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Random Walks on Inhomogeneous Lattices

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For lattices with two kinds of points ("black" and "white"), distributed according to a translation-invariant joint probability distribution, we study statistical properties of the sequence of consecutive colors encountered by a random walker moving through the lattice. The probability distribution for the single steps of the walk is considered to be independent of the colors of the points. Several exact results are presented which are valid in any number of dimensions and for arbitrary probability distributions for the coloring of the points and the steps of the walk. They are used to derive a few general properties of random walks on lattices containing traps.

KEY WORDS: Random walks; inhomogeneous lattice; perfect and imperfect traps; average number of steps until trapping; probability of return to the origin; FKG inequality.

1. INTRODUCTION

Random walks on inhomogeneous lattices—i.e., lattices containing *special* points, where the stepping probabilities of the walker differ from those on other, *regular*, points—form the subject of a rapidly growing branch of random-walk theory.[1] The special points may be traps (sinks, absorbing points), imperfect traps (partially absorbing points), points where the walker has at each step a probability of pausing, or points where the probability distribution for single steps deviates in any other way from that on regular points.

Quantities on which interest has centered are: the average number of steps made until trapping, the probability of return to the origin, the mean square displacement after a given number of steps, and a number of related quantities.

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The special points are usually assumed to be arranged in a fixed periodic pattern or to be distributed at random. Only recently more general arrangements of special and regular points have been considered.[2–4] For periodic arrangements exact results can be obtained without too much labor provided the number of special points in a unit cell of the pattern is sufficiently small. For random and other arrangements the situation is much more complicated and, with a few exceptions, one resorts to approximations valid for small concentrations of special points (or of regular points).

The systems mentioned have one feature in common. The walker, having started at a given point, moves through the lattice until, after a certain number of steps (which may be zero), he visits a special point. If this point is a perfect trap his walk comes to an end, but in other cases he has a possibility to continue his walk and to visit new (or old) regular and special points. Thus the walker samples the lattice in his own characteristic way. In doing so he visits a sequence of points of two (or more) different kinds, in an order determined by the stepping probabilities and the arrangement of the special and regular points.

It is the aim of this paper to study the stochastic properties of this sequence in a relatively simple case, where there are only two kinds of lattice points, which we call black and white, and where the stepping probabilities are the same for all lattice points, i.e., where the steps of the walk are independent of the colors of the points. So we forget about perfect and imperfect traps, pausing points or scatterers and we follow the walker, registering only the colors of the points visited. Of course, this is only a first step towards understanding the properties of walks that *are* influenced by the colors, but, as we shall see, some applications can already be given. In addition, we feel that the problems discussed here are interesting in their own right.

2. BLACK–WHITE SEQUENCES

Let us consider an infinite d-dimensional lattice L of which the points are colored black and white according to a given joint probability distribution $\mathscr{P}$. Thus, the lattice is *inhomogeneous*, but we assume that it is *statistically homogeneous* in that $\mathscr{P}$ is *translation invariant*. This assumption, which is in line with what one usually assumes, will be seen to be of crucial importance. Examples of translation-invariant distributions are (a) the *random* distribution; (b) *periodic* distributions (obtained by dividing L into identically shaped and identically colored finite unit cells and assigning equal probability to all distinct colorings of L obtained from the given one by a translation; this is equivalent to the more usual procedure of taking a fixed periodic arrangement of the two kinds of points and allowing the walker to start with equal probability at any point of a unit cell) and convex linear combinations of these; (c) (translation-invariant) canonical distributions (Gibbs states) of lattices consisting of black and white points with a given interaction (binary alloys, Ising models).

We next consider a random walk on L starting at the origin and proceeding according to a probability distribution p for single steps which is independent of the coloring of L [and translation invariant as usual: $p(l' \to l' + l) = p(0 \to l) =: p(l)$].

If we register the colors of the points which the walker successively visits we get a sequence such as $WWWWBBBWBWWB\ldots$ with B = black, W = white. Such a sequence is the realization of a stochastic process $(X_0, X_1, X_2, \ldots)$, where X_n, the color of the point visited at step n, is a random variable taking the values B and W. The process is, of course, entirely determined by the probability distributions $\mathscr{P}$ and p.

