RANDOM WALKS ON RANDOM LATTICES

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RANDOM

CONTENTS

PREFACE

Over the years random-walk models have been extensively and successfully applied in many fields ranging from solid-state physics and polymer chemistry to photosynthesis, economics and the social sciences. The motives for the choice of a random-walk model to describe a particular empirical situation may vary considerably, but even so, the approaches followed for different applications are built on the same formalism.

Random-walk theory has its roots in the 17th- and 18th-century analysis of games of chance [1,2]. Its underlying concepts have played an important role in the early studies of Brownian motion and diffusion [3,4;cf.5] and have been instrumental in the development of the basic principles of nonequilibrium statistical mechanics [6;cf.2]. In the past fifty years random walks have emerged as a significant tool for the understanding of a variety of transport processes occurring in physical systems. In mathematics random walks occupy a place as a special class of Markov chains [7] and have become an important element of modern probability theory. The field has reached a high level of mathematical sophistication due to the interplay with Fourier analysis, generating-function techniques, potential theory and ergodic theory [8,9].

For a recent historical account of the subject the reader is referred to the review paper by Montroll and Shlesinger [2]. A very thorough and complete treatment of the mathematical foundations of random-walk theory has been laid down in the monograph by Spitzer [8]. A wide range of applications is discussed in the book by Barber and Ninham [10] and in the review paper by Weiss and Rubin [11]. Also, for an overview of the present state of the art the reader may find it useful to browse through the proceedings of the symposium on random walks that was held in Gaithersburg (Maryland, USA) in 1982 [12].

The formulation of a random walk as a statistical problem per se is a product of the early 20th century [13,14]. A random walk in discrete space and time may be defined as follows. Consider an infinite d-dimensional lattice L with points

$$\ell := (\ell^1, \ldots, \ell^d) = \ell^1\vec{e}_1 + \ldots + \ell^d\vec{e}_d \, , \; \ell^i \in \mathbb{Z}, \; i=1,\ldots,d \, , \tag{1}$$

where $\{\vec{e}_1, \ldots, \vec{e}_d\}$ is a set of independent unit vectors. Suppose that a walker starts at a given point ℓ_0 and makes a succession of random steps on L, visiting a random sequence of points

$$(\ell_0, \ell_1, \ell_2, \dots), \tag{2}$$

such that the successive displacements $\ell_{n+1}-\ell_n$, n=0,1,2,... , are *independent* and *identically distributed* random variables with a given probability distribution

$$p(\ell) \ , \ \ell \epsilon L. \tag{3}$$

In other words, the probability $p(\ell \rightarrow \ell')$ for the walker when finding himself on ℓ to make a step to ℓ' is independent of previous steps (the history of the walk) and depends only on the difference $\ell'-\ell$:

$$p(\ell \rightarrow \ell') = p(0 \rightarrow \ell'-\ell) =: p(\ell'-\ell) \ , \ \ell,\ell' \epsilon L. \tag{4}$$

The function $p : L \rightarrow \mathbb{R}$ is the single-step probability distribution function and has the properties

$$p(\ell) \geq 0 \ , \ \Sigma_{\ell \epsilon L} p(\ell) = 1. \tag{5}$$

This defines a *random walk* on L. Characteristic in the definition are the *independence* of the steps and the *translation invariance of the transition probabilities* as expressed by Eq.(4). Similar definitions may be given for a random walk in continuous space and/or time [2,5,11]. We shall be concerned only with the discrete case.

The aim of random-walk theory is, in short, to study the probability laws that govern the various properties associated with the walk as a function of the number of steps. Typical questions which are addressed are, for instance: (1) What is the asymptotic form of the probability distribution for the position of the walker in the limit of a very large number of steps? (2) What is the probability that the walker in the course of his walk returns to his starting point, or similarly, reaches an arbitrary point in a specified subset of L? (3) What is the probability distribution for the number of distinct points visited by the walker in a given number of steps? The answers to these questions will generally depend on the dimensionality and structure of L and on the detailed properties of p, such as range, symmetry, existence of moments, etc.

Since the 1960's a new branch of random-walk theory has developed in which the object of study carries the name of a *random walk in a random medium* (or *random environment*). Here the random-walk problem is generalized by allowing the *transition probabilities* to be (static) *random variables themselves*, i.e., the set of probabilities $\{p(\ell \to \ell')\}_{\ell,\ell' \in L}$ is determined by a given (joint) probability distribution. In this case $p(\ell \to \ell')$ depends both on ℓ *and* ℓ', so that there is *no longer translation invariance* as in Eq.(4). This is sometimes expressed by saying that the *medium* or *lattice* itself is random (disordered, inhomogeneous). Thus there are now two types of randomness in play: randomness in the walk and randomness in the medium (the lattice), and so the problem is one of a *doubly random* nature. In the general case the transition probabilities between different pairs of points may be *correlated*.

Models of a random walk in a random medium have been used to describe a variety of transport processes occurring in random physical systems, i.e., systems with *structural disorder on a microscopic scale*. Examples are: transfer of excitations in photosynthetic membranes, diffusion of vacancies or selfinterstitials in deformed metals, electrical conductivity in random-resistor networks, hopping conductivity in amorphous semiconductors, and diffusion of particles in composite materials such as alloys (see e.g. Refs. 11,12 and 15). Since completely pure (ordered, homogeneous) systems are rather rare in nature and most physical systems are structurally random in some form or other, it is not surprising that a lot of attention has been given to understanding the role of randomness in such systems in general. Transport processes are an important class of phenomena in this field.

A rich variety of models of the above type have been investigated in the past 20 years. These include models with lattices containing scatterers, traps, anisotropy points, pausing points, open and closed columns, etc. A selection of papers devoted to various areas in this field are listed in References 16-39. It will be clear that, because of the random character of the transition probabilities, the questions which are addressed here are in general much harder to handle than those which are encountered in standard random-walk theory. A typical problem arising in this context is that certain powerful techniques, such as Fourier analysis and generating-function techniques, turn out to be fruitless because of the lack of translation invariance. Many fundamental questions therefore still remain open. To mention two: (1) Under what conditions is the behaviour of a random walk on a lattice with a given type of impurity diffusion-like? (2) If it is diffusion-like, then under what conditions does the diffusion constant depend only on the density of impurities and not on their arrangement? The new techniques which have been developed over the years to deal with these types of problems have made the field especially lively from a theoretical point of view. Another interesting aspect is that certain results which have been found are of a somewhat unexpected nature, so it turns out, the randomness inherent in these models leading to new types of behaviour which seem to run against plain intuition. This situation makes careful and systematic techniques, as opposed to approximative techniques, sometimes indispensable.

In this thesis we shall be mainly concerned with *trapping problems*, i.e., we shall study models of a random walk on a lattice with points where the walk may come to an end (traps, absorbers, sinks). Trapping problems have a long history and many properties have, in some form or other, been discussed in the literature (see e.g. Refs.11,12,29-36). The model that we shall investigate is the following. We consider again an infinite d-dimensional lattice L and let a certain fraction of its points act as traps. We assume a given *joint probability distribution* $\mathcal{P}$ for the positions of the traps (which in principle may allow for *correlations* between the trap positions) with a given trap density $q>0$. Next we consider a random walk that starts at a given point and proceeds according to a given single-step probability distribution p satisfying Eqs.(4) and (5), as in the original random-walk problem. The walk continues *until a trap is hit* and the walk ends. In the following we shall study the case of *perfect* traps, where absorption is certain, but also consider the extension that is obtained by letting the traps be *imperfect*, i.e., by allowing the walker, whenever stepping on a trap, to remain free with a given probability $\eta<1$ and to continue his walk as prescribed (η is the "escape" parameter). For many applications this extension is necessary (see e.g. Refs. 40 and 41).

In the sequel much of our attention will focus on a detailed study of the following two quantities:

$$f = \text{the total probability that the walker is trapped,} \tag{6}$$

$$\langle n \rangle = \text{the average number of steps made until trapping (given that this happens),} \tag{7}$$

and related quantities. The question to be settled is how these quantities depend on L, d, $\mathcal{P}$, q, p and η.

Trapping models are relatively easy because the traps do not influence the walk "spatially". The transition probabilities are random only in the sense that whether or not at a given stage the walker continues his walk depends on the character of the point he finds himself on. Our model with η arbitrary is a special case of the general problem formulated above, with the transition probabilities taking the values

$$p(\ell\to\ell') = \begin{cases} \eta p(\ell'-\ell) \text{ , if } \ell \text{ is a trap,} \\ p(\ell'-\ell) \text{ , if } \ell \text{ is not a trap.} \end{cases} \tag{8}$$

Note that when ℓ is a trap, $\Sigma_{\ell' \in L} p(\ell\to\ell') = \eta < 1$.

In Chapter 1 we begin with a study of the case where the trap distribution $\mathcal{P}$ is *periodic*, i.e., the traps are placed in such a way that the lattice can be divided into identical finite blocks ("unit cells") each of which contains traps and nontrapping points at identical positions (in other words, there is a fixed repeating trap pattern). The shape and structure of the blocks will be arbitrary. Also the single-step distribution p will be arbitrary. The periodic case is the easiest and f and $\langle n \rangle$ can be calculated *exactly*. We also consider mixtures of different types of imperfect traps, each with a different escape parameter. Models with two types of imperfect traps are of particular interest in the theory of photosynthesis [40,41]. Our results are an extension of earlier work by Montroll (for perfect traps) [30]. In this Chapter we further allow the walker to have a fixed probability $\varepsilon<1$ per step to disappear from the lattice. This is put in with the aim of application of our results to fluorescence experiments conducted with photosynthetic bacteria [42,43]. This extension will be dropped in the subsequent Chapters.

In Chapter 2 the case of a *random* trap distribution is investigated, where each point of L has probability q to be a trap *independently* of the character of other points. This case is considerably harder and only few rigorous results are known from the literature (except in d=1) [29-31,44,45]. We consider several classes of random walks of varying dimensionality and derive a systematic asymptotic expansion in the trap density for $\langle n \rangle$. For most random walks this expansion is accurate up to relatively high densities. (We also show that for the random case f=1 for all q, p and η, provided $p(0)<1$.) A large part of the analysis in this Chapter centers on a careful study of the probability distribution for the number of points the walker visits a given number of times in a given number of steps, i.e., the "amount" and "degree of occupancy" of space covered by the walk. Again, we also consider (random) mixtures of different types of imperfect traps. Our results are an extension of earlier work by Rosenstock (for perfect traps in the limit as $q \to 0$) [29]. (See also Refs.32-36.)

For many physical applications the assumption of a periodic or a random trap distribution is not so realistic and too much of an idealization of physical reality. For more general trap distributions, however, little is known in detail. In Chapters 3 and 4 we attempt to approach the problem as generally as seems possible and allow $\mathcal{T}$ to be *completely arbitrary*, assuming only that $\mathcal{T}$ is *translation invariant*, i.e., the trap distribution is such that, loosely speaking, two trap configurations which can be obtained from each other by a translation have equal probability. Thus the lattice is inhomogeneous, but it is assumed to be *statistically homogeneous*. This property restores part of the translation invariance that was lost by randomizing the transition probabilities, and will be seen to play a crucial role in the analysis. Physically this assumption amounts to assuming that the system is *homogeneous on a macroscopic scale*. Our approach is different from that followed in the previous Chapters in that, instead of a lattice consisting of traps and nontrapping points, we now consider a lattice that consists of points of two *colours*, black and white, and on this lattice a random walk that is *independent* of the colours. The aim of this approach is partly to simplify the discussion; as we shall see, the model can be directly applied to the original trapping problem by identifying one of the colours with an imperfect trap. Thus $\mathcal{T}$ now plays the role of a colour distribution. We investigate the statistical properties of the sequence of consecutive colours encountered by the walker. More in particular our attention will focus on the following set of quantities:

f_i = the total probability that at least $i+1$ black points are visited; $i \geq 0$; (9)

$\langle n_i \rangle$ = the average number of steps made between the ith and the $(i+1)$st visit of a black point (given that these take place); $i > 0$. (10)

The successive subwalks over white points ending with a visit to a black point we call "the successive runs". In Chapter 3 we derive a number of exact relations, which are valid for arbitrary p. In Chapter 4 these relations are used to calculate the f_i, and further to derive a set of *rigorous inequalities* for the $\langle n_i \rangle$ (the average lengths of the successive runs) under the assumption that the random walk is *symmetric*, i.e., $p(\ell) = p(-\ell)$ for all ℓ. The origin of these inequalities and their "sharpness" are discussed at length, as well as the role that $\mathcal{P}$ and p play in the final results. In the calculations a number of interesting problems arise which are solved by using certain theorems from ergodic theory. Here again the translation invariance of $\mathcal{P}$ plays a crucial role. Our results are especially interesting because they have a number of *unexpected aspects*, which come to light as a result of the exact approach that is followed in the analysis.

As noted earlier, the colour model can be directly applied to the original trapping problem by identifying one of the colours, e.g. black, with an imperfect trap. In particular it is easily seen from Eqs.(6) and (7) that

$$f = f_0 - \Sigma_{i\geq 1} \eta^i (f_{i-1} - f_i), \tag{11}$$

$$\langle n \rangle = \langle n_0 \rangle + \Sigma_{i\geq 1} \eta^i \langle n_i \rangle. \tag{12}$$

Because of its somewhat abstract set-up the colour model can be applied to a few other physical problems as well. Actually, this was part of the reason why we investigated the model; however, we shall not pursue other applications here. In addition, we feel that the colour model is interesting in its own right. Because the random walk is independent of the colours, an appropriate name for the model would be a random walk in a *random scenery*, rather than in a *random environment*. The former expression is sometimes used in the literature to allude to the independence of random walk and medium (though in a somewhat different context) [46,47].

The thesis will be concluded with a list of some additional results for the colour model (without derivation or discussion) and a few conjectures, which we feel are worth investigating. It might be added that throughout the thesis the emphasis is on mathematical rigour and that many of the results which we present have sprung from the wish to approach the problem as generally as seems possible. Especially Chapters 3 and 4 were felt as a "voyage of discovery".

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Chapter I

Random walks with "spontaneous emission" on lattices with periodically distributed imperfect traps

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RANDOM WALKS WITH 'SPONTANEOUS EMISSION' ON LATTICES WITH PERIODICALLY DISTRIBUTED IMPERFECT TRAPS

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We study random walks on d-dimensional lattices with periodically distributed traps in which the walker has a finite probability per step of disappearing from the lattice and a finite probability of escaping from a trap. General expressions are derived for the total probability that the walk ends in a trap and for the moments of the number of steps made before this happens if it does happen. The analysis is extended to lattices with more types of traps and to a model where the trapping occurs during special steps. Finally, the Green's function at the origin $G(0;z)$ for a finite lattice with periodic boundary conditions, which enters into the main expressions, is studied more closely. A generalization of an expression for $G(0;1)$ for the square lattice given by Montroll to values of z different from, but close to, 1 is derived.

1. Introduction

Random walks on lattices containing traps can serve as a model for various processes occurring in molecular crystals, ionic crystals, polymers and photosynthetic units[1,2]). In the simplest case one assumes a certain distribution of traps over the lattice and one supposes that the walker steps on this lattice according to a given step probability distribution until he arrives at a trap and ends his walk. Properties of such walks have been studied by several authors[3,4]).

In some applications the walk represents the migration of a molecular excitation which can at any time disappear spontaneously through the emission of a photon. This phenomenon can be taken into account in the random-walk model by introducing a fixed probability for the walker not to survive a step[5,6]).

In other applications it is required to take into account the phenomenon, well known in photosynthesis[7]), that an excitation can, with a certain probability, escape from a trapping site and resume its migration.

It is easy to extend the theory formally so as to incorporate spontaneous emission and/or trap imperfection[8-10]). The effects of these extensions and their interplay have, however, not been investigated in detail (except in one dimension[8])).

In this paper we study some of these effects for a model with periodically distributed traps as introduced by Montroll[3]). We consider an infinite lattice, divided into identical unit cells each of which contains one trapping point at a fixed position. A walker carries out a random walk on this lattice subject to the extended conditions mentioned above. For this model we study in particular the total probability of trapping and the first and second moment of the number of steps made before trapping. For the calculation of such quantities it suffices to consider a single unit cell with periodic boundary conditions.

After having given the formal analysis in section 2, we show in section 3 how these quantities can be built up in a simple manner from quantities referring to a unit cell without a trap. In section 4 we consider lattices with different types of imperfect traps. Models with two types of imperfect traps are important in the theory of photosynthesis[11]). In section 5 we study the problem where trapping can occur not at a specific point but during a specific step. Section 6, finally, is devoted to a closer analysis of the Green's function at the origin, which plays a central role in the preceding sections, and to a discussion of some numerical results.

2. General formalism

Consider a d-dimensional simple cubic lattice L of $m \times \cdots \times m = m^d = N$ points on which periodic boundary conditions are imposed and a special point ℓ^* in L to be called the trap. Suppose that a walker W, starting from a given point ℓ_0, executes a random walk on L in which at any step the probability of a displacement by a vector ℓ is $p(\ell)$, with $\Sigma_{\ell \in L} p(\ell) = 1$. Suppose further that whenever W is at ℓ^* there is a fixed probability $1-\eta$ that W is trapped (i.e. that the walk ends) and a probability η that W remains free and continues the walk as prescribed. If $\eta = 0$ ($\eta > 0$) the trap is called perfect (imperfect).

Note that the case $\ell_0 = \ell^*$ is not excluded (as is done by some authors). Note also that 'pausing' at the trap is possible when $p(0) > 0$, but that the probability of trapping is supposed to be independent of the number of steps spent at the trap (which makes the trapping process Markovian).

We denote the probability that after n steps W is at ℓ and still free by $P_n(\ell)$, suppressing the dependence on N, ℓ^*, ℓ_0 and η. According to our assumptions

$P_n(\ell)$ satisfies the following recurrence relation:

$$P_{n+1}(\ell) = \sum_{\ell' \neq \ell^*} p(\ell - \ell')P_n(\ell') + \eta p(\ell - \ell^*)P_n(\ell^*) \tag{2.1}$$

for all $n \geq 0$, with initial condition $P_0(\ell) = \delta_{\ell\ell_0}$.

Finally suppose, in addition, that with every step the walker has a probability $\epsilon < 1$, independent of the walk performed, to disappear from the lattice ('spontaneous emission').

Now consider the probability T_n that W is trapped after exactly n steps. Obviously, since W has to 'survive' until trapping,

$$T_n = (1-\epsilon)^n(1-\eta)P_n(\ell^*). \tag{2.2}$$

If we define the generating function

$$P(\ell; z) := \sum_{n=0}^{\infty} z^n P_n(\ell) \tag{2.3}$$

and write $(1-\eta)P(\ell^*; z) = :f(z)$, then the probability f that W is eventually trapped, the average $\langle n \rangle$, the second moment $\langle n^2 \rangle$, etc. of the number of steps made before this happens (if it does happen) are given by

$$f = \sum_{n=0}^{\infty} T_n = [f(z)]_{z=1-\epsilon}, \tag{2.4}$$

$$\langle n^k \rangle = f^{-1} \sum_{n=0}^{\infty} n^k T_n = f^{-1}\left[\left(z\frac{\mathrm{d}}{\mathrm{d}z}\right)^k f(z)\right]_{z=1-\epsilon} \quad (k = 1, 2, \ldots). \tag{2.5}$$

The function $f(z)$, which we shall call 'the generating function for trapping' and always write down with its argument z, can be found by solving $P(\ell^*; z)$ in the usual manner in terms of the Green's function for the lattice and the walk chosen. From eq. (2.1) it follows that

$$P(\ell; z) - z\sum_{\ell'} p(\ell - \ell')P(\ell'; z) = \delta_{\ell\ell_0} - zp(\ell - \ell^*)(1-\eta)P(\ell^*; z). \tag{2.6}$$

Let $G(\ell; z)$ be the Green's function defined by

$$G(\ell; z) - z\sum_{\ell'} p(\ell - \ell')G(\ell'; z) = \delta_{\ell 0}, \quad \ell \in \mathrm{L}, \tag{2.7}$$

then $P(\ell; z)$ satisfies the equation

$$P(\ell; z) = G(\ell - \ell_0; z) - \{G(\ell - \ell^*; z) - \delta_{\ell\ell^*}\}(1-\eta)P(\ell^*; z). \tag{2.8}$$

Substituting $\ell = \ell^*$ and solving eq. (2.8) for $P(\ell^*; z)$ we find the following expression for $f(z)$:

$$f(z) = \frac{G(\ell^* - \ell_0; z)}{G(0;z) + \eta/(1-\eta)}. \tag{2.9}$$

As is well known, the solution of eq. (2.7) is

$$G(\ell; z) = N^{-1} \sum_\theta \frac{e^{-i\ell\cdot\theta}}{1 - z\hat{p}(\theta)}, \tag{2.10}$$

where the summation runs over $\theta = 2\pi(k_1, \dots, k_d)/m$ with $k_i = 0, 1, \dots, m-1$ $(i = 1, \dots, d)$ and where $\hat{p}(\theta)$ is the structure function of the walk:

$$\hat{p}(\theta) := \sum_\ell e^{i\ell\cdot\theta} p(\ell). \tag{2.11}$$

Although we have considered only walks on simple cubic lattices, the results derived can be applied to other lattices as well since there is no restriction on the function $p(\ell)$ (cf. ref. 3).

Up to now the walk has been supposed to start at a given point ℓ_0. If we now assume that the walk can start with equal probability at any point of L, eq. (2.9) is to be replaced by

$$f(z) = \{N(1-z)[G(0;z) + \eta/(1-\eta)]\}^{-1}, \tag{2.12}$$

which is obtained by averaging eq. (2.9) over ℓ_0, using the relation

$$\sum_\ell G(\ell; z) = (1-z)^{-1}. \tag{2.13}$$

The results thus obtained constitute the formal solution of the problem stated in the introduction. The study of $f, \langle n \rangle, \langle n^2 \rangle$ etc. as functions of the parameters N, ϵ and η is seen to reduce to that of $G(0;z)$ as a function of N and z. The dependence on η is simple: evidently, allowing imperfect traps does not substantially complicate the trapping problem. Why this is so will become more clear in the next section in which we present an alternative derivation.

In some applications of the model one is interested in the process of spontaneous emission rather than in that of trapping. The statistics of this process is equally well contained in the generating function $f(z)$. Let E_n be the probability that W disappears from the lattice after exactly n steps. Then clearly, $E_n = \epsilon(1-\epsilon)^n Q_n$, where $Q_n := \Sigma_{\ell\neq\ell^*} P_n(\ell) + \eta P_n(\ell^*)$. From eqs. (2.8) and (2.13) it follows that the generating function $Q(z) := \Sigma_{n=0}^{\infty} z^n Q_n$ is equal to $\{1 - f(z)\}/(1-z)$.

3. Alternative solution

Since the walks in which we are interested all end in the trap at ℓ^* they can be divided into one subwalk running from the starting point ℓ_0 to ℓ^* and a number of subwalks starting and ending at ℓ^*. Because of the Markovian character of the trapping process these subwalks are independent and it is a simple matter to combine them to a 'composite' walk passing through ℓ^*. Since the subwalks themselves do not pass through ℓ^*, they can be treated as walks made in the absence of the trap: it is only in combining them that the variable η characterizing the trap comes into play. Conceptually this is a simplification.

We define

f_0:= probability that W, starting at ℓ_0, reaches the trap (= 1 if $\ell_0 = \ell^*$);

f_1:= probability that W, having escaped from the trap, returns to it;

f_∞:= probability that W, having escaped from the trap, is eventually trapped.

Note that f_0 and f_1 do not depend on η, whereas f_∞ does.

Now when the walker disappears from the lattice he is lost for trapping. Since this loss can happen either before or after ℓ^* is reached, the total probability that W is not trapped is

$$1 - f = 1 - f_0 + f_0\eta(1 - f_\infty). \tag{3.1}$$

To find f_∞ we apply the same argument to walks starting at ℓ^*:

$$1 - f_\infty = 1 - f_1 + f_1\eta(1 - f_\infty). \tag{3.2}$$

Combining eqs. (3.1) and (3.2) we can express f in terms of f_0 and f_1:

$$f = f_0 \frac{1-\eta}{1-\eta f_1}. \tag{3.3}$$

By a similar reasoning we can express $\langle n \rangle$ in terms of the two averages $\langle n \rangle_0$ and $\langle n \rangle_1$ that correspond to f_0 and f_1. Thus,

$$\langle n \rangle = \langle n \rangle_0 + \eta f_1 \langle n \rangle_\infty, \tag{3.4}$$

$$\langle n \rangle_\infty = \langle n \rangle_1 + \eta f_1 \langle n \rangle_\infty, \tag{3.5}$$

where ηf_1 is the probability that the walker escapes from the trap but returns to it again, and hence

$$\langle n \rangle = \langle n \rangle_0 + \frac{\eta f_1}{1-\eta f_1} \langle n \rangle_1. \tag{3.6}$$

Higher moments can in principle be found in a similar way. This leads to increasingly more complicated expressions involving all the lower moments. For the second moment we find

$$\langle n^2\rangle = \langle n^2\rangle_0 + \eta f_1(\langle n^2\rangle_\infty + 2\langle n\rangle_0\langle n\rangle_\infty), \tag{3.7}$$

$$\langle n^2\rangle_\infty = \langle n^2\rangle_1 + \eta f_1(\langle n^2\rangle_\infty + 2\langle n\rangle_1\langle n\rangle_\infty), \tag{3.8}$$

and hence

$$\langle n^2\rangle = \langle n^2\rangle_0 + \frac{\eta f_1}{1-\eta f_1}(\langle n^2\rangle_1 + 2\langle n\rangle_0\langle n\rangle_1) + 2\left(\frac{\eta f_1}{1-\eta f_1}\right)^2\langle n\rangle_1^2. \tag{3.9}$$

The next step is to find expressions for f_0, f_1 and the corresponding first and second moments. This is essentially a first-passage problem on the lattice L without the trap. Hence f_0, $\langle n\rangle_0$ and $\langle n^2\rangle_0$ are given by eqs. (2.4) and (2.5) with $f(z)$ replaced by

$$f_0(z) = \begin{cases} F(\ell^* - \ell_0; z) & (\ell_0 \neq \ell^*) \\ 1 & (\ell_0 = \ell^*) \end{cases}, \tag{3.10}$$

where $F(\ell; z)$ is the generating function for first passage[12])

$$F(\ell; z) = \frac{G(\ell; z) - \delta_{\ell 0}}{G(0; z)}. \tag{3.11}$$

Using this expression, we can write eq. (3.10) as

$$f_0(z) = \frac{G(\ell^* - \ell_0; z)}{G(0; z)}. \tag{3.12}$$

Similarly, f_1, $\langle n\rangle_1$ and $\langle n^2\rangle_1$ are found after replacing $f(z)$ by

$$f_1(z) = F(0; z) = \frac{G(0; z) - 1}{G(0; z)}. \tag{3.13}$$

The eqs. (3.3), (3.6) and (3.9) together with (3.12) and (3.13) can be shown to imply the expressions for f, $\langle n\rangle$ and $\langle n^2\rangle$ derived in section 2. However, they give more details about the problem studied. Observe that, since ϵ is arbitrary, eq. (3.3) can also be considered as a relation between the generating functions $f(z)$, $f_0(z)$ and $f_1(z)$.

If we now assume again that ℓ_0 may with equal probability be any lattice point, the eqs. (3.3), (3.6) and (3.9) are formally not affected, but eq. (3.12) is to be replaced by

$$f_0(z) = \{N(1-z)G(0; z)\}^{-1}. \tag{3.14}$$

For $\epsilon = 0$ (i.e. $z = 1$) the results simplify considerably. Writing[3])

$$G(0; z) = \{N(1-z)\}^{-1} + \phi(0; z), \tag{3.15}$$

taking the limit $z \to 1$ and noting that $\phi(0;1) < \infty$ for $N < \infty$, one finds $f_0 = f_1 = 1$, $\langle n \rangle_0 = N\phi(0;1)$, $\langle n \rangle_1 = N$, and hence $f = 1$ and

$$\langle n \rangle = N\phi(0;1) + \frac{\eta}{1-\eta} N. \tag{3.16}$$

The fact that $\langle n \rangle_1$ equals the number of points of L reflects the well-known theorem on the recurrence time in Markov chains[12]).

4. Lattices with more traps per unit cell

If, instead of one, more imperfect traps are present in L, the generating function for trapping can be found by a straightforward generalization of the methods used in sections 2 and 3. In the most general case each trap can have a different escape probability.

We first discuss the generalization of section 2. Suppose that there are t traps in L and that trap i is located at position ℓ_i and has escape probability $\eta_i (i = 1, \ldots, t)$. If the walk starts at ℓ_0, eq. (2.8) is easily seen to generalize to

$$P(\ell;z) = G(\ell - \ell_0;z) - \sum_{i=1}^{t} \{G(\ell - \ell_i;z) - \delta_{\ell\ell_i}\}(1-\eta_i)P(\ell_i;z), \tag{4.1}$$

and if we now successively let ℓ be $\ell_1, \ldots, \ell_t$ we get the following closed set of t equations:

$$\sum_{i=1}^{t} \left\{G_{ji} + \frac{\eta_j}{1-\eta_j}\delta_{ji}\right\}(1-\eta_i)P_i = G_{j0}, \tag{4.2}$$

where $G_{ji} := G(\ell_j - \ell_i;z)$, $G_{j0} := G(\ell_j - \ell_0;z)$ and $P_i := P(\ell_i;z)$. Solving this set of equations we find the generating function for trapping at trap i to be

$$f_i(z) = (1-\eta_i)P_i = \frac{\det \mathbf{G}_i}{\det \mathbf{G}}, \tag{4.3}$$

where $\mathbf{G}$ is the $t \times t$-matrix

$$\begin{bmatrix} G_{11} + \frac{\eta_1}{1-\eta_1} & G_{12} & \cdots & G_{1t} \\ G_{21} & G_{22} + \frac{\eta_2}{1-\eta_2} & \cdots & G_{2t} \\ \vdots & \vdots & \ddots & \vdots \\ G_{t1} & G_{t2} & \cdots & G_{tt} + \frac{\eta_t}{1-\eta_t} \end{bmatrix},$$

and $\mathbf{G}_i$ is the matrix obtained from $\mathbf{G}$ by replacing, for fixed i, the ji-elements by $G_{j0}(j = 1, \ldots, t)$.

