta \exp(x \cos \theta) \cos(m\theta)$ ,  $m \in \mathbb{Z}$ , is the modified Bessel function of order  $m$ , and if we substitute the expansion  $I_m(x) = (\frac{1}{2}x)^m \sum_{k=0}^\infty (\frac{1}{2}x)^k / k!(m+k)!$ ,  $m \geq 0$ , we can find an asymptotic series for  $G(l; 1)$  for any  $l$ . Doing so for a few lattice points close to 0 and noting that  $G(l; 1) = O[(1/2d)^{\sum_i |l_i|}]$  we readily find Eq. (2.26).

**APPENDIX B**

To study  $U_n$  it is convenient to write Eq. (3.3a) in the form

$$U_n = \sum_{k \geq 1} \mu_k \sum_{l \geq k} V_n^{(l)} \tag{B1}$$

with  $\mu_1 := \lambda_1$  and  $\mu_k := \lambda_k - \lambda_{k-1}$ ,  $k \geq 2$ . By Eq. (3.4)  $\mu_k \geq 0$  for all  $k$ . To prove Eq. (3.5) we introduce stochastic variables  $V_{mn}^{(k)} :=$  the number of distinct lattice points visited exactly  $k$  times *on* or *between* steps  $m$  and  $n$  ( $0 \leq m \leq n$ ), and put

$$W_{mn} := \sum_{k \geq 1} \mu_k \sum_{1 \leq l < k} V_{mn}^{(l)} \tag{B2}$$

By Eqs. (3.4), (B1), and (B2)  $U_n = \lambda S_n - W_{0n}$ .

The variables  $W_{mn}$  have the following properties: (i)  $W_{mn} \leq W_{mi} + W_{in}$  for all  $m < i < n$ , (ii) the process  $\{W_{mn}\}$  is strictly stationary (i.e., the joint probability distributions of the sets  $\{W_{mn}\}$  and  $\{W_{m+1 n+1}\}$  are identical), (iii)  $\langle W_{0n} \rangle$  is finite and  $\langle W_{0n} \rangle \geq -An$  for some constant  $A$  and all  $n$ . This is easily seen by inspection; (i) follows from the fact that for any  $k$  the sum  $\sum_{l < k} V_{mn}^{(l)}$  satisfies the inequality while  $\mu_k \geq 0$ , (ii) is an immediate consequence of the independence of the individual steps in a random walk, and (iii) is trivial because  $0 \leq \mu_k \leq \lambda < \infty$  and  $V_{mn}^{(k)} \geq 0$  for all  $k$ .

Stochastic variables that satisfy (i)–(iii) are said to form a subadditive process and by an ergodic theorem of Kingman<sup>(51)</sup> the (finite) limit

$$\lim_{n \rightarrow \infty} n^{-1} W_{0n} = \xi \tag{B3}$$

exists with probability 1 and in mean, and  $\langle \xi \rangle = \inf_{n \geq 1} n^{-1} \langle W_{0n} \rangle = \lim_{n \rightarrow \infty} n^{-1} \langle W_{0n} \rangle$ . The last equality follows from (i), by which  $\langle W_{02n} \rangle \leq 2 \langle W_{0n} \rangle$ .

To prove Eq. (3.5) it remains to show that  $\xi = \langle \xi \rangle$  with probability 1. From Eqs. (3.4) and (B2) one easily deduces that  $-\lambda i \leq W_{0n} - W_{in} \leq \lambda i$  for any  $0 < i \leq n$  and this implies that for a given  $i > 0$

$$\lim_{n \rightarrow \infty} n^{-1} W_{in} = \lim_{n \rightarrow \infty} n^{-1} W_{0n} \tag{B4}$$

Equation (B4) means that for any given  $i > 0$  the limit  $\xi$  depends on the walk only through the steps  $i + 1, i + 2, \dots$  and not through any of the previous steps (i.e.,  $\xi$  is a so-called “tail” event). Since the individual steps are independent it follows from Kolmogorov’s zero–one law (see Ref. 60, p. 102) that  $\xi$  is equal to a constant with probability 1 and hence  $\xi = \langle \xi \rangle$  with



probability 1, as asserted. Since  $U_n = \lambda S_n - W_{0n}$  and since it is known that  $\lim_{n \rightarrow \infty} n^{-1} S_n = \lim_{n \rightarrow \infty} n^{-1} \langle S_n \rangle (= 1 - F)$  with probability 1 (Ref. 33, p. 38), this proves Eq. (3.5).

**APPENDIX C**

In this Appendix we consider the following two classes of random walks: (I) random walks in  $d = 3$  with  $\sum_{l \in L} G^2(l; 1) G(-l; 1) = \infty$ ; (II) random walks with  $d \geq 3$  not in class I and strongly transient random walks in  $d = 1$  and  $2$  (for all random walks in this class  $\sum_{l \in L} G^2(l; 1) G(-l; 1) < \infty$ ).<sup>(26,28,31)</sup>

We calculate  $\text{Var } U_n$  to leading order in  $q$  and  $n$ . We further calculate the term of order  $q^2$  in  $\langle U_n \rangle$  and show that Eqs. (3.12b) and (3.16a, b) hold. Finally we show that  $\text{Var } U_n \sim \text{Var } S_n$  for all  $0 < q < 1$  and  $0 \leq \eta < 1$ . We assume that the random walk is aperiodic and that  $F > 0$ .