We shall study this process, in particular the stochastic properties of the following two sequences of integers derived from it:

I. The numbers $n_0, n_1, n_2, \ldots$ ($n_0 \geqslant 0$, $n_i \geqslant 1$ for $i \geqslant 1$) with the property that $X_{n_0} = X_{n_0+n_1} = X_{n_0+n_1+n_2} = \cdots = B$, whereas $X_n = W$ for all other n. In other words, n_0 is the number of steps made by the walker until his first visit to a black point and n_i ($i \geqslant 1$) is the number of steps made between the ith and $(i+1)$th visit to a black point; for all i we call n_i "the length of the ith run."

II. The numbers $s_0, s_1, s_2, \ldots$ ($s_i \geqslant 1$ for all i) with the property that $X_{s_0} \neq X_{s_0-1}$, $X_{s_0+s_1} \neq X_{s_0+s_1-1}, \ldots$, whereas $X_s = X_{s-1}$ for all other s. In other words, s_0 is the number of steps made until the first change in color and s_i ($i \geqslant 1$) is the number of steps between the ith and the $(i+1)$th change in color. Equivalently, s_i is the length of the $(i+1)$th sequence of equal consecutive colors.

Obviously, the sequence of numbers $(n_0, n_1, \ldots)$ determines the sequence $(s_0, s_1, \ldots)$; the converse is equally true if we also specify the color of the starting point. Observe that these sequences, unlike the basic sequence $(X_0, X_1, \ldots)$, may be finite: if there is a number n such that $X_{n'} = X_n$ for all $n' \geqslant n$, then the sequence (s_i) is finite, and if moreover $X_n = W$ then also the sequence (n_i) is finite. Averages such as $\langle n_i \rangle$ and $\langle s_i \rangle$ should therefore always be understood as conditional averages given that the numbers involved are finite.

I. We first investigate the sequence (n_i). Let $F_{n_0 n_1 \ldots n_i}$ be the probability that at least $i+1$ runs, of lengths $n_0, n_1, \ldots, n_i$, are completed, and $P_{n; n_1 \ldots n_i}$ the probability that at step n a black point (not necessarily the first one) is visited and that subsequently i runs, of lengths $n_1, \ldots, n_i$, are completed.

Since a walker visiting a black point does so either for the first time or, say, m steps after his previous visit to a black point, we have

$$P_{n;n_1 \dots n_i} = F_{nn_1 \dots n_i} + \sum_{m=1}^{n} P_{n-m;mn_1 \dots n_i} \tag{1}$$

For $n = 0$ the sum in the right-hand side is empty.

Now the subwalk beginning with the $(n + 1)$th step may be considered as a complete walk in itself. By the translation invariance of the probability distributions $\mathscr{P}$ and p, however, the probability distribution for the sequence $(X_n, X_{n+1}, \dots)$ is identical to that for $(X_0, X_1, \dots)$. Hence, $P_{n;n_1 \dots n_i}$ is independent of n, so that we may replace n by 0 and write

$$P_{0;n_1 \dots n_i} = F_{nn_1 \dots n_i} + \sum_{m=1}^{n} P_{0;mn_1 \dots n_i}$$

which for $n = 0$ reduces to $P_{0;n_1 \dots n_i} = F_{0n_1 \dots n_i}$. Eliminating the P's we obtain the following relation for the F's:

$$F_{nn_1 \dots n_i} = F_{0n_1 \dots n_i} - \sum_{m=1}^{n} F_{0mn_1 \dots n_i} \tag{2}$$

From this relation, in particular that for $i = 0$:

$$F_n = F_0 - \sum_{m=1}^{n} F_{0m} \tag{3}$$

one can draw a number of interesting conclusions, of which we mention the following ones.

1. Subtracting Eq. (3) for two consecutive values of n we get

$$F_{n-1} - F_n = F_{0n} \geqslant 0 \tag{4}$$

Thus, F_n is a *monotonically nonincreasing function* of n. This result is not easily extracted from the expressions for F_n which have been derived for periodic distributions[5] and the random distribution.[6] It excludes distributions for F_n with a maximum at a certain value of n. It is further obvious that the F_n tend to zero for $n \to \infty$, since the total probability of visiting at least one black point, $F^f := \sum_{n=0}^{\infty} F_n$, is $\leqslant 1$.