Observe that the parameters η_i simply occur in the combination $\eta_i/(1-\eta_i)$ added to $G_{ii} = G(0; z)$ on the diagonal. Eq. (4.3) generalizes a result by Montroll[13]) for perfect traps and, of course, eq. (2.9).

If the walk may with equal probability start at any lattice point, G_{j0} is to be replaced in $\mathbf{G}_i$ by $\{N(1-z)\}^{-1}$ for all j. If, furthermore, 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 the total generating function for trapping

$$f(z) = \sum_{i=1}^{t} f_i(z). \tag{4.4}$$

If one wants to have more information on the itinerary of the walker, one can follow the lines indicated in section 3, dividing the walk into subwalks. However, as the number of traps increases this soon becomes cumbersome. To illustrate the procedure we shall discuss one special case with two types of traps, which is relatively simple because of its symmetry. To define it we go back to the infinite lattice, divided into (identical) unit cells with one trap each, considered in the introduction.

Suppose now that the traps are of two types, with escape probabilities η and η', distributed in such a way that traps in adjacent unit cells are of different type (so that on the sublattice with lattice spacing m, which is formed by the trapping points, the two types alternate). This new lattice with traps is again periodic but on a larger scale.

To calculate the total probability of trapping f we next divide the lattice into new unit cells of $(2m)^d = 2^d N$ points and consider one unit cell on which we impose periodic boundary conditions. This finite lattice, to be denoted by $\tilde{\mathrm{L}}$, contains 2^{d-1} traps of either type. Note that a smaller unit cell, with only one trap of either type, can be chosen, but this has the disadvantage of requiring less practical boundary conditions. For brevity we suppose at once that W may start with equal probability at any point of $\tilde{\mathrm{L}}$. We define

f_0: = probability that W reaches a trap or starts at a trap;

$f_2(f_3)$: = probability that W, having escaped from a trap, reaches a trap of the same (other) type without having visited traps of the other (same) type.

To express f in terms of f_0, f_2, f_3, η and η' we proceed in the following way. We define

$p_r(p_r')$: = probability that W visits r times a trap without being trapped and then reaches a trap with parameter $\eta(\eta')$.

The p_r and p'_r satisfy the following recurrence relation, written in matrix form:

$$\begin{pmatrix} p_{r+1} \\ p'_{r+1} \end{pmatrix} = \begin{pmatrix} f_2\eta & f_3\eta' \\ f_3\eta & f_2\eta' \end{pmatrix} \begin{pmatrix} p_r \\ p'_r \end{pmatrix} =: \mathbf{T} \begin{pmatrix} p_r \\ p'_r \end{pmatrix} \tag{4.5}$$

for all $r \geq 0$, with initial conditions

$$p_0 = p'_0 = \tfrac{1}{2} f_0. \tag{4.6}$$

The probability that W, having escaped from a trap, never reaches one anymore is $1 - f_2 - f_3$. Hence the total probability that W is not caught in a trap is

$$1 - f = 1 - f_0 + (1 - f_2 - f_3) \sum_{r=0}^{\infty} (\eta p_r + \eta' p'_r). \tag{4.7}$$

Using eqs. (4.5) and (4.6) one can write

$$\sum_{r=0}^{\infty} (\eta p_r + \eta' p'_r) = (\eta\ \eta') \sum_{r=0}^{\infty} \mathbf{T}^r \begin{pmatrix} 1 \\ 1 \end{pmatrix} = (\eta\ \eta')(\mathbf{E} - \mathbf{T})^{-1} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \tag{4.8}$$

where $\mathbf{E}$ is the 2×2 unit matrix, and it follows that

$$f = f_0 \left[1 - (1 - f_2 - f_3) \frac{\tfrac{1}{2}(\eta + \eta') - \eta\eta'(f_2 - f_3)}{(1 - \eta f_2)(1 - \eta' f_2) - \eta f_3 \eta' f_3} \right]. \tag{4.9}$$

It is clear from the definition that f_0 is the same probability that is found from eq. (3.14) and that $f_2 + f_3$ is equal to f_1 obtained from eq. (3.13) (both f_0 and f_1 referring to the original unit cell L). If we set $\eta = \eta'$, eq. (4.9) reduces to eq. (3.3).

Explicit expressions for the probabilities f_2 and f_3 can be obtained by solving a first-passage problem for sets of points on the lattice $\tilde{L}$ without traps (cf. ref. 14) as follows. Let $G_n(\ell)$ be the probability that W, having started at a chosen point 0 (the origin), is at ℓ after n steps. By definition, $G(\ell; z) := \sum_{n=0}^{\infty} z^n G_n(\ell)$ is the Green's function for $\tilde{L}$ (not to be confused with that for L). For any set $S \subset \tilde{L}$ and $n > 0$ let $P_n^S(\ell)$ be the probability that W, having started at 0, is at ℓ after n steps without having 'hit' S at any intermediate step; let further $P_0^S(\ell) = 0$ for all ℓ. Clearly, since every walk from 0 to ℓ either avoids S altogether or hits it for the first time at some step, we have for $n > 0$

$$G_n(\ell) = P_n^S(\ell) + \sum_{\ell' \in S} \sum_{m=0}^{n-1} P_m^S(\ell') G_{n-m}(\ell - \ell'). \tag{4.10}$$

For the generating function $P^S(\ell; z) := \sum_{n=0}^{\infty} z^n P_n^S(\ell)$ it now follows that

$$G(\ell; z) - \delta_{\ell 0} = P^S(\ell; z) + \sum_{\ell' \in S} \{G(\ell - \ell'; z) - \delta_{\ell\ell'}\} P^S(\ell'; z). \tag{4.11}$$

For $\ell \in S$ this reduces to

$$G(\ell;z)-\delta_{\ell 0}=\sum_{\ell'\in S} G(\ell-\ell';z)P^S(\ell';z). \tag{4.12}$$

If desired, $P^S(\ell;z)$ can be solved from eq. (4.12) for $\ell \in S$ and then from eq. (4.11) for $\ell \notin S$. We shall, however, not consider $\ell \notin S$. Note that eq. (4.12) closely resembles eq. (4.2) with all η_i equal to zero and $S=\{\ell_1,\ldots,\ell_l\}$. The difference lies in the term $\delta_{\ell 0}$ in the left-hand side of eq. (4.12). Like the one in eq. (3.11) it arises from the fact that the start at 0 is not considered as a first visit to 0 (i.e. $P_0^S(0)=0$).

To find f_2 and f_3 we let S be the set of all trapping points in $\tilde{L}$, and $0 \in S$. Let further $S_A(S_B)$ be the set of all points in $\tilde{L}$ where traps of the same (other) type as the one at 0 are located ($S_A \cup S_B = S$). Then it is clear that

$$f_2(z)=\sum_{\ell\in S_A} P^S(\ell;z), \tag{4.13}$$

$$f_3(z)=\sum_{\ell\in S_B} P^S(\ell;z). \tag{4.14}$$

We define

$$C_A(z):=\sum_{\ell\in S_A} G(\ell;z), \tag{4.15}$$

$$C_B(z):=\sum_{\ell\in S_B} G(\ell;z). \tag{4.16}$$

Because of translational symmetry we have $\ell-\ell' \in S_A$ if ℓ and ℓ' belong both to S_A or both to S_B but $\ell-\ell' \in S_B$ otherwise. Then, summing eq. (4.12) successively over all $\ell \in S_A$ and over all $\ell \in S_B$, we obtain

$$C_A(z)f_2(z)+C_B(z)f_3(z)=C_A(z)-1,$$
$$C_B(z)f_2(z)+C_A(z)f_3(z)=C_B(z),$$

and hence

$$f_2(z)=1-\frac{C_A(z)}{C_A^2(z)-C_B^2(z)}, \tag{4.17}$$

$$f_3(z)=\frac{C_B(z)}{C_A^2(z)-C_B^2(z)}; \tag{4.18}$$

f_2 and f_3 follow by setting $z=1-\epsilon$, and f from (4.9).

Lattices with a more complicated pattern of traps of two types can of course be treated in a similar way as long as the pattern has a certain periodicity. Accordingly, the unit cell will be more complicated and actual calculation soon becomes unfeasible.

5. Trapping during a step

An interesting variant of the models discussed so far is obtained if we suppose that the walker W can be trapped not while visiting a special *point* but while making a special *step*. The effect of this change in the trapping model is not, as one might expect, marginal.

For simplicity, as well as with a view to applications, we restrict ourselves to simple random walks, representing the possible steps by lines between nearest-neighbour points of L. Now suppose that there is one special line such that when W steps along this line (in either direction) there is a probability $1-\eta$ that he gets trapped ('line trapping'). By a direct generalization of the type of calculations made in section 2 we find the generating function for trapping to be

$$f(z)=\left\{N(1-z)\left[\frac{1+z}{2}G(0;z)+\frac{c-1}{2}+\frac{\eta}{1-\eta}\frac{c}{2}\right]\right\}^{-1}, \tag{5.1}$$

where we have averaged over all possible starting points of W and not counted the step during which W is trapped; c is the coordination number of L.

The corresponding expression for $\langle n\rangle$, obtained by substituting eq. (5.1) into (2.5), is not very transparent but becomes so in the limit $\epsilon\to 0$. Using eq. (3.15) we find

$$\langle n\rangle=\{N\phi(0;1)-\tfrac{1}{2}\}+\frac{(c-1)N}{2}+\frac{\eta}{1-\eta}\frac{cN}{2}. \tag{5.2}$$

This is to be compared with eq. (3.16) for 'point trapping'.

First we note the appearance in eq. (5.2) of the factor $\frac{1}{2}cN$ in the last term. This is evidently the average number of steps by which the walk is prolonged every time W 'successfully' traverses the trapping line and continues his walk starting from one of its endpoints. It is the total number of lines drawn in L and reflects again the theorem on the recurrence time in Markov chains mentioned in section 3.

More interesting is the term $\frac{1}{2}(c-1)N$, which has no counterpart in eq. (3.16). To begin with, it is, unlike the first term, independent of the structure of L. Its origin lies in the fact that when W reaches for the first time an endpoint of the trapping line (which, for reasons of symmetry, can be seen to require on the average $N\phi(0;1)-\frac{1}{2}$ steps), there is a probability $(c-1)/c =: \gamma$ that he does not step along it but prolongs his walk. Since in this case too W continues his walk starting from one of the endpoints, the average number of steps by which the walk is then prolonged is again $\frac{1}{2}cN$, which multiplied by γ gives just the term considered.

Secondly, this term can be of considerable numerical importance. For the s.c. $d = 3$ lattice we have $\phi(0;1) \approx 1.5$ for large N, while $\frac{1}{2}(c-1) = 5/2$. For the b.c.c. and f.c.c. lattice and for lattices with $d > 3$ the difference is even more pronounced, and $\langle n \rangle$ is to a large extent determined solely by c and η.

It is instructive to consider also what happens if W can only be trapped while stepping along the trapping line in one direction. In this case we find

$$\langle n \rangle = N\phi(0;1) + \gamma c N + \frac{\eta}{1-\eta} cN, \tag{5.3}$$

the interpretation of which is obvious.

Thus it is clear that although 'point trapping' and 'line trapping' are closely related (especially for simple random walks), the difference between the two is sufficiently interesting to be stressed.

6. The function $G(0;z)$

We have expressed a number of quantities of interest in terms of the function $G(0;z)$, which we shall henceforth denote by $G_N(0;z)$ in order to display also its dependence on N, the number of lattice points in the unit cell (i.e. its dependence on the density of traps). From eq. (2.10) one can evaluate $G_N(0;z)$ and its derivatives numerically for N not too large. In addition one can study the asymptotic behaviour of $G_N(0;z)$ for large N, but care is to be taken since the summand in eq. (2.10) has, for $\theta = 0$, a pole at $z = 1$.

If, for z close to 1, we expand $G_N(0;z)$ in powers of $1-z$, we find that two regimes are to be distinguished, characterized by the product $N(1-z)\phi_N(0;1)$ which, by eq. (3.15), is the ratio of the first two terms in the expansion in question. If this product is $\ll 1$ the expansion is expected to make sense; if it is $\gg 1$, however, one has to resort to other approximation methods.

Returning to the trapping model considered in sections 2 and 3, we see that the product $N(1-z)\phi_N(0;1)$ has a simple interpretation: it is equal to ϵ times $\langle n \rangle_0^{(\epsilon=0)}$; its order of magnitude largely controls the qualitative aspects of the walk in that it indicates whether or not the walker has an appreciable chance to reach the trap at all. For simple random walks Montroll[3]) has shown that, to leading order in N:

$$\langle n \rangle_0^{(\epsilon=0)} \simeq \begin{cases} (1/6)N^2 & (d=1) \\ bN \log N & (d=2) \\ cN & (d \geq 3), \end{cases} \tag{6.1}$$

where b and c are lattice-dependent constants.

From the expansion of $G_N(0;z)$ in powers of $1-z$ we can get corresponding expansions in powers of ϵ for the quantities of interest. This is straightforward, but finding the asymptotic behaviour for large N of the coefficients in this expansion is in general far from easy.

To derive expressions for the relative standard deviations $\tau_i = (\langle n^2\rangle_i - \langle n\rangle_i^2)^{1/2}/\langle n\rangle_i$ $(i = 0, 1)$ to leading order we have to expand $G_N(0;z)$ up to first order in $1-z$. On expanding

$$G_N(0;z) = \{N(1-z)\}^{-1} + \phi_N - \phi'_N(1-z) + \cdots, \tag{6.2}$$

where we write $\phi_N(0;1) = :\phi_N$ and $\phi'_N(0;1) = :\phi'_N$, it follows that for $\epsilon = 0$:

$$\langle n\rangle_0 = N\phi_N, \langle n\rangle_1 = N,$$

and

$$\tau_0^2 = 1 + 1/N\phi_N + 2\phi'_N/N\phi_N^2, \tag{6.3}$$

$$\tau_1^2 = 2\phi_N - 1 + 1/N. \tag{6.4}$$

For the simple random walk on the linear chain and square lattice we have evaluated ϕ_N and ϕ'_N.

For the linear chain it can easily be shown that $\phi_N = (N^2-1)/6N$ [3]) and $\phi'_N = (N^4 - 20N^2 + 19)/180N$. This leads, for $N \to \infty$, to

$$\tau_0^2 \simeq 7/5, \tag{6.5}$$

$$\tau_1^2 \simeq (1/3)N. \tag{6.6}$$

For the square lattice no closed expressions can be obtained but one can derive asymptotic expressions, valid for large N, using the Euler–Maclaurin summation formula. The results are:

$$\phi_N = a_1 \log N + a_2 + a_3N^{-1} + a_4N^{-2} + \cdots, \tag{6.7a}$$

$$\phi'_N = b_1N + b_2 \log N + b_3 + b_4N^{-1} + b_5N^{-2} + \cdots \tag{6.7b}$$

with

$$\begin{aligned} a_1 &= \pi^{-1}, & b_1 &= 0.061871145451\ldots, \\ a_2 &= 0.195062532\ldots, & b_2 &= -(2\pi)^{-1}, \\ a_3 &= -0.116964779\ldots, & b_3 &= -0.1347623119\ldots, \\ a_4 &= 0.484065704\ldots, & b_4 &= 0.2005850758\ldots, \\ & & b_5 &= 0.4283683639\ldots. \end{aligned}$$

Details of the calculation of ϕ'_N and a comment on Montroll's result for ϕ_N[3])

are given in the appendix. In this case it follows that for large N

$$\tau_0^2 \simeq 1 + 2\pi^2 b_1/\log^2 N, \tag{6.8}$$

$$\tau_1^2 \simeq (2/\pi)\log N + 2a_2 - 1. \tag{6.9}$$

Eq. (6.8) differs from the result obtained by Hatlee and Kozak[15]). Some errors seem to have slipped into their calculations; moreover they chose not to include the trapping point as a possible starting point, but the effect of this choice is of order N^{-1}. By Monte-Carlo simulation, however, they correctly found that τ_0 is slightly larger than 1.

Observe that for both cases τ_0 is of order 1 whereas τ_1 diverges as $N \to \infty$; this divergence is related to the well-known fact that the simple random walk on the infinite one- or two-dimensional lattice is recurrent.

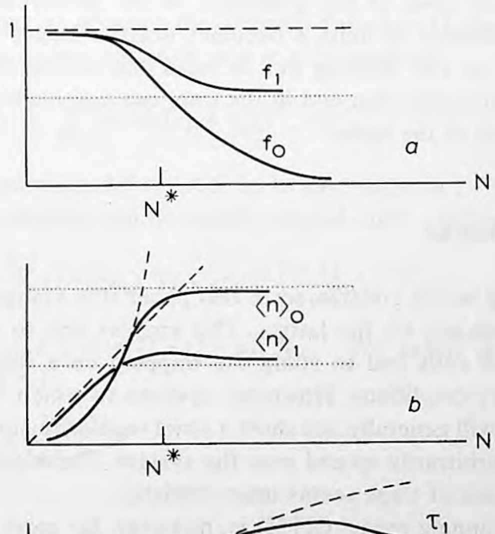

Fig. 1. Sketch of the behaviour of the quantities f_0 and f_1 (a), $\langle n\rangle_0$ and $\langle n\rangle_1$ (b), τ_0 and τ_1 (c) for the simple random walk on a square lattice of N points as functions of N for fixed ϵ. The value of N^* is such that $\pi^{-1}N^*\epsilon\log N^* = 1$ and marks the transition between the two regimes. The dotted lines are the theoretical asymptotes for $N \to \infty$ and the dashed lines indicate the behaviour of the quantities for $\epsilon = 0$.

For $d \geq 3$ so far no comparable results for large but finite N have been derived. It would require much hard labour to apply the Euler–Maclaurin summation formula to these cases. If $N = \infty$ it is easily seen that $\tau_0^2 = 1$ and $\tau_1^2 = 2\phi_\infty - 1 < \infty$.

We have not investigated the regime where $N(1-z)\phi_N(0; 1) \gg 1$. In the limit $N \to \infty$ for $z < 1$, however, $G_N(0; z)$ tends to a d-fold integral, the behaviour of which for z close to 1 has been extensively investigated for $d = 1, 2, 3$[12]).

For the simple random walk on the square lattice we have evaluated $G_N(0; z)$ numerically and computed f_0, f_1, $\langle n \rangle_0$, $\langle n \rangle_1$, τ_0 and τ_1 for a number of values of N (ranging from $N = 2 \times 2$ to $N = 22 \times 22$) and ϵ (ranging from $\epsilon = 10^{-5}$ to $\epsilon = 10^{-1}$). The general qualitative behaviour of these quantities as a function of N for fixed ϵ is sketched in fig. 1. This figure clearly shows the transition between the two regimes. An unexpected aspect is the non-monotonic behaviour of some of the quantities. In the intermediate region, as N increases, the influence of finite ϵ becomes drastic: longer walks tend to be more and more cut off. Bearing this in mind and noting that we have only taken into account walks that end in the trap, one can readily understand the qualitative aspects of the figure.

7. Concluding remarks

In the trapping model considered in this paper it is assumed that the traps are placed periodically on the lattice. This enables one to divide the lattice into identical unit cells and to study the trapping on a single unit cell with periodic boundary conditions. However, systems to which one would like to apply the model will generally not show a strict regularity and traps will rather be more or less arbitrarily spread over the system. Therefore, a model with a random distribution of traps seems more realistic.

The random trapping model (RTM) is, however, far more difficult than the periodic trapping model (PTM), at least for $d \geq 2$. It is obviously related to other models with a random structure such as the percolation model and the random Ising model. So far, hardly any rigorous results have been obtained for the RTM, except in one dimension (see ref. 5 for a solvable model in more dimensions which has essentially one-dimensional features).

On the other hand, several authors have discussed approximative methods to deal with the RTM. Rosenstock[4,6]) has derived asymptotic expressions for f_0 and $\langle n \rangle_0^{(\epsilon=0)}$ valid for small q, where q is the density of traps. In the analysis of f_0 the same 'competition' between ϵ and the density of traps is encountered that we discussed in section 6. A comparison of Rosenstock's expressions for

$\langle n\rangle_0^{(\epsilon=0)}$ with the corresponding ones of Montroll for the PTM (with N replaced by q^{-1}) shows that for $d \geq 2$ and $q \ll 1$ the RTM and the PTM do not differ substantially. Weiss[16]) has shown that for $d = 3$ corrections to Rosenstock's approximation are quite small for $q \leq 0.01$. No other moments of the probability distribution of the number of steps before trapping than f_0 and $\langle n\rangle_0^{(\epsilon=0)}$ have been studied explicitly.

The influence of imperfect traps in the RTM has received relatively little interest. This is a problem which cannot be treated by Rosenstock's approximation. Hemenger et al.[8]) have applied a different approximative method in the context of a master equation approach; their results, too, are restricted to small q.

Appendix

In this appendix we expand the Green's function $G_N(0;z)$ for a simple random walk on a square lattice of $m \times m = N$ points:

$$G_N(0;z) = \frac{1}{m^2}\sum_{k_1=0}^{m-1}\sum_{k_2=0}^{m-1}\{1-\tfrac{1}{2}z(c_{k_1}+c_{k_2})\}^{-1}, \tag{A.1}$$

where $c_k := \cos(2\pi k/m)$ and $0 \leq z \leq 1$, up to first order in $1-z$.

One of the summations can be readily carried out[3]), yielding

$$G_N(0;z) = \frac{1}{m}\sum_{k=0}^{m-1}(1-\tfrac{1}{2}zc_k)^{-1}(1-\rho_k^2)^{-1/2}\frac{1+x_k^m}{1-x_k^m}, \tag{A.2}$$

where $\rho_k := z(2-zc_k)^{-1}$, $x_k := \{1-(1-\rho_k^2)^{1/2}\}\rho_k^{-1}$. We define $\alpha := (1-z)^{1/2}$. For fixed $k \ll m$ and $\alpha \ll 1$:

$$x_k = 1 - 2\left(\alpha^2 + \frac{\pi^2k^2}{m^2}\right)^{1/2} + \cdots,$$

and hence

(i) $\lim\limits_{m\to\infty}\lim\limits_{\alpha\to 0} x_k^m = e^{-2\pi k}$,

(ii) $\lim\limits_{\alpha\to 0}\lim\limits_{m\to\infty} x_k^m = 0$.

In the limit $m \to \infty$, $\alpha \to 0$, $m\alpha = \pi c$ constant

$$x_k^m \to e^{-2\pi(c^2+k^2)^{1/2}},$$

and it follows that for $c \ll 1$ the factor x_k^m rapidly goes to zero with increasing k, so that in sums of terms containing this factor only the lowest few values of k contribute significantly. We therefore restrict ourselves to this regime.

In expanding $G_N(0;z)$, as given in eq. (A.2), in powers of α, we find, expressing c_k in terms of $\sigma_k := \sin(\pi k/m)$:

$$(1-\tfrac{1}{2}zc_k)^{-1}(1-\rho_k^2)^{-1/2} = \{\sigma_k^2(1+\sigma_k^2)+(1-2\sigma_k^4)\alpha^2-\sigma_k^2(1-\sigma_k^2)\alpha^4\}^{-1/2}$$

$$= \begin{cases} \alpha^{-1} & (k=0) \\ \sigma_k^{-1}(1+\sigma_k^2)^{-1/2} - \tfrac{1}{2}\sigma_k^{-3}(1+\sigma_k^2)^{-3/2}(1-2\sigma_k^4)\alpha^2 + \cdots & (k>0) \end{cases}$$

and

$$\frac{1+x_k^m}{1-x_k^m} = \begin{cases} (m\alpha)^{-1}\{1+\tfrac{1}{3}(m^2-1)\alpha^2 - \tfrac{1}{45}(m^2-1)(m^2-4)\alpha^4+\cdots\} & (k=0) \\ \left(1+\dfrac{2\lambda_k^m}{1-\lambda_k^m}\right) - \sigma_k^{-1}(1+\sigma_k^2)^{-1/2}\dfrac{2m\lambda_k^m}{(1-\lambda_k^m)^2}\alpha^2+\cdots, & (k>0) \end{cases}$$

where $\lambda_k := 1+2\sigma_k^2 - 2\sigma_k(1+\sigma_k^2)^{1/2}$. Hence

$$G_{m^2}(0;1-\alpha^2) = (m\alpha)^{-2} + \left\{\frac{m^2-1}{3m^2} + \psi(m)\right\}$$
$$- \left\{\frac{(m^2-1)(m^2-4)}{45m^2} + \psi'(m)\right\}\alpha^2 + \cdots, \qquad \text{(A.3)}$$

where

$$\psi(m) := \frac{1}{m}\sum_{k=1}^{m-1} \sigma_m^{-1}(1+\sigma_k^2)^{-1/2}\left(1+\frac{2\lambda_k^m}{1-\lambda_k^m}\right), \qquad \text{(A.4a)}$$

$$\psi'(m) := \frac{1}{m}\sum_{k=1}^{m-1}\left[\tfrac{1}{2}\sigma_k^{-3}(1+\sigma_k^2)^{-3/2}(1-2\sigma_k^4)\left(1+\frac{2\lambda_k^m}{1-\lambda_k^m}\right)\right.$$
$$\left. - \sigma_k^{-2}(1+\sigma_k^2)^{-1}\frac{2m\lambda_k^m}{(1-\lambda_k^m)^2}\right]. \qquad \text{(A.4b)}$$

Montroll[3]) has derived an asymptotic expression for the zeroth order term $\psi(m)$, valid for large m, using the Euler–Maclaurin summation formula in the form

$$\frac{1}{m}\sum_{k=1}^{m-1} f\left(\frac{\pi k}{m}\right) = \frac{1}{\pi}\int_0^\pi \mathrm{d}y\, f(y) - \frac{1}{2m}[f(0)+f(\pi)] + \frac{\pi}{12m^2}[f'(\pi)-f'(0)]$$
$$- \frac{\pi^3}{720m^4}[f'''(\pi)-f'''(0)] + \cdots. \qquad \text{(A.5)}$$

We proceed along the same line and derive an expression for the first order term. To this end we split the sum in eq. (A.4b) into several parts. First we write $\psi'(m) = S_1 + S_2$ with $S_1 := (2m)^{-1}\Sigma_{k=1}^{m-1}\sigma_k^{-3}(1+\sigma_k^2)^{-3/2}(1-2\sigma_k^4)$, so that S_2 consists of the terms containing $\lambda_k^m (= \lim_{\alpha\to 0} x_k^m)$.

A.1. Evaluation of S_1

We find it expedient to split S_1 as follows:

$$S_1 = \frac{1}{2m}\sum_{k=1}^{m-1}\left\{\sigma_k^{-3}(1+\sigma_k^2)^{-1/2} - \sigma_k^{-1}(1+\sigma_k^2)^{-1/2} - \sigma_k(1+\sigma_k^2)^{-3/2}\right\}$$
$$=: S_{11} + S_{12} + S_{13}$$

and to split S_{11} further into two parts to which we apply eq. (A.5):

$$\text{(i)}\quad \frac{1}{2m}\sum_{k=1}^{m-1}\sigma_k^{-3}\{(1+\sigma_k^2)^{-1/2} - 1 + \tfrac{1}{2}\sigma_k^2\} = \frac{1}{4\pi} - \frac{\pi}{32m^2} - \frac{\pi^3}{320m^4} + \cdots,$$

$$\text{(ii)}\quad \frac{1}{2m}\sum_{k=1}^{m-1}\{\sigma_k^{-3} - \tfrac{1}{2}\sigma_k^{-1}\} = \frac{1}{2m}\sum_{k=1}^{m-1}\left\{\sigma_k^{-3} - \tfrac{1}{2}\sigma_k^{-1} - \left[\left(\frac{\pi k}{m}\right)^{-3} + \left(\frac{\pi(m-k)}{m}\right)^{-3}\right]\right\}$$
$$+ \frac{1}{m}\sum_{k=1}^{m-1}\left(\frac{\pi k}{m}\right)^{-3} = \left(\frac{1}{2\pi^3} - \frac{1}{12\pi}\right) + \frac{1}{2\pi^3 m} + \left(\frac{1}{4\pi^3} - \frac{7\pi}{1440}\right)\frac{1}{m^2}$$
$$+ \left(\frac{31\pi^3}{181440} - \frac{1}{12\pi^3}\right)\frac{1}{m^4} + \cdots + \frac{m^2}{\pi^3}\sum_{k=1}^{m-1} k^{-3}.$$

The remaining sum over k can be evaluated by using a slightly different form of the Euler–Maclaurin formula. We find

$$\sum_{k=1}^{m-1} k^{-3} = \zeta(3) - \frac{1}{2m^2} - \frac{1}{2m^3} - \frac{1}{4m^4} + \frac{1}{12m^6} + \cdots,$$

where ζ is Riemann's zeta function and $\zeta(3) = 1.202056903159\ldots$ and hence

$$S_{11} = \frac{\zeta(3)}{\pi^3}m^2 + \frac{1}{6\pi} - \frac{13\pi}{360m^2} - \frac{67\pi^3}{22680m^4} + \cdots.$$

The sum S_{12} has been evaluated by Montroll:

$$S_{12} = -\frac{1}{2m}\sum_{k=1}^{m-1}\sigma_k^{-1}(1+\sigma_k^2)^{-1/2}$$
$$= -\frac{1}{\pi}\log m - \left(\frac{\gamma}{\pi} + \frac{1}{2\pi}\log\frac{2}{\pi^2}\right) - \frac{\pi}{36m^2} - \frac{43\pi^3}{10800m^4} + \cdots,$$

where γ is Euler's constant: $\gamma = 0.5772156649\ldots$. For the sum S_{13} the application of eq. (A.5) yields

$$S_{13} = -\frac{1}{2m}\sum_{k=1}^{m-1}\sigma_k(1+\sigma_k^2)^{-3/2} = -\frac{1}{2\pi} + \frac{\pi}{12m^2} + \frac{\pi^3}{72m^4} + \cdots,$$

so that, finally,

$$S_1 = \frac{\zeta(3)}{\pi^3}m^2 - \frac{1}{\pi}\log m - \left(\frac{1}{3\pi} + \frac{\gamma}{\pi} + \frac{1}{2\pi}\log\frac{2}{\pi^2}\right) + \frac{7\pi}{360m^2} + \frac{1577\pi^3}{226800m^4} + \cdots. \tag{A.6}$$

A.2. *Evaluation of* S_2

Application of the Euler–Maclaurin formula to the sum

$$S_2 = \frac{1}{m}\sum_{k=1}^{m-1}\left[\sigma_k^{-3}(1+\sigma_k^2)^{-3/2}(1-2\sigma_k^4)\frac{\lambda_k^m}{1-\lambda_k^m} - \sigma_k^{-2}(1+\sigma_k^2)^{-1}\frac{2m\lambda_k^m}{(1-\lambda_k^m)^2}\right]$$

is not possible since λ_k^m depends on m not only through the ratio $\pi k/m$. An expansion of S_2 in powers of $1/m$ with closed expressions for the coefficients is therefore not found. Following ref. 3 we can, however, write these coefficients as quickly converging series in powers of $e^{-2\pi}$. Because of the symmetry relation $\sigma_k = \sigma_{m-k}$ we replace $\Sigma_{k=1}^{m-1}$ by $2\Sigma_{k=1}^{[m/2]}$.