We start from Eq. (B1) and write

$$U_n = \sum_{k \geq 1} \mu_k S_n^{(k)} \tag{C1a}$$

$$\text{Var } U_n = \sum_{k, k' \geq 1} \mu_k \mu_{k'} \text{Cov}(S_n^{(k)}, S_n^{(k')}) \tag{C1b}$$

where  $S_n^{(k)}$  is the number of lattice points visited *at least*  $k$  times after  $n$  steps and  $\mu_k = \log(1 - q + \eta^{k-1}q) - \log(1 - q + \eta^kq)$ . Let  $l_n$  denote the position of the walker at step  $n$  and consider the following *indicator* stochastic variables:

$$\begin{aligned} Z_{i_1 \dots i_k} &:= I[l_{i_1} = \dots = l_{i_k}; l_{i_1} \neq l_\alpha, \alpha \in \{i_1 + 1, \dots, \infty\} \setminus \{i_2, \dots, i_k\}] \\ Z_{i_1 \dots i_k; n} &:= I[l_{i_1} = \dots = l_{i_k}; l_{i_1} \neq l_\alpha, \alpha \in \{i_1 + 1, \dots, n\} \setminus \{i_2, \dots, i_k\}] \\ W_{i_1 \dots i_k; n} &:= Z_{i_1 \dots i_k; n} - Z_{i_1 \dots i_k} \\ &:= I[l_{i_1} = \dots = l_{i_k}; l_{i_1} \neq l_\alpha, \alpha \in \{i_1 + 1, \dots, n\} \setminus \{i_2, \dots, i_k\}; \\ &\quad \exists \beta > n: l_{i_1} = l_\beta] \\ &k \geq 1, \quad 1 \leq i_1 < \dots < i_k, \quad n \geq i_k \end{aligned}$$

A little reflection shows that

$$S_n^{(k)} = \sum_{0 \leq i_1 < \dots < i_k \leq n} Z_{i_1 \dots i_k; n} \tag{C2}$$

(For  $k > n + 1$  the sum in the right-hand side is empty.) We split  $S_n^{(k)}$  into two parts:

$$S_n^{(k)} = Y_n^{(k)} + W_n^{(k)} \tag{C3}$$

with

$$Y_n^{(k)} := \sum_{0 \leq i_1 < \dots < i_k \leq n} Z_{i_1 \dots i_k} \tag{C3a}$$

$$W_n^{(k)} := \sum_{0 \leq i_1 < \dots < i_k \leq n} W_{i_1 \dots i_k; n} \tag{C3b}$$

and further split  $Y_n^{(k)}$ , writing

$$Y_n^{(k)} = X_n^{(k)} - \sum_{l=1}^{k-1} \sum_{0 \leq i_1 < \dots < i_l \leq n < i_{l+1} < \dots < i_k < \infty} Z_{i_1 \dots i_l i_{l+1} \dots i_k} \tag{C4}$$

with

$$X_n^{(k)} := \sum_{0 \leq i \leq n} Z_i^{(k)} \tag{C5}$$

where for fixed  $i$

$$\begin{aligned} Z_i^{(k)} &:= \sum_{i < i_2 < \dots < i_k < \infty} Z_{ii_2 \dots i_k} \\ &= I[\text{after step } i \text{ the walker returns to } i \text{ exactly } k - 1 \text{ times}] \end{aligned} \tag{C5a}$$

The reason for choosing to split  $S_n^{(k)}$  in this way lies in the two inequalities

$$W_n^{(k+1)} \leq W_n^{(k)} \tag{C6a}$$

$$X_n^{(k)} - Y_n^{(k)} \leq \sum_{l=1}^{k-1} W_n^{(l)} \tag{C6b}$$

which, as we shall see in a moment, play a key role in the calculations. Equation (C6a) is not much deeper than the obvious inequality  $S_n^{(k+1)} \leq S_n^{(k)}$ . To see that it holds, write  $W_{i_1 i_2 \dots i_{k+1}; n} = Z_{i_1 i_2; i_2} W_{i_2 \dots i_{k+1}; n}$ , substitute this product into Eq. (C3b) and use  $\sum_{i_1=0}^{i_2-1} Z_{i_1 i_2; i_2} \leq 1$ . To see that Eq. (C6b) holds, use  $\sum_{n < i_{l+1} < \dots < i_k < \infty} Z_{i_1 \dots i_l i_{l+1} \dots i_k} \leq W_{i_1 \dots i_l; n}$ .

In the following we shall calculate  $\text{Cov}(X_n^{(k)}, X_n^{(k')})$  to leading order in  $n$ . We shall show that  $\text{Cov}(X_n^{(k)}, X_n^{(k')})$  for all pairs  $k, k'$  and the two sums  $(\sum_k \mu_k \text{Var}^{1/2} X_n^{(k)})^2$  and  $\sum_{k, k'} \mu_k \mu_{k'} \text{Cov}(X_n^{(k)}, X_n^{(k')})$  for all  $0 < q < 1$  and  $0 \leq \eta < 1$  are all of the same order in  $n$  and have the property that they grow faster than  $n$  in class I and proportional to  $n$  in class II. This will be seen to imply that in both classes

$$\text{Cov}(S_n^{(k)}, S_n^{(k')}) \simeq \text{Cov}(X_n^{(k)}, X_n^{(k')}) \tag{C7a}$$

$$\sum_k \mu_k \text{Var}^{1/2} S_n^{(k)} \simeq \sum_k \mu_k \text{Var}^{1/2} X_n^{(k)} \tag{C7b}$$

and, with Eq. (C1b),

$$\text{Var } U_n \simeq \sum_{k,k'} \mu_k \mu'_k \text{Cov}(X_n^{(k)}, X_n^{(k')}) \tag{C7c}$$