2. Summing Eq. (4) over n we obtain

$$F_0^f := \sum_{n=1}^{\infty} F_{0n} = F_0 = q$$

where q denotes the probability that a point is black, which we assume to be > 0. Hence the conditional probability F_0^f / F_0 that at least one more black point is visited given that the walk starts at a black point, equals one. More generally it can be shown that $\sum_{n_i=1}^{\infty} F_{n_0 n_1 \dots n_i} / F_{n_0 \dots n_{i-1}} = 1$, i.e., that if i visits to a black point have taken place, then another visit to a black point will occur with probability one.[4] Hence the probability that the sequence (n_i) is infinite equals F^f.

3. The average number of steps made until the next visit to a black point given that the walk starts at a black point is

$$\langle n_1 | B \rangle := \sum_{n=1}^{\infty} nF_{0n} \Big/ \sum_{n=1}^{\infty} F_{0n} = F_0^{-1} \sum_{n=1}^{\infty} n(F_{n-1} - F_n) = F_0^{-1} \sum_{n=0}^{\infty} F_n = \frac{F^f}{q} \tag{5}$$

It can further be shown that $\langle n_i | B \rangle = \langle n_1 | B \rangle$ for all $i > 1$.[4] The probability F^f can be expressed in terms of L, $\mathscr{P}$, and $p^{(7)}$; in most cases of physical interest it is equal to 1, so that we have the simple result

$$\langle n_1 | B \rangle = 1/q \tag{6}$$

This relation is a generalization of a result derived by Montroll[8] for periodic trap distributions with one trap per unit cell of N points (where $q^{-1} = N$). For the random distribution it is one of the few exact results.

II. We now consider the sequence (s_i). Let $B_{s_0 s_1 \ldots s_i}$ be the probability that the sequence (X_n) starts with s_0 successive B's, followed by i more sequences of equal colors, alternately W's and B's, of lengths $s_1, \ldots, s_i$; $W_{s_0 s_1 \ldots s_i}$ is defined analogously by interchanging B and W.

By the same argument that led to Eq. (3) we can now derive the following relation:

$$W_{s s_1 \ldots s_i} = W_{1 s_1 \ldots s_i} - \sum_{r=1}^{s-1} B_{1 r s_1 \ldots s_i} \tag{7}$$

and a similar equation for $B_{s s_1 \ldots s_i}$. We mention some of the consequences of these equations.

1. $$W_{s-1} - W_s = B_{1\,s-1}, \qquad B_{s-1} - B_s = W_{1\,s-1}$$

The first equation is identical with Eq. (4), since $W_s = F_s$ and $B_{1s} = F_{0\,s+1}$. The second equation is new, however; in this connection we mention that

$$B_s = F_{0\underbrace{11\ldots1}_{s-1}} - F_{0\underbrace{11\ldots11}_{s}}$$

2. $$\sum_{s=1}^{\infty} B_{1s} = W_1, \qquad \sum_{s=1}^{\infty} W_{1s} = B_1 \tag{8}$$

Since $\sum_s B_{1s} \leqslant B_1$ and $\sum_s W_{1s} \leqslant W_1$ we conclude from Eq. (8) that $W_1 = B_1$. It thus follows that the probability of beginning the sequence (X_n) by two different colors is independent of the first color, X_0; we denote it by Q. From the translation invariance it then follows that the probability of having $X_n \neq X_{n-1}$ is equal to Q for all n. Note that the value of Q depends on L, $\mathscr{P}$, and p.