Noting that λ_k is the smaller root of the equation $\lambda_k + \lambda_k^{-1} = 2 - \cos(2\pi k/m)$, we can derive

$$\lambda_k = \exp -\left\{2\frac{\pi k}{m} - \frac{2}{3}\left(\frac{\pi k}{m}\right)^3 + \frac{1}{3}\left(\frac{\pi k}{m}\right)^5 - \frac{79}{315}\left(\frac{\pi k}{m}\right)^7 + \cdots\right\},$$

and hence

$$\lambda_k^m = e^{-2\pi k}\left\{1 + \frac{2(\pi k)^3}{3}\frac{1}{m^2} + \left(-\frac{(\pi k)^5}{3} + \frac{2(\pi k)^6}{9}\right)\frac{1}{m^4} + \left(\frac{79(\pi k)^7}{315} - \frac{2(\pi k)^8}{9} + \frac{4(\pi k)^9}{81}\right)\frac{1}{m^6} + \cdots\right\}. \quad \text{(A.7)}$$

Using this expression for λ_k^m and expanding σ_k in powers of $\pi k/m$ we find, after going through a good deal of algebra:

$$S_2 = s_2 m^2 + s_0 + s_{-2}m^{-2} + s_{-4}m^{-4} + \cdots, \quad \text{(A.8)}$$

where

$$s_r = \sum_{k=1}^{[m/2]} s_r(k), \quad \text{(A.9)}$$

with

$$s_2(k) = 4(\pi k)^{-2}\frac{e_k}{(1-e_k)^2} + 2(\pi k)^{-3}\frac{e_k}{1-e_k},$$

$$s_0(k) = \frac{8}{3}\pi k\frac{e_k(1+e_k)}{(1-e_k)^3} - \frac{4}{3}\frac{e_k}{(1-e_k)^2} - 2(\pi k)^{-1}\frac{e_k}{1-e_k},$$

$$s_{-2}(k) = \frac{8}{9}(\pi k)^4\frac{e_k(1+4e_k+e_k^2)}{(1-e_k)^4} - \frac{24}{9}(\pi k)^3\frac{e_k(1+e_k)}{(1-e_k)^3} + \frac{34}{15}(\pi k)^2\frac{e_k}{(1-e_k)^2} - \frac{7}{15}\pi k\frac{e_k}{1-e_k},$$

$$s_{-4}(k)=\frac{16}{81}(\pi k)^7\frac{e_k(1+11e_k+11e_k^2+e_k^3)}{(1-e_k)^5}-\frac{112}{81}(\pi k)^6\frac{e_k(1+4e_k+e_k^2)}{(1-e_k)^4}$$
$$+\frac{404}{105}(\pi k)^5\frac{e_k(1+e_k)}{(1-e_k)^3}-\frac{838}{189}(\pi k)^4\frac{e_k}{(1-e_k)^2}+\frac{1577}{945}(\pi k)^3\frac{e_k}{1-e_k},$$

where $e_k:=\mathrm{e}^{-2\pi k}$. Expanding these expressions in powers of e_k, replacing the upper limit in eq. (A.9) by ∞ (thus neglecting terms of order $\mathrm{e}^{-\pi m}$) and introducing

$$\mu(i,j):=\sum_{k,l=1}^{\infty}(\pi k)^i l^j\,\mathrm{e}^{-2\pi kl}\quad\text{for integer } i \text{ and } j,$$

we obtain

$$\begin{aligned}
s_2&=4\mu(-2,1)+2\mu(-3,0)\\
&=0.000880743626\ldots,\\
s_0&=\frac{8}{3}\mu(1,2)-\frac{4}{3}\mu(0,1)-2\mu(-1,0)\\
&=0.0121245076\ldots,\\
s_{-2}&=\frac{8}{9}\mu(4,3)-\frac{8}{3}\mu(3,2)+\frac{34}{15}\mu(2,1)-\frac{7}{15}\mu(1,0)\\
&=0.0506096631\ldots,\\
s_{-4}&=\frac{16}{81}\mu(7,4)-\frac{112}{81}\mu(6,3)+\frac{404}{105}\mu(5,2)-\frac{838}{189}\mu(4,1)-\frac{1577}{945}\mu(3,0)\\
&=0.2127735741\ldots\ldots
\end{aligned}\tag{A.10}$$

Combining eqs. (A.3), (A.4b), (A.6) and (A.8) we find the expression for ϕ'_N in eq. (6.7b).

Note that the values of a_2, a_3 and a_4 in eq. (6.7a) differ from those given by Montroll[3]). In going through his calculation of a_4 we found that in his eq. (B.31) a term, corresponding to the second term in the coefficient of m^{-4} in our eq. (A.7), is missing; for a_2 and a_3 we came to slightly different numerical values*. The fact that the values given by Montroll might not be entirely correct has already been observed by Sanders et al.[17]); they doubted, however, in particular the value of a_3.

A comparison of the values of ϕ_N found from eq. (6.7a) for values of N from 14×14 to 22×22 with those obtained from direct numerical evaluation shows an agreement of 1 to 10^7 or better. For ϕ'_N an equally good agreement is found. From the results we can even systematically estimate the next coefficients: $a_5\approx 2.6$, $b_6\approx 4.4$. The values of a_1 through a_5 and b_1 through b_6 strongly suggest that the series in eqs. (6.7a, b) are asymptotic.

* We remark in passing that the various series in powers of $\mathrm{e}^{-2\pi}$ occurring in the derivation of eq. (6.7a) can also be written in terms of the $\mu(i,j)$.

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Chapter II

Random walks on lattices with randomly distributed traps
I. The average number of steps until trapping

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Random Walks on Lattices with Randomly Distributed Traps I. The Average Number of Steps Until Trapping

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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,[1] of charge carriers in an anisotropic molecular crystal in an electric field[2] and of electrons in an amorphous material.[3]

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

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

Many authors have studied various properties of this *random trap model.*[4–24] 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[21,23] (see also Ref. 25), except in one dimension.[4,5,7,10,20] 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,[4] was the first to find an expression, valid for $q \to 0$, for the average number of steps until trapping $\langle n \rangle$ for simple random walks.[14] 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[15] 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[17,18] 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[5] and by Jain *et al.*[26–31] 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.(32)

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 $\hat{p}(\theta) := \sum_{l \in L} e^{il \cdot \theta} p(l)$, $\theta \in \mathbb{R}^d$, 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 $d' \leqslant d$) 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 $F = 1 - G^{-1}(0; 1) = 1$,(34) 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 $d \geqslant 3$ 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,(35) plays an important role in the work of Jain *et al.*(26–31) All random walks with $d \geqslant 5$ or with $\sum_{l \in L} |l|^2 p(l) < \infty$ and $\sum_{l \in L} l p(l) \neq 0$ are strongly transient.(29)

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 $z \to 1$ (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[36]

$$f_n = \langle (1-q)^{S_n} \rangle, \qquad n \geqslant 0 \tag{2.1}$$

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 $S_n \to \infty$ with probability 1 as $n \to \infty$, and hence $f_n \to 0$, 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

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

(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[5]

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

where

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

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

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 $S_n \to \infty$ with probability 1 as $n \to \infty$. The asymptotic behavior for large n of $\langle S_n \rangle$ can be extracted from Eq. (2.3). Furthermore, for simple random walks with $d \geqslant 2$ Dvoretsky and Erdös[38] proved that the stochastic variables S_n satisfy the so-called weak law of large numbers:

$$\lim_{n\to\infty} P[|S_n - \langle S_n \rangle| / \langle S_n \rangle > \varepsilon] = 0, \qquad \text{for } \varepsilon > 0 \tag{2.5}$$

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

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

($\text{Var } S_n := \langle S_n^2 \rangle - \langle S_n \rangle^2$) and using the Chebyshev inequality. They further improved Eq. (2.5) by proving that $S_n/\langle S_n \rangle \to 1$, $n \to \infty$, 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.[29] For recurrent random walks in $d = 1$ the asymptotic behavior is in general more complicated[29] and Eqs. (2.5) and (2.6) do not hold.

Jain *et al.*[26–31] 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 $d \geqslant 3$ 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):

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

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, $f_\infty := \lim_{n \to \infty} f_n$ 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[39] that R is of order $f'(\infty) - f'(0)$, where obviously $f'(\infty) := \lim_{n \to \infty} f'(n) = 0$. 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 $K_{n1} := \langle S_n \rangle$, $K_{n2} := \mathrm{Var}\, S_n$ and $K_{nj} (j \geqslant 3)$ is the jth 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

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

In order to find dn/dx we construct a systematic expansion in terms of λ (for a *given finite* x) for the inverse function $n(x)$ of $x(n)$, valid for small λ, 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 λ, 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 λ 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 λ 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 $\mathrm{Var}\, S_n$ contributes. If Eq. (2.6) holds this term is certainly *not* the leading term in q. Since only the leading term in n for $\mathrm{Var}\, S_n$ 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[40–41] (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 $j \geqslant 3$ is not known we shall also have to neglect contributions arising from these cumulants. However, it can be rigorously shown that if

$$\frac{\langle (S_n - \langle S_n \rangle)^j \rangle}{\langle S_n \rangle^{j-2}\, \mathrm{Var}\, S_n} \to 0, \qquad n \to \infty, \qquad \text{for all } j \geqslant 3 \tag{2.10}$$

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 Pruit[31] have proved that for all random walks with $d \geqslant 3$ 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) $\langle (S_n - \langle S_n \rangle)^4 \rangle = O(\mathrm{Var}^2\, S_n)$. 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 $1 \leqslant S_n \leqslant n + 1$ and $\langle S_n \rangle \simeq (1 - F)n \sim n$[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 $\mu := \sum_{l \in \mathrm{L}} l p(l) = 0$ and $m_2 := \sum_{l \in \mathrm{L}} |l|^2 p(l) < \infty$ (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 $\hat{p}(\theta) = 1 - \frac{1}{2} \sum_{i,j} C_{ij} \theta_i \theta_j + o(|\theta|^2)$, $\theta \to 0$, with $C_{ij} := \sum_{l \in \mathrm{L}} l_i l_j p(l)$, $i, j = 1,..., d$. 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 $d \geqslant 5$. 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 $m_3 := \sum_{l \in \mathrm{L}} |l|^3 p(l) < \infty$ 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[7] (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 $q \to 0$ as follows. Jain and Pruitt[29] have proved that the probability distribution of $S_n/\langle S_n \rangle$ converges for $n \to \infty$ to a limit distribution of which we merely note that it is *independent* of the random walk. They have also proved that $\langle S_n^k \rangle / \langle S_n \rangle^k$, $k \geqslant 2$, converges to the kth moment of this limit distribution. Using this result, together with the fact that $\langle S_n \rangle \simeq C(8n/\pi)^{1/2}$,[34] 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

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

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

$$G(0; z) = -u_1 \log(1-z) + u_1 u_2 + o((1-z)^{1/2}) \tag{2.13}$$

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[34,43]; e.g., for the simple random walk $u_2 = \log 8$. From Eqs. (2.3) and (2.13) it follows, as Henyey and Seshadri[43] 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 $c_k := (-d/dx)^k \Gamma^{-1}(x)|_{x=2}$ (Γ 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 $c_2 = (1-\gamma)^2 + 1 - \frac{1}{6}\pi^2$ (γ is Euler's constant).

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

$$\langle n \rangle = \frac{u_1}{q}\left[\log\left(\frac{u_1 u}{q}\right) + \log\log\left(\frac{u_1 u}{q}\right) + \frac{\log\log(u_1 u/q)}{\log(u_1 u/q)} + \frac{2K}{\log(u_1 u/q)} + \cdots\right] + \cdots \tag{2.16}$$

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 $j \geqslant 3$ 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

$\langle (S_n - \langle S_n \rangle)^j \rangle = O(\langle S_n \rangle^{j-3} \operatorname{Var}^{3/2} S_n)$ 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 $1 - \operatorname{Re} \hat{p}(\theta) \leq \frac{1}{2} \sum_{i,j} C_{ij} \theta_i \theta_j$ 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, $\hat{p}(\theta) - 1 + \frac{1}{2} \sum_{i,j} C_{ij} \theta_i \theta_j = o(|\theta|^2/\log^2 |\theta|)$, $\theta \to 0$, 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 $z \to 1$ 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[34,44–48]; e.g., for the simple random walk $u_0 = 1.516386....$ 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[28] have found that $\operatorname{Var} S_n \simeq \{(1-F)^4/2\pi^2 C^2\} n \log n$. Using this together with Eq. (2.18) we find

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

Since $\langle (S_n - \langle S_n \rangle)^4 \rangle = O(\operatorname{Var}^2 S_n)$,[28] 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 $z \to 1$ we have

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

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

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 $d \geqslant 5$. For $d=4$, but not for $d \geqslant 5$, we have assumed $m_3 < \infty$.

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

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

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

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

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

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

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

$$\langle n \rangle = \frac{u_0}{q} - \{1 + u_2 u_0^{-1} - u_0^2 a\} + \cdots, \qquad d \geqslant 5 \qquad (2.23\text{b})$$

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

For the simple random walk Montroll[34] has derived the following asymptotic series for u_0 in powers of $1/2d$:

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

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

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

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

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

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 $\hat{p}(\theta)-1+\frac{1}{2}\sum_{i,j} C_{ij}\theta_i\theta_j = o(|\theta|^2/\log|\theta|)$, $\theta \to 0$, 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).[2] Jain and Pruitt[29] 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[26] have proved that for all strongly transient random walks $\operatorname{Var} S_n \simeq \{F(1-F)+2a\}n$. As mentioned earlier, $\langle (S_n - \langle S_n \rangle)^4 \rangle = O(\operatorname{Var}^2 S_n)$ for random walks with $d \geqslant 3$ 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 $G(l; 1) \leqslant G(0; 1)$ 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 $m_1 = \infty$, μ 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 $d \geqslant 5$, $\langle n \rangle$ 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 $\mu \neq 0$ [33] or when $d \geqslant 3$, 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 $d \geqslant 3$ $\operatorname{Var} S_n \simeq \{F(1-F)+2a\}n$, except when $d=3$ *and* $\sum_{l \in L} G^2(l; 1)\, G(-l; 1) = \infty$ in which case $a=\infty$ and $\operatorname{Var} S_n = O(n \log n)$.[28] 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 $z \to 1$. 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

[2] 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 η 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 than 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

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

where $V_n^{(k)}$, $k = 1, \ldots, n + 1$, 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 $f_n(q, \eta) \leqslant f_n((1 - \eta)q, 0)$, so that $f_n \to 0$ as $n \to \infty$ 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

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

which was derived by Montroll and Weiss.[5]

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

$$f_n = \langle e^{-U_n}\rangle \tag{3.3}$$

with

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

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

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

$$0 < \lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_{n+1} \leqslant \lambda < \infty \tag{3.4}$$

(Note also that in the symbol U_n we suppress the dependence on q and η.) 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,[51] together with Eq. (3.4), we prove in Appendix B that for an arbitrary random walk $\lim_{n\to\infty} n^{-1}\langle U_n\rangle =: \zeta$ exists and

$$\lim_{n\to\infty} n^{-1} U_n = \zeta, \qquad \text{with probability 1} \tag{3.5}$$

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 $\lim_{n\to\infty} n^{-1}\langle V_n^{(k)}\rangle = 0$ for all k. Since $0 < U_n \leqslant \lambda S_n$, 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

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

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

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

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

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

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

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

We need Eq. (3.8) to calculate $\langle n\rangle$ for $q \to 0$. 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 η. 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 $q \to 0$ and $n \to \infty$ 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 $\{V_n^{(k)}\}_{k\geqslant 1}$. 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 $k, k' \geqslant 1$. 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),

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

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 $d \geqslant 3$ and for strongly transient random walks in $d = 1$ and 2. It is the work of Jain *et al.*[26–31] that has inspired this calculation.

For *strongly transient* random walks we find

$$\phi(n) = v_0^{-1} n + (v_0^{-1} + u_2 v_0^{-2}) + o(1) \tag{3.12a}$$

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

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

$$\langle n \rangle = \frac{v_0}{q} - \left\{ 1 + u_2 v_0^{-1} - v_0^2 a + \frac{\eta F}{1-\eta F} \right\} + \cdots \tag{3.14}$$

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

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

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

and we arrive at

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

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

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 $z\to 1$ 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 $0\leqslant\eta<1$. 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*

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

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

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

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

$$\langle n\rangle = \frac{u_1}{q}\left[\log\left(\frac{u_1 u}{q}\right) + \log\log\left(\frac{u_1 u}{q}\right) + \frac{\log\log(u_1 u/q)}{\log(u_1 u/q)} + \cdots\right] + \frac{\eta}{1-\eta}\frac{1}{q} + \cdots \qquad (3.20)$$

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 $0\leqslant\eta<1$, then it is clear that the contribution to $\langle n\rangle$ coming from Var U_n is $O(1/q \log q)$ because Var $S_n \sim n^2/\log^4 n$. We expect that it is possible to prove Var $U_n \sim$ 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) $G(0;z)\to\infty$ as $z\to 1$] 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 $p_i q$, $i=1,\ldots,t$, it is a trap with "escape" parameter $0 \leqslant \eta_i < 1$. 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

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

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

$$\langle n\rangle \simeq v_0/q, \qquad q\to 0 \tag{3.23}$$

with

$$v_0^{-1} := \sum_l p_l[u_0 + n_l/(1-\eta_l)]^{-1} \tag{3.24a}$$

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 η in Eq. (3.10a), we see from Eqs. (3.22a, b) that $\phi(n;\eta)$ generalizes to $\sum_l p_l \phi(n;\eta_l)$. 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

$$w_0^{-2} := \sum_l p_l[u_0 + n_l/(1-\eta_l)]^{-2} \tag{3.24b}$$

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 $\sum_l p_l \eta_l/(1-\eta_l)$ 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 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 $n\to\infty$.

In this connection it is worth mentioning a strong result on the asymptotic behavior of f_n for $n\to\infty$ found by Donsker and Varadhan[25] (see also Refs. 52–55). They proved that for aperiodic random walks, either with the property that $1-\hat{p}(\theta) \simeq A(e_\theta)\,|\theta|^\alpha$, $\theta\to 0$, 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 $\lambda > 0$:

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

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 $q \to 0$, the other with $n \to \infty$ 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 $q \to 0$. 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 $f_n \geqslant (1-q)^{\langle S_n \rangle}$, which follows from Eq. (2.1) and Jensen's inequality and which is the approximation to f_n originally used by Rosenstock.[14]

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 $d \geqslant 3$ 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 $p(1) = \gamma$, $p(-1) = 1 - \gamma$ ($\frac{1}{2} < \gamma \leqslant 1$) 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 $m_0 < m_1 < m_2 < \cdots$ at which a new point is visited (such that visits to old points occur at intermediate steps). Let $R_n = 1$ for $n = m_0, m_1, m_2, \ldots$, 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 $S = 1 + \sum_{n=1}^{\infty} R_n(1-q)^{R_0+R_1+\cdots+R_{n-1}}$, where the 1 counts the origin. Obviously, $m_0 = 0$ and $S = 1 + R_{m_1}(1-q) + R_{m_2}(1-q)^{1+R_{m_1}} + \cdots = 1 + (1-q) + (1-q)^2 + \cdots = q^{-1}$. This is true for any walk with the required property. But any nondegenerate random walk has this property with probability 1 (as $S_n \to \infty$ with probability 1) and hence we have the simple result

$$\langle S \rangle = q^{-1} \tag{4.2}$$

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 $d = 1$:

$$\langle S_{\langle n \rangle} \rangle \simeq q^{-1} \tag{4.3}$$

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[57] 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 ith and $(i+1)$th visit to a trap (given that these take place) is $\simeq 1/q$, $q \to 0$, for all $i \geqslant 1$; this follows from Eq. (3.9). If the walker "escapes" from a trap there is a probability $\leqslant F$ that he returns to that trap before hitting another one. As $q \to 0$ 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_l one with escape parameter η_l, 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 $q \geqslant u_1 u$ 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 η 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 η in which for the Bernoulli random walk the power η 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 $\tilde{\mathrm{L}}$ and place identical imperfect traps at identical position $l_i \in \tilde{\mathrm{L}}$, $i = 1, 2, \ldots$. 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 $T_{l;n}$ denote the probability that he is trapped by trap i at step n and let $f_i(z) := \sum_{n=0}^{\infty} z^n T_{l;n}$. A simple argument shows that

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

[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.

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APPENDIX A

For strongly transient random walks $G(0; z)$ behaves for $z \to 1$ 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[34] 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.[59] Substituting the expansion $I_0(x) = \sum_{k=0}^\infty (\frac{1}{2}x)^k/(k!)^2$ we find

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

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 $d \geqslant 3$ 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 $F(l; z) = [G(l; z) - \delta_{l0}]/G(0; z)$.[34] 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 $I_m(x) = (\frac{1}{2}x)^m \sum_{k=0}^\infty (\frac{1}{2}x)^k/k!(m+k)!$, $m \geqslant 0$, 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[51] the (finite) limit

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

exists with probability 1 and in mean, and $\langle \xi \rangle = \inf_{n\geq 1} n^{-1} \langle W_{0n} \rangle = \lim_{n\to\infty} n^{-1} \langle W_{0n} \rangle$. 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 $i > 0$

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

Equation (B4) means that for any given $i > 0$ the limit ξ depends on the walk only through the steps $i+1$, $i+2$,... and not through any of the previous steps (i.e., ξ 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 ξ 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 $\lim_{n\to\infty} n^{-1} S_n = \lim_{n\to\infty} n^{-1}\langle S_n\rangle$ $(=1-F)$ 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 $d\geqslant 3$ not in class I and strongly transient random walks in $d=1$ and 2 (for all random walks in this class $\sum_{l\in L} G^2(l;1)\,G(-l;1)<\infty$).[26,28,31]

We calculate 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 Var $U_n \sim$ Var S_n for all $0<q<1$ and $0\leqslant \eta<1$. We assume that the random walk is aperiodic and that $F>0$.

We start from Eq. (B1) and write

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

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

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

$$\begin{aligned}
Z_{i_1\cdots i_k} &:= I[l_{i_1}=\cdots=l_{i_k};\, l_{i_1}\neq l_\alpha,\, \alpha\in\{i_1+1,\ldots,\infty\}\backslash\{i_2,\ldots,i_k\}]\\
Z_{i_1\cdots i_k;n} &:= I[l_{i_1}=\cdots=l_{i_k};\, l_{i_1}\neq l_\alpha,\, \alpha\in\{i_1+1,\ldots,n\}\backslash\{i_2,\ldots,i_k\}]\\
W_{i_1\cdots i_k;n} &:= Z_{i_1\cdots i_k;n} - Z_{i_1\cdots i_k}\\
&:= I[l_{i_1}=\cdots=l_{i_k};\, l_{i_1}\neq l_\alpha,\, \alpha\in\{i_1+1,\ldots,n\}\backslash\{i_2,\ldots,i_k\};\\
&\qquad \exists\beta>n\colon l_{i_1}=l_\beta]\\
&\qquad k\geqslant 1,\quad 1\leqslant i_1<\cdots<i_k,\quad n\geqslant i_k
\end{aligned}$$

A little reflection shows that

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

(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

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

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

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

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

with

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

where for fixed i

$$Z_i^{(k)} := \sum_{i < i_2 < \cdots < i_k < \infty} Z_{i i_2 \cdots i_k}$$

$$= I[\text{after step } i \text{ the walker returns to } l_i \text{ exactly } k-1 \text{ times}] \tag{C5a}$$

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

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

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

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 $S_n^{(k+1)} \leqslant S_n^{(k)}$. To see that it holds, write $W_{i_1 i_2 \cdots i_{k+1}; n} = Z_{i_1 i_2; i_2} W_{i_2 \cdots i_{k+1}; n}$, substitute this product into Eq. (C3b) and use $\sum_{i_1=0}^{i_2-1} Z_{i_1 i_2; i_2} \leqslant 1$. To see that Eq. (C6b) holds, use $\sum_{n < i_{l+1} < \cdots < i_k < \infty} Z_{i_1 \cdots i_l i_{l+1} \cdots i_k} \leqslant W_{i_1 \cdots i_l; n}$.

In the following we shall calculate $\mathrm{Cov}(X_n^{(k)}, X_n^{(k')})$ to leading order in n. We shall show that $\mathrm{Cov}(X_n^{(k)}, X_n^{(k')})$ for *all* pairs k, k' and the two sums $(\sum_k \mu_k \mathrm{Var}^{1/2} X_n^{(k)})^2$ and $\sum_{k,k'} \mu_k \mu_{k'} \mathrm{Cov}(X_n^{(k)}, X_n^{(k')})$ for *all* $0 < q < 1$ and $0 \leqslant \eta < 1$ 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

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

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

and, with Eq. (C1b),

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

Our calculation will thus provide us with the leading order behavior in n of $\operatorname{Var} U_n$ and also make it evident that $\operatorname{Var} U_n \sim \operatorname{Var} S_n$ $(=\operatorname{Var} S_n^{(1)})$ and $\sum_k \mu_k \operatorname{Var}^{1/2} S_n^{(k)} \sim \operatorname{Var}^{1/2} S_n$. 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 $\langle W_n^{(1)^2} \rangle = o(\operatorname{Cov}(X_n^{(k)}, X_n^{(k')}))$ 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) $\operatorname{Var}(X_n^{(k)} - Y_n^{(k)}) \leqslant (k-1)^2 \langle W_n^{(1)^2} \rangle$, and together with the Schwarz inequality this implies that $\operatorname{Cov}(Y_n^{(k)}, Y_n^{(k')}) \simeq \operatorname{Cov}(X_n^{(k)}, X_n^{(k')})$. Second, by Eq. (C6a) $\operatorname{Var}(S_n^{(k)} - Y_n^{(k)}) \leqslant \langle W_n^{(1)^2} \rangle$ and hence $\operatorname{Cov}(S_n^{(k)}, S_n^{(k')}) \simeq \operatorname{Cov}(Y_n^{(k)}, Y_n^{(k')})$, 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 $0 \leqslant \eta < 1$.