Our calculation will thus provide us with the leading order behavior in  $n$  of  $\text{Var } U_n$  and also make it evident that  $\text{Var } U_n \sim \text{Var } S_n (= \text{Var } S_n^{(1)})$  and  $\sum_k \mu_k \text{Var}^{1/2} S_n^{(k)} \sim \text{Var}^{1/2} S_n$ . We shall need the latter two relations in Appendix D. To prove Eqs. (C7a, b) we use Eqs. (C6a, b) and a bound obtained for  $\langle W_n^{(1)2} \rangle$ . In Refs. 29 (p. 376) and 32 (p. 97) it is shown that in class I  $\langle W_n^{(1)2} \rangle = O(n)$ , while in class II  $\langle W_n^{(1)2} \rangle = o(n)$ . This means that in both classes  $\langle W_n^{(1)2} \rangle = o(\text{Cov}(X_n^{(k)}, X_n^{(k')}))$  for any pair  $k, k'$  and similarly for the two sums in the right-hand side of Eqs. (C7b, c). Equation (C7a) follows in two steps. First, by Eqs. (C6a, b)  $\text{Var}(X_n^{(k)} - Y_n^{(k)}) \leq (k-1)^2 \langle W_n^{(1)2} \rangle$ , and together with the Schwarz inequality this implies that  $\text{Cov}(Y_n^{(k)}, Y_n^{(k')}) \simeq \text{Cov}(X_n^{(k)}, X_n^{(k')})$ . Second, by Eq. (C6a)  $\text{Var}(S_n^{(k)} - Y_n^{(k)}) \leq \langle W_n^{(1)2} \rangle$  and hence  $\text{Cov}(S_n^{(k)}, S_n^{(k')}) \simeq \text{Cov}(Y_n^{(k)}, Y_n^{(k')})$ , leading to Eq. (C7a). Equations (C7b, c) do *not* follow straight from Eq. (C7a). They follow from a similar argument plus the fact that  $\sum_k (k-1)\mu_k < \infty$  for all  $0 < q < 1$  and  $0 \leq \eta < 1$ .

Equation (C7c) is important because the right-hand side is easier to evaluate than the left-hand side. From now on we shall concentrate on the calculation of this right-hand side.

By Equation (C5)

$$\text{Cov}(X_n^{(k)}, X_n^{(k')}) = \sum_{i=0}^n \text{Cov}(Z_i^{(k)}, Z_i^{(k')}) + \sum_{j=1}^n (a_j^{(k,k')} + a_j^{(k',k)}) \tag{C8}$$

with

$$a_j^{(k,k')} := \sum_{i=0}^{j-1} \text{Cov}(Z_i^{(k)}, Z_j^{(k')}) \tag{C8a}$$

The first sum in Eq. (C8) is easy. Indeed, for  $k \neq k'$  we have  $\langle Z_i^{(k)} Z_i^{(k')} \rangle = 0$ , by Eq. (C5a), and thus  $\text{Cov}(Z_i^{(k)}, Z_i^{(k')}) = -\langle Z_i^{(k)} \rangle \langle Z_i^{(k')} \rangle$ . Furthermore,  $\text{Cov}(Z_i^{(k)}, Z_i^{(k)}) = \text{Var } Z_i^{(k)} = \langle Z_i^{(k)} \rangle - \langle Z_i^{(k)} \rangle^2$ . Since  $\langle Z_i^{(k)} \rangle = \langle Z_0^{(k)} \rangle = F^{k-1}(1-F)$  this gives us

$$\sum_{i=0}^n \text{Cov}(Z_i^{(k)}, Z_i^{(k')}) = [F^{k-1}(1-F) \delta_{kk'} - F^{k-1} F^{k'-1} (1-F)^2](n+1) \tag{C9}$$

To write out the second sum in Eq. (C8) we define

$T_l^{(k)}$  := the number of the step at which the walker visits  $l$  for the  $k$ th time;

$P_n^{(k)}(l)$  := the probability that the walker returns to 0 exactly  $k-1$  times during steps 1, ...,  $n$  and visits  $l$  at step  $n$ .

In Eq. (C8a)  $\text{Cov}(Z_i^{(k)}, Z_j^{(k')}) = \text{Cov}(Z_0^{(k)}, Z_{j-i}^{(k')})$ ,  $j > i$ , and we write out

$$a_j^{(k,k')} = \sum_{l=0}^{j-1} \sum_{m=0}^{k-1} P_{j-i}^{(m+1)}(l) b_l^{(k-m,k')} \tag{C10}$$

with

$$b_l^{(k,k')} := P_l[T_0^{(k-1)} < \infty, T_0^{(k)} = \infty, T_l^{(k'-1)} < \infty, T_l^{(k')} = \infty] \\ - P_l[T_0^{(k-1)} < \infty, T_0^{(k)} = \infty] P_l[T_l^{(k'-1)} < \infty, T_l^{(k')} = \infty] \tag{C11}$$

where  $P_l$  stands for probability with respect to the random walk starting in  $l$ . In Eq. (C10) we sum over the position  $l = l_{j-i}$  of the walker at step  $j - i$ . If  $Z_0^{(k)} = 1$  the walker returns to 0 exactly  $k - 1$  times. Of these returns  $m = 0, \dots, k - 1$  may take place during the first  $j - i$  steps. If  $Z_{j-i}^{(k')} = 1$  the walker returns to  $l$  exactly  $k' - 1$  times after step  $j - i$ .

To find the probability  $P_n^{(m+1)}(l)$  it is convenient to introduce the generating function

$$P^{(m+1)}(l; z) := \sum_{n=0}^{\infty} z^n P_n^{(m+1)}(l) \tag{C12}$$

First we take  $l = 0$ .  $P_n^{(m+1)}(0)$  is the probability that the walker returns to 0 for the  $m$ th time at step  $n$ . A standard type of argument shows that therefore

$$P^{(m+1)}(0; z) = F^m(0; z), \quad m \geq 1 \tag{C13a}$$

and  $P^{(1)}(0; z) = 0$ , where  $F(0; z)$  is the generating function for first return to 0. For  $l \neq 0$ , on the other hand,  $P_n^{(m+1)}(l)$  is the probability that the walker returns to 0 for the  $m$ th time at some step  $n' < n$  and in the remaining  $n - n'$  steps walks from 0 to  $l$  *without* returning to 0, arriving in  $l$  at step  $n$  and possibly visiting  $l$  at some earlier step. Now it is easily recognized that the probability for the latter event is equal to the probability that the walker after the remaining  $n - n'$  steps reaches  $l$  for the *first* time with *returns* to 0 *allowed*. Therefore we have

$$P^{(m+1)}(l; z) = F^m(0; z) F(l; z), \quad l \neq 0 \tag{C13b}$$

where  $F(l; z)$  is the generating function for first passage in  $l$ .

