Mean number of distinct sites visited by correlated walks. I. Perfect lattices

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The mean number of distinct sites visited by correlated walks on one-, two-, and three-dimensional lattices is studied by numerical simulations and by generating-function techniques. The random walks include correlations over two consecutive steps. The asymptotic behavior is derived analytically in $d = 1$, and in $d = 2, 3$ for the model with restricted reversals, and good agreement with the simulations is found. The model with increased probability for forward steps is studied numerically in $d = 2, 3$ and analyzed. It is found in all cases that the mean number of visited sites cannot be simply obtained by rescaling the step number n with the correlation factor f, but there are additional correction terms that do not obey scaling.

I. INTRODUCTION

The mean number of distinct sites visited by a random walk of a particle on a lattice is an important quantity, both in random walk theory and in applications. The asymptotic behavior of this quantity with large step numbers is well understood for ordinary random walks in one, two, and three dimensions.[1–5] Here we investigate the asymptotic behavior of the mean number of distinct sites visited by correlated walks, where the particle retains a memory to the preceding step. We were motivated to this work by the applications to diffusion experiments where a description with correlated walk is appropriate. One important example is the coherent motion of excitons at low temperatures which can be modeled[6,7] by random walks of the excitons including strong forward correlations. There are other instances of correlated motion in crystals, e.g., of hydrogen in group VB metals at higher temperatures,[8] and of vacancies in solids as seen in computer simulations.[9] Generally, stochastic processes where a memory plays a role are abundant in various fields, in particular in chemical physics.

We intend to show that the study of the mean number of sites visited by correlated walks is also interesting from the point of view of random walk theory. Correlated random walk—often also called persistent random walk—has been studied for a long time.[10–15] The diffusional properties, such as mean-square displacements of a particle, are well understood. Much less attention has been directed towards the first-passage properties, under which the mean number of distinct sites visited can be subsumed. The leading asymptotic behavior of the mean number of distinct sites visited by correlated walk has been derived in one dimension.[16] Further, two publications[17] are known to us where moments of first-passage times for correlated random walks are derived in a general manner.

In this article we study the mean number of distinct sites visited by correlated walks in one, two, and three dimensions both by analytical methods and by numerical simulations. We restrict ourselves to perfect lattices where analytical methods for the correlated walk are available. The case of mixed binary lattices where a portion of sites is inaccessible is also of great interest; this case was already investigated by simulations.[6] We plan to address this more complicated problem in detail in a later publication.

As already mentioned the models of correlated walks discussed in this article comprise a memory to the preceding step of the random walk. Thus in one dimension the particle has a probability p_f for a step in the same direction as the preceding one which is different from the probability $p_b = 1 - p_f$ for a step in the reverse direction. Various extensions of this model are possible in higher dimensions. We select two variants, (i) the model with a reduced probability of reversal p_b, but equal probabilities for steps in the other directions, and (ii) the "forward stepping model" where the probability p_f for a step in the same direction as the previous one is increased compared to the steps in the other directions.

In Sec. II we describe the models in more detail and give details on the method used for the numerical simulations. In Sec. III the one-dimensional case is treated analytically and compared to the simulations. Section IV is devoted to the analytical treatment of the model with reduced probability of reversal and its comparison with the simulations in $d = 2$ and 3. Section V contains the simulation results of the forward stepping model and their analysis in $d = 2$ and 3. The results are summarized in Sec. VI.

II. METHOD OF SIMULATION

The simulations were performed slightly different in one and higher dimensions. In $d = 1$ computer memory was no concern. Ensembles of typically 10^4 particles were introduced and the position and direction of the last step of each particle was stored. In discrete random walk one particle is taken after the other, a random number $0 < r < 1$ is generated and compared with the forward stepping probability p_f. If $r < p_f$ a step is performed in the same direction as the previous step, if $r > p_f$ the step is taken in the opposite direction. The positive and negative extrema of the random walk of each particle are monitored; the mean number of distinct sites visited follows immediately. Also the mean-square displacement of the correlated walk is computed. This serves as

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a test for the correctness of the simulations.

In two and three dimensions our method is based on previous work on uncorrelated random walk,[18] where we now introduce the correlation effects. We utilize the new algorithm of the cluster growth technique that generates only those lattice portions that are used at any moment of the execution, but we avoid generating and keeping in memory portions that are never used. We perform random walks monitoring different walk properties such as $\langle S_n \rangle$, the mean number of distinct sites visited in an n step; $\langle R_n^2 \rangle$, the mean-square displacement in an n-step walk; P_0, the probability of return to the origin.