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)

$$\operatorname{Cov}(X_n^{(k)}, X_n^{(k')}) = \sum_{l=0}^{n} \operatorname{Cov}(Z_l^{(k)}, Z_l^{(k')}) + \sum_{j=1}^{n} (a_j^{(k,k')} + a_j^{(k',k)}) \tag{C8}$$

with

$$a_j^{(k,k')} := \sum_{l=0}^{j-1} \operatorname{Cov}(Z_l^{(k)}, Z_j^{(k')}) \tag{C8a}$$

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

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

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 kth 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) $\mathrm{Cov}(Z_i^{(k)}, Z_j^{(k')}) = \mathrm{Cov}(Z_0^{(k)}, Z_{j-i}^{(k')})$, $j > i$, and we write out

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

with

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

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 $m = 0,..., k-1$ 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 mth time at step n. A standard type of argument shows that therefore

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

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 mth 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 remainig $n - n'$ steps reaches l for the *first* time with *returns* to 0 *allowed*. Therefore we have

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

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 $\mathrm{Var}\, U_n$. Noting that $\mu_k \simeq (1-\eta)\eta^{k-1} q$, $q \to 0$, we have

$$\mathrm{Var}\, U_n \simeq \phi_n q^2, \qquad q \to 0 \tag{C14}$$

with

$$\phi_n := (1-\eta)^2 \sum_{k,k'\geqslant 1} \eta^{k-1}\eta^{k'-1} \operatorname{Cov}(S_n^{(k)}, S_n^{(k')})$$

$$\simeq (1-\eta)^2 \sum_{k,k'\geqslant 1} \eta^{k-1}\eta^{k'-1} \operatorname{Cov}(X_n^{(k)}, X_n^{(k')}) =: \phi'_n \tag{C15}$$

where we use Eq. (C7c). We shall calculate ϕ'_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

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

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

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

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

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

with

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

Similarly,

$$c_l^{(k,k')} = d_l^{(k,k')} - d_l^{(k,k'-1)}, \qquad k' \geqslant 2, \qquad c_l^{(k,1)} = d_l^{(k,1)} \tag{C20}$$

with

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

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

$$\sum_{k,k' \geqslant 1} \eta^{k-1}\eta^{k'-1} b_l^{(k,k')} = (1-\eta)^2 \sum_{k,k' \geqslant 1} \eta^{k-1}\eta^{k'-1} d_l^{(k,k')} \tag{C21}$$

To evaluate the right-hand side we write

$$d_l^{(k,k')} = p_l^{(k,k')} + q_l^{(k,k')} - F_{-l}F^{k+k'-1} \tag{C22}$$

where we introduce the probabilities

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

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

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

$$\begin{aligned} p_l^{(k,k')} &= P_l[T_0^{(k)} < T_l^{(k'-1)} < T_l^{(k')} < \infty] \\ &\quad + P_l[T_l^{(k'-1)} < T_0^{(k)} < T_l^{(k')} < \infty] \end{aligned} \tag{C24}$$

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 $Fp_l^{(k,k'-1)}$. The second term factorizes into $P_l[T_l^{(k'-1)} < T_0^{(k)} < \infty,\, T_0^{(k)} < T_l^{(k')}]\, P_0[T_l^{(1)} < \infty]$, of which the first factor can be written as $q_l^{(k,k'-1)} - q_l^{(k,k')}$. Together this gives

$$p_l^{(k,k')} = Fp_l^{(k,k'-1)} + F_l[q_l^{(k,k'-1)} - q_l^{(k,k')}], \qquad k' \geqslant 2 \tag{C25a}$$

A similar reasoning shows that

$$q_l^{(k,k')} = Fp_l^{(k-1,k')} + F_{-l}[p_l^{(k-1,k')} - p_l^{(k,k')}], \qquad k \geqslant 2 \tag{C25b}$$

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

$$\begin{aligned} p_l^{(k,1)} &= P_l[T_0^{(k)} < T_l^{(1)} < \infty] \\ &= P_l[T_0^{(1)} < T_l^{(1)}, T_0^{(1)} < \infty] \\ &\quad \times \{P_0[T_0^{(1)} < T_l^{(1)} < \infty]\}^{k-1} P_0[T_l^{(1)} < \infty] \\ &= \{F_{-l} - q_l^{(1,1)}\}\{F - p_{-l}^{(1,1)}\}^{k-1} F_l, \qquad k \geqslant 1 \end{aligned} \tag{C26a}$$

and similarly

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

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

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

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

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

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

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

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

Equations (C18) and (C34) are exact expressions from which the coefficients ϕ_n' in Eq. (C16) can be deduced. We are now ready to use Eq. (C15) and find the leading order behavior in n of ϕ_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 $\sum_{l\in L} G^2(l;1)\,G(-l;1)<\infty$ we deduce from Eq. (C34) that

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

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

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

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

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

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

For random walks with $d = 3$, $\mu = 0$ and $m_2 < \infty$ it is shown in Ref. 29 (p. 379) that $\sum_{l \neq 0} G_l G_{-l} G_l^j \simeq (2\pi C)^{-2} \log j$, $j \to \infty$, 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 $\mathrm{Cov}(X_n^{(k)}, X_n^{(k')})$ for all k and k', and the two sums $(\sum_k \mu_k \mathrm{Var}^{1/2} X_n^{(k)})^2$ and $\sum_{k,k'} \mu_k \mu_{k'} \mathrm{Cov}(X_n^{(k)}, X_n^{(k')})$ for all $0 < q < 1$ and $0 \leqslant \eta < 1$, 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 $\sum_{k,k'} \eta^{k-1} \eta^{k'-1} \mathrm{Cov}(X_n^{(k)}, X_n^{(k')})$ and found that it has the mentioned property for all $0 \leqslant \eta < 1$. Now with the analysis given above it is not hard to calculate also the sums $\sum_k z^{k-1} \mathrm{Var}^{1/2} X_n^{(k)} =: \rho_n(z)$, $0 \leqslant z < 1$, and $\sum_{k,k'} z_1^{k-1} z_2^{k'-1} \mathrm{Cov}(X_n^{(k)}, X_n^{(k')}) =: \rho_n(z_1, z_2)$, $0 \leqslant z_1, z_2 < 1$. 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 $\sum_k \mu_k \mathrm{Var}^{1/2} X_n^{(k)} = -\sum_{r \geqslant 1} (1/r)[-q/(1-q)]^r (1-\eta^r) \rho_n(\eta^r)$ and $\sum_{k,k'} \mu_k \mu_{k'} \mathrm{Cov}(X_n^{(k)}, X_n^{(k')}) = \sum_{r,r' \geqslant 1} (1/rr')[-q/(1-q)]^{r+r'} (1-\eta^r)$ $(1-\eta^{r'})\, \rho_n(\eta^r, \eta^{r'})$ 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 $(\sum_k \mu_k \mathrm{Var}^{1/2} X_n^{(k)})^2 \geqslant \sum_{k,k'} \mu_k \mu_{k'} \mathrm{Cov}(X_n^{(k)}, X_n^{(k')})$.) From the result for $\rho_n(z_1, z_2)$ one further easily deduces (cf. Ref. 37, p. 232) that also the individual $\mathrm{Cov}(X_n^{(k)}, X_n^{(k')})$ 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 Var U_n and shall need in the next appendix.

APPENDIX D

The purpose of this appendix is to prove that

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

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

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

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

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

where μ_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 $\langle (x+y)^4 \rangle^{1/4} \leqslant \langle x^4 \rangle^{1/4} + \langle y^4 \rangle^{1/4}$ for any pair of stochastic variables x, y and hence by Eq. (C1a) $\langle (U_n - \langle U_n \rangle)^4 \rangle^{1/4} \leqslant \sum_k \mu_k \langle (S_n^{(k)} - \langle S_n^{(k)} \rangle)^4 \rangle^{1/4}$, so that

$$\langle (U_n - \langle U_n \rangle)^4 \rangle \leqslant t_n^4 \, \mathrm{Var}^2 \, S_n$$

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

We start from Eq. (C2) and write

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

with

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

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

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

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

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

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

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

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 $n^{-1}\operatorname{Var} S_n$ is asymptotically a monotone, nondecreasing and slowly varying function of n. Thus $\operatorname{Var} S_{2n+1} \simeq 2 \operatorname{Var} S_n$ and it now follows from Eqs. (C6a), (D2), (D3), and (D6) that there is a constant $M < \infty$ such that

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

where we use that $\sum_k \mu_k \operatorname{Var}^{1/2} S_n^{(k)} \sim \operatorname{Var}^{1/2} S_n$ (which was shown in Appendix C) and that $\sum_k k\mu_k < \infty$ for all $0 < q < 1$ and $0 \leqslant \eta < 1$. [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 $2^{-1/8} + (M/\gamma) \leqslant 1$. Suppose that for some integer m we have $t_m \geqslant \gamma$. Then it follows from Eq. (D7) that $(t_{2n+1}/t_m) \leqslant 2^{-1/8}(t_n/t_m) + (M/\gamma)$ for $n \geqslant m$. This implies that $t_{2m+1} \leqslant t_m$ and it follows by induction that $t_n \leqslant t_m$ for n in the subsequence of integers of the form $n = 2^j(m+1) - 1 =: n_j, j \geqslant 0$. Next, consider $n_{j-1} < n < n_j$ for some j. Trivially,

$$\langle (S_n^{(k)} - \langle S_n^{(k)} \rangle)^4 \rangle^{1/4} \leqslant [\langle (S_n^{(k)} - \langle S_n^{(k)} \rangle)^4 \rangle + \langle (S_{n_j-n-1}^{(k)} - \langle S_{n_j-n-1}^{(k)} \rangle)^4 \rangle + 6 \operatorname{Var} S_n^{(k)} \cdot \operatorname{Var} S_{n_j-n-1}^{(k)}]^{1/4}$$

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

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

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

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Chapter III

Random walks on lattices with points of two colours
I.

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RANDOM WALKS ON LATTICES WITH POINTS OF TWO COLOURS. I

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This paper is concerned with random walks on lattices with two kinds of points, black and white. The colours of the points are random variables with a translation invariant, but otherwise arbitrary, joint probability distribution. The steps of the walk are independent of the colours. We study the stochastic properties of the length of the subwalk from the starting point to a first black point and of subwalks between black points visited in succession, and establish a number of exact relations. These relations can be applied to a trapping problem by identifying the black points with imperfect traps. An example is discussed.

1. Introduction

The theory of random walks on lattices with traps has developed into a well-established branch of random-walk theory. Calculations have been made on quantities such as the mean value and higher moments of the number of steps the walker makes before being trapped[1-5]), the probability that the walker returns to the starting point without having been trapped[6]) and the mean square displacement after a given number of steps (diffusion)[7,8]). One can extend the theory by letting the traps be imperfect, i.e. by allowing the walker to escape with finite probability when stepping on a trap[9-13]).

As a rule, the traps are assumed to be distributed either periodically or randomly over the lattice. Except for one dimension, rigorous results have been obtained only for periodic trap distributions. The case of a random trap distribution is much harder to treat and the results obtained are approximations valid for trap concentrations that are either small or close to unity. Other trap distributions have not been studied, to the best of our knowledge.

The aim of this paper is to present a number of exact relations which are valid for all walks and for a large class of trap distributions, including the periodic and random distribution. In section 2 we temporarily disregard the effect of trapping and instead consider a random walk on a lattice with points of two colours, called black and white. The colours of the points are assumed to be random variables, distributed according to a joint probability distribution which is translation invariant but otherwise completely arbitrary. The colours, once chosen, are considered to be frozen in and the steps of the walk are assumed to be independent of the colours. We study the stochastic properties of the length of the subwalk from the starting point to a first black point and of subwalks between successive visits to black points, and we establish a number of useful relations. These relations are applied in section 3 by identifying the black points with imperfect traps. More applications will be presented in a subsequent paper. Section 4 is devoted to a discussion.

2. Exact relations

Consider an infinite d-dimensional lattice L. Suppose that the points of L are coloured "black" and "white" according to some joint probability distribution $\mathcal{P}$. More precisely, to each *local* configuration of black and white points (i.e. to each finite set of points $\Lambda \subset L$ and each partition of Λ into a set of black points and a set of white points) a probability is attributed. If this is done in a consistent way, these probabilities determine a unique probability distribution $\mathcal{P}$ for the infinite lattice (see ref. 14, p. 34).

We assume that $\mathcal{P}$ is *translation invariant* or, equivalently, that two local configurations obtained from each other by a translation have equal probability. The probability that a given point $l \in L$ is black is then independent of l; we denote it by q and assume that $q > 0$.

Simple examples are the following distributions: (i) the *random* distribution, in which the colours of different points are independently and identically distributed; (ii) distributions obtained by choosing an arbitrary periodic configuration of black and white points on L (i.e. a configuration such that L can be divided into identical *finite* unit cells having identical local configurations) and assigning equal probability to all distinct configurations obtained from the given one by a translation; distributions of this type we call *periodic*; (iii) the *uniform* distribution where L is entirely black with probability q or entirely white with probability $1-q$; (iv) a (translation invariant) *grand canonical* distribution (Gibbs state) of a lattice gas of black points with a given interaction and chemical potential (see ref. 15, pp. 4.1 and 5.1).

Now consider a random walk on L starting at the origin 0 and proceeding according to some probability distribution p for single steps, with $\Sigma_{l\in L}\, p(l) = 1$, which is *independent* of the colouring of L (and translation invariant as usual). We are interested in the walker's visits to black points ("hits"), in particular in the stochastic properties of the number of steps made before the first hit and between successive hits. A subwalk between successive hits we call a run. Two black points hit in succession may or may not be identical.

We consider the following two stochastic processes:

(0) The process $(n_0, n_1, n_2, \ldots)$, where n_0 is the number of steps made before the first hit ($n_0 \geqslant 0$) and $n_i (i = 1, 2, \ldots)$ is the length of the ith run ($n_i > 0$); for convenience we call the subwalk to the first black point hit the 0th run;

(1) The process $(0, n_1, n_2, \ldots)$ obtained from (0) by the restriction that n_0 be zero, i.e. that the origin be black.

These processes are based on the two independent probability distributions $\mathscr{P}$ and p for the colouring of the lattice and the single steps of the walk. They are both processes in a generalized sense in that the number of black points visited may be finite (i.e. only a finite number of runs is completed). Consequently, averages such as $\langle n_i \rangle$ should be understood as conditional averages given that the ith run is completed. Furthermore, averages in process 1 are in turn conditional averages in process 0 given that $n_0 = 0$. Nevertheless we prefer to speak of 0 and 1 as separate processes; accordingly, we denote averages by $\langle\,\rangle_0$ and $\langle\,\rangle_1$, respectively.

We shall show that the stochastic properties of either process can be expressed rigorously in terms of those of the other process. From this relationship we derive the following results:

A) In process 0, the probability that for the first time a black point is hit at step n_0 is a monotonically decreasing function of n_0.

B) In process 0, the probability f_i that at least $i+1$ black points are hit is, for all $i > 0$, equal to the probability f_0 that at least one black point is hit. In process 1, the corresponding probabilities p_i equal one. In other words, once the walker has hit a first black point he almost surely will hit arbitrarily many.

C) Process 1 is stationary; hence the stochastic variables n_i are identically distributed in this process. Furthermore, $\langle n_1 \rangle_1 = f_0 q^{-1}$. More generally, each of the moments of n_1 in process 1 can be linearly expressed in terms of lower moments of n_0 in process 0.

D) In process 0, the moments of n_i with $i > 0$ can be expressed in terms of correlations in process 1: $\langle n_i^k \rangle_0 = \langle n_1 n_{i+1}^k \rangle_1 / f_0 q^{-1} (k = 1, 2, \ldots)$.

The proof runs as follows. We define for $i \geqslant 0$, $n \geqslant 0$ and $n_i > 0 (i = 1, 2, \ldots)$:

$P_{nn_1 \ldots n_i}$:= the probability that a black point is hit at step n and that subsequently at least i runs, of lengths $n_1, \ldots, n_i$, are completed;

$F_{nn_1 \ldots n_i}$:= the probability that for the *first* time a black point is hit at step n and that subsequently at least i runs, of lengths $n_1, \ldots, n_i$, are completed.

(For $i = 0$ these symbols are to be replaced by P_n and F_n, respectively). Process 0 is described by the set of all probabilities $F_{n_0 n_1 \dots n_i}$ with $i \geqslant 0$, process 1 by $F_{0 n_1 \dots n_i}$ with $i > 0$.

Now the translation invariance of both $\mathscr{P}$ and p entails a crucial property: $P_{nn_1 \dots n_i}$ is independent of n (in particular, $P_n = P_0 = q$). To see this, observe that for $P_{nn_1 \dots n_i}$ (but not for $F_{nn_1 \dots n_i}$) each point that can be reached from the origin in one step could equally well have been considered as the point from where the walk has started. Thus, for all $n > 0$, $P_{nn_1 \dots n_i} = P_{n-1\, n_1 \dots n_i}$, and hence

$$P_{nn_1 \dots n_i} = P_{0n_1 \dots n_i}. \tag{2.1}$$

This argument is easily written out in terms of the probability distributions $\mathscr{P}$ and p.

If the walker hits a black point he either does so for the first time or there has been a last preceding hit. Hence, for $n > 0$

$$P_{nn_1 \dots n_i} = F_{nn_1 \dots n_i} + \sum_{m=1}^{n} P_{n-m\, mn_1 \dots n_i}. \tag{2.2}$$

Using eq. (2.1) we may write

$$F_{nn_1 \dots n_i} = P_{0n_1 \dots n_i} - \sum_{m=1}^{n} P_{0mn_1 \dots n_i}. \tag{2.3a}$$

For $n = 0$

$$F_{0n_1 \dots n_i} = P_{0n_1 \dots n_i}. \tag{2.3b}$$

Eqs. (2.3) are the basic equations from which we derive the properties A to D.

A) From eq. (2.3a) it follows that for all $n_0 > 0$

$$F_{n_0 - 1\, n_1 \dots n_i} - F_{n_0 n_1 \dots n_i} = P_{0n_0 n_1 \dots n_i} \geqslant 0. \tag{2.4a}$$

In particular for $i = 0$

$$F_{n_0 - 1} - F_{n_0} \geqslant 0. \tag{2.4b}$$

(We remark in passing that a similar inequality does in general not hold for P_n).

To prove B to D we introduce the following generating functions:

$$f_i(z_0, z_1, \dots, z_i) := \sum_{n_0=0}^{\infty} z_0^{n_0} \sum_{n_1, \dots, n_i = 1}^{\infty} z_1^{n_1} \dots z_i^{n_i} F_{n_0 n_1 \dots n_i}, \tag{2.5}$$

$$p_i(z_1, \dots, z_i) := \sum_{n_1, \dots, n_i = 1}^{\infty} z_1^{n_1} \dots z_i^{n_i} P_{0n_1 \dots n_i} P_0^{-1}, \tag{2.6}$$

($|z_j| \leqslant 1$, $j = 0, \dots, i$). Using eqs. (2.3) and noting that $P_0 = q$, we find

$$q^{-1}(1 - z_0) f_0(z_0) = 1 - p_1(z_0), \tag{2.7a}$$

and for $i>0$

$$q^{-1}(1-z_0)f_i(z_0, z_1, \ldots, z_i) = p_i(z_1, \ldots, z_i) - p_{i+1}(z_0, z_1, \ldots, z_i). \tag{2.7b}$$

The sets of generating functions defined by eqs. (2.5) and (2.6) contain all the information on the statistical properties of the two processes; eqs. (2.7) relate these properties and from them one can deduce relations between the moments of the n_i.

B) The probabilities f_i and p_i are obtained from the generating functions (2.5) and (2.6), respectively, by setting all arguments equal to one. Making this substitution in eqs. (2.7) and noting that $f_i \leq 1 < \infty$, we find by induction:

$$p_i = 1 \quad (i = 1, 2, \ldots). \tag{2.8}$$

If instead we now set all arguments equal to one except z_0 then, on account of this result, eqs. (2.7) reduce to

$$q^{-1}(1-z_0)f_i(z_0, 1, \ldots, 1) = 1 - p_{i+1}(z_0, 1, \ldots, 1). \tag{2.9}$$

Whenever a black point is hit, the probability that a next run is completed is, of course, ≤ 1. It follows that for $0 \leq z_0 \leq 1$

$$f_{i+1}(z_0, 1, \ldots, 1, 1) \leq f_i(z_0, 1, \ldots, 1), \tag{2.10}$$

$$p_{i+2}(z_0, 1, \ldots, 1, 1) \leq p_{i+1}(z_0, 1, \ldots, 1). \tag{2.11}$$

Using eq. (2.9), we see that both these equations reduce to equalities. Then, by setting finally $z_0 = 1$, we find

$$f_i = f_0 (i = 1, 2, \ldots). \tag{2.12}$$

C) The moments $\langle n_i^k \rangle_0$ and $\langle n_i^k \rangle_1$ (which are conditional averages given that the ith run is completed) are given by

$$\langle n_i^k \rangle_0 = f_i^{-1}\left[\left(z_i \frac{d}{dz_i}\right)^k f_i(z_0, \ldots, z_i)\right]_{z_0 = \cdots = z_i = 1}, \tag{2.13}$$

$$\langle n_i^k \rangle_1 = p_i^{-1}\left[\left(z_i \frac{d}{dz_i}\right)^k p_i(z_1, \ldots, z_i)\right]_{z_1 = \cdots = z_i = 1}. \tag{2.14}$$

Setting $z_0 = 1$ in eq. (2.7b) we find that

$$p_i(z_1, \ldots, z_i) = p_{i+1}(1, z_1, \ldots, z_i). \tag{2.15}$$

This equation expresses the stationarity of process 1. From this it follows that $\langle n_i^k \rangle_1 = \langle n_1^k \rangle_1$, for all $i > 0$. From eq. (2.7a) we deduce

$$\langle n_1 \rangle_1 = f_0 q^{-1}, \tag{2.16}$$

$$\langle n_1^2 \rangle_1 = f_0 q^{-1}(1 + 2\langle n_0 \rangle_0) \tag{2.17}$$

and similar relations in which $\langle n_1^k \rangle_1$ is expressed in terms of the moments $\langle n_0^j \rangle_0$ with $0 \leq j < k$.

D) Differentiating eq. (2.7b) once with respect to z_0 and k times with respect to $z_i (i > 0)$ we find

$$\langle n_i^k \rangle_0 = \langle n_1 n_{i+1}^k \rangle_1 / f_0 q^{-1}. \tag{2.18}$$

This completes the proof.

One can also easily derive a number of inequalities for the moments. We give two examples. Obviously, $\langle n_1^2 \rangle_1 \geq \langle n_1 \rangle_1^2$. By combining this with eqs. (2.16) and (2.17) we get

$$\langle n_0 \rangle_0 \geq \tfrac{1}{2}(f_0 q^{-1} - 1). \tag{2.19}$$

Also, noting that $\langle n_1 n_{i+1} \rangle_1 \leq \frac{1}{2}\langle n_1^2 + n_{i+1}^2 \rangle_1 = \langle n_1^2 \rangle_1$ and using eqs. (2.17) and (2.18), we find

$$\langle n_0 \rangle_0 \geq \tfrac{1}{2}(\langle n_i \rangle_0 - 1), \tag{2.20}$$

for all $i > 0$.

Eqs. (2.19) and (2.20) reduce to equalities for several special cases, e.g. for a 'one-sided' nearest-neighbour walk in $d = 1$ (with $p(1) = 1$) and a strictly periodic colour distribution (i.e. with one black point per unit cell). Therefore they represent the strongest bounds generally valid.

3. An application to lattices with traps

Suppose that the black points considered in section 2 are traps characterized by a probability of escape η, i.e. whenever the walker visits a black point there is a fixed probability $1 - \eta$ that he is trapped (forever) and a probability η that he remains free. If $\eta = 0$ ($\eta > 0$) the trap is called perfect (imperfect).

One is usually interested in the stochastic properties of process 0 modified by trapping. Let T_n be the probability that the walker is trapped after exactly n steps and let $T(z) := \Sigma_{n=0}^{\infty} z^n T_n$ be the generating function for trapping. Then a simple argument shows that

$$T(z) = (1 - \eta) \sum_{i=0}^{\infty} \eta^i f_i(z), \tag{3.1}$$

where $f_i(z)$ is the generating function defined by eq. (2.5) with all arguments equal to z. Eq. (3.1) shows that in order to calculate $T(z)$ one has to know all the functions $f_i(z)$ characterizing process 0.

Without knowing $T(z)$ explicitly we can prove a simple result, namely that T_n is a monotonically decreasing function of n. Indeed, noting that $T_0 =$

$q(1-\eta)$ and using eqs. (3.1) and (2.7), we find

$$\sum_{n=1}^{\infty} z^n (T_{n-1} - T_n) = q(1-\eta) - (1-z)T(z) = q(1-\eta)^2 \sum_{i=1}^{\infty} \eta^{i-1} p_i(z), \tag{3.2}$$

with $p_i(z)$ defined in analogy with $f_i(z)$. Since the coefficients in each $p_i(z)$ are nonnegative it follows that

$$T_{n-1} - T_n \geqslant 0, \tag{3.3}$$

for all $n > 0$. A consequence of this inequality (which reduces to eq. (2.4b) for $\eta = 0$) is that $T_{n'} = 0$ implies that $T_n = 0$ for all $n > n'$. Conversely, if there are arbitrarily large values of n for which $T_n > 0$, then $T_n > 0$ for each n.

We further remark that, by eqs. (2.12) and (3.1), the total probability of trapping $\Sigma_{n=0}^{\infty} T_n$ equals f_0 for all $\eta < 1$.

For process 1 modified by trapping a relation similar to eq. (3.1) can be written down and the results of section 2 can be carried over in a similar way.

4. Discussion

In section 2 we have introduced two stochastic processes and established a rigorous relationship between them. This relationship was then used to derive several properties of the separate processes. The results derived are valid for all types of lattices, all translation invariant colour distributions and all walks, and therefore are necessarily of a modest nature. Stronger results may be obtained as more specific assumptions are introduced. Examples will be given in subsequent papers. However, it is a challenge to see what can be derived without making such assumptions.

Process 0 is perhaps physically the more interesting one and some of its properties (almost exclusively the stochastic properties of n_0) have, in some form or other, been discussed in the literature for the random distribution and for periodic distributions. In the latter case one usually considers what we call the black points as having fixed positions and one assumes that the walk may start with equal probability at any point of a unit cell. Obviously, this is equivalent to our assumption of a fixed starting point and a translation invariant colour distribution.

The properties of process 1 seem not to have received any attention thus far. One may conceive of physical situations which can be described by this process and we expect that actual applications can be found.

As was derived in section 2, process 1 is stationary. Process 0, on the other hand, is in general not stationary. Furthermore, both in process 0 and in process 1 the n_i are in general *not* independently distributed (nor are the processes Markovian). This stems from the fact that different black points may have different 'environments'. Conversely, it is the reason why the stochastic properties of the $n_i (i > 0)$ in process 0 are not identical to those in process 1, in other words why process 1 does not describe the runs in process 0 made after the first black point has been hit. It is the correlation between successive runs that presents the great difficulty in studying the processes in detail.

In spite of the existing differences the processes 0 and 1 are, of course, similar in nature. Thus one may expect that under suitable circumstances (notably for $d \geqslant 2$ and $q \ll 1$) and for a large class of distributions, the effect of the zeroth run on subsequent runs in process 0 is relatively small and, consequently, that e.g. $\langle n_i \rangle_0 \approx \langle n_i \rangle_1 = f_0 q^{-1}$, $i > 0$.

The case of a strictly periodic distribution is special because there, obviously, all black points have the same environment. As a consequence, the n_i are independent and the generating functions (2.5) and (2.6) factorize as follows:

$$f_i(z_0, z_1, \dots, z_i) = f_0(z_0) p_1(z_1) \dots p_1(z_i), \tag{4.1a}$$

$$p_i(z_1, \dots, z_i) = p_1(z_1) \dots p_1(z_i). \tag{4.1b}$$

The set of equations (2.7b) reduces to eq. (2.7a) and both processes are completely described by $f_0(z_0)$ or, alternatively, by $p_1(z_1)$. From eqs. (3.1), (4.1a) and (2.7a) we then find

$$T(z) = (1-\eta) f_0(z)[1 - \eta p_1(z)]^{-1} = f_0(z)\left[1 + \frac{\eta}{1-\eta} q^{-1}(1-z) f_0(z)\right]^{-1}, \tag{4.2}$$

(cf. ref. 12, eq. (3.3)). Thus, in this case the extension to imperfect traps presents no difficulty at all.

We conclude the discussion by commenting on a few specific results.

(a) The monotonicity of T_n expressed by eq. (3.3) may seem to be somewhat surprising. Neither for periodic distributions (where an explicit expression for $T(z)$ is known[12]), nor for a random distribution (where at least for $\eta = 0$ a formal expression for $T(z)$ in terms of the number of distinct lattice points visited can be given[5]) is this result otherwise obvious. It means that short walks are (equally or) more probable than long walks, no matter how small q is or how close to unity η. Thus all distributions of T_n with a maximum (such as the one suggested in ref. 16 for strictly periodic distributions and $\eta = 0$) are excluded.

(b) Whereas p_1 always equals 1, f_0 may take values in the interval $[q, 1]$ depending on the particular choice of the probability distributions $\mathcal{P}$ and p. For example, in the uniform distribution, where L is entirely black with probability q or entirely white with probability $1-q$, obviously $f_0 = q$ for all walks. However, one can show that in almost all cases of physical interest $f_0 = 1$.

For instance, in the case of a random colour distribution it suffices to exclude the degenerate walk where $p(0) = 1$ (i.e. the walker stays forever at 0), since for all other walks the number of distinct lattice points visited goes to infinity with probability 1 as the number of steps increases. The latter statement may be proved as follows. If $d > 1$, suppose that there is a lattice point $l \neq 0$ such that $p(l) > 0$. Consider the line through 0 and l and the projection of the random walk on this line, parallel to some $(d-1)$-dimensional lattice plane containing 0 but not l. This projection is itself a (translation invariant) non-degenerate random walk on a one-dimensional lattice L'. Clearly, the number of distinct points visited on L' is not larger than that visited on L. Hence, it is sufficient to give the proof for $d = 1$. In this case consider the event that the walker remains forever in an interval of length $M < \infty$. In order to do so he has to reverse his direction infinitely often, each time after at most M steps, chosen from a finite collection. Since each of these reversals has a probability bounded above by some constant $C_M < 1$, the event has probability zero, which completes the proof.