Before we come to  $b_l^{(k,k')}$  in Eqs. (C10) and (C11) we return to Eq. (C1b). Our first aim is to find the term of leading order in  $q$  and  $n$  of  $\text{Var } U_n$ . Noting that  $\mu_k \simeq (1 - \eta)\eta^{k-1}q$ ,  $q \rightarrow 0$ , we have

$$\text{Var } U_n \simeq \phi_n q^2, \quad q \rightarrow 0 \tag{C14}$$

with

$$\begin{aligned} \phi_n &:= (1 - \eta)^2 \sum_{k, k' \geq 1} \eta^{k-1} \eta^{k'-1} \text{Cov}(S_n^{(k)}, S_n^{(k')}) \\ &\simeq (1 - \eta)^2 \sum_{k, k' \geq 1} \eta^{k-1} \eta^{k'-1} \text{Cov}(X_n^{(k)}, X_n^{(k')}) =: \phi'_n \end{aligned} \tag{C15}$$

where we use Eq. (C7c). We shall calculate  $\phi'_n$ . From Eqs. (C8)–(C10) it follows that the generating function

$$\phi'(z) := \sum_{n=0}^{\infty} z^n \phi'_n \tag{C16}$$

is given by

$$\begin{aligned} \phi'(z) &= \frac{(1 - \eta)^4 F(1 - F)}{(1 - \eta F)^2 (1 - \eta^2 F)} (1 - z)^{-2} \\ &\quad + 2(1 - \eta)^2 (1 - z)^{-2} \sum_l \left( \sum_{m=0}^{\infty} \eta^m P^{(m+1)}(l; z) \right) \left( \sum_{k, k' \geq 1} \eta^{k-1} \eta^{k'-1} b_l^{(k, k')} \right) \end{aligned} \tag{C17}$$

The term with  $l=0$  in Eq. (C17) is easy. Indeed, by Eq. (C11)  $b_0^{(k, k')} = F^{k-1}(1 - F)\delta_{kk'} - F^{k-1}F^{k'-1}(1 - F)^2$  and using Eq. (C13a) we find that this term equals  $2\eta F(0; z)/(1 - \eta F(0; z))$  times the first term in Eq. (C17). We may therefore write

$$\phi'(z) = \frac{(1 - \eta)^4 F(1 - F)}{(1 - \eta F)^2 (1 - \eta^2 F)} (1 - z)^{-2} \frac{1 + \eta F(0; z)}{1 - \eta F(0; z)} + 2\phi''(z) \tag{C18}$$

with

$$\phi''(z) := (1 - \eta)^2 (1 - z)^{-2} \sum_{l \neq 0} \frac{F(l; z)}{1 - \eta F(0; z)} \left[ \sum_{k, k' \geq 1} \eta^{k-1} \eta^{k'-1} b_l^{(k, k')} \right] \tag{C18a}$$

where we use Eq. (C13b). It remains to find the double sum in Eq. (C18a). We shall need most of the rest of this appendix to calculate this sum.

Equation (C11) can be simplified a little bit. An easy calculation shows that

$$b_l^{(k, k')} = c_l^{(k, k')} - c_l^{(k-1, k')}, \quad k \geq 2, \quad b_l^{(1, k')} = c_l^{(1, k')} \tag{C19}$$

with

$$\begin{aligned} c_l^{(k, k')} &:= P_l[T_0^{(k)} < \infty] P_l[T_l^{(k'-1)} < \infty, T_l^{(k')} = \infty] \\ &\quad - P_l[T_0^{(k)} < \infty, T_l^{(k'-1)} < \infty, T_l^{(k')} = \infty] \end{aligned} \tag{C19a}$$

Similarly,

$$c_i^{(k,k')} = d_i^{(k,k')} - d_i^{(k,k'-1)}, \quad k' \geq 2, \quad c_i^{(k,1)} = d_i^{(k,1)} \quad (\text{C20})$$

with

$$d_i^{(k,k')} := P_l[T_0^{(k)} < \infty, T_l^{(k')} < \infty] - P_l[T_0^{(k)} < \infty] P_l[T_l^{(k')} < \infty] \quad (\text{C20a})$$

From Eqs. (C19) and (C20) we get

$$\sum_{k,k' \geq 1} \eta^{k-1} \eta^{k'-1} b_i^{(k,k')} = (1-\eta)^2 \sum_{k,k' \geq 1} \eta^{k-1} \eta^{k'-1} d_i^{(k,k')} \quad (\text{C21})$$

To evaluate the right-hand side we write

$$d_i^{(k,k')} = p_i^{(k,k')} + q_i^{(k,k')} - F_{-l} F^{k+k'-1} \quad (\text{C22})$$

where we introduce the probabilities

$$p_i^{(k,k')} := P_l[T_0^{(k)} < T_l^{(k')} < \infty] \quad (\text{C23a})$$

$$q_i^{(k,k')} := P_l[T_l^{(k')} < T_0^{(k)} < \infty] \quad (\text{C23b})$$

and where  $F_l := F(l; 1)$  is the total probability that the walker reaches  $l$  from 0. To find  $p_i^{(k,k')}$  and  $q_i^{(k,k')}$  we derive a set of recursion relations in  $k$  and  $k'$  valid for  $l \neq 0$ . Write

$$p_i^{(k,k')} = P_l[T_0^{(k)} < T_l^{(k'-1)} < T_l^{(k')} < \infty] \\ + P_l[T_l^{(k'-1)} < T_0^{(k)} < T_l^{(k')} < \infty] \quad (\text{C24})$$

The first term factorizes into  $P_l[T_0^{(k)} < T_l^{(k'-1)} < \infty] P_l[T_l^{(1)} < \infty]$  and is seen to be equal to  $F p_i^{(k,k'-1)}$ . The second term factorizes into  $P_l[T_l^{(k'-1)} < T_0^{(k)} < \infty, T_0^{(k)} < T_l^{(k')} < \infty] P_0[T_l^{(1)} < \infty]$ , of which the first factor can be written as  $q_i^{(k,k'-1)} - q_i^{(k,k')}$ . Together this gives

$$p_i^{(k,k')} = F p_i^{(k,k'-1)} + F_l [q_i^{(k,k'-1)} - q_i^{(k,k')}], \quad k' \geq 2 \quad (\text{C25a})$$