3. If $Q > 0$, the average values of s_1 under the conditions $X_0 = B$, $X_1 = W$ and $X_0 = W$, $X_1 = B$ are, respectively,

$$\langle s_1 \mid BW \rangle = \sum_{s=1}^{\infty} sB_{1s} \Big/ \sum_{s=1}^{\infty} B_{1s} = Q^{-1} \sum_{s=1}^{\infty} s(W_s - W_{s+1})$$

$$= Q^{-1} \sum_{s=1}^{\infty} W_s =: \frac{W^f}{Q}$$

$$\langle s_1 \mid WB \rangle = Q^{-1} \sum_{s=1}^{\infty} B_s =: \frac{B^f}{Q}$$

More generally, it can be shown that

$$\begin{aligned} \langle s_{2j+1} \mid BW \rangle = \langle s_{2j} \mid WB \rangle = \frac{W^f}{Q} \\ \langle s_{2j+1} \mid WB \rangle = \langle s_{2j} \mid BW \rangle = \frac{B^f}{Q} \end{aligned} \tag{9}$$

Observe that W^f, the probability of starting with a finite sequence of W's, is $\leqslant 1 - q$, and that $B^f \leqslant q$. In most cases we have $W^f = 1 - q$, $B^f = q$. For the random distribution and walks with $p(0) = 0$ we further have $Q = q(1 - q)$, and hence $\langle s_1 \mid BW \rangle = q^{-1}$, $\langle s_1 \mid WB \rangle = (1 - q)^{-1}$, etc.

The results obtained thus far are valid for lattices of any dimensionality, for all (translation-invariant) color distributions and all walks (simple or nonsimple, recurrent or transient, with finite or infinite step variance). As such they are in sharp contrast with some results which have been, or may be, found if no condition is imposed on the initial color(s) of the sequence. For the averages $\langle n_i \rangle$ and $\langle s_i \rangle$, e.g., one can obtain wildly varying results, depending on L, $\mathscr{P}$, and p. Still, it is possible to derive some exact relations for these averages by making use of the simple results of the present analysis.[7]

3. APPLICATIONS

Let us now identify the black points with imperfect traps, i.e., with traps that are such that the walker, when stepping on one, has a probability $\eta > 0$ of remaining free (i.e., of continuing the walk) and a probability $1 - \eta$ of being trapped forever (i.e., of terminating the walk). Let T_n be the probability that the walker is trapped at the nth step. It is easily seen that the generating function for trapping, $T(z) := \sum_{n=0}^{\infty} T_n z^n$, is given by

$$T(z) = (1-\eta) \sum_{i=0}^{\infty} \eta^i \sum_{n_0=0}^{\infty} \sum_{n_1,\ldots,n_i=1}^{\infty} F_{n_0 \ldots n_i} z^{n_0 + \cdots + n_i} \tag{10}$$

Now consider the function

$$\Delta(z) := \sum_{n=1}^{\infty} (T_{n-1} - T_n) z^n = T_0 - (1-z) T(z)$$

Noting that $T_0 = q(1-\eta)$ and using Eq. (2) we find, after a little algebra,

$$\Delta(z) = q(1-\eta)^2 \sum_{i=1}^{\infty} \eta^{i-1} \sum_{n_1,\ldots,n_i=1}^{\infty} F_{0 n_1 \ldots n_i} z^{n_1 + \cdots + n_i}$$

Since the coefficients of all powers of z in the right-hand side are nonnegative, we have $T_{n-1} - T_n \geqslant 0$ for all $n > 0$. This is a generalization of Eq. (4).

For a more specific application we interpret the black points as perfect traps ($\eta = 0$) and we restrict ourselves to the *random* distribution. We consider in particular two quantities: $\langle n_0 \rangle$, the average number of steps made before trapping, and r, the probability that the walker returns to the starting point without having been trapped. We first summarize some results mentioned in the literature and the extension of these results which can be obtained by a careful analysis of known data.[9]

Both $\langle n_0 \rangle$ and r have been related to the number of distinct sites visited in n steps on the lattice without traps, S_n. The connection between $\langle n_0 \rangle$ and S_n runs via the probability f_n that during the first n steps the walker has not yet visited a trap. Since

$$\langle n_0 \rangle = \sum_{n=1}^{\infty} n (f_{n-1} - f_n) = \sum_{n=0}^{\infty} f_n$$

and $f_n = \langle (1-q)^{S_n} \rangle$ (where the average is taken over all walks) we have

$$\langle n_0 \rangle = \sum_{n=0}^{\infty} \langle (1-q)^{S_n} \rangle \tag{11}$$