The correlation in the random walk is introduced through the fractions p_f or p_b, the forward or backward stepping probabilities, respectively. In the forward stepping model p_f is specified with $1/z < p_f < 1$; where z is the lattice coordination number. The p_f fraction gives the probability that after a particular step took place the next step will also be in the same direction. In the case of $p_f = 1$ we have a completely correlated walk, and $S_n = n$; if $p_f = 1/z$ (lower limit considered here) we have a totally uncorrelated (stochastic) case. The model with restricted reversals is introduced by use of the p_b fraction. In this case we assign a p_b value in the range $0 \leqslant p_b < 1/z$ which means that steps to the previously occupied position of the lattice are less probable, but jumps in all the other directions are equally probable. Again here when $p_b = 0$ no backward steps are allowed (lower limit) and when $p_f = 1/z$, equivalent to $p_f = 1/z$, the totally stochastic random walk is obtained. One could also consider values $p_b > 1/z$ (as well as $p_f < 1/z$ in the first model), but we restrict ourselves to models with an effective persistence of the walks, where the diffusion coefficient is larger than in the purely stochastic case.

In the forward stepping model everytime a step is taken $1 - p_f$ gives the overall scattering probability, while $(1 - p_f)/(z - 1)$ is the scattering probability in a particular direction. In the computational algorithm we use a uniform random number generator to choose the direction of motion. Before the first step, the probability interval (0, 1) is divided into a section given by p_f and $z - 1$ sections given by $(1 - p_f)/(z - 1)$, each section specifying a fixed given direction. These sections should be randomly distributed on the interval (0, 1), but the first step has negligible influence in the limit of many steps. The first random number generated determines a particular direction for the motion, which means forward motion if it falls in the p_f section, otherwise it means that there is a scattering event. In the first case the same subdivision of the probability interval is kept in memory for the next step, thus signifying correlated motion; in the latter case of scattering the random walk changes direction, but also the subdivision of the probability interval is rearranged according to this event. The section corresponding to the new direction now contains the p_f fraction with the rest being equally divided between the other directions, and this new distribution now stays in memory. The process continues in this fashion for a given number of n steps. In the case of the model with restricted reversals, a similar subdivision of the probability interval (0, 1) is made. Now a section of length p_b is assigned to the direction corresponding to reversed steps, while the other $z - 1$ sections each have the length $(1 - p_b)/(z - 1)$. Otherwise the correlated walk is performed in analogy to the forward model.

The same mechanism is applied to all topologies in two or three dimensions. However, for computational speed all such topologies are reduced to a one-dimensional array, in which case adjacent positions on the plane are given, for the square lattice topology, by $+1$, -1, $+L$, $-L$ (where L is the lattice size), and for the simple cubic lattice by $+L^2$, $-L^2$ for out-of-plane interactions. In these calculations the total lattice size was $N = 4 \times 10^6$, where $L = 2000$ ($d = 2$) and $L = 158$ ($d = 3$). This is attained in FORTRAN language by the breaking up of each computer word (as discussed in Ref. 18) but without byte manipulation.

Notice that this method is applicable to the cases of a pure (one-component) lattice discussed in this article, but it can be extended directly to the case of binary lattices, where the second component constitutes blocking (nonallowed) sites, a topic we plan to discuss in a separate publication.

III. ONE-DIMENSIONAL LATTICE

A. Theory

We shall derive the asymptotic behavior of $\langle S_n \rangle$, the mean number of distinct sites visited by a correlated walk of n steps, by using generating function techniques.[2] The generating function of $\langle S_n \rangle$ is defined by

$$\langle S \rangle(z) := \sum_{n=0}^{\infty} z^n \langle S_n \rangle, \tag{1}$$

where $|z| < 1$. Montroll[1,2] has related $\langle S \rangle(z)$ to the generating function $P(\mathbf{0}; z)$ of finding the particle at the origin,

$$\langle S \rangle(z) = 1/(1 - z)^2 P(\mathbf{0}; z). \tag{2}$$

This relation holds generally, in particular also for the case of correlated walk. Hence we require the generating function $P(\mathbf{0}, z)$ for correlated walk, which is easily derived in one dimension.

The generating function is obtained by analogous methods as used, e.g., in Ref. 14. It is in Fourier space

$$P(k; z) = \frac{1 + z(1 - 2p_f)\cos k}{1 - 2zp_f \cos k + z^2(2p_f - 1)}. \tag{3}$$

We have put the lattice constant $a = 1$. Equation (3) is also the special case of random walk with restricted reversals in $d = 1$.[13] From Eq. (3) follows the asymptotic mean-square displacement of the particle:

$$\langle x^2 \rangle_n \underset{n \to \infty}{\to} fn, \tag{4}$$

where f is the correlation factor for one-dimensional correlated random walk,

$$f = p_f/(1 - p_f). \tag{5}$$

The inverse Fourier transform of Eq. (3) is elementary, with the result

$$P(0; z) = (a^2 - b^2)^{-1/2} + z(1 - 2p_f)\frac{(a^2 - b^2)^{1/2} - a}{b(a^2 - b^2)^{1/2}},$$

where

$$a(z) = 1 + z^2(2p_f - 1),$$
$$b(z) = -2p_f z. \tag{6}$$

The asymptotic behavior of $\langle S_n \rangle$ for large n is determined by that of $\langle S \rangle(z)$ for $z \to 1$; hence it