A similar reasoning shows that

$$q_i^{(k,k')} = F p_i^{(k-1,k')} + F_{-l} [p_i^{(k-1,k')} - p_i^{(k,k')}], \quad k \geq 2 \quad (\text{C25b})$$

To complete Eqs. (C25a, b) we also need to know  $p_i^{(k,1)}$ ,  $k \geq 1$ , and  $q_i^{(1,k')}$ ,  $k' \geq 1$ . These probabilities are easily calculated. Indeed,

$$p_i^{(k,1)} = P_l[T_0^{(k)} < T_l^{(1)} < \infty] \\ = P_l[T_0^{(1)} < T_l^{(1)}, T_0^{(1)} < \infty] \\ \times \{P_0[T_0^{(1)} < T_l^{(1)} < \infty]\}^{k-1} P_0[T_l^{(1)} < \infty] \\ = \{F_{-l} - q_l^{(1,1)}\} \{F - p_{-l}^{(1,1)}\}^{k-1} F_l, \quad k \geq 1 \quad (\text{C26a})$$

and similarly

$$q_l^{(1,k')} = \{F - p_l^{(1,1)}\}^{k'} F_{-l}, \quad k' \geq 1 \tag{C26b}$$

from which we deduce

$$p_l^{(k,1)} = p_l^{(1,1)} X_l^{k-1} \tag{C27a}$$

$$q_l^{(1,k')} = q_l^{(1,1)} X_l^{k'-1} \tag{C27b}$$

with

$$p_l^{(1,1)} = \frac{(1-F)F_l F_{-l}}{1-F_l F_{-l}} \tag{C28a}$$

$$q_l^{(1,1)} = \frac{F - F_l F_{-l}}{1 - F_l F_{-l}} F_{-l} \tag{C28b}$$

$$X_l := \frac{F - F_l F_{-l}}{1 - F_l F_{-l}} \tag{C28c}$$

From Eqs. (C25a, b) it follows that the two sums

$$P_l(\eta) := \sum_{k,k' \geq 1} \eta^{k-1} \eta^{k'-1} p_l^{(k,k')} \tag{C29a}$$

$$Q_l(\eta) := \sum_{k,k' \geq 1} \eta^{k-1} \eta^{k'-1} q_l^{(k,k')} \tag{C29b}$$

satisfy the set of equations

$$(1 - \eta F)P_l = I_l - (1 - \eta)F_l Q_l \tag{C30a}$$

$$(1 - \eta F)Q_l = J_l - (1 - \eta)F_{-l} P_l \tag{C30b}$$

with

$$I_l(\eta) := p_l^{(1,1)} / (1 - \eta X_l) + F_l \sum_{k=1}^{\infty} \eta^{k-1} q_l^{(k,1)} \tag{C31a}$$

$$J_l(\eta) := q_l^{(1,1)} / (1 - \eta X_l) + F_{-l} \sum_{k'=1}^{\infty} \eta^{k'-1} p_l^{(1,k')} \tag{C31b}$$

where Eqs. (C27a, b) are used. The two sums in Eqs. (C31a, b) can be found from Eqs. (C25b) and (C25a), respectively, with Eqs. (C27a, b) and (C28a, b, c). This leads to

$$I_l = F_l F_{-l} / (1 - \eta F) \tag{C32a}$$

$$J_l = F F_{-l} / (1 - \eta F) \tag{C32b}$$

Substituting this into Eqs. (C30a, b) we can solve  $P_l(\eta)$  and  $Q_l(\eta)$ , and from Eqs. (C21), (C22), and (C29) we then get

$$\sum_{k, k' \geq 1} \eta^{k-1} \eta^{k'-1} b_l^{(k, k')} = \frac{(1-\eta)^2(1-F)}{(1-\eta F)^3} F_l F_{-l} \left[ 1 - \left( \frac{1-\eta}{1-\eta F} \right) F_{-l} \right] \times \left[ 1 - \left( \frac{1-\eta}{1-\eta F} \right)^2 F_l F_{-l} \right]^{-1}, \quad l \neq 0 \quad (C33)$$

Using Eq. (C18a), noting that  $F(l; z) = [G(l; z) - \delta_{l0}]/G(0; z)$  <sup>(34)</sup> and writing  $G_l := G(l; 1)$  and  $(1-\eta F)/(1-\eta)(1-F) = G_0 + \eta/(1-\eta)$  we finally arrive at

$$\phi''(z) = (1-z)^{-2} \sum_{l \neq 0} \frac{G_l G_{-l} \{ [G_0 + \eta/(1-\eta)] - G_{-l} \}}{[G_0 + \eta/(1-\eta)]^2 \{ [G_0 + \eta/(1-\eta)]^2 - G_l G_{-l} \}} \times \frac{G(l; z)}{[G(0; z) + \eta/(1-\eta)]} \quad (C34)$$

Equations (C18) and (C34) are exact expressions from which the coefficients  $\phi'_n$  in Eq. (C16) can be deduced. We are now ready to use Eq. (C15) and find the leading order behavior in  $n$  of  $\phi_n$ . At this point we have to distinguish between the two classes of random walks I and II introduced earlier. Class II is the easiest one. Because in this class  $\sum_{l \in \mathbb{L}} G^2(l; 1) G(-l; 1) < \infty$  we deduce from Eq. (C34) that

$$\phi''(z) \simeq a(1-z)^{-2}, \quad z \rightarrow 1 \quad (C35)$$

with  $a$  given by Eq. (3.13b). Equation (C.35) implies that the coefficients of  $\phi''(z)$  have a leading order behavior in  $n$  that is  $an$ . With Eqs. (C14)–(C16) and (C18) this explains the term  $2an$  in Eqs. (3.12b) and (3.16b). The first term in each of these equations is a sum of two contributions. One comes from the first term in Eq. (C18), the other from the term of order  $q^2$  in the expansion of  $\langle U_n \rangle$ , which is

$$\frac{1}{2} \sum_{k \geq 1} (1-\eta^k)^2 \langle V_n^{(k)} \rangle \simeq \frac{1}{2} \frac{(1-\eta)^2(1-F)(1+\eta F)}{(1-\eta F)(1-\eta^2 F)} n$$

by Eq. (3.2) and Darboux’s theorem. The two contributions become transparent in their combination.