Expanding the right-hand side of Eq. (11) in powers of q, using asymptotic expressions for $\langle S_n \rangle$ and $\langle S_n^2 \rangle$ for $n \to \infty$ together with a certain amount of information on the asymptotic behavior of the probability distribution for S_n, and applying the Euler–Maclaurin formula one can derive expressions for $\langle n_0 \rangle$ valid for small q. For (aperiodic) d-dimensional symmetric walks with finite step (co)variance [i.e., walks with $p(l) = p(-l)$ and $C_{ij} := \sum_{l \in L} l_i l_j p(l) < \infty$ for all pairs of components $i, j = 1, \ldots, d$]

and if $d = 2, 3$, or 4 also with $\sum_{l \in L} l_i l_j l_k l_l (l) < \infty$ one finds

$$d = 2: \quad \langle n_0 \rangle = \frac{u_1}{q}\left[\log\left(\frac{u_1 u}{q}\right) + \log\log\left(\frac{u_1 u}{q}\right) + \frac{\log\log(u_1 u/q)}{\log(u_1 u/q)} + \frac{2K}{\log(u_1 u/q)} + \cdots\right] + \cdots \tag{12a}$$

$$d = 3: \quad \langle n_0 \rangle = \frac{u_0}{q} - u_1 u_0^{-1}\left(\frac{u_0}{q}\right)^{1/2} + \frac{1}{2} u_1^2 u_0^{-2} \log\left(\frac{u_0}{q}\right) + \cdots \tag{12b}$$

$$d = 4: \quad \langle n_0 \rangle = \frac{u_0}{q} - u_1 u_0^{-1} \log\left(\frac{u_0}{q}\right) - v + \cdots \tag{12c}$$

$$d \geqslant 5: \quad \langle n_0 \rangle = \frac{u_0}{q} - w + \cdots \tag{12d}$$

where $u_1 = 1/2\pi C,\ 1/2^{1/2}\pi C,\ 1/4\pi^2 C$ for $d = 2$, 3, and 4, respectively, with $C^2 := \det\{C_{ij}\}$, $u_0 = G(0; 1) = (1 - F)^{-1}$, with $G(l; z)$ the Green's function (F is the probability of return to the origin in the absence of traps) and u, v, w are constants (e.g. for the simple random walk $u = 8$) that are related in a somewhat more complicated way to the Green's function; further, $K = -\int_0^1 dx\,(1 - x + x^2)^{-1} \log x = 1.171953\ldots$. By a different line of reasoning one finds

$$d = 1: \quad \langle n_0 \rangle = \frac{1}{C^2 q^2} + \cdots \tag{12e}$$

Equation (12d) can be shown to be equally valid for all asymmetric walks with finite step variance in all dimensions and for all walks with infinite step variance in $d \geqslant 5$. Altogether Eqs. (12a)–(12e) express a rich variety in behavior.

A similar variety is found for r, where an additional argument is required before the results obtained for S_n can be applied. For symmetric random walks with finite step variance one finds

$$d = 3: \quad r = F - u_1 u_0^{-5/2} q^{1/2} + \cdots \tag{13a}$$

$$d = 4: \quad r = F - u_1 u_0^{-3} q \log\left(\frac{u_0}{q}\right) + \cdots \tag{13b}$$

$$d \geqslant 5: \quad r = F - w' q + \cdots \tag{13c}$$

where w' is related to the Green's function. Further it is known that for simple random walks in $d = 1$

$$r = 1 - \frac{q}{1 - q} \log \frac{1}{q} \tag{13d}$$

For $d = 2$ and for nonsimple random walks in $d = 1$ no expression for r is known. Again, Eq. (13c) is also valid for asymmetric walks with finite step variance and for all walks in $d \geqslant 5$.