In the case of a periodic colour distribution f_0 equals 1 if the walk is *aperiodic* (in the sense of Spitzer, ref. 17, p. 20). This is easily extracted from the analysis given in ref. 2, using the fact that in terms of the structure function of the walk $\hat{p}(\theta) := \Sigma_{l \in L} e^{il \cdot \theta} p(l)$ aperiodicity is equivalent to $\hat{p}(\theta) = 1$ iff $\theta = 0 \pmod{2\pi}$; this equivalence is proved in ref. 17, p. 67. If the walk is not aperiodic, the walker can only visit points in a proper sublattice $L_0 \subset L$. In such a case f_0 may be smaller than 1, but this is not necessarily the case. Since the walk is aperiodic on L_0, it follows from the argument given above that $1 - f_0$ is equal to the probability that the entire sublattice L_0 is white. To see this, it suffices to observe that if L_0 is not white, it certainly contains some periodic configuration of black and white points. Examples are easily constructed.

We shall discuss f_0 for general distributions in a subsequent paper.

(c) The result $\langle n_i \rangle_1 = f_0 q^{-1}$, for all $i > 0$, is the direct generalization of a well-known result derived by Montroll for strictly periodic distributions (ref. 18, eq. (III. 16)). A striking feature of our result is its generality: for all cases where $f_0 = 1$, $\langle n_i \rangle_1$ equals q^{-1} independently of the dimension of the lattice and all further details of the walk and the colour distribution. In particular for the random distribution it is one of the rare *exact* results. Its simplicity is in sharp contrast with what may be found for $\langle n_i \rangle_0$. One can, for instance, easily find simple (though extreme) one-dimensional examples where $\langle n_1 \rangle_0$ takes any value $\geqslant 1$ for given q.

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Chapter IV

Random walks on lattices with points of two colours
II. Some rigorous inequalities for symmetric random walks

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Random Walks on Lattices with Points of Two Colors. II. Some Rigorous Inequalities for Symmetric Random Walks

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We continue our investigation of a model of random walks on lattices with two kinds of points, "black" and "white." The colors of the points are stochastic variables with a translation-invariant, but otherwise arbitrary, joint probability distribution. The steps of the random walk are independent of the colors. We are interested in the stochastic properties of the sequence of consecutive colors encountered by the walker. In this paper we first summarize and extend our earlier general results. Then, under the restriction that the random walk be symmetric, we derive a set of rigorous inequalities for the average length of the subwalk from the starting point to a first black point and of the subwalks between black points visited in succession. A remarkable difference in behavior is found between subwalks following an odd-numbered and subwalks following an even-numbered visit to a black point. The results can be applied to a trapping problem by identifying the black points with imperfect traps.

KEY WORDS: Random walks; inhomogeneous lattice; colored points; average length of successive runs; ergodic theorems; perfect and imperfect traps.

1. INTRODUCTION

In a previous paper[1] we have introduced a model of a random walk on a lattice of which the points can carry two different colors, "black" and "white." The colors are (not necessarily independent) frozen-in stochastic variables. We have obtained rigorous results for a number of stochastic properties of the sequence of consecutive colors encountered by the walker while stepping through the lattice. The model may serve to describe certain transport processes in disordered media, such as the diffusion and trapping

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of "particles" in a medium with static traps. Our aim is to obtain results which are valid for a broad range of different types of diffusion and disorder, and therefore we have kept the model as general as possible. In addition, this model is an example of a doubly stochastic process which we feel is interesting in its own right.

The definitions are as follows. Consider an infinite d-dimensional lattice L and suppose that the points of L are colored *black* and *white* according to a given joint probability distribution $\mathscr{P}$. $\mathscr{P}$ is assumed to be *translation invariant*. The probability that a given point $l \in L$ is black is thereby independent of l; we denote it by q and assume that $q > 0$. Next consider a random walk on L, starting at the origin and proceeding according to a given probability distribution p for single steps. It is assumed that p is *independent* of the coloring of L (and translation invariant as usual).

A color distribution $\mathscr{P}$ may be defined by attributing probabilities to *local* configurations of black and white points, i.e., partitions of *finite* subsets of L into a set of black points and a set of white points with the colors of points outside the subset unspecified. If this is done in a consistent way, these probabilities determine a unique probability distribution for the infinite lattice (as is guaranteed by the so-called extension theorem; see Ref. 2, Vol. 2, p. 118). Two local configurations that are obtained from each other by a translation must be assigned equal probability in order to acquire translation invariance. $\mathscr{P}$ is otherwise completely arbitrary. Examples are (see Ref. 1): (i) the *random* distribution; (ii) (translation-invariant) *periodic* distributions; (iii) the *uniform* distribution; (iv) (translation-invariant) *grand canonical* distributions (Gibbs states).

The step distribution p may be chosen to be any function $p: L \to \mathbb{R}$ with $p(l) \geq 0$ and $\sum_{l \in L} p(l) = 1$, where $p(l)$ is the probability of a step over the lattice vector l; p assigns probabilities to the individual steps of the walker, independent of the colors by assumption and, of course, independent of previous steps.

We are interested in the walker's visits to black points, called "hits," more in particular in the stochastic properties of the number of steps made before the first hit and between successive hits. A subwalk between successive hits we call a *run* and, for convenience, we call the subwalk to the first hit the zeroth run. In Ref. 1 we have considered the following two stochastic processes:

(0) The process $(n_0, n_1, n_2, \ldots)$, where n_i is the length of the ith run, $i \geq 0 (n_0 \geq 0;\ n_i \geq 1,\ i \geq 1)$.

(1) The process $(0, n_1, n_2, \ldots)$ obtained from (0) by the restriction that n_0 be zero, i.e., that the origin be black.

Both processes are entirely determined by the two independent probability distributions $\mathscr{P}$ and p. The number of black points visited may be finite, i.e., it may happen that only a finite number of runs is completed. Averages such as $\langle n_i \rangle$ will, however, be understood as conditional averages given that the ith run is *completed* (i.e., given that at least $i+1$ black points are visited). Furthermore, averages in process 1 are in turn *conditional* averages in process 0 given that $n_0 = 0$. Nevertheless, we prefer to speak of 0 and 1 as separate processes; accordingly we denote averages by $\langle \cdots \rangle_0$ and $\langle \cdots \rangle_1$, respectively.

In Ref. 1 we have shown, using a simple "renewal-type" argument (of the type used, e.g., in Ref. 2, Vol. 1, Chap. 13) in combination with our assumption of translation invariance, that the stochastic properties of either process can be expressed rigorously in terms of those of the other. From this relationship we have derived several general properties. Here is a list of the main results:

A. In process 0 the probability that a first black point is hit at step n_0 is a *monotone* nonincreasing function of n_0.

B. Let f_i, $i \geqslant 0$, be the probability that in process 0 at least the ith run is completed. Let p_i, $i \geqslant 1$, be the corresponding probability in process 1. Then

$$f_i = f_0, \qquad \text{for all } i \geqslant 1 \tag{1.1}$$

$$p_i = 1, \qquad \text{for all } i \geqslant 1 \tag{1.2}$$

C. Process 1 is *stationary*; hence the stochastic variables n_i are identically distributed in this process. Furthermore, each of the moments of n_1 in process 1 can be linearly expressed in terms of lower moments of n_0 in process 0. In particular,

$$\langle n_1 \rangle_1 = f_0 q^{-1} \tag{1.3}$$

$$\langle n_1^2 \rangle_1 = f_0 q^{-1}(1 + 2\langle n_0 \rangle_0) \tag{1.4}$$

D. In process 0 the moments of n_i with $i \geqslant 1$ can be expressed in terms of *correlations* in process 1. In particular,

$$\langle n_i \rangle_0 = \langle n_1 n_{i+1} \rangle_1 / \langle n_1 \rangle_1, \qquad i \geqslant 1 \tag{1.5}$$

E. In process 0 the following inequalities hold:

$$\langle n_0 \rangle_0 \geqslant \tfrac{1}{2}(f_0 q^{-1} - 1) \tag{1.6}$$

$$\langle n_0 \rangle_0 \geqslant \tfrac{1}{2}(\langle n_i \rangle_0 - 1), \qquad \text{for all } i \geqslant 1 \tag{1.7}$$

In process 0 the n_i with $i \geq 1$ are in general *not* identically distributed. Furthermore, both in process 0 and in process 1 the lengths of the successive runs are in general *correlated*. This stems from the fact that different black points may have different "environments," which is the reason why it is difficult to study the processes in detail. Process 0 is physically the more interesting one and has our main interest. Process 1 serves more or less as an "auxiliary" process.

The above remarks summarize the results of Ref. 1. The outline of this paper is as follows. In Section 2 we study the probability f_0 in more detail. The result is:

F. In process 0

$$f_0 = 1 - \mathscr{P}[\bar{L} \text{ is white}] \tag{1.8}$$

where $\bar{L}$ is the smallest sublattice of L to which the random walk is confined.

The results obtained thus far are valid for arbitrary L, $\mathscr{P}$, and p and are therefore necessarily of a modest nature. Stronger results can be obtained as more specific assumptions are introduced. In Section 3, which constitutes the main part of the paper, we focus on one such specific assumption, viz. that the random walk is *symmetric*, i.e., that $p(l) = p(-l)$ for all l. Under this assumption we derive the following set of inequalities, assuming (without loss of generality) that (a) the color distribution is *extremal* (i.e., $\mathscr{P}$ cannot be decomposed into two distinct translation-invariant components), (b) the random walk covers the *whole* lattice (i.e., $\bar{L} = L$), so that $f_0 = 1$:

G. For the zeroth run in process 0

$$\langle n_0 \rangle_0 \geq (1-q)^2/q(1-X) \tag{1.9}$$

where $X := \text{Prob}[n_1 = 1 \mid n_0 = 0] = q^{-1} \sum_{l \in L} p(l)\, \mathscr{P}[0 \text{ and } l \text{ are black}]$.

H. For the higher runs in process 0 let $\Delta_i := \langle n_i \rangle_0 - q^{-1}$. Then

$$\Delta_1 \geq \Delta_3 \geq \Delta_5 \geq \Delta_7 \geq \cdots \geq 0$$

$$\Delta_1 \geq |\Delta_2|,\ \Delta_3 \geq |\Delta_4|,\ \Delta_5 \geq |\Delta_6|, \ldots \tag{1.10}$$

We further show:

I. For periodic color distributions $\Delta_i \to 0$ as $i \to \infty$, exponentially fast, irrespective of the random walk. For general color distributions decay is expected to occur in most cases, but it may be slower than exponential.

In Section 3.1 we first consider periodic color distributions. The unit cell of the periodic pattern will be completely arbitrary. The arguments used are essentially probabilistic and are based on simple matrix algebra. The derivation presented for this case will set the stage for the extension to arbitrary (translation-invariant) color distributions, which is given in Section 3.2 and requires the use of certain ergodic theorems. In Section 4 we apply our results by identifying the black points with imperfect traps. Section 5 is devoted to a discussion, including some examples and a few references to related results in the literature.

The reader who is not interested in the derivation of F–I may wish to skip Sections 2 and 3 and go straight to Section 4.

When in the following we speak of runs we shall mean runs in process 0, unless stated otherwise. As in the previous paper, the assumption of translation invariance will play a key role in the calculations.

2. THE PROBABILITY f_0

The probability f_0 that the zeroth run is completed plays an important part in Ref. 1 and appears in many of the formulas. Of course, this probability may depend on L, $\mathscr{P}$, and p. In this section we shall study f_0 in more detail.

Let us use the symbol $P_n(l)$ to denote the probability that the walker visits point $l \in L$ at step n. Let further

$$L^+ := \{l \in L: P_n(l) > 0 \text{ for some } n \geqslant 0\}$$

L^+ is the set of all points that can be reached by the walker in a finite number of steps; it depends on p. We shall first prove that

$$f_0 = 1 - \mathscr{P}[L^+ \text{ is white}] \tag{2.1}$$

Proof. When L^+ is white there are no black points that the walker can reach and the zeroth run cannot be completed ($n_0 = \infty$). To prove Eq. (2.1) we must show that $n_0 < \infty$ with probability 1 when it is given that L^+ contains a black point.

The plan of the proof is to use Eq. (1.2). Now Eq. (1.2) states that given that the origin is black the walker will with probability 1 hit arbitrarily many black points, or in other words, there exists with probability 1 an infinite sequence of steps at which the walker hits a black point. By the translation invariance of $\mathscr{P}$ it immediately follows that also the following is true: given that l is black there exists with probability 1 an infinite sequence of step numbers $k_0(=0) < k_1 < k_2 < \dots$ such that $l_{k_j} + l$ is black, where l_n stands for the point visited at step n. These step numbers are, of course, stochastic variables. It is important that the above statement is true for *all* $l \in L$.

Next, let $l \in L^+$ and let m be the smallest integer with $P_m(l) > 0$. Assume that l is black and let $m_0(=0) < m_1 < m_2 < \dots$ be the infinite sequence of the smallest elements of $(k_j)_{j \geq 0}$ with the property that $m_{j+1} - m_j \geq m$ for all j. We define the following sequence of events: E_j, $j \geq 0$, is the event $\{m_i < \infty$ for $i \leq j$ and $l_{m_j+m} = l_{m_j} + l\}$, or in other words, the event that the first $j+1$ step numbers in the sequence $(m_j)_{j \geq 0}$ indeed exist and that the visit to l_{m_j} is followed by a visit to the black point $l_{m_j} + l$ at the mth subsequent step. Clearly, the event E_j has probability $\rho_j = P_m(l) > 0$, independent of j. Moreover, since $m_{j+1} - m_j \geq m$ the events are independent. It follows from the second Borel–Cantelli lemma[2] that, as $\sum_j \rho_j = \infty$, with probability 1 arbitrarily many among the events E_j will occur.

We have now reached the following result: given that some point of L^+ is black the walker will with probability 1 hit arbitrarily many black points. But, trivially, this implies that $f_i = \mathscr{P}[L^+$ contains a black point$]$ for all $i \geq 0$. Equation (2.1) is the special case for $i = 0$ (note that from Eq. (1.1) we already knew that all the f_i are equal). This completes the proof. ∎

Equation (2.1) may be slightly strengthened. Let

$$\bar{L} := \{l \in L: l = l' - l'' \text{ for some } l', l'' \in L^+\}$$

$\bar{L}$ is the smallest sublattice of L that contains L^+ (see Ref. 3, p. 15); it is the lattice on which the random walk "actually takes place." In many cases $\bar{L} = L$, but not in all. We shall now prove that

$$f_0 = 1 - \mathscr{P}[\bar{L} \text{ is white}] \tag{2.2}$$

Proof. Since $L^+ \subset \bar{L}$ it follows that $\mathscr{P}[\bar{L}$ is white$] \leq \mathscr{P}[L^+$ is white$]$. To prove Eq. (2.2) we must show that the equality sign holds. To do so we shall again use the translation invariance of $\mathscr{P}$.

The proof will depend on the following remarkable property. Let $L' := \{l_k\}$, $k \in \mathbb{Z}$, be *any* line of points in L, i.e., $l_k = l_a + k l_b$ for some $l_a, l_b \in L$ with $l_b \neq 0$. If L' contains *one* black point then with probability 1 it contains *infinitely many*, extending in both directions. Indeed, let $c_k := \mathscr{P}[l_k$ is black, $l_{k'}$ is white for all $k' > k]$. Then we have $\mathscr{P}[L'$ contains a black point and a white positive half-line$] = \sum_{k \in Z} c_k$. Now obviously $\sum_{k \in Z} c_k \leq 1$. By the translation invariance of $\mathscr{P}$, however, c_k is independent of k and so it must be that $c_k = 0$. Hence $\sum_{k \in Z} c_k = 0$, which proves that if

L' contains one black point it contains with probability 1 infinitely many on the positive half-line $k \geqslant 0$. For the negative half-line the argument, of course, runs the same. This proves the statement.

We shall use the above-mentioned property in combination with some elementary properties of the structure of L^+. When $L^+ = \bar{L}$ there is nothing to prove as then Eqs. (2.1) and (2.2) are identical. For the rest of the proof we shall therefore assume that $L^+ \neq \bar{L}$. We want to show that $\mathscr{P}[L^+ \text{ is white}] - \mathscr{P}[\bar{L} \text{ is white}] = \mathscr{P}[L^+ \text{ is white}, \bar{L} \setminus L^+ \text{ contains a black point}] = 0$.

Let us begin by specializing to the case $d = 1$. We may assume that $\bar{L} = L(= \mathbb{Z})$, since it will be clear that there is no loss of generality in doing so. (Note that the *degenerate* random walk with $p(0) = 1$ has $L^+ = \bar{L} = \{0\}$ and is therefore excluded by our assumption that $L^+ \neq \bar{L}$.) Let $\Sigma := \{l \in L: p(l) > 0\}$. L^+ is the set of all finite sums of elements of Σ (i.e., L^+ is the additive semigroup generated by Σ). Suppose first that $p(l) = 0$ for $l < 0$. Then all elements of L^+ are nonnegative. Because L^+ is not contained in any proper sublattice of $\mathbb{Z}$, the greatest common divisor of the elements of Σ is 1. This implies that $l \in L^+$ for l sufficiently large, so that L^+ contains a positive half-line. It now follows that $\mathscr{P}[L^+ \text{ is white}, L \setminus L^+ \text{ contains a black point}] \leqslant \mathscr{P}[\mathbb{Z} \text{ contains a black point and a white positive half-line}] = 0$, which is the required equality. When $p(l) = 0$ for $l > 0$ the result is the same. When, finally, Σ has both positive and negative elements it is readily seen that $L^+ = \bar{L}$, which is the trivial case excluded. This proves Eq. (2.2) for $d = 1$.

The proof for $d \geqslant 2$ follows almost as a corollary. L^+ may have a variety of forms depending on L and p, but since L and $\mathscr{P}$ are completely arbitrary there is again no loss of generality in assuming that $\bar{L} = L$. To get the desired result it now suffices to observe that for any point $l \in L$ there exists a line through l that has a half-line in common with L^+ (this derives, in fact, from a simple group-theoretical property). It follows that given that l is black there are with probability 1 infinitely many black points in L^+. Since l is arbitrary this again implies that $\mathscr{P}[L^+ \text{ is white}, L \setminus L^+ \text{ contains a black point}] = 0$, which completes the proof of Eq. (2.2). ∎

Equation (2.2) is a strong result: once it is known that there is *some* black point in $\bar{L}$ it follows that with probability 1 *some* black point is hit. For recurrent random walks this is not surprising, for in this case always $L^+ = \bar{L}$ and *each* point of L^+ is hit with probability 1 (see Ref. 3, p. 19), but for transient random walks it is. It should be emphasized, however, that the generality of Eq. (2.2) is due entirely to the translation invariance of $\mathscr{P}$. The proof shows that $\bar{L}$ is either white or contains infinitely many black points extending in *all* directions. This property explains some of the background of Eqs. (1.2) and (2.2). In Section 3.2 we shall take a closer look at the effect of the translation invariance on the coloring of L and show that with probability 1 an "asymptotic density" of black points exists.

From Eq. (2.2) it follows that in almost all cases of physical interest $f_0 = 1$. Indeed, when the random walk is *aperiodic* (in the sense of Spitzer, Ref. 3, p. 20) we have $\bar{L} = L$ (by definition), in which case $f_0 = 1$ if the possibility that L is white has zero probability. For the random distribution $f_0 = 1$ if only we exclude the degenerate random walk which has $f_0 = q$ (in all other cases $|\bar{L}| = \infty$). It will be clear that when $\bar{L} \neq L$ the problem is in a sense "ill posed" and, instead of $\mathscr{P}$, one may then as well consider the restriction of $\mathscr{P}$ to $\bar{L}$, which is obviously translation invariant on $\bar{L}$.

Finally, Eq. (2.2) shows that cases with $f_0 < 1$ are in a sense nothing but trivial extensions of cases with $f_0 = 1$. Assume $\bar{L} = L$. If $f_0 < 1$ there is a positive probability that L is white, but then it is always possible to reduce the problem by writing $\mathscr{P}$ as the (unique) *convex linear combination* of two translation-invariant color distributions $\mathscr{P}'$ and $\mathscr{P}''$, viz. $\mathscr{P} = f_0 \mathscr{P}' + (1 - f_0)\mathscr{P}''$, with $\mathscr{P}'[L \text{ is white}] = 0$ and $\mathscr{P}''[L \text{ is white}] = 1$. Since we are interested in completed runs only, $\mathscr{P}''$ is the "irrelevant" part that does not contribute to the averages in our model. $\mathscr{P}'$, on the other hand, covers all relevant events and thus one may reduce the problem by "scaling" $\mathscr{P}$ to $\mathscr{P}'$. This also explains why the probabilities q and f_0 always appear in the combination f_0/q: for $\mathscr{P}'$ we have the corresponding probabilities $q' = q/f_0$ and $f_0' = f_0/f_0 = 1$, and q' is the "effective" probability that a point is black once the problem is reduced by scaling.

In the following we shall assume, for reasons which will become clear later, that $\mathscr{P}[L \text{ is black}] = 0$. By the same argument it will be clear that this minor restriction involves no loss of generality.

3. RIGOROUS INEQUALITIES FOR SYMMETRIC RANDOM WALKS

We shall henceforth center interest on the *moments* $\langle n_i \rangle_0$, $i \geq 0$. Whereas the probabilities f_i equal 1 for practically all choices of L, $\mathscr{P}$, and p, these moments depend strongly on this choice.

As observed in Ref. 1, one may derive from Eqs. (1.3)–(1.5), noting that $\langle n_1^2 \rangle_1 \geq \langle n_1 \rangle_1^2$ and $\langle n_1 n_{i+1} \rangle_1 \leq \frac{1}{2}\langle n_1^2 + n_{i+1}^2 \rangle_1 = \langle n_1^2 \rangle_1$, the following two inequalities mentioned in the Introduction:

$$\langle n_0 \rangle_0 \geq \tfrac{1}{2}(f_0 q^{-1} - 1) \tag{3.1}$$

$$\langle n_0 \rangle_0 \geq \tfrac{1}{2}(\langle n_i \rangle_0 - 1), \qquad \text{for all } i \geq 1 \tag{3.2}$$

These equations reduce to equalities for a few special cases.

With a simple scaling argument Eq. (3.1) may be slightly refined to obtain a stronger bound that depends on p:

$$\langle n_0 \rangle_0 \geq \tfrac{1}{2}(f_0 q^{-1} - 1)/[1 - p(0)] \tag{3.1a}$$

Unfortunately, however, it does not seem easy to do better in general. No upper bound was found in Ref. 1. Furthermore, for the runs with number $i \geq 1$ no lower bound was found. Here it should be noted that for *any given* $q > 0$ [and $p(0)$ fixed] one easily constructs simple (though somewhat extreme) examples where $\langle n_0 \rangle_0$ can take *arbitrarily large* values or $\langle n_i \rangle_0$ can take *any* value > 1 for *given* $i \geq 1$. Thus Eqs. (3.1a) and (3.2) are by nature weak. One may expect stronger results if one places restrictions on $\mathscr{P}$ or on p, or both.

In the following we shall investigate the case where p is *symmetric*. We shall derive a set of rigorous inequalities which are valid for arbitrary (translation-invariant) color distributions. In Section 3.1 we first consider periodic color distributions. The extension to arbitrary color distributions is given in Section 3.2.

3.1. Periodic Color Distributions

We begin with some definitions. A periodic color *configuration* is an arrangement of black and white points in L such that L can be divided into identical *finite* unit cells ("blocks") having identical (local) color configurations (in other words, there is a periodic pattern of colors). A *translation-invariant* periodic color *distribution* is obtained by choosing an arbitrary periodic color configuration and assigning equal probability to all distinct configurations obtained from the chosen one by a translation. Examples are: (i) a *strictly* periodic distribution, where the black points form a sublattice of L and the (smallest) unit cell contains one black point; (ii) a *pair*-periodic distribution, where the (smallest) unit cell contains two black points.

Consider first an *arbitrary* random walk p on L. We shall find it convenient to change our point of view in two ways. First, since we are not interested in the positions at which the walker hits the black points we shall consider the random walk as taking place on a single unit cell with *periodic boundary conditions* imposed. This unit cell we denote by $\tilde{L}$. Second, rather than sticking to our description with a fixed starting point for the walker and a translation-invariant color distribution, we shall fix the positions of the colors and, instead, allow the walker to start with equal probability at any point of $\tilde{L}$. The two descriptions are obviously equivalent; however, the latter description facilitates the discussion somewhat.

Let, then, N be the number of points in $\tilde{L}$, $B = \{l_1, ..., l_t\} \subset \tilde{L}$ the set of black points in $\tilde{L}(1 \leqslant t < N)$ and $W = \tilde{L} \backslash B$ the set of white points. $\tilde{L}$ and the sets B and W are *completely arbitrary*. The results which we derive depend only on the existence of a unit cell. We may assume that $t < N$, i.e., that W is not empty, as otherwise the model is trivial. Of course, $q = t/N$.

(I) The Zeroth Run. The zeroth run plays a special role in that it may start either on a black or on a white point. If the walker starts in B then $n_0 = 0$; if he starts in W then he can go through a succession of visits to points of W before hitting a point of B. We define

$$p_{ll'} := \text{probability of a step from } l \text{ to } l';\ l, l' \in \tilde{L}$$

(taking into account the periodic boundary conditions!). Further, let $\boldsymbol{p} := (p_{ll'})_{l,l' \in W}$ denote the $(N-t) \times (N-t)$ matrix that has as elements the stepping probabilities between the *white* points. Of course, $\boldsymbol{p}$ depends on p as well as on the shape and the coloring of $\tilde{L}$.

Now the average $\langle n_0 \rangle_0$ can be expressed in terms of $\boldsymbol{p}$ as follows. Let

$$w_n := \text{probability that after } n \text{ steps the walker has not yet hit a black point; } n \geqslant 0.$$

In order not to hit B the walker must start in W and make steps between points of W only. Recalling that with probability N^{-1} the walker may start at any point of $\tilde{L}$, we therefore have

$$w_n = N^{-1} \sum_{l,l' \in W} (\boldsymbol{p}^n)_{ll'}, \qquad n \geqslant 0 \tag{3.3}$$

We shall assume that $f_0 = 1$. (This condition will be removed later.) Then $w_n \to 0$ as $n \to \infty$ and by the monotonicity of w_n

$$\langle n_0 \rangle_0 = \sum_{n=1}^{\infty} n(w_{n-1} - w_n) = \sum_{n=0}^{\infty} w_n \tag{3.4}$$

(see Ref. 2, Vol. 1, p. 265). Hence by Eq. (3.3)

$$\langle n_0 \rangle_0 = N^{-1} \sum_{l,l' \in W} (\mathbf{1} + \boldsymbol{p} + \boldsymbol{p}^2 + \cdots)_{ll'} \tag{3.5}$$

where $\mathbf{1}$ denotes the $(N-t) \times (N-t)$ unit matrix. Note that $\boldsymbol{p}$ does *not* include any steps from W to B that are needed by the walker to reach a black point. These steps will appear in the calculation at a later stage.

Obviously, $\sum_{l' \in W} p_{ll'} \leqslant 1$ for all $l \in W$. This property is expressed by saying that the matrix $\boldsymbol{p}$ is *substochastic*. The condition $f_0 = 1$ implies that strict inequality holds for *at least one* $l \in W$ (as otherwise the walker could never escape from W once he had started in W), and thus p is *strictly substochastic*. Now it is well known that the eigenvalues of a (nonnegative) strictly substochastic matrix are all strictly smaller in modulus than unity (see, e.g., Refs. 4 and 5). Since we shall need this property later we give the proof.

Proof. First assume that p is irreducible. Then the well-known Perron–Frobenius theorem for nonnegative (square) matrices[4,5] states that p has a real eigenvalue $\lambda_1 > 0$ with the following properties:

(i) λ_1 is nondegenerate and with it are associated strictly positive left and right eigenvectors.

(ii) $|\lambda| \leqslant \lambda_1$ for any other eigenvalue λ of p.

(iii) $\lambda_1 \leqslant \max_{l \in W}(\sum_{l' \in W} p_{ll'})$ and $\lambda_1 \leqslant \max_{l' \in W}(\sum_{l \in W} p_{ll'})$.

By (iii) one has $\lambda_1 \leqslant 1$. However, $\lambda_1 = 1$ is excluded, since if $x := (x_l)_{l \in W}$ is the left eigenvector associated with λ_1 then $\lambda_1 = 1$ would imply that

$$\sum_{l' \in W} x_{l'} = \sum_{l \in W} x_l \left(\sum_{l' \in W} p_{ll'} \right) \leqslant \sum_{l \in W} x_l$$

and hence, by (i), that $\sum_{l' \in W} p_{ll'} = 1$ for all $l \in W$. With (ii) this completes the proof for irreducible p. When p is reducible one can through a permutation of its rows and columns obtain a matrix of the form

$$\begin{bmatrix} p_{11} & 0 \\ p_{21} & p_{22} \end{bmatrix}$$

where p_{11} and p_{22} are square matrices and p_{11} is either zero or irreducible. A repetition of the above argument shows that p_{11} cannot have an eigenvalue 1, and the proof is completed by induction. ∎

Thus it is seen that the condition $f_0 = 1$ entails that $|\lambda| < 1$ for all eigenvalues λ of p. This in turn implies that the inverse of $1 - p$ exists, so that we may write for Eq. (3.5)

$$\langle n_0 \rangle_0 = N^{-1}(e, (1-p)^{-1} e) \tag{3.6}$$

where e denotes the $(N-t)$-vector with all elements equal to 1 and $(.,.)$ stands for the vector inner product. An important consequence of the existence of $(1-p)^{-1}$ is that $\langle n_0 \rangle_0 < \infty$.