Class I is harder. In this class  $\sum_{l \in \mathbb{L}} G^2(l; 1) G(-l; 1) = \infty$  and  $(1-z)^2 \phi''(z) \rightarrow \infty$  as  $z \rightarrow 1$ . Since for transient random walks with  $d \geq 2$   $G(l; 1) \rightarrow 0, |l| \rightarrow \infty$  (Ref. 34, p. 281), we get from Eq. (C18)

$$\phi'(z) \simeq 2\phi''(z) \simeq 2 \left( G_0 + \frac{\eta}{1-\eta} \right)^{-4} (1-z)^{-2} \sum_{l \neq 0} G_l G_{-l} G(l; z), \quad z \rightarrow 1 \quad (C36)$$



For random walks with  $d = 3$ ,  $\mu = 0$  and  $m_2 < \infty$  it is shown in Ref. 29 (p. 379) that  $\sum_{l \neq 0} G_l G_{-l} G_l^j \simeq (2\pi C)^{-2} \log j$ ,  $j \rightarrow \infty$ , where  $G_l^j$  is the sum of the first  $j$  coefficients in the power series in  $z$  of  $G(l; z)$ . With Eqs. (C14)–(C16) and (C36) this explains Eq. (3.16a).

It remains to show what we used earlier to prove Eqs. (C7a, b, c), viz. that  $\text{Cov}(X_n^{(k)}, X_n^{(k')})$  for all  $k$  and  $k'$ , and the two sums  $(\sum_k \mu_k \text{Var}^{1/2} X_n^{(k)})^2$  and  $\sum_{k,k'} \mu_k \mu_{k'} \text{Cov}(X_n^{(k)}, X_n^{(k')})$  for all  $0 < q < 1$  and  $0 \leq \eta < 1$ , are all of the same order in  $n$  and have the property that they grow faster than  $n$  in class I and proportional to  $n$  in class II. This may be done as follows. We have calculated the sum  $\sum_{k,k'} \eta^{k-1} \eta^{k'-1} \text{Cov}(X_n^{(k)}, X_n^{(k')})$  and found that it has the mentioned property for all  $0 \leq \eta < 1$ . Now with the analysis given above it is not hard to calculate also the sums  $\sum_k z^{k-1} \text{Var}^{1/2} X_n^{(k)} =: \rho_n(z)$ ,  $0 \leq z < 1$ , and  $\sum_{k,k'} z_1^{k-1} z_2^{k'-1} \text{Cov}(X_n^{(k)}, X_n^{(k')}) =: \rho_n(z_1, z_2)$ ,  $0 \leq z_1, z_2 < 1$ . This is straightforward but tedious and is left to the reader. One finds that  $\rho_n^2(z)$  has the same asymptotic behavior in  $n$  for all  $z$  and so does  $\rho_n(z_1, z_2)$  for all  $z_1, z_2$ . Writing  $\sum_k \mu_k \text{Var}^{1/2} X_n^{(k)} = -\sum_{r \geq 1} (1/r) [-q/(1-q)]^r (1-\eta^r) \rho_n(\eta^r)$  and  $\sum_{k,k'} \mu_k \mu_{k'} \text{Cov}(X_n^{(k)}, X_n^{(k')}) = \sum_{r,r' \geq 1} (1/rr') [-q/(1-q)]^{r+r'} (1-\eta^r)(1-\eta^{r'}) \rho_n(\eta^r, \eta^{r'})$  and carrying out the summation over  $r$  one can then show that the two sums over  $k$  and  $k'$  have the required property, as asserted. (Note that by the Schwarz inequality  $(\sum_k \mu_k \text{Var}^{1/2} X_n^{(k)})^2 \geq \sum_{k,k'} \mu_k \mu_{k'} \text{Cov}(X_n^{(k)}, X_n^{(k')})$ .) From the result for  $\rho_n(z_1, z_2)$  one further easily deduces (cf. Ref. 37, p. 232) that also the individual  $\text{Cov}(X_n^{(k)}, X_n^{(k')})$  have this property. The attentive reader will observe that we do not really need Eq. (C7a). Nevertheless this equation stands at the basis of Eqs. (C7b, c), which we have used in the calculation of  $\text{Var} U_n$  and shall need in the next appendix.

**APPENDIX D**

The purpose of this appendix is to prove that

$$\langle (U_n - \langle U_n \rangle)^4 \rangle = O(\text{Var}^2 U_n), \quad \text{for all } 0 < q < 1 \text{ and } 0 \leq \eta < 1 \quad (D1)$$

for random walks in the classes I and II introduced in Appendix C, subject to the condition

$$\langle W_n^{(1)4} \rangle = O(\text{Var}^2 S_n) \quad (D2)$$

where  $W_n^{(1)}$  is defined in Eq. (C3b). In Ref. 32, Eq. (D2) is proved for both classes, with the exception of random walks with  $d = 1$  or  $2$  and  $G''(0; 1) = \infty$  (see Ref. 32, p. 117). For the latter subclass a proof of Eq. (D2) is not known.

Let

$$t_n := \sum_k \mu_k \langle (S_n^{(k)} - \langle S_n^{(k)} \rangle)^4 \rangle^{1/4} / \text{Var}^{1/2} S_n \tag{D3}$$

where  $\mu_k$  and  $S_n^{(k)}$  are defined below Eqs. (C1a, b). We shall show that  $t_n$  is bounded. By Minkowski's inequality we have  $\langle (x + y)^4 \rangle^{1/4} \leq \langle x^4 \rangle^{1/4} + \langle y^4 \rangle^{1/4}$  for any pair of stochastic variables  $x, y$  and hence by Eq. (C1a)  $\langle (U_n - \langle U_n \rangle)^4 \rangle^{1/4} \leq \sum_k \mu_k \langle (S_n^{(k)} - \langle S_n^{(k)} \rangle)^4 \rangle^{1/4}$ , so that

$$\langle (U_n - \langle U_n \rangle)^4 \rangle \leq t_n^4 \text{Var}^2 S_n$$

Since  $\text{Var} U_n \sim \text{Var} S_n$ , the boundedness of  $t_n$  will imply Eq. (D1).