We now return to the language of colorings and introduce the analogs of $\langle n_0 \rangle$ and r for each fixed configuration C of black points, to be denoted by $\langle n_0 \rangle^{(C)}$ and $r^{(C)}$. If we average these quantities under the random distribution over the set $\mathscr{C}$ of all configurations on L, we obviously have

$$\langle n_0 \rangle = \overline{\langle n_0 \rangle^{(C)}}^{\mathscr{C}}, \qquad r = \overline{r^{(C)}}^{\mathscr{C}}$$

Let now $\mathscr{C}^B (\mathscr{C}^W)$ be the set of all configurations containing (not containing) the origin 0. If $C \in \mathscr{C}^W$, the walker may return to the origin before visiting a black point. To take this fact into account, we first consider the average number of steps required to reach *either* a black point *or* 0. This number may be denoted by $\langle n_1 \rangle^{(C \cup 0)}$, where $C \cup 0$ is the configuration obtained from C by adding 0, i.e., by changing the color of 0 from white to black. If the walker returns to 0 he can continue his walk as if he has just started; the probability that this happens is $r^{(C)}$. Thus we have

$$\langle n_0 \rangle^{(C)} = \langle n_1 \rangle^{(C \cup 0)} + r^{(C)} \langle n_0 \rangle^{(C)} \tag{14}$$

and hence, with an obvious extension of notation,

$$\overline{(1 - r^{(C)}) \langle n_0 \rangle^{(C)}}^{\mathscr{C}^W} = \overline{\langle n_1 \rangle^{(C \cup 0)}}^{\mathscr{C}^W} \tag{15}$$

Since the color distribution is random, the probability of any coloring of a neighborhood of 0 is independent of the color of 0 and therefore

$$\overline{\langle n_1 \rangle^{(C \cup 0)}}^{\mathscr{C}^W} = \overline{\langle n_1 \rangle^{(C)}}^{\mathscr{C}^B} = \langle n_1 \mid B \rangle = q^{-1} \tag{16}$$

where the latter equality follows from Eq. (6) [provided we exclude the degenerate walk with $p(0) = 1$, which for this distribution can be shown to be the only walk for which $F^f < 1$[4]].

If we combine Eqs. (15) and (16) and extend the averaging so as to include the $C \in \mathscr{C}^B$, using the fact that $\langle n_0 \rangle^{(C)} = 0$ for $C \in \mathscr{C}^B$, we finally obtain

$$\overline{(1 - r^{(C)}) \langle n_0 \rangle^{(C)}}^{\mathscr{C}} = \frac{1 - q}{q} \tag{17}$$

The simplicity of this result, which is exact and valid for all (nondegenerate) walks and all $q > 0$, is in striking contrast with the specificity of the results (12a)–(12e) and (13a)–(13d).

Equation (17) has interesting consequences. For example, since $0 \leqslant r^{(C)} \leqslant F$ we find immediately the following bounds for $\langle n_0 \rangle$:

$$\frac{1 - q}{q} \leqslant \langle n_0 \rangle \leqslant \frac{1 - q}{(1 - F) q} \tag{18}$$

The upper bound (which makes sense only if $F < 1$) is not trivial; the lower bound, however, is, for it also follows immediately from the obvious inequality $S_n \leqslant n + 1$. To find a sharper lower bound we observe that both $r^{(C)}$ and $\langle n \rangle^{(C)}$ decrease (or at most remain unaltered) if black points (traps) are added to C. Together with the fact that the colors of the points are independent random variables this ensures that the so-called FKG inequality[10] holds for the correlation between $r^{(C)}$ and $\langle n_0 \rangle^{(C)}$:

$$\overline{r^{(C)}\langle n_0\rangle^{(C)}}^{\mathscr{C}} - \overline{r^{(C)}}^{\mathscr{C}}\,\overline{\langle n_0\rangle^{(C)}}^{\mathscr{C}} \geqslant 0$$

From this inequality we obtain, using Eq. (17),

$$(1 - r)\langle n_0\rangle \geqslant (1 - q)/q \tag{19}$$

so that we end up with the following bounds for $\langle n_0 \rangle$:

$$\frac{1 - q}{(1 - r)q} \leqslant \langle n_0\rangle \leqslant \frac{1 - q}{(1 - F)q} \tag{20}$$

where it is to be noted that $r = r(q)$ and $F = r(0)$. Conversely, Eq. (19) can be considered to yield an upper bound for the quantity r, which is less well known than $\langle n_0 \rangle$:

$$r \leqslant 1 - \frac{1 - q}{q\langle n_0\rangle}$$

It can be shown that the inequality (19) is not restricted to the random distribution alone but has a wider domain of validity. Furthermore, Eqs. (17) and (19) can be extended to the case of imperfect traps.[9]

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