So far we have not yet made any assumption concerning the random walk p. Even though Eq. (3.6) may not be a very suitable starting point for a detailed calculation of $\langle n_0 \rangle_0$, it will serve us here to obtain a bound in the case of a symmetric random walk. Therefore we now, as promised, assume that p is *symmetric*, i.e.,

$$p(l) = p(-l), \qquad \text{for all } l \in L \tag{3.7}$$

Equation (3.7) implies that the matrix $\boldsymbol{p}$ is symmetric (because a step and its reverse between any two points of $\tilde{L}$ are equally probable by symmetry). Therefore all eigenvalues of $\boldsymbol{p}$ are real and it immediately follows that $\mathbf{1} - \boldsymbol{p}$ is *positive definite*. This is the crucial property in the argument: we can now use a matrix inequality known as the Kantorovich inequality (see Ref. 6, p. 117 and Ref. 7, p. 69), which gives in our case

$$(e, (\mathbf{1} - \boldsymbol{p})\, e)(e, (\mathbf{1} - \boldsymbol{p})^{-1}\, e) \geqslant (e, e)^2 \tag{3.8}$$

and yields with Eq. (3.6)

$$\langle n_0 \rangle_0 \geqslant (e, e)^2 / N(e, (\mathbf{1} - \boldsymbol{p})\, e) \tag{3.9}$$

The right-hand side of Eq. (3.9) is easy to evaluate. Indeed, we have $(e, e) = N - t$ and $(e, \boldsymbol{p}e) = \sum_{l,l' \in W} p_{ll'} = N - 2t + \sum_{l,l' \in B} p_{ll'}$, where now the probabilities of steps to and from *black* points appear as we use that $\sum_{l \in \tilde{L}} p_{ll'} = 1$ for all $l' \in \tilde{L}$ and $\Sigma_{l' \in \tilde{L}} p_{ll'} = 1$ for all $l \in \tilde{L}$; the latter equalities follow from the condition $\sum_{l \in L} p(l) = 1$. Thus we finally arrive at

$$\langle n_0 \rangle_0 \geqslant (1 - q)^2 / q(1 - X) \tag{3.10}$$

with $q = t/N$ and $X := t^{-1} \sum_{l,l' \in B} p_{ll'}$.

The condition $f_0 = 1$ is easily removed. As observed at the end of Section 2, cases with $f_0 < 1$ are trivial extensions of cases with $f_0 = 1$, and a simple scaling argument has made it clear that in the general case q should be replaced by q/f_0. In our setting $\tilde{L}$ may be partitioned into two sets S' and S'' from which the walker has probability 1 and 0, respectively, to reach B. S' is a sublattice of $\tilde{L}$ (or a union of sublattices), $B \subset S'$ and $f_0 = |S'|/N$. Because $\langle n_0 \rangle_0$ is a conditional average given that the zeroth run is completed, only those walks that start from S' will contribute. S' takes over the role of $\tilde{L}$, $f_0' = 1$, and $q' = |B|/|S'| = q/f_0$. Hence the general result is

$$\langle n_0 \rangle_0 \geqslant (f_0 q^{-1} - 1)^2 / f_0 q^{-1} (1 - X) \tag{3.11}$$

Equation (3.11) is the first of a series of inequalities that are the object of this section. Note that the connection between process 0 and process 1, as seen in Eq. (1.4), reappears through X: X is the probability that $n_1 = 1$ given that $n_0 = 0$. Note further that $X < 1$. X depends on p as well as on the shape and the coloring of $\tilde{L}$. In all cases, however, $X \geqslant p(0)$ so that we have the weaker but simpler bound

$$\langle n_0 \rangle_0 \geqslant (f_0 q^{-1} - 1)^2 / f_0 q^{-1} [1 - p(0)] \tag{3.12}$$

which is to be compared with Eq. (3.1a). Here only the variable q appears as prominent and the dependence on $\mathscr{P}$ and p has disappeared nearly altogether.

Equation (3.11) is stronger than Eq. (3.1a). When $f_0 = 1$ this is obvious for $q \leqslant \frac{1}{2}$. For $q > \frac{1}{2}$, on the other hand, note that $X \geqslant 1 + (1 - q^{-1})[1 - p(0)]$ and hence $\langle n_0 \rangle_0 \geqslant (1 - q)/[1 - p(0)]$. Incidentally, the latter inequality is trivial.

For several special cases Eq. (3.11) reduces to an equality, e.g., for any unit cell and a random walk that is "indifferent" with respect to $\tilde{L}$, in the sense that from any point of $\tilde{L}$ the probability of a jump to any other point is $1/(N-1)$ [here $f_0 = 1$ and $p(0) = 0$]. An example is the case with $L = \mathbb{Z}$, the strictly periodic distribution with $q = 1/3$ and the simple random walk (where steps to nearest-neighbor points have equal probability and other steps are not allowed). In the derivation of Eq. (3.11) we have used of $\boldsymbol{p}$ only its symmetry. Obviously, the translation invariance of p places *additional restrictions* on $\boldsymbol{p}$ (to be more specific, $\boldsymbol{p}$ is obtained from a cyclic stochastic matrix by deleting certain rows and columns). If this fact were exploited Eq. (3.11) could perhaps be strengthened further.

(II) The Runs with Number $i \geqslant 1$. The runs with number $i \geqslant 1$ all start from a black point. This is, however, all that they have in common. As pointed out earlier, the n_i are in general *not* independent *nor* are they identically distributed, to the effect that the moments $\langle n_i \rangle_0$ for different i take different values.

To study $\langle n_i \rangle_0$, $i \geqslant 1$, we shall make explicit use of the relations between process 0 and process 1 established in Ref. 1. We define

$$\Delta_i := \langle n_i \rangle_0 - f_0 q^{-1}, \qquad i \geqslant 1 \tag{3.13}$$

$$\gamma_i := \langle n_1 n_{i-1} \rangle_1 - \langle n_1 \rangle_1 \langle n_{i+1} \rangle_1, \qquad i \geqslant 1 \tag{3.14}$$

With Eqs. (1.3) and (1.5) we have

$$\Delta_i = \gamma_i / f_0 q^{-1} \tag{3.15}$$

This relation says that the amount by which $\langle n_i \rangle_0$ differs from $f_0 q^{-1}$ is directly related to the *correlation* of the runs 1 and $i+1$ in process 1. By studying γ_i we shall be able to get information about Δ_i. In particular, since $f_0 q^{-1} > 0$ either Δ_i and γ_i have the same sign or they are both zero.

Process 1 is in a sense easier than process 0 because it is stationary. Also in process 1, however, the n_i are in general *not* independent to the effect that the γ_i, and hence the Δ_i, are $\neq 0$. Note that in Eq. (3.13) the term $f_0 q^{-1}$ is, by Eq. (1.3), the average of n_i in process 1 (!). Thus one could say that in process 0 the zeroth run, through its mere existence, has an effect on all subsequent runs. Note that $\langle n_i \rangle_0 < \infty$ for all $i \geqslant 1$ by Eq. (3.2), as $\langle n_0 \rangle_0 < \infty$.

(a) The First Run. Let us consider the first run to begin with. Again we first assume that p is arbitrary and begin with some definitions:

$T_n(i \to j) :=$ probability for the walker, when starting from $l_i \in B$, to make a run of exactly n steps to $l_j \in B$; $n \geqslant 1$; $i, j = 1, \dots, t$.

$p_{n_1 n_2} :=$ probability that in process 1 the first run has length n_1 and the second run length n_2. (3.16)

With these definitions we shall write out γ_1.

In process 1 the walker may start with probability t^{-1} at any point of B and so

$$p_{n_1 n_2} = t^{-1} \sum_{i,j,k} T_{n_1}(i \to j)\, T_{n_2}(j \to k) \tag{3.17}$$

From Eq. (3.16) we get

$$\begin{aligned} \langle n_1 n_2 \rangle_1 &= \sum_{n_1, n_2} n_1 n_2\, p_{n_1 n_2} \Big/ \sum_{n_1, n_2} p_{n_1 n_2} \\ &= t^{-1} \sum_{i,j,k} S_{ij} S_{jk} \Big/ t^{-1} \sum_{i,j,k} T_{ij} T_{jk} \end{aligned} \tag{3.18}$$

where we introduce

$$T_{ij} := \sum_n T_n(i \to j) \tag{3.19a}$$

$$S_{ij} := \sum_n n T_n(i \to j) \tag{3.19b}$$

The probabilities T_{ij}, $i, j = 1, \dots, t$, form a matrix of what may be called "transition" probabilities between different "states": T_{ij} is the total probability of a run from l_i to l_j. Because $\bar{L}$ is finite

$$\sum_j T_{ij} = 1, \qquad \text{for all } i \tag{3.20a}$$

[See also Eq. (1.2).] Also the following is true:

$$\sum_i T_{ij} = 1, \qquad \text{for all } j \tag{3.20b}$$

This is seen by comparing the random walk p with the *reversed* random walk $\tilde{p}$ obtained from p by defining $\tilde{p}(l) = p(-l)$, $l \in L$. For each $n \geqslant 1$ the probabilities $T_n(i \to j)[p]$ and $T_n(i \to j)[\tilde{p}]$ in Eq. (3.16), corresponding to p and $\tilde{p}$, are related as

$$T_n(i \to j)[\tilde{p}] = T_n(j \to i)[p]$$

This gives $T_{ij}[\tilde{p}] = T_{ji}[p]$, so that Eq. (3.20b) follows from Eq. (3.20a), which is valid for all p. In all cases therefore $\boldsymbol{T} := (T_{ij})$ is what is called a *doubly stochastic* matrix.

Using Eq. (3.20a) we may simplify Eq. (3.18) a little bit to

$$\langle n_1 n_2 \rangle_1 = t^{-1} \sum_{i,j,k} S_{ij} S_{jk} \tag{3.21}$$

The product $\langle n_1 \rangle_1 \langle n_2 \rangle_1$, which is the second term of γ_1 in Eq. (3.14), is known from Eq. (1.3), but we shall want for it an expression similar to Eq. (3.21). Following a similar line of reasoning as above we get

$$\langle n_1 \rangle_1 = t^{-1} \sum_{i,j} S_{ij} \tag{3.22a}$$

$$\langle n_2 \rangle_1 = t^{-1} \sum_{i,j,k} T_{ij} S_{jk} = t^{-1} \sum_{j,k} S_{jk} \tag{3.22b}$$

where we use Eq. (3.20b). Combining with Eq. (3.21) we thus arrive at

$$\gamma_1 = t^{-1} \sum_{i,j,k} S_{ij} S_{jk} - \left\{ t^{-1} \sum_{i,j} S_{ij} \right\}^2 \tag{3.23}$$

Now we are ready to use the *symmetry* of p, which will again be seen to be of crucial importance. From Eq. (3.7) it follows that $p = \tilde{p}$ and hence that $\boldsymbol{T}$ and $\boldsymbol{S} := (S_{ij})$ are symmetric. Defining

$$S_i := \sum_j S_{ij}, \qquad i = 1, \ldots, t \tag{3.24}$$

and noting that by the symmetry also $S_j = \sum_i S_{ij}$, we may then write

$$\gamma_1 = t^{-1} \sum_i S_i^2 - \left\{ t^{-1} \sum_i S_i \right\}^2 \tag{3.25}$$

Now the right-hand side of this equation has the pleasant property that it can be written as a sum of squares (!):

$$\gamma_1 = t^{-2} \sum_{i<j} (S_i - S_j)^2 \tag{3.26}$$

and it thus immediately follows that $\gamma_1 \geqslant 0$ and, by Eq. (3.15), $\Delta_1 \geqslant 0$ or with Eq. (3.13)

$$\langle n_1 \rangle_0 \geqslant f_0 q^{-1} \tag{3.27}$$

This is the desired inequality for the first run.

The equality sign in Eq. (3.27) holds *if and only if* the S_i in Eq. (3.24) are *all equal*. S_i has a simple interpretation: it is *the average length of a run starting from black point labeled i*. When $t = 1$ the sum in Eq. (3.26) is empty and the equality sign holds. This is the case of a *strictly* periodic distribution. [Note that it follows from Eq. (3.23) that for this particular case $\langle n_1 \rangle_0 = f_0 q^{-1}$ also for asymmetric random walks; here the equality for general p is a well-known result found by Montroll[8].] When $t = 2$ the sum in Eq. (3.26) is not empty; in this case, however, we have not only $T_n(1 \to 2) = T_n(2 \to 1)$ by the symmetry of the random walk but also $T_n(1 \to 1) = T_n(2 \to 2)$ by the inversion symmetry of the unit cell, so that both $S_{12} = S_{21}$ and $S_{11} = S_{22}$ hence $S_1 = S_2$ and again $\langle n_1 \rangle_0 = f_0 q^{-1}$. This is the case of a *pair*-periodic distribution. When $t \geqslant 3$ we do in general *not* have equality (unless of course the arrangement of black points is strictly or pair-periodic on a smaller scale); equality then holds only for special choices of p, $\tilde{L}$, and B.

(b) The Runs 2,3,.... Further inequalities follow from simple matrix algebra. Equations (3.13)–(3.15) serve as our starting point.

With arguments similar to those presented above it is found that Eq. (3.23) generalizes to

$$\gamma_k = t^{-1} \sum_{i,j,m,n} S_{ij} (T^{k-1})_{jm} S_{mn} - \left\{ t^{-1} \sum_{i,j} S_{ij} \right\}^2, \qquad k \geqslant 1 \tag{3.28}$$

Here the power T^{k-1} "bridges the gap" between the first and the $(k+1)$st run in the first term of Eq. (3.14). When we use the *symmetry* of the random walk this equation simplifies further to

$$\gamma_k = t^{-1}(s, (T^{k-1} - t^{-1}E)\, s) \tag{3.29}$$

where s is the t vector with components S_i, $i = 1, \ldots, t$, as given by Eq. (3.24), E is the $t \times t$ matrix with all elements equal to 1 and $(.,.)$ again denotes the vector inner product.

To proceed we make the following observations.

(i) $TE = ET = E$ by Eqs. (3.20a, b), so T^{k-1} and $t^{-1}E$ have a common base of eigenvectors. Hence each eigenvalue of $T^{k-1} - t^{-1}E$ is the difference of the corresponding eigenvalues of T^{k-1} and $t^{-1}E$.

(ii) Both T and E are symmetric and have real eigenvalues. By the Perron–Frobenius theorem the eigenvalues of T fall in the interval $[-1, 1]$. The largest eigenvalue is 1 (which may be degenerate if T is reducible) and one eigenvalue 1 corresponds to the eigenvector (1,..., 1). E has an eigenvalue t corresponding to the same eigenvector and a $(t-1)$-fold degenerate eigenvalue 0. Thus, when $1 = \tau_1 \geqslant \tau_2 \geqslant \cdots \geqslant \tau_t \geqslant -1$ are the eigenvalues of T, the eigenvalues of $T^{k-1} - t^{-1}E$ are 0 and the powers $\tau_2^{k-1}, ..., \tau_t^{k-1}$.

(iii) Because T and E are symmetric there exists a matrix O, which is orthogonal, such that $O(T^{k-1} - t^{-1}E)\, O^{-1} = D^{k-1}$, with the diagonal matrix

$$D = \begin{bmatrix} 0 & & \cdots & 0 \\ & \tau_2 & & \\ \vdots & & \ddots & \vdots \\ 0 & & \cdots & \tau_t \end{bmatrix}$$

When we now define $u = Os$ we get from Eq. (3.29)

$$\gamma_k = t^{-1}(u, D^{k-1}u) = t^{-1} \sum_{i=2}^{t} U_i^2 \tau_i^{k-1}, \qquad k \geqslant 1 \tag{3.30}$$

$$1 \geqslant \tau_2 \geqslant \cdots \geqslant \tau_t \geqslant -1$$

where the U_i are the components of u.

From Eq. (3.30) a number of interesting inequalities can be deduced. We use Eq. (3.15), and read off for *k odd*:

(1) $\Delta_k \geqslant 0$; for $k \geqslant 3$ the Δ_k are either all $=0$ or all >0;

(2) $\Delta_k \geqslant \Delta_m$ for all $m > k$ (m both odd and even);

(3) $\Delta_k + \Delta_{k+1} \geqslant 0$ and hence with (2): $\Delta_k \geqslant |\Delta_{k+1}|$;

(4) When $\tau_2 \neq 1$ and $\tau_t \neq -1$ then $\Delta_k \to 0$ exponentially fast with k as $k \to \infty$, including the even-numbered runs.

Thus we have as a general result the set of inequalities

$$\Delta_1 \geqslant \Delta_3 \geqslant \Delta_5 \geqslant \Delta_7 \geqslant \cdots \geqslant 0,$$
$$\Delta_1 \geqslant |\Delta_2|,\ \Delta_3 \geqslant |\Delta_4|,\ \Delta_5 \geqslant |\Delta_6|, ... \tag{3.31}$$

Whereas the Δ_k for k *odd* display a "smooth" *monotonic* decay, surprisingly enough the *even*-numbered runs show *no such general behavior*. In fact, examples show that there is a *rich variety* (!) in behavior for Δ_{2k}, depending on the choice of the colors in the unit cell and the step distribution of the random walk. In some cases all Δ_{2k} are positive, in others all are negative, but there exist cases where different signs occur. As an example for the latter situation, take for $\tilde{L}$ a ring of six lattice points (the ring structure takes care of the periodic boundary conditions) with three black points, two of which are neighbors and the third at a nonneighboring position, and take for the random walk one with steps of probability 3/7 over one lattice spacing and 1/14 over two. A straightforward calculation shows that for this particular example $\Delta_2 > \Delta_4 > 0$, whereas $\Delta_6 < \Delta_8 < \cdots < 0$.

In many cases one has the smooth behavior

$$\Delta_1 \geqslant \Delta_2 \geqslant \Delta_3 \geqslant \Delta_4 \geqslant \Delta_5 \geqslant \cdots \geqslant 0 \tag{3.31a}$$

From Eq. (3.30) it is clear that this will certainly occur in all cases where the eigenvalues of T are all $\geqslant 0$. From the so-called Gerchgorin theorem[9] together with Eqs. (3.20a, b) it follows that the eigenvalues fall in the set

$$\bigcup_{i=1}^{r} \{\tau \in [-1, 1] : |\tau - T_{ii}| \leqslant 1 - T_{ii}\} = [2(\min_i T_{ii}) - 1, 1]$$

For Eq. (3.31a) to hold it therefore suffices that $T_{ii} \geqslant \frac{1}{2}$ for all i. This is so, for instance, in the following two cases: (i) $p(0) \geqslant \frac{1}{2}$, irrespective of *all* other details; (ii) the simple random walk on any ring of points with *any* color arrangement that does *not* have two black points as neighbors.

In some cases where Eq. (3.31a) does not hold one encounters an *oscillating* decay of the type

$$\Delta_1 \geqslant -\Delta_2 \geqslant \Delta_3 \geqslant -\Delta_4 \geqslant \Delta_5 \geqslant \cdots \geqslant 0 \tag{3.31b}$$

This may appear, for instance, when there is some underlying symmetry in the arrangement of the colors and some of the U_i in Eq. (3.30) are zero. As an example consider a simple random walk on a ring of six points with three black points next to each other. One finds after a short calculation: $\Delta_k = (-\frac{1}{2})^{k+1}, k \geqslant 1$.

To classify the different types of behavior for the even-numbered runs one would need more detailed information about T and S. It turns out that this presents a very complicated problem, since in general little is known about these matrices in detail. Although Eqs. (3.31a, b) appear only as special cases of Eq. (3.31), examples tend to show that the monotonic decay and, to a lesser extent, the oscillating decay are predominant. In most cases the decay becomes asymptotically either monotonic or oscillating as $k \to \infty$.

A special situation occurs when $\tau_2 = 1$ (and $U_2 \neq 0$): in that case the Δ_k do *not* decay to zero. This, however, is possible only when T is reducible, since when T is irreducible the eigenvalue 1 is always nondegenerate (see Ref. 5, p. 120). Irreducibility of T means that from each black point the walker can eventually reach all other black points (i.e., there are no disjoint sets of black points between which the walker cannot "cross over"). It will be clear that in the reducible case the problem is in a sense "ill posed" and can always be reduced to the irreducible case. In the latter case also the eigenvalue -1 is nondegenerate. From the Gerchgorin theorem one sees that $\tau_i = -1$ can occur only when $T_{ii} = 0$ for *some i*. By the irreducibility it can occur only when $T_{ii} = 0$ for *all i* (see Ref. 5, p. 121). Together with the symmetry of the random walk the latter condition is so strong that it is fulfilled only in the trivial case where the walker cannot make any step between a black and a white point.

Finally, in Eq. (3.31) the equality signs hold in a few special cases, notably for the strictly and the pair-periodic distribution. (In the latter case $U_2 = 0$ due to the symmetry.) A remarkable situation occurs when $\Delta_1 > 0$ and $\Delta_k = 0$ for $k \geqslant 2$. This happens when T has an eigenvalue zero and all other eigenvalues carry a coefficient zero. This may be illustrated by the following example: a ring of five points with three black points, two of which are neighbors and the third at the remaining nonneighboring position, and a random walk with steps of probability $[1 + (13)^{1/2}]/12$ over one lattice spacing and $[5 - (13)^{1/2}]/12$ over two. In this example T is not invertible (!) and, so to say, *projects* the Δ_k, $k \geqslant 2$, onto zero, in the sense that for any given $k \geqslant 2$, but *not* for $k = 1$, the three black points each have probability $\frac{1}{3}$ to be hit as the kth black point, which brings the result back to Eq. (1.3).

3.2. Extension to Arbitrary Color Distributions

So far we have only considered periodic color distributions. The fact that the unit cell of the periodicity was completely arbitrary makes one suspect that the results of the previous section may be generalized. As we shall see, this is indeed the case and the extension can be made to arbitrary (translation-invariant) color distributions. It turns out, however, that the extension is far from trivial. In fact, the approach followed in Section 3.1 will serve only as a guide and on our way we shall encounter some new and interesting problems that have to be dealt with. Thus the extension is more than just a piece of formalism.

In the general case there is no unit cell and we return to our original description with a fixed starting point for the walker (at the origin) and a translation-invariant color distribution. For simplicity we shall from now on assume that $L = \mathbb{Z}^d$; the arguments are easily generalized to arbitrary lattices.

(I) The Zeroth Run. Our aim is to generalize Eq. (3.10). Let $\mathscr{B} := \{B: B \subset L\}$ be the set of all subsets of L. A color configuration in L will henceforth be *identified* with the set that consists of all the black points and $\mathscr{B}$ may therefore represent the set of all color configurations. For a given B let $W := L \backslash B$ and let $p^{(B)} := (p(l' - l))_{l,l' \in W}$ be the matrix of stepping probabilities between the white points. The set W is either finite or (countably) infinite. By the translation invariance, W is empty with probability 1 when it is finite (see Section 2). Since, however, we have assumed that $\mathscr{P}[L \text{ is black}] = \mathscr{P}[W \text{ is empty}] = 0$, it follows that with probability 1 the matrix $p^{(B)}$ is (countably) infinite.

Let $I[E] \in \{0, 1\}$ denote the indicator stochastic variable of the event E. A little reflection shows that instead of Eq. (3.5) we now have

$$\langle n_0 \rangle_0 = \overline{I[0 \in W] \sum_{l \in W} (\mathbf{1} + p^{(B)} + p^{(B)2} + \cdots)_{0l}}^{\mathscr{B}} \tag{3.32}$$

where the bar denotes the average over $\mathscr{B}$ with respect to $\mathscr{P}$ and $\mathbf{1}$ is the (countably) infinite unit matrix. Here we must again assume that $f_0 = 1$. Because of the translation invariance we may choose instead of 0 any point of L as the starting point for the walker and we are therefore free to write

$$\langle n_0 \rangle_0 = \overline{I[l \in W] \sum_{l' \in W} (\mathbf{1} + p^{(B)} + p^{(B)2} + \cdots)_{ll'}}^{\mathscr{B}} \qquad \text{for any } l \in L \tag{3.33}$$

The powers of $p^{(B)}$ are well-defined (see, e.g., Ref. 4, p. 161). It is not at all clear, however, whether or not the inverse of $\mathbf{1} - p^{(B)}$ exists with probability 1 and thus whether or not $\langle n_0 \rangle_0 < \infty$. This is a problem not encountered in the periodic case. We shall return to this point in the discussion.

We shall arrive at our result by a *truncation* method together with a suitable limit procedure. Let

$$L_n := \{l \in L: |l^i| \leqslant n, i = 1, \ldots, d\}, \qquad n \geqslant 0$$

and let $p_n^{(B)}$ be the truncation of $p^{(B)}$ obtained by deleting all rows and columns that correspond to white points *outside* L_n, i.e., $p_n^{(B)}$ is the matrix of stepping probabilities between the white points that fall in L_n. Clearly we have

$$\langle n_0 \rangle_0 \geqslant |L_n|^{-1} \overline{\sum_{l,l' \in L_n} I[l \in W]\, I[l' \in W](1_n^{(B)} + p_n^{(B)} + p_n^{(B)2} + \cdots)_{ll'}}^{\mathscr{B}} \qquad \text{for any } n \qquad (3.34)$$

where $1_n^{(B)}$ is the unit matrix of the same order as $p_n^{(B)}$, i.e., of order $|L_n \cap W|$. To get Eq. (3.34) one first averages in Eq. (3.33) over l in L_n and then truncates $p^{(B)}$ (observe that the elements of $p^{(B)}$ are nonnegative). The advantage of Eq. (3.34) over Eq. (3.33) is not only that l and l' appear symmetrically but also that $p_n^{(B)}$ is a *finite* matrix. Working with Eq. (3.34) we shall avoid some difficulties that are connected with infinite matrices (see, e.g., Ref. 4, Chap. 6) and that would, at least for our purpose, unnecessarily complicate the calculations.

As we shall see in a moment, the right-hand side of Eq. (3.34) is finite for all n. It is also monotone nondecreasing in n. We shall derive for this right-hand side an inequality valid for all n and then take the limit $n \to \infty$ to obtain the desired inequality for $\langle n_0 \rangle_0$. For finite n there may be a positive probability that $L_n \cap W$ is empty, in which case $p_n^{(B)}$ is not defined. However, since the sequence $(L_n)_{n \geqslant 0}$ is monotone and $\lim_{n \to \infty} L_n = L$ it follows that $\lim_{n \to \infty} \mathscr{P}[L_n \text{ is black}] = \mathscr{P}[L \text{ is black}]$, and as the latter probability is zero by assumption the probability that $L_n \cap W$ is empty tends to zero as $n \to \infty$.

If we exclude the degenerate random walk ($p(0) = 1$), then because L_n is finite there is for all $B \in \mathscr{B}$ a step of positive probability that will bring the walker from a point inside $L_n \cap W$ (if not empty) to a point outside. Therefore $p_n^{(B)}$ is for all B and n strictly substochastic so that the inverse of $1_n^{(B)} - p_n^{(B)}$ exists. Thus we may write for Eq. (3.34)

$$\begin{aligned}\langle n_0 \rangle_0 &\geqslant |L_n|^{-1} \overline{\sum_{l,l' \in L_n \cap W} (1_n^{(B)} - p_n^{(B)})_{ll'}^{-1}}^{\mathscr{B}} \\ &= |L_n|^{-1} \overline{(e_n^{(B)}, (1_n^{(B)} - p_n^{(B)})^{-1} e_n^{(B)})}^{\mathscr{B}} \qquad \text{for any } n \qquad (3.35)\end{aligned}$$

where $e_n^{(B)}$ is the vector of order $|L_n \cap W|$ with all elements equal to 1. Note that the right-hand side of Eq. (3.35) is finite for all n.

Now we are ready to use the *symmetry* of the random walk. This property implies that for all B and n the matrix $p_n^{(B)}$ is symmetric, so that $1_n^{(B)} - p_n^{(B)}$ is positive definite. The Kantorovich inequality gives

$$\langle n_0 \rangle_0 \geqslant |L_n|^{-1} \overline{(e_n^{(B)}, e_n^{(B)})^2 / (e_n^{(B)}, (1_n^{(B)} - p_n^{(B)})\, e_n^{(B)})}^{\mathscr{B}} \qquad \text{for all } n \qquad (3.36)$$

We proceed as follows. Let

$$q_n^{(B)} := |L_n \cap B| / |L_n| \tag{3.37a}$$

denote the fraction of black points in L_n for given B. We have $(e_n^{(B)}, e_n^{(B)}) = |L_n \cap W|$ and

$$(e_n^{(B)}, p_n^{(B)} e_n^{(B)}) = \sum_{l,l' \in L_n \cap W} p(l-l')$$

$$= |L_n \cap W| - |L_n \cap B| + \sum_{l,l' \in L_n \cap B} p(l-l') + R_n^{(B)}$$

where

$$R_n^{(B)} := \sum_{l \notin L_n} \sum_{l' \in L_n \cap B} p(l-l') - \sum_{l \in L_n \cap W} \sum_{l' \notin L_n} p(l-l') \tag{3.37b}$$

plays the role of a rest term. Defining

$$X_n^{(B)} := |L_n \cap B|^{-1} \sum_{l,l' \in L_n \cap B} p(l-l') \tag{3.37c}$$

we thus get

$$\langle n_0 \rangle_0 \geqslant \overline{(1-q_n^{(B)})^2 / (q_n^{(B)}[1 - X_n^{(B)}] - |L_n|^{-1} R_n^{(B)})}^{\mathscr{B}} \qquad \text{for all } n \tag{3.38}$$

Now we consider the limit $n \to \infty$ of Eq. (3.38). First we show that

$$\lim_{n \to \infty} |L_n|^{-1} R_n^{(B)} = 0, \qquad \text{for all } B \in \mathscr{B} \tag{3.39a}$$

Proof. By the symmetry of the random walk it follows from Eq. (3.37b) that $|R_n^{(B)}| \leqslant \sum_{l \in L_n} \sum_{l' \notin L_n} p(l-l')$ for all B. The latter sum does not depend on B. Let $c_m := \sum_{l \in L, |l| \geqslant m} p(l)$, $m \geqslant 0$, and $L_{m,n} := L_n \backslash L_{n-m}$, $m < n$ (the "shell" of thickness m between the cubes L_n and L_{n-m}). Then one writes

$$\sum_{l \in L_n} \sum_{l' \notin L_n} p(l-l') = \sum_{l \in L_{n-m}} \sum_{l' \notin L_n} p(l-l') + \sum_{l \in L_{m,n}} \sum_{l' \notin L_n} p(l-l')$$

$$\leqslant |L_{n-m}| \, c_m + |L_{m,n}|$$

and for m fixed this gives

$$\lim_{n \to \infty} |L_n|^{-1} |R_n^{(B)}| \leqslant \lim_{n \to \infty} |L_n|^{-1} \{ |L_{n-m}| \, c_m + |L_{m,n}| \} = c_m$$

Noting that $c_m \to 0$ as $m \to \infty$ one sees that Eq. (3.39a) follows. ∎

Having thus disposed of the rest term we are next faced with the question whether or not also the limits

$$q^{(B)} := \lim_{n\to\infty} q_n^{(B)} \tag{3.39b}$$

and

$$X^{(B)} := \lim_{n\to\infty} X_n^{(B)} \tag{3.39c}$$

exist. This is not immediately obvious. Indeed, it is easy to construct color configurations for which these limits do *not* exist. However, the translation invariance entails, as we shall show in a moment, that $q^{(B)}$ and $X^{(B)}$ *exist with probability 1*. This is weaker but enough for our purpose, and we can now safely take the limit in Eq. (3.38) to obtain

$$\langle n_0\rangle_0 \geqslant \overline{(1-q^{(B)})^2/q^{(B)}[1-X^{(B)}]}^{\mathscr{B}} \tag{3.40}$$

thus completing the generalization of Eq. (3.10).