We start from Eq. (C2) and write

$$\begin{aligned} S_{2n+1}^{(k)} &= \sum_{0 \leq i_1 < \dots < i_k \leq 2n+1} Z_{i_1 \dots i_k; 2n+1} \\ &= \sum_{0 \leq i_1 < \dots < i_k \leq n} Z_{i_1 \dots i_k; n} \\ &\quad + \sum_{n+1 \leq i_1 < \dots < i_k \leq 2n+1} Z_{i_1 \dots i_k; 2n+1} + R_n^{1(k)} - R_n^{2(k)} \end{aligned} \tag{D4}$$

with

$$R_n^{1(k)} := \sum_{l=1}^{k-1} \sum_{0 \leq i_1 < \dots < i_l \leq n < i_{l+1} < \dots < i_k \leq 2n+1} Z_{i_1 \dots i_l i_{l+1} \dots i_k; 2n+1} \tag{D4a}$$

$$R_n^{2(k)} := \sum_{0 \leq i_1 < \dots < i_k \leq n} (Z_{i_1 \dots i_k; n} - Z_{i_1 \dots i_k; 2n+1}) \tag{D4b}$$

Obviously,  $0 \leq \sum_{n < i_{l+1} < \dots < i_k \leq 2n+1} Z_{i_1 \dots i_l i_{l+1} \dots i_k; 2n+1} \leq W_{i_1 \dots i_l; n}$  and  $0 \leq Z_{i_1 \dots i_k; n} - Z_{i_1 \dots i_k; 2n+1} \leq W_{i_1 \dots i_k; n}$ , and thus with Eq. (C3b)

$$0 \leq R_n^{1(k)} \leq \sum_{l=1}^{k-1} W_n^{(l)} \tag{D5a}$$

$$0 \leq R_n^{2(k)} \leq W_n^{(k)} \tag{D5b}$$

The two sums in Eq. (D4) are independent and have the same distribution as  $S_n^{(k)}$ . Hence, subtracting averages, we get

$$\begin{aligned} \langle (S_{2n+1}^{(k)} - \langle S_{2n+1}^{(k)} \rangle)^4 \rangle^{1/4} &\leq [2 \langle (S_n^{(k)} - \langle S_n^{(k)} \rangle)^4 \rangle + 6 \text{Var}^2 S_n^{(k)}]^{1/4} \\ &\quad + 2 \sum_{l=1}^k \langle W_n^{(l)4} \rangle^{1/4} \end{aligned} \tag{D6}$$

where we use Eqs. (D5a, b) and repeatedly apply Minkowski's inequality. In Ref. 32 it is shown that both in class I and in class II  $n^{-1} \text{Var } S_n$  is asymptotically a monotone, nondecreasing and slowly varying function of  $n$ . Thus  $\text{Var } S_{2n+1} \simeq 2 \text{Var } S_n$  and it now follows from Eqs. (C6a), (D2), (D3), and (D6) that there is a constant  $M < \infty$  such that

$$t_{2n+1} \leq 2^{-1/8} t_n + M, \quad \text{for all } n \tag{D7}$$

where we use that  $\sum_k \mu_k \text{Var}^{1/2} S_n^{(k)} \sim \text{Var}^{1/2} S_n$  (which was shown in Appendix C) and that  $\sum_k k \mu_k < \infty$  for all  $0 < q < 1$  and  $0 \leq \eta < 1$ . [The number  $2^{-1/8}$  in Eq. (D7) may be replaced by any number  $> 2^{-1/4}$ ; it is chosen  $< 1$  to suit the proof.]

We follow the line of reasoning in Ref. 32 (p. 114). Now there is a  $\gamma < \infty$  so large that  $2^{-1/8} + (M/\gamma) \leq 1$ . Suppose that for some integer  $m$  we have  $t_m \geq \gamma$ . Then it follows from Eq. (D7) that  $(t_{2n+1}/t_m) \leq 2^{-1/8}(t_n/t_m) + (M/\gamma)$  for  $n \geq m$ . This implies that  $t_{2m+1} \leq t_m$  and it follows by induction that  $t_n \leq t_m$  for  $n$  in the subsequence of integers of the form  $n = 2^j(m+1) - 1 =: n_j, j \geq 0$ . Next, consider  $n_{j-1} < n < n_j$  for some  $j$ . Trivially,

$$\begin{aligned} \langle (S_n^{(k)} - \langle S_n^{(k)} \rangle)^4 \rangle^{1/4} &\leq [\langle (S_n^{(k)} - \langle S_n^{(k)} \rangle)^4 \rangle + \langle (S_{n_j-n-1}^{(k)} - \langle S_{n_j-n-1}^{(k)} \rangle)^4 \rangle \\ &\quad + 6 \text{Var } S_n^{(k)} \cdot \text{Var } S_{n_j-n-1}^{(k)}]^{1/4} \end{aligned}$$

and through an argument similar to that given above we find that there are constants  $N_1, N_2 < \infty$  such that

$$t_n \leq N_1 t_{n_j} + N_2, \quad \text{for all } j \tag{D8}$$

This proves the boundedness of  $t_n$  for all  $n$ , and hence Eq. (D1) subject to Eq. (D2), as asserted.