The existence with probability 1 of the limits in Eqs. (3.39b, c) follows from an *ergodic theorem* for so-called (super)additive stochastic processes[10-12]. Consider first Eq. (3.39b). For any finite set $S \subset L$ let $N_S^{(B)} := |S \cap B|$ denote the number of black points of B that fall in S. The random variable $N_S^{(B)}$ has the following three properties:

(i) By the translation invariance the probability distributions of $N_S^{(B)}$ and $N_{S+l}^{(B)}$ are identical for all $l \in L$, where $S+l$ is the set obtained from S after a translation over l ("stationarity").

(ii) For any two disjoint sets S and S': $N_{S\cup S'}^{(B)} = N_S^{(B)} + N_{S'}^{(B)}$, for all $B \in \mathscr{B}$ ("additivity").

(iii) $0 \leqslant \overline{N_S^{(B)}}^{\mathscr{B}} \leqslant |S|$, for all $B \in \mathscr{B}$ ("integrability").

From a theorem by Pitt[10] (which is a generalization to higher dimensions of the well-known ergodic theorem of Birkhoff) it then follows that $\lim_{n\to\infty} |S_n|^{-1} N_{S_n}^{(B)}$ exists with probability 1 for any sequence of finite sets $(S_n)_{n\geqslant 0}$ such that $\lim_{n\to\infty} |S_n| = \infty$, provided this sequence satisfies the following *regularity* conditions: (1) $S_n \subset L_n$ for all n; (2) $|S_n|/|L_n|$ is bounded from below; (3) S_n is convex in L for all n. Furthermore, under these conditions the limit does *not* depend on the sequence chosen. Obviously, if we choose $S_n = L_n$ the regularity is guaranteed and this proves the existence with probability 1 of $q^{(B)}$. In general $q^{(B)}$ will be a stochastic variable.

Next consider Eq. (3.39c). For any finite set $S \subset L$ we now define $M_S^{(B)} := \sum_{l,l' \in S\cap B} p(l-l')$. This random variable has properties similar to those of $N_S^{(B)}$, except that (ii) is replaced by the following:

(ii)′ For any two disjoint sets S and S': $M^{(B)}_{S\cup S'} \geqslant M^{(B)}_{S} + M^{(B)}_{S'}$, for all $B \in \mathscr{B}$ ("superadditivity").

The existence with probability 1 of $\lim_{n\to\infty} |S_n|^{-1} M^{(B)}_{S_n}$ now follows from a generalization of Pitt's theorem due to Nguyen[11] (see also Akcoglu and Krengel[12]). By the regularity the limit is again independent of the sequence chosen. This proves the existence with probability 1 of $q^{(B)}X^{(B)}$ and hence of $X^{(B)}$ (it is easy to prove that $q^{(B)} > 0$ with probability 1 when B is nonempty). Also $X^{(B)}$ will in general be a stochastic variable.

Thus we have now firmly established Eq. (3.40). As we have seen, except for the translation invariance only the regularity of the sequence $(L_n)_{n\geqslant 0}$ is required. This is a very weak condition (which, incidentally, may still be slightly relaxed[12]) and it is, of course, reassuring that we could have chosen instead of our L_n any other regular sequence of sets without affecting $q^{(B)}$ and $X^{(B)}$ [and Eq. (3.39a)]. Our choice of the cubes L_n is standard.

Equation (3.40) is the formal generalization of Eq. (3.10). The stochastic variables $q^{(B)}$ and $X^{(B)}$ are formally defined as limits, $q^{(B)}$ being the "asymptotic" density of black points corresponding to B and $X^{(B)}$ the "asymptotic" mean probability of a jump between two black points. In general, these limits will *not* be constant on $\mathscr{B}$, not even with probability 1. The simplest example for this situation is a color distribution which is a convex linear combination of two periodic color distributions with different densities of black points. We know only that

$$\overline{q^{(B)}}^{\mathscr{B}} = q \tag{3.41a}$$

$$\overline{q^{(B)}X^{(B)}}^{\mathscr{B}} = \overline{I[0\in B] \sum_{l\in B} p(l)}^{\mathscr{B}} = q \operatorname{Prob}[n_1 = 1 \mid n_0 = 0] =: qX \tag{3.41b}$$

as may readily be shown.

In many cases of physical interest the limits $q^{(B)}$ and $X^{(B)}$ *are* constant with probability 1. These cases include all so-called *extremal* color distributions, which are distributions that cannot be written as a convex linear combination of two different (translation-invariant) color distributions. This follows from the easily established fact that $q^{(B)}$ and $X^{(B)}$ are translation invariant. Examples include all periodic distributions and all (translation-invariant) grand canonical distributions with "short-range correlations", i.e., having the property that the colorings of any two finite blocks become independent as the blocks are separated to infinity (see Ref. 13, Chap. 11). The random distribution falls in the latter class. In such cases Eq. (3.40) reduces to Eq. (3.10) through Eqs. (3.41a, b), so that again we end up with

$$\langle n_0\rangle_0 \geqslant (1-q)^2/q(1-X) \tag{3.42}$$

To get this result we used $f_0 = 1$. When $f_0 < 1$ the generalization is, of course, given by Eq. (3.11).

In the random case obviously $X = p(0) + q[1 - p(0)]$ and we get the result $\langle n_0 \rangle_0 \geqslant (1-q)/q[1-p(0)]$. This is precisely the bound which for this case was known already from other arguments (see, e.g., Ref. 14) and happens to be valid also for asymmetric random walks. The fact that the bound obtained here is not stronger is not at all surprising. In Ref. 14 we proved that for the random case $\langle n_0 \rangle_0 \leqslant (1-q)/(1-F)q$, where F is the (total) probability of return to the origin. F can be arbitrarily close to $p(0)$ for lattices of large enough dimensionality, such that even within the class of symmetric random walks the lower bound obtained can be arbitrarily sharp.

(II) The Runs with Number $i \geqslant 1$. Our aim is to show that the inequalities in Eq. (3.31) remain valid in the general case. We shall not spell out the generalization in full detail but rather indicate the main parts of the proof.

First we introduce the analogs of Eqs. (3.19a, b) for given nonempty $B \in \mathscr{B}$:

$T_n^{(B)}(l \to l') :=$ probability for the walker, when starting from $l \in B$, to make a run of exactly n steps to $l' \in B$; $n \geqslant 1$; $l, l' \in B$.

$$T_{ll'}^{(B)} := \sum_n T_n^{(B)}(l \to l') \tag{3.43a}$$

$$S_{ll'}^{(B)} := \sum_n n T_n^{(B)}(l \to l') \tag{3.43b}$$

In the following we shall assume that $\mathscr{P}[B \text{ is empty}] = 0$. The probabilities $T_{ll'}^{(B)}$, $l, l' \in B$, form a matrix $T^{(B)}$ of "transition" probabilities between the black points; $T^{(B)}$ is (countably) infinite with probability 1. For given $l \in L$ let $\mathscr{B}_l := \{B \in \mathscr{B} : l \in B\}$. By the translation invariance and by Eq. (1.2)

$$\overline{\sum_{l' \in B} T_{ll'}^{(B)}}^{\mathscr{B}_l} = \overline{\sum_{l \in B} T_{0l'}^{(B)}}^{\mathscr{B}_0} = 1 \qquad \text{for any given } l$$

Since obviously $\sum_{l' \in B} T_{ll'}^{(B)} \leqslant 1$ for all $l \in B$ and all $B \in \mathscr{B}$, this shows that

$$\sum_{l' \in B} T_{ll'}^{(B)} = 1 \qquad \text{for all } l \in B \text{ with probability } 1 \tag{3.44a}$$

A comparison of the random walk with its reversed counterpart shows that also

$$\sum_{l \in B} T_{ll'}^{(B)} = 1 \qquad \text{for all } l' \in B \text{ with probability 1} \tag{3.44b}$$

so that $T^{(B)}$ is with probability 1 *doubly stochastic.*

Using Eqs. (3.43a, b) and Eq. (3.44a) we write out

$$\langle n_1 n_{k+1} \rangle_1 = \overline{\sum_{l_1, l_2, l_3 \in B} S_{0l_1}^{(B)} (T^{(B)k-1})_{l_1 l_2} S_{l_2 l_3}^{(B)}}^{\mathscr{B}_0}, \qquad k \geqslant 1 \tag{3.45}$$

Next, using the translation invariance as well as the inversion symmetry of the lattice, we may write this in the following slightly different form:

$$\langle n_1 n_{k+1} \rangle_1 = \overline{\sum_{l_1, l_2, l_3 \in B} S_{l_1 0}^{(B)} (T^{(B)k-1})_{0 l_2} S_{l_2 l_3}^{(B)}}^{\mathscr{B}_0} \tag{3.46}$$

The proof is left to the reader. Then, defining

$$S_l^{(B)} := \sum_{l' \in B} S_{ll'}^{(B)}, \qquad l \in B \tag{3.47}$$

and using the *symmetry* of the random walk, we get

$$\langle n_1 n_{k+1} \rangle_1 = \overline{\sum_{l \in B} S_0^{(B)} (T^{(B)k-1})_{0l} S_l^{(B)}}^{\mathscr{B}_0} \tag{3.48}$$

Together with Eqs. (1.3) and (1.5) this gives

$$\langle n_k \rangle_0 = f_0^{-1} \overline{I[0 \in B] \sum_{l \in B} S_0^{(B)} (T^{(B)k-1})_{0l} S_l^{(B)}}^{\mathscr{B}}, \qquad k \geqslant 1 \tag{3.49}$$

Equation (3.49) serves as the starting point for our calculation. In the following we shall *assume* that $\langle n_k \rangle_0 < \infty$ for all k. We shall return to this point in the discussion.

To arrive at our result we again use a truncation method. Consider Eq. (3.49). By the translation invariance the point 0 may be replaced by any given point l and if we then average over l in L_n we get

$$\langle n_k \rangle_0 = f_0^{-1} |L_n|^{-1} \overline{\sum_{l \in L_n \cap B} \sum_{l' \in L \cap B} S_l^{(B)} (T^{(B)k-1})_{ll'} S_{l'}^{(B)}}^{\mathscr{B}} \qquad \text{for any } n \tag{3.50}$$

The second sum runs over the black points in the *whole* lattice. To obtain a symmetric expression we first restrict this sum to L_n and then take the limit

$n \to \infty$. Let $T_n^{(B)}$ be the *truncation* of $T^{(B)}$ obtained by deleting all rows and columns that correspond to black points *outside* L_n. Then

$$\langle n_k \rangle_0 = f_0^{-1} \lim_{n \to \infty} |L_n|^{-1} \overline{\sum_{l,l' \in L_n \cap B} S_l^{(B)} (T_n^{(B)k-1})_{ll'} S_{l'}^{(B)}}^{\mathscr{B}} \qquad (3.51)$$

The equality sign is guaranteed by the fact that $L_n \to L$ monotonically in n.

We proceed by defining the following counterparts of Eqs. (3.13)–(3.14):

$$\Delta_k := \langle n_k \rangle_0 - \kappa, \qquad k \geqslant 1 \qquad (3.52)$$

$$\gamma_k := \langle n_1 n_{k+1} \rangle_1 - \langle n_1 \rangle_1 \kappa, \qquad k \geqslant 1 \qquad (3.53)$$

where

$$\kappa := f_0^{-1} \lim_{n \to \infty} |L_n|^{-1} \overline{|L_n \cap B|^{-1} \sum_{l,l' \in L_n \cap B} S_l^{(B)} S_{l'}^{(B)}}^{\mathscr{B}} \qquad (3.54)$$

Equations (3.52)–(3.54) differ from Eqs. (3.13)–(3.14) for reasons which will become clear later. It will be seen that in the periodic case $\kappa = f_0 q^{-1} = \langle n_k \rangle_1$, so that the two sets of definitions coincide. Note that Eq. (3.15) remains valid and thus we can again investigate Δ_k by looking at γ_k.

Using Eqs. (3.15), (3.51), and (3.54) we write

$$\gamma_k = q^{-1} \lim_{n \to \infty} |L_n|^{-1} \overline{(s_n^{(B)}, (T_n^{(B)k-1} - |L_n \cap B|^{-1} E_n^{(B)}) s_n^{(B)})}^{\mathscr{B}} \qquad (3.55)$$

where $E_n^{(B)}$ is the matrix with all elements equal to 1 of the same order as $T_n^{(B)}$, i.e., of order $|L_n \cap B|$, and $s_n^{(B)}$ is the vector with components $S_l^{(B)}$, $l \in L_n \cap B$. Now Eq. (3.55) is in form very similar to Eq. (3.29) and we shall use this fact to show that the γ_k satisfy *exactly the same* set of inequalities that were found in the periodic case. To that end let us write

$$\gamma_k = \overline{\gamma_k^{(B)}}^{\mathscr{B}} \qquad (3.56)$$

with

$$\gamma_k^{(B)} := \lim_{n \to \infty} \gamma_{k;n}^{(B)} \qquad (3.57a)$$

$$\gamma_{k;n}^{(B)} := q^{-1} |L_n|^{-1} (s_n^{(B)}, (T_n^{(B)k-1} - |L_n \cap B|^{-1} E_n^{(B)}) s_n^{(B)}) \qquad (3.57b)$$

Here it is important that the limit in Eq. (3.57a) exists with probability 1. This is a consequence of the ergodic theorems used below Eq. (3.40) (note that $\gamma_k < \infty$, because $\langle n_k \rangle_0 < \infty$ by assumption), both the translation invariance and the regularity of our sequence $(L_n)_{n \geq 0}$ playing again an essential role. We shall show that with probability 1 the following inequalities hold:

$$\gamma_1^{(B)} \geq \gamma_3^{(B)} \geq \gamma_5^{(B)} \geq \gamma_7^{(B)} \geq \cdots \geq 0$$

$$\gamma_1^{(B)} \geq |\gamma_2^{(B)}|, \gamma_3^{(B)} \geq |\gamma_4^{(B)}|, \gamma_5^{(B)} \geq |\gamma_6^{(B)}|, \ldots \tag{3.58}$$

Together with Eqs. (3.15) and (3.56) this will immediately yield the desired generalization of Eq. (3.31).

Proof. As announced, to prove Eq. (3.58) we shall exploit the close resemblance between Eqs. (3.29) and (3.57b). Now for all B and n the matrix $T_n^{(B)}$ is finite and, by the symmetry of the random walk, symmetric. Therefore we can imitate most of the argument that led from Eq. (3.29) to (3.30). The only difference is that, unlike $T^{(B)}$, $T_n^{(B)}$ is *not* doubly stochastic, as is required to follow the argument. According to Eqs. (3.44a, b) the doubly stochastic property is recovered in the limit as $n \to \infty$ and we have somehow to use this fact in Eqs. (3.57a, b). This is a technical problem which may be solved as follows.

Let $T_n'^{(B)}$ be the matrix obtained from $T_n^{(B)}$ by defining

$$(T_n'^{(B)})_{ll'} := \begin{cases} (T_n^{(B)})_{ll'}, & l' \neq l \\ 1 - \sum\limits_{l'' \neq l} (T_n^{(B)})_{ll''}, & l' = l \end{cases} \tag{3.59}$$

i.e., by simply adding the "missing part" of the row sum (=column sum) to the diagonal elements. Like $T_n^{(B)}$ this matrix is finite and symmetric, but by construction it is *also* doubly stochastic for *all n*. The point in introducing this matrix is that in the limit as $n \to \infty$ we may, as we shall show in a moment, simply replace $T_n^{(B)}$ by $T_n'^{(B)}$ in Eq. (3.57b) *without* affecting $\gamma_k^{(B)}$. But then $\gamma_{k:n}^{(B)}$ can be written in a diagonalized form which is similar to Eq. (3.30), $T_n'^{(B)}$ having all the properties required to copy the proof, and Eq. (3.58) can immediately be read off. The details are left to the reader.

It thus only remains to show that the substitution of $T_n'^{(B)}$ for $T_n^{(B)}$ is indeed justified, in other words, that

$$d_k := \lim_{n \to \infty} |L_n|^{-1} \overline{(s_n^{(B)}, [T_n'^{(B)k-1} - T_n^{(B)k-1}] s_n^{(B)})}^{\#} = 0 \qquad \text{for all } k \geq 1 \tag{3.60}$$

This is done as follows. For $k=1$ there is nothing to prove, as then the term between the square brackets in Eq. (3.60) is zero. For $k=2$ we use Eqs. (3.44a) and (3.59) to write

$$d_2 = \lim_{n\to\infty} |L_n|^{-1} \overline{\sum_{l \in L_n \cap B} S_l^{(B)2} \left\{ \sum_{l' \in (L \setminus L_n) \cap B} T_{ll'}^{(B)} \right\}}^{\mathscr{B}}$$

The following reasoning is similar in spirit to the one used to prove Eq. (3.39a). Let

$$\varepsilon_{l;m}^{(B)} := \sum_{l' \in B, |l'-l| \geqslant m} T_{ll'}^{(B)}, \qquad l \in B$$

then for fixed m

$$d_2 \leqslant \lim_{n\to\infty} |L_n|^{-1} \overline{\sum_{l \in L_{n-m} \cap B} S_l^{(B)2} \varepsilon_{l;m}^{(B)}}^{\mathscr{B}} + \lim_{n\to\infty} |L_n|^{-1} \overline{\sum_{l \in L_{m,n} \cap B} S_l^{(B)2}}^{\mathscr{B}}$$

By the translation invariance it follows that for any $\varepsilon > 0$

$$d_2 \leqslant q\, \overline{S_0^{(B)2}(\varepsilon_{0;m}^{(B)} + \varepsilon)}^{\mathscr{B}_0} \qquad \text{for all } m$$

When we now let $m \to \infty$ and observe that by Eq. (3.44a)

$$\lim_{m\to\infty} \varepsilon_{0;m}^{(B)} = 0 \qquad \text{with probability 1 in } \mathscr{B}_0$$

we find that

$$d_2 \leqslant \varepsilon q\, \overline{S_0^{(B)2}}^{\mathscr{B}_0} = \varepsilon q \langle n_1 n_2 \rangle_1 = \varepsilon f_0 \langle n_1 \rangle_0$$

[see Eq. (3.48)]. Here we have applied the *Lebesgue bounded convergence theorem* (see Ref. 15, p. 110) to interchange the limit and the average, using the fact that the average in the right-hand side is finite by assumption. Since ε is arbitrary this proves that $d_2 = 0$.

The proof for $k \geqslant 3$ proceeds in a similar way. We first note that $T_n'^{(B)} \leqslant T_n^{(B)} + 1_n^{(B)}$ and write

$$\begin{aligned} T_n'^{(B)k} - T_n^{(B)k} &= \sum_{k'=0}^{k-1} T_n'^{(B)k'} (T_n'^{(B)} - T_n^{(B)})\, T_n^{(B)k-k'-1} \\ &\leqslant \sum_{k'=0}^{k-1} \sum_{k''=0}^{k'} \binom{k'}{k''} T_n^{(B)k''} (T_n'^{(B)} - T_n^{(B)})\, T_n^{(B)k-k'-1} \end{aligned}$$

We substitute this inequality into Eq. (3.60) and follow the same type of reasoning as before, using the translation invariance. After a little manipulation we then find that

$$d_{k+1} \leqslant \varepsilon q \sum_{k'=0}^{k-1} \sum_{k''=0}^{\kappa} \binom{k'}{k''} \langle n_1 n_{k-k'+k''+1} \rangle_1$$
$$= \varepsilon f_0 \sum_{m=0}^{k-1} \binom{k}{m} \langle n_{m+1} \rangle_0$$

The details are left to the reader. The boundedness of the moments implies that $d_k = 0$ for all k. This proves Eq. (3.60) and hence Eq. (3.58). ∎

We have thus established the desired generalization of Eq. (3.31), except that it remains to identify κ in Eq. (3.54). Let

$$Y_n^{(B)} := |L_n \cap B|^{-1} \sum_{l \in L_n \cap B} S_l^{(B)} \tag{3.61}$$

then κ takes the form

$$\kappa = f_0^{-1} \lim_{n \to \infty} \overline{q_n^{(B)} Y_n^{(B)2}}^{\mathscr{B}}$$

where Eq. (3.37a) is used. We already showed that the limit in Eq. (3.39b) exists with probability 1. The same ergodic theorems imply that also

$$Y^{(B)} := \lim_{n \to \infty} Y_n^{(B)} \tag{3.62}$$

exists with probability 1 (note that $q^{(B)} > 0$ with probability 1), so that we arrive at

$$\kappa = f_0^{-1} \overline{q^{(B)} Y^{(B)2}}^{\mathscr{B}} \tag{3.63}$$

Like $q^{(B)}$, $Y^{(B)}$ will in general be a stochastic variable. A simple calculation shows that

$$\overline{q^{(B)} Y^{(B)}}^{\mathscr{B}} = q \overline{S_0^{(B)}}^{\mathscr{B}_0} = q \langle n_1 \rangle_1 = f_0 \tag{3.64}$$

Since $q^{(B)} \geqslant 0$ for all B we have

$$\overline{q^{(B)} Y^{(B)2}}^{\mathscr{B}} \cdot \overline{q^{(B)}}^{\mathscr{B}} - \{\overline{q^{(B)} Y^{(B)}}^{\mathscr{B}}\}^2 \geqslant 0$$

and therefore

$$\kappa \geqslant f_0 q^{-1} \tag{3.65}$$

Thus our earlier bounds remain valid in the general case. For *extremal* color distributions $q^{(B)}$ and $Y^{(B)}$ are constant with probability 1 and the equality sign holds in Eq. (3.65).

The above calculation completes the generalization of the bounds obtained in Section 3.1. What seems harder than in the periodic case, though, is to determine under what conditions $\Delta_k \to 0$ as $k \to \infty$ (it is not even obvious that $\Delta_k < \infty$) and, if so, how fast. In the periodic case we found that the decay, if present, is *always exponential* in k. In the general case we expect this *not* to be so. The decay depends on the eigenvalues of $T^{(B)}$ in the neighborhood of 1 and -1, the spectrum of $T^{(B)}$ can have both a discrete and a continuous part and the decay, if present, may generally be *slower* than exponential. What also seems harder than in the periodic case is to find examples where the equality signs hold in Eqs. (3.31) and (3.42). For the first run, however, we note the following. Returning to Eq. (3.49) we have

$$\langle n_1 \rangle_0 = \overline{S_0^{(B)2}}^{\mathscr{B}_0} / \overline{S_0^{(B)}}^{\mathscr{B}_0} \tag{3.66}$$

which is the counterpart of Eq. (3.26) (note that $\langle n_1 \rangle_0 - f_0 q^{-1}$ can be written as a variance), and it follows that $\langle n_1 \rangle_0 = f_0 q^{-1}$ *if and only if* within the set of color configurations that include the origin the average length of the first run is constant with probability 1. This may be used to construct new examples of equality for the first run, but it will be clear that the restriction on the color distribution and the random walk is rather strong, showing that in general there will be strict inequality.

4. AN APPLICATION TO LATTICES WITH TRAPS

Suppose now that the black points are *traps* characterized by a probability of escape η, i.e., whenever the walker visits a black point there is a probability $1-\eta$ that he is trapped (forever) and a probability η that he remains free ("escapes"). If $\eta = 0$ ($\eta > 0$) the trap is called *perfect (imperfect)*. We assume that $\eta < 1$.

Let

$T_n :=$ probability that the walker is trapped after exactly n steps; $n \geqslant 0$.

In Ref. 1 it is shown that T_n is monotone nonincreasing in n for *arbitrary* L, $\mathscr{P}$, and p. From Eq. (1.1) it may further be deduced that for all η the total probability of trapping $f := \sum_n T_n$ equals f_0. Thus by Eq. (2.2) $f = 1$

in almost all cases of physical interest. The average number of steps before trapping $\langle n\rangle := \sum_n nT_n/\sum_n T_n$ follows from

$$\langle n\rangle = \langle n_0\rangle_0 + \sum_{i\geq 1} \eta^i \langle n_i\rangle_0 \tag{4.1}$$

Equation (4.1) shows that in order to calculate $\langle n\rangle$ one has to know all the moments $\langle n_i\rangle_0$, $i\geq 0$.

Our results in Section 3 give a lower bound for $\langle n\rangle$ for symmetric random walks. For perfect traps we have the bound given by Eq. (3.42) (assuming without loss of generality that $f=1$ and that the trap distribution is extremal):

$$\langle n\rangle|_{\eta=0} \geq (1-q)^2/q(1-X) \tag{4.2a}$$

From Eq. (3.31), using that $\sum_{i=1}^{k} \langle n_i\rangle_0 \geq kq^{-1}$ for all k, we can further deduce that for imperfect traps $\langle n\rangle$ is prolonged by an amount

$$\langle n\rangle - \langle n\rangle|_{\eta=0} \geq \frac{\eta}{1-\eta}\frac{1}{q} \tag{4.2b}$$

Except for a few rather special cases, the equality sign in Eq. (4.2b) holds only for strictly and pair-periodic trap distributions.

5. DISCUSSION

In Ref. 1 and the present paper we have studied statistical properties of the sequence of consecutive colors encountered by a random walker on a lattice of which the points are colored black and white according to a translation-invariant joint probability distribution. The relevance of our results to trapping problems in particular will be evident. Trapping problems have a long history and many properties have, in some form or other, been discussed in the literature (see, e.g., Refs. 3, 16, and 17). Usually, however, the traps are assumed to be distributed either periodically or randomly over the lattice. Except in one dimension, little is known in detail for other trap distributions. Reference 1 and the present paper are an attempt to bring out some of the characteristic features of trapping problems in a more general setting.

Earlier Results for Traps. For periodic trap distributions an *exact* solution for $\langle n\rangle$ (see Section 4) was found in Ref. 18. The approach followed in that paper is a generalization of earlier work by Montroll,[19] who derived an expression for $\langle n\rangle|_{\eta=0}$. The final result, however, appears in a form that is not very practical for analytical purposes unless the unit cell of the periodicity contains a very limited number of traps. To be more specific, when N is the number of points in the unit cell and t the number of traps, $\langle n \rangle$ is expressed in terms of $t \times t$ determinants of which the elements are Green's functions that are N-fold sums depending on the positions of the traps and on the random walk. As an illustration of the difficulties that one encounters in this context the fact may serve that we have been unable to rederive Eqs. (4.2a, b) for any unit cell with more than two traps starting from the results of Refs. 18 and 19. Thus in practice to get detailed results one should have recourse to the computer.

For the random distribution asymptotic expansions for $\langle n \rangle$ valid for small q were obtained in Ref. 20 for several classes of random walks of varying dimensionality. Earlier work by Rosenstock[21] included a study of $\langle n \rangle |_{\eta=0}$ for $q \to 0$. So far, only few rigorous results have been obtained for the random case, except in one dimension. On the other hand, several approximative methods have been developed, one more sophisticated than the other, all for values of q that are either small or close to unity (see, e.g., Refs. 16 and 17).

Higher Runs, Odd/Even Effect. In this paper we have centered interest on the probabilities f_i and the moments $\langle n_i \rangle_0$. A particularly striking aspect of our results for the runs with number $i \geq 1$ is that for i odd $\langle n_i \rangle_0$ is always monotone in i whereas for i even a variety in behavior is displayed depending on the choice of $\mathscr{P}$ and p. This difference must essentially come from our assumption of symmetry, but it is not intuitively obvious why then the odd-numbered runs should be so special. To get some feeling for the situation, let us look at the first few runs in some more detail. For the sake of the argument we consider a *simple* random walk on a large unit cell, with periodic boundary conditions, in which the black points occur in several *large* compact "clusters" surrounded by a large "sea" of white points. Now if all black points would have equal probability to be the starting point for the first run we would have $\langle n_1 \rangle_0 = \langle n_1 \rangle_1 = q^{-1}$ by Eq. (1.3), but obviously the probability in question differs for different black points: by the translation invariance black points that are on the edge of a cluster are much more likely to be hit first than others. On the other hand, by the symmetry the average length of a run starting from the edge of a cluster is larger than that of one starting from the interior. Together this leads to $\langle n_1 \rangle_0 > q^{-1}$. The second black point hit is one that with a large probability lies either on the edge of a cluster or one layer deeper. This gives $q^{-1} < \langle n_2 \rangle_0 < \langle n_1 \rangle_0$. As more and more black points are visited, the "excess" in probability of points on the outer part of a cluster to be the next black point hit gradually "diffuses" into the cluster, so that $\langle n_i \rangle_0 \to q^{-1}$ *monotonically* as $i \to \infty$. When, instead of large clusters, we have clusters of *small size*, say, only one interior point and one boundary layer, then the following happens: after the first run the excess in probability of points on the edge is all transferred to the single interior point, so that now we get $\langle n_2 \rangle_0 < q^{-1}$. By the symmetry this effect will be reversed by an extra run, so that again $\langle n_3 \rangle_0 > q^{-1}$ etc. and the decay is in this case *oscillating*.

To illustrate this argument one may consider a simple random walk on a ring of arbitrary length with one compact cluster of black points of size M. An easy calculation shows that as M varies one gets the following types of behavior: (a) $M = 1, 2$: $\langle n_i \rangle_0 = q^{-1}$ for all $i \geqslant 1$; (b) $M = 3$: oscillating decay; (c) $M = 4$: $\langle n_1 \rangle_0 > q^{-1}$, equality for all other i; (d) $M \geqslant 5$: monotonic decay.

The extreme example considered above brings out the origin of our results for the runs with number $i \geqslant 1$. More generally it will be clear that the bounds obtained all arise from the fact that (i) *different black points may have different environments*, (ii) black points in certain environments are *more easily accessible* than others, i.e., are favoured over others to be hit at a given stage in the process, (iii) those black points which are most easily accessible are *also* the ones from which a run takes longest, simply because they are surrounded by more white points. The "clumping" of black points, or to phrase it differently, the spatial fluctuation in local ordering of colors generally tends to increase the lengths of the runs and to favor monotonic behavior, but certain special conditions may cause a shortening of the even-numbered runs. It is interesting to note that the first run in a sense "sets the stage" for all the subsequent runs.

The bounds obtained for the runs with number $i \geqslant 1$ are probably fairly strong. In Eqs. (3.31) and (4.2b) the equality signs hold for *all* strictly and pair-periodic distributions, regardless of the random walk and the size of the unit cell, and so there is every reason to expect that the inequalities will be sharp in many other cases of physical interest. Moreover, in Ref. 20 it is shown that for the random distribution $\langle n \rangle - \langle n \rangle|_{\eta=0} \simeq \eta/(1-\eta)\, q$ as $q \to 0$ for a very large class of random walks, including all transient random walks (which include all aperiodic random walks with $d \geqslant 3$). Since η is arbitrary this implies that $\langle n_i \rangle_0 \simeq 1/q$, $q \to 0$, for all $i \geqslant 1$, so that equality in Eqs. (3.31) and (4.2b) holds asymptotically in this case.

Zeroth Run. The zeroth run differs in character from all the subsequent runs and the bound obtained in Eq. (3.42) is in practice, unfortunately, not so strong. For strictly periodic distributions, for instance, it can be shown that the equality sign holds *only* for a very special type of random walk, which we have called "indifferent" with respect to the unit cell, and that for most other random walks the bound is numerically rather weak when the unit cell is large. Moreover, for the random distribution it is known that $\langle n_0 \rangle_0 \simeq 1/(1-F)q$, $q \to 0$, for transient random walks, where F is the (total) probability of return to the origin (in the absence of traps), and thus for small q the bound is in this case "off" by a factor $1/(1-F)$.

Our result for the zeroth run becomes more transparent when we rewrite Eq. (3.42) as an inequality relating two conditional averages:

$$\langle n_0 \,|\mathrm{W} \rangle \geqslant \langle n_1 - 1 \,|\mathrm{BW} \rangle \tag{5.1}$$

Here Eq. (1.3) is used and W (BW) is a condition on the first (two) color(s) encountered by the walker. Returning to our example of a simple random walk on a unit cell with clusters of black points, we see that Eq. (5.1) is quite clear: when the walker may start anywhere in the sea of white points it takes him longer to reach a black point than when he must first step on a black point, next step to a white point and *then* start to go for a black point, simply because in the latter case he starts next to a cluster. In the general case Eq. (5.1) comes from the fact that (i) different *white* points may have different environments, (ii) white points in certain environments are *more easily hit* from a black point than others, (iii) those white points which are most easily hit are *also* the ones from which a run takes shortest. This is very similar to what we listed earlier with respect to the behavior of the other runs. It now also becomes clear why our bound is not so strong when q is small: in the case of a strictly periodic distribution, for instance, black points *do* but white points generally *do not* have the same environment, and in particular when the unit cell is large (and hence $\langle n_0 \rangle_0$ large) this will have a substantial effect. Equation (5.1) tends to become better as q increases. Thus it remains a challenge for the zeroth run in particular to look for ways of obtaining a better bound. It is amusing to note that Eq. (5.1) reduces to an equality for all color distributions which are complementary to a strictly or pair-periodic distribution, i.e., obtained from the latter ones after changing black into white and vice versa. Note also that Eq. (3.42) is the only inequality obtained that depends explicitly on $\mathscr{P}$ and p.

Finiteness of Moments. A question which we have postponed so far is whether or not the averages that we consider are finite [see below Eqs. (3.33) and (3.49)]. For periodic distributions all moments are finite because of the finite size of the unit cell. For general distributions, however, Eq. (1.3) is exceptional in that $\langle n_1 \rangle_1$ is the only moment that is always finite, and there are examples where *all* other moments are infinite. In such cases the bounds obtained are, of course, trivial though still correct. (It is not hard to show that the moments $\langle n_i \rangle_0$, $i \geqslant 1$, are either all finite or all infinite.) As an example, take a simple random walk on $\mathbb{Z}$ and let the color distribution be such that, loosely described, the lengths of white intervals between black points are independently and identically distributed. Let $C(m)$ denote the probability that an interval has length m. We have $\sum_m C(m) = 1$ and $\sum_m mC(m) = q^{-1}$, but C is otherwise arbitrary. Following the approach of Ref. 19 it may then be shown that $\langle n_0 \rangle_0 = \sum_m (m^3 - m)\, C(m)/6\sum_m mC(m)$, which can be made infinite by choosing C such that $\sum_m m^3 C(m) = \infty$. It may further be shown that when C is such that $\sum_m m^2 C(m) = \infty$, also all the next runs have infinite first moment. This example is, of course, highly special and it seems reasonable to expect that in most cases of physical interest the moments considered are finite. In particular for the random distribution one should be able to establish finiteness for arbitrary random walk.

Assumptions Used. The assumption of symmetry of the random walk plays a crucial role in most of the present paper. Once the symmetry is dropped one may get "wildly varying" results [see the remarks below Eq. (3.1a)] and each of the inequalities obtained may be seriously violated. To illustrate this let us consider a pair-periodic color distribution. It follows from Eqs. (3.20a, b) that $T_{11} = T_{22} = 1 - T_{12} = 1 - T_{21}$. Since there are only two traps in the unit cell it further follows that $S_{11} = S_{22}$ (!) [see below Eq. (3.27)], and with Eqs. (3.13)–(3.15) and (3.28) this gives $\langle n_i \rangle_0 = q^{-1} - \frac{1}{4}q(S_{12} - S_{21})^2 (T_{11} - T_{12})^{i-1}$, $i \geqslant 1$ (assume $f_0 = 1$). Now for symmetric random walks $S_{12} = S_{21}$ and $\langle n_i \rangle_0 = q^{-1}$, as found earlier. For asymmetric random walks, however, we have in general $S_{12} \neq S_{21}$, so that $\langle n_1 \rangle_0 < q^{-1}$ and when $T_{11} \neq T_{12}$ also $\langle n_i \rangle_0 < q^{-1}$ for all i odd. This is just the *opposite* of what we found in Eq. (3.31). Thus, for our bounds the symmetry is necessary.

By the translation invariance of $\mathscr{P}$ and p the sequence of colors encountered by the walker is a *stationary* stochastic process. We have derived the results in Ref. 1 on the basis of this property *alone*, without referring to the detailed background of the process, i.e., without using the fact that the color sequence is actually constructed from a random walk taking place on a stochastically colored lattice. Therefore Eqs. (1.1)–(1.7) reflect only this stationarity and, viewed in retrospect, they could also have been derived starting from certain theorems on stationary stochastic processes known from the mathematical literature. The reader is referred to Breiman[22] (Chap. 6) and Berbee[23] (Chap. 3).

For the present paper the situation is quite different: in deriving our results we have made frequent use of properties of the underlying model such as lattice structure, existence of asymptotic density of black points, independence of successive steps of the walker, symmetry of steps and paths, etc. Therefore the various inequalities obtained in the present paper reflect more of the specific features of our model.

To conclude the discussion it seems appropriate to ask: "How restrictive are the basic assumptions in our model in view of actual applications?,, The model may be used to describe physical processes such as the diffusion and trapping of "particles" in a medium with static traps. In such processes the translation invariance enters as a very natural assumption: the system, though microscopically inhomogeneous, is assumed to be *statistically homogeneous*, and hence homogeneous on a macroscopic level. As to the symmetry, this assumption should be realistic for a system *without external field*, where the stepping probability distribution of the "particles" is expected to exhibit the symmetries of the underlying lattice structure.

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SOME ADDITIONAL RESULTS AND CONJECTURES

In this section we list a few additional results for the colour model (without derivation or discussion) and mention a few conjectures, which we feel are worth investigating. We take $L=\mathbb{Z}^d$ and assume that $\mathcal{P}$ is extremal, p is aperiodic and $q>0$ (so that $f_i=1$ for all $i>0$; see Chapter 4).

RESULTS:

I. For $\mathcal{P}$ *random* and for *arbitrary* d, p, q and η the following inequalities can be shown to hold:

$$\langle n\rangle\big|_{\eta=0} > \frac{1-q}{q(1-r)}, \tag{1}$$

$$\langle n\rangle - \langle n\rangle\big|_{\eta=0} > \frac{\eta}{1-\eta}\,\frac{1}{q}, \tag{2}$$

$$\langle n\rangle < \frac{1-q}{q(1-F)} + \frac{\eta}{1-\eta}\,\frac{1}{q}, \tag{3}$$

where $\langle n\rangle$ is given by Eq.(4.1) of Chapter 4, F is the total probability for the walker to return to the origin, and r is the total probability for the walker to return to the origin *without* hitting a black point. Note that Eq.(3) only makes sense when $F<1$, i.e., when the random walk is transient (see Chapter 2). Eqs.(1) and (2) hold for more general $\mathcal{P}$, in particular for all grand canonical distributions of a lattice gas of black points with attractive interactions.

II. Let $\Delta_i = \langle n_i\rangle_0 - q^{-1}$, $i>1$, as in Eq.(1.10) of Chapter 4. Under the condition that $\Delta_i<\infty$ for all i it can be shown that for *arbitrary* $\mathcal{P}$ and p:

$$\lim_{j\to\infty} \frac{1}{j}\,\Sigma_{i=1}^{j}\,\Delta_i = 0. \tag{4}$$

III. Let $w_n = \mathrm{Prob}[n_0>n]$ as in Eq.(3.3) of Chapter 4. When $\mathcal{P}$ is *periodic*, either $w_n\to 0$ *exponentially* fast as $n\to\infty$ or there exists some n' such that $w_n=0$ for $n>n'$. The latter occurs only in the exceptional case when the walker can never return to a white point without hitting a black one. When $\mathcal{P}$ is *nonperiodic* the decay of w_n may be *slower* than exponential (see e.g. Eq.(4.1) of Chapter 2). When p is *symmetric* the following exponential lower bound is valid for *arbitrary* $\mathcal{P}$:

$$w_n > w_0 (w_1/w_0)^n , n>0. \quad (5)$$

After summation over n this immediately gives the bound for $\langle n_0 \rangle_0$ that we derived in Chapter 4 (Eq.(1.9)).

IV. The sequence $(X_0, X_1, X_2, \dots)$, with X_n the colour encountered by the walker at step n, is for *arbitrary* $\mathcal{P}$ and p a *stationary and ergodic* stochastic process. By the well-known individual ergodic theorem this entails a number of interesting limiting properties; for instance:

$$\lim_{n\to\infty} \frac{1}{n} \sum_{m=0}^{n-1} I[X_m \text{ is black}] = q \quad \text{with probability } 1, \quad (6)$$

where I is the indicator random variable.

CONJECTURES:

I. Let S_n be the number of distinct points visited by the walker in n steps, and let U_n and λ be defined as in Eqs.(2.8a) and (3.3a,b) of Chapter 2. For *arbitrary* d, p, q and η:

$$\text{Var } U_n < \lambda^2 \text{ Var } S_n , n>0. \quad (7)$$

This should hold in virtue of Eq.(3.4) of Chapter 2.

II. Let p(0)=0. For all n and n' the probability Prob[S_n<n'] has its *maximum* value when the random walk is simple and d=1. This would imply, by Eq.(2.1) of Chapter 2, that when $\mathcal{P}$ is *random*:

$$w_n < w_n[\text{simple random walk, d=1}], n>0. \quad (8)$$

The right-hand side can be calculated exactly. Eq.(8) implies that for the random colour distribution all the moments of n_0 are finite for arbitrary d and p (see Eq.(4.1) of Chapter 2, and section 5 of Chapter 4).

III. When *either* $\mathcal{P}$ is nonperiodic *or* p is such that F>0, then:

$$\lim_{i\to\infty} \Delta_i = 0. \tag{9}$$

In particular this would hold when p is symmetric (see Chapter 4).

IV. Let p be the simple random walk of arbitrary dimensionality. Among the colour distributions with a fixed value $q=m^{-d}$, where m is some integer, the probability w_n, for any fixed n, has its *minimum* value when the colour distribution is *strictly periodic* with a hypercubic unit cell of size m. This would imply that for arbitrary η the average $\langle n\rangle$ in Eq.(4.1) of Chapter 4 is bounded below by the corresponding average for the strictly-periodic case, by Eqs.(3.4) and (4.2b) of Chapter 4. The latter average is known exactly (see Chapter 1). For d=1 the proof of this conjecture is easy. The same bound will presumably hold for a large class of other random walks; however, it is not clear how large one should expect this class to be. It is, for instance, not enough to assume that p is symmetric, nor is it enough to assume that p has the full point symmetry of the lattice.

SAMENVATTING

In dit proefschrift worden modellen bestudeerd van een stochastische wandeling op een puntrooster met stochastisch geplaatste vallen (absorberende punten). Het onderzoek vormt een bijdrage tot de studie van transportprocessen in systemen die structureel wanordelijk zijn op microscopische schaal.

Een stochastische wandeling op een puntrooster is een stapproces tussen de punten van dit rooster, waarbij de achtereenvolgens gemaakte stappen onafhankelijke en identiek verdeelde stochastische variabelen zijn, met een gegeven stapwaarschijnlijkheidsverdeling. In de bestudeerde modellen start de wandeling op een gekozen punt en duurt voort totdat een val wordt bereikt en de wandeling stopt. Ook de posities van de vallen zijn stochastisch bepaald, volgens een gegeven ruimtelijke valwaarschijnlijkheidsverdeling. De modellen zijn derhalve van een dubbelstochastisch karakter. Bestudeerd worden, in het bijzonder, de totale vangstkans en het gemiddeld aantal stappen tot vangst, en onderzocht wordt in detail hoe deze beide grootheden afhangen van de gekozen waarschijnlijkheidsverdelingen. Naast het geval van perfecte vallen, waar vangst zeker is, wordt ook de uitbreiding beschouwd naar imperfecte vallen, van waaruit bij aankomst ontsnapping met zekere kans is toegestaan.

In hoofdstuk 1 wordt eerst het speciale geval bestudeerd waarbij de vallen periodiek op het rooster geplaatst zijn. Dit geval is relatief eenvoudig en kan exact worden aangepakt. In hoofdstuk 2 wordt vervolgens het geval van een random (ongecorreleerde) valverdeling onder de loep genomen. Dit geval is veel lastiger te behandelen en weinig exacte resultaten zijn hiervoor tot nu toe bekend. Voor verschillende klassen van stochastische wandelingen van verschillende dimensionaliteit wordt voor het gemiddeld aantal stappen tot vangst een systematische reeksontwikkeling in de valdichtheid afgeleid, die bruikbaar is voor relatief hoge dichtheden. De afleiding berust op een analyse van de waarschijnlijkheidsverdeling voor de aantallen roosterpunten die de wandeling in een gegeven aantal stappen een gegeven aantal keren bezoekt. De resultaten leiden tot een dieper inzicht in de structuur van het probleem en maken tevens duidelijk waar de verschillen met het periodieke geval liggen.

Valmodellen zijn veelvuldig onderzocht en hebben een breed gebied van toepassingen, waaronder bijvoorbeeld het onderzoek van de fotosynthese, van elektrische geleiding in legeringen en van diffusie van roosterfouten in vervormde metalen. Veelal wordt uitgegaan van een periodieke of random

valstructuur. Voor de beschrijving van reële fysische systemen is dit echter te zeer een idealisatie van de werkelijkheid. Het doel van dit proefschrift is mede om na te gaan wat kan worden afgeleid voor meer algemene valverdelingen.

In hoofdstukken 3 en 4 wordt daartoe als uitgangspunt een model gekozen met een rooster bestaande uit punten van tweeërlei kleur, verdeeld volgens een translatie-invariante, maar verder geheel willekeurige waarschijnlijkheidsverdeling, en op dit rooster een stochastische wandeling die niet door de kleuren wordt beïnvloed. Deze aanpak heeft voor een deel tot doel de discussie van het probleem te vereenvoudigen. Het model kan direkt worden gebruikt voor het oorspronkelijke valprobleem door een van de kleuren, b.v. zwart, te identificeren met een imperfecte val. Daarnaast heeft het model nog enkele andere toepassingen (welke echter niet nader worden besproken). Bestudeerd worden de statistische eigenschappen van de reeks van kleuren die de wandelaar achtereenvolgens ontmoet. In hoofdstuk 3 worden eerst enkele exacte relaties afgeleid, die geldig zijn voor een willekeurige stochastische wandeling. In hoofdstuk 4 worden deze relaties gebruikt voor de afleiding van een aantal exacte ongelijkheden voor de gemiddelde lengte van de achtereenvolgens door de wandeling afgelegde etappen over witte punten eindigend met een bezoek aan een zwart punt, en wel onder de aanname dat de stapwaarschijnlijkheidsverdeling symmetrisch is. Dit geeft o.a. een exacte ondergrens voor het gemiddeld aantal stappen tot vangst in het valprobleem. Voor de afleiding worden wiskundige technieken uit de ergodentheorie gebruikt. De resultaten hebben een aantal verrassende aspecten, die vooral dankzij de exacte behandeling van het probleem aan het licht komen.

Terwijl de resultaten van hoofdstukken 1 en 2 vrij gedetailleerd zijn, zijn die van hoofdstukken 3 en 4 noodzakelijkerwijze bescheiden door de hoge graad van algemeenheid. De hoop is dat deze resultaten een uitgangspunt kunnen vormen voor verdere studie van het valprobleem, dat in de hier beschouwde zeer algemene vorm tot nu toe in de literatuur vrijwel onbehandeld was gebleven.

De in dit proefschrift bestudeerde modellen maken deel uit van een grote klasse van verwante en in het algemeen zeer moeilijke modellen, die bekend staan onder de verzamelnaam van stochastische wandelingen in stochastische media. Systemen met een stochastische ruimtelijke structuur staan de laatste jaren erg in de belangstelling. Valmodellen, als beschrijving van bepaalde transportprocessen in deze systemen, behoren tot de meest eenvoudige en meest bestudeerde modellen in dit gebied.

CURRICULUM VITAE

van Frank den Hollander, geboren te Voorburg op 1 december 1956.

Op verzoek van de Faculteit der Wiskunde en Natuurwetenschappen volgt hier een overzicht van mijn studie.

Na mijn eindexamen Atheneum B aan het Sint Maartenscollege te Voorburg begon ik in 1975 met mijn studie aan de Rijksuniversiteit Leiden. In januari 1978 legde ik het kandidaatsexamen Natuurkunde en Wiskunde met bijvak Sterrenkunde af. Het doctoraal examen volgde met lof in november 1980. Tijdens het praktische gedeelte van mijn doctorale studie was ik werkzaam op het Kamerlingh Onnes Laboratorium in de werkgroep "Magnetische Resonantie en Relaxatie", o.l.v. Prof.dr.ir. N.J. Poulis. Het onderzoek voor mijn theoretische doctoraalscriptie verrichtte ik op het Instituut-Lorentz voor Theoretische Natuurkunde, o.l.v. Prof.dr. P.W. Kasteleyn. Hierbij werd een aanvang gemaakt met een onderzoek van stochastische wandelingen op roosters met vallen. Dit onderzoek werd voortgezet en uitgebreid na december 1980, toen ik in dienst kwam bij de universiteit als wetenschappelijk assistent. Sinds medio april 1984 ben ik in dienst van de "Stichting voor Fundamenteel Onderzoek der Materie" (FOM) als wetenschappelijk medewerker. Een deel van de resultaten van het onderzoek is neergelegd in dit proefschrift. Naast mijn promotie-onderzoek heb ik samengewerkt met de vakgroepen Biofysica van de Rijksuniversiteit Leiden en de Vrije Universiteit te Amsterdam. In het onderzoek van de fotosynthese, dat in deze vakgroepen wordt verricht, vindt mijn promotie-onderzoek een belangrijke toepassing.

Aan het onderwijs droeg ik bij door in het academisch jaar 1984/1985 een werkcollege te geven bij het college statistische fysica. Verder hielp ik bij het afnemen van tentamens en het geven van enkele colleges.

Tijdens mijn studie heb ik deelgenomen aan een aantal conferenties en zomerscholen, te weten de NUFFIC zomerscholen over "Fundamental Problems in Statistical Mechanics" V en VI (Enschede, 1980 en Trondheim, Noorwegen, 1984), het "Symposium on Random Walks and Their Application to the Physical and Biological Sciences" (Gaithersburg, Maryland, USA, 1982) en de "Fifteenth IUPAP International Conference on Thermodynamics and Statistical Mechanics" (Edinburgh, Schotland, 1983). In het najaar van 1984 heb ik, in het kader van een Koninklijke/Shell Studiereis mij aangeboden door Shell Nederland BV, een bezoek gebracht aan het I.H.E.S. te Bures-sur-Yvette in Frankrijk en voorts een reis gemaakt langs aan een aantal wetenschappelijke instituten in de Verenigde Staten, waar ik een serie lezingen over mijn werk heb gegeven.

Vanaf 1 september 1985 zal ik voor een periode van vier jaar verbonden zijn aan de Technische Hogeschool Delft, in de vakgroep "Statistiek, Stochastiek en Operationele Analyse" van de Onderafdeling der Wiskunde en Informatica, als medewerker van Prof.dr. M. S. Keane.

LIST OF PUBLICATIONS

(1) Random walks with "spontaneous emission" on lattices with periodically distributed imperfect traps,
W.Th.F. den Hollander and P.W. Kasteleyn,
Physica 112A (1982) 523-543.

(2) Random walks on lattices with points of two colours. I,
W.Th.F. den Hollander and P.W. Kasteleyn,
Physica 117A (1983) 179-188.

(3) Random walks on inhomogeneous lattices,
P.W. Kasteleyn and W.Th.F. den Hollander,
J. Stat. Phys. 30 (1983) 363-372.

(4) Trapping, loss and annihilation of excitations in a photosynthetic system. I. Theoretical aspects,
W.Th.F. den Hollander, J.G.C. Bakker and R. van Grondelle,
Biochim. Biophys. Acta 725 (1983) 492-507.

(5) Trapping, loss and annihilation of excitations in a photosynthetic system. II. Experiments with the purple bacteria Rhodospirillum rubrum and Rhodopseudomonas capsulata,
J.G.C. Bakker, R. van Grondelle and W.Th.F. den Hollander,
Biochim. Biophys. Acta 725 (1983) 508-518.

(6) Random walks on lattices with randomly distributed traps.
I. The average number of steps until trapping,
W.Th.F. den Hollander,
J. Stat. Phys. 37 (1984) 331-367.

(7) Random walks on lattices with points of two colours.
II. Some rigorous inequalities for symmetric random walks,
W.Th.F. den Hollander and P.W.Kasteleyn,
J. Stat. Phys. 39 (1985) 15-52.

(8) Comment on a paper by G.H. Weiss, S. Havlin and A. Bunde,
W.Th.F. den Hollander,
J. Stat. Phys. (to appear).

(9) A random-walk calculation of the quantum yield of photosynthetic processes as a function of molecular-excitation transfer parameters,
W.Th.F. den Hollander and L.N.M. Duysens,
Physiol. Vég. (to appear).

"Je ne suis qu'un artiste de variété et ne peux rien dire qui ne puisse être dit de variété, car on pourrait me reprocher de parler de choses qui ne me regardent pas." (Leo Ferré)

STELLINGEN

(1) De hyperbolische relatie tussen het fluorescentierendement en de fractie van reactiecentra in de fotochemisch actieve toestand, zoals die voor purperbacteriën experimenteel gevonden werd door Vredenberg en Duysens, kan analytisch worden afgeleid uit het door Duysens voorgestelde matrixmodel. Essentieel daarbij is slechts dat de totale dichtheid van reactiecentra en het verlies op antennemoleculen klein zijn.

W.J. Vredenberg en L.N.M. Duysens, Nature 197 (1963) 355.
L.N.M. Duysens, in: Brookhaven Symposium in Biology 19 (1967) 71.
W.Th.F. den Hollander en L.N.M. Duysens, Physiol. Vég. (verschijnt).

(2) De conclusie van Otten, dat de benaderingsmethoden gebruikt door Vredenberg en Duysens (1963) en door Duysens (1967) ter verklaring van de in stelling 1 genoemde hyperbolische relatie equivalent zijn, is fysisch weinig zinvol.

H.A. Otten, Proefschrift Leiden (1973).

(3) Weiss, Havlin en Bunde hebben laten zien dat de overlevingskans van een stochastische wandeling op een eindig rooster met periodieke randvoorwaarden en één valpunt asymptotisch exponentieel vervalt als functie van het aantal gemaakte stappen. Eenvoudig kan worden aangetoond dat hetzelfde type verval optreedt voor een willekeurig rooster met willekeurige randvoorwaarden en een willekeurig aantal valpunten. Essentieel daarbij is slechts dat het rooster eindig is.

G.H. Weiss, S. Havlin en A. Bunde, J. Stat. Phys. (verschijnt).
W.Th.F. den Hollander, J. Stat. Phys. (verschijnt).

(4) De door Rosenstock gegeven berekening van de totale kans op terugkeer naar de oorsprong in een stochastische wandeling op een rooster met random geplaatste valpunten in de limiet van kleine dichtheid van deze valpunten is op alle fronten incorrect.

H.B. Rosenstock, J. Math. Phys. 11 (1970) 487.

(5) De drie door Shuler geformuleerde "Ansätze", die betrekking hebben op het asymptotische gedrag van een symmetrische stochastische wandeling tussen naaste buren op een kwadratisch rooster met stochastisch verdeelde "open" en "gesloten" kolommen, kunnen exact bewezen worden voor een willekeurige translatie-invariante extremale waarschijnlijkheidsverdeling van deze kolommen onder een conditie die lange-drachtscorrelaties tussen de kolommen uitsluit.

K.E. Shuler, Physica 95A (1979) 12.

(6) Zij Γ een oneindige k-reguliere graaf en zij $\tilde{\Gamma}$ de overdekkingsgraaf van Γ. Wanneer $G(\Gamma)$ het gemiddeld aantal bezoeken aan de oorsprong is in een simpele stochastische wandeling op de punten van Γ, en $G(\tilde{\Gamma})$ hetzelfde gemiddelde voor $\tilde{\Gamma}$, dan geldt:

$$G(\tilde{\Gamma}) = \frac{(k-1)(k-2)}{k^2} + \frac{4(k-1)}{k^2} G(\Gamma).$$

(7) In tegenstelling tot hetgeen door Reichl wordt beweerd hebben interne rotatievrijheidsgraden van een vloeistof géén invloed op het leidende-orde lange-tijdsgedrag van de snelheidsautocorrelatiefunctie van een zich in deze vloeistof bevindend Browns deeltje.

L.E. Reichl, Phys. Rev. Lett. 49 (1982) 85.

(8) Het scenario voorgesteld door Holdom om het anomale Z_0-verval te verklaren kan de experimenteel daarbij gevonden hoekverdeling tussen het lepton en het foton niet verklaren. Dit manco wordt veroorzaakt door het ontbreken in de theorie van een propagatorstructuur.

B. Holdom, Phys. Lett. 143B (1984) 241.

(9) In het oorspronkelijke manuscript van Debussy's twaalf études voor piano uit 1915 is een groot aantal schrijffouten geslopen. Het is opmerkelijk dat in géén van de latere edities die van dit werk zijn uitgegeven deze fouten gecorrigeerd zijn.

edities: Durand (1916), Broekmans & van Poppel (1969), Peters (1970).

(10) In het algemeen wordt Rodin beschouwd als de kunstenaar die de belangrijkste aanzet heeft gegeven tot de moderne beeldhouwkunst. Bij dit oordeel echter worden de vernieuwende elementen in de sculptuur van Degas te zeer ondergewaardeerd.

(11) In de theorie van stochastische wandelingen is elke dimensie bijzonder.

W.Th.F. den Hollander
Leiden, 25 juni 1985