## REFERENCES

1. R. M. Pearlstein, in *Photosynthesis: Energy Conversion by Plants and Bacteria*, Vol. I (Academic Press, New York, 1982), p. 293.
2. H. Scher, S. Alexander, and E. W. Montroll, *Proc. Natl. Acad. Sci.* **77**:3758 (1980).
3. G. Pfister and H. Scher, *Adv. Phys.* **27**:747 (1978).
4. H. B. Rosenstock, *J. Soc. Indust. Appl. Math.* **9**:169 (1961).
5. E. W. Montroll and G. H. Weiss, *J. Math. Phys.* **6**:167 (1965).
6. M. Rudemo, *SIAM J. Appl. Math.* **14**:1293 (1966).
7. E. W. Montroll, *J. Phys. Soc. Japan Suppl.* **26**:6 (1969).
8. H. B. Rosenstock, *Phys. Rev.* **187**:1166 (1969).
9. H. B. Rosenstock, *J. Math. Phys.* **11**:487 (1970).
10. K. Lakatos-Lindenberg, R. P. Hemenger, and R. M. Pearlstein, *J. Chem. Phys.* **56**:4852 (1972).

11. R. P. Hemenger, R. M. Pearlstein, and K. Lakatos-Lindenberg, *J. Math. Phys.* **13**:1056 (1972).
12. H. B. Rosenstock, *SIAM J. Appl. Math.* **27**:457 (1974).
13. R. H. J. Fastenau, C. M. van Baal, P. Penning, and A. van Veen, *Phys. Stat. Sol.* **A52**:577 (1979).
14. H. B. Rosenstock, *J. Math. Phys.* **21**:1643 (1980).
15. G. H. Weiss, *Proc. Natl. Acad. Sci.* **77**:4391 (1980).
16. H. B. Rosenstock and J. P. Straley, *Phys. Rev. B* **24**:2540 (1981).
17. G. Zumofen and A. Blumen, *J. Chem. Phys.* **76**:3713 (1982).
18. A. Blumen and G. Zumofen, *J. Chem. Phys.* **77**:5127 (1982).
19. R. H. J. Fastenau, thesis, Delft (1982).
20. B. Movaghar, G. W. Sauer, and D. Würtz, *J. Stat. Phys.* **27**:473 (1982).
21. W. Th. F. den Hollander and P. W. Kasteleyn, *Physica* **117A**:179 (1983).
22. D. L. Huber, *J. Stat. Phys.* **30**:345 (1983).
23. P. W. Kasteleyn and W. Th. F. den Hollander, *J. Stat. Phys.* **30**:363 (1983).
24. A. Blumen and G. Zumofen, *J. Stat. Phys.* **30**:487 (1983).
25. M. D. Donsker and S. R. S. Varadhan, *Commun. Pure Appl. Math.* **32**:721 (1979).
26. N. C. Jain and S. Orey, *Isr. J. Math.* **6**:1373 (1968).
27. N. C. Jain and W. E. Pruitt, *Z. Wahrscheinlichkeitstheorie Verw. Gebiete* **16**:279 (1970).
28. N. C. Jain and W. E. Pruitt, *J. Analyse Math.* **24**:369 (1971).
29. N. C. Jain and W. E. Pruitt, in *Proceedings of the Sixth Berkeley Symposium*, (University of California Press, Berkeley, 1971), p. 31.
30. N. C. Jain and W. E. Pruitt, *Ann. Math. Statist.* **43**:1692 (1972).
31. N. C. Jain and W. E. Pruitt, *J. Analyse Math.* **27**:94 (1974).
32. R. van Grondelle and L. N. M. Duysens, *Plant Physiol.* **65**:751 (1980).
33. F. Spitzer, *Principles of Random Walk* (Van Nostrand, Princeton, 1964).
34. E. W. Montroll, *Proc. Symp. Appl. Math.* **16**:193 (1964).
35. S. C. Port, *J. Comb. Theory* **2**:107 (1967).
36. G. H. Weiss and R. J. Rubin, *Adv. Chem. Phys.* **52**:363 (1982).
37. W. Feller, *An Introduction to Probability Theory and Its Applications*, Vol. 1 (Wiley, New York, 1950).
38. A. Dvoretzky and P. Erdős, in *Proceedings of the Second Berkeley Symposium* (University of California Press, Berkeley, 1951), p. 353.
39. N. G. de Bruijn, *Asymptotic Methods in Analysis* (North-Holland, Amsterdam, 1961).
40. J. G. Darboux, *J. de Math.* **4**:1 (1878).
41. J. G. Darboux, *J. de Math.* **4**:377 (1878).
42. R. B. Dingle, *Asymptotic Expansions: Their Derivation and Interpretation* (Academic Press, London, 1973).
43. F. S. Henyey and V. Seshadri, *J. Chem. Phys.* **76**:5530 (1982).
44. E. W. Montroll, *J. Soc. Indust. Appl. Math.* **4**:241 (1956).
45. G. S. Joyce, *J. Math. Phys.* **12**:1390 (1971).
46. G. S. Joyce, *J. Phys.* **C4**:L53 (1971).
47. G. S. Joyce, *J. Phys.* **A5**:L65 (1972).
48. S. Ishioka and M. Koiwa, *Philos. Mag.* **A37**:5176 (1978).
49. J. E. Gillis and G. H. Weiss, *J. Math. Phys.* **11**:1307 (1970).
50. B. D. Hughes, E. W. Montroll, and M. F. Shlesinger, *J. Stat. Phys.* **28**:111 (1982).
51. J. F. C. Kingman, *Ann. Probab.* **6**:883 (1973).
52. M. D. Donsker and S. R. S. Varadhan, *Commun. Pure Appl. Math.* **28**:525 (1975).
53. P. Grassberger and I. Procaccia, *Phys. Rev. A* **26**:3683 (1982).
54. P. Grassberger and I. Procaccia, *J. Chem. Phys.* **77**:6281 (1982).

55. R. F. Kayser and J. Hubbard, *Phys. Rev. Lett.* **51**:79 (1983).
56. E. W. Montroll, *J. Math. Phys.* **10**:753 (1969).
57. K. E. Shuler, H. Silver, and K. Lindenberg, *J. Stat. Phys.* **15**:393 (1976).
58. W. Th. F. den Hollander and P. W. Kasteleyn, *Physica* **112A**:523 (1982).
59. M. Abramowitz and I. A. Stegun, eds. *Handbook of Mathematical Functions* (Dover, New York, 1972).
60. J. L. Doob, *Stochastic Processes* (Wiley, New York, 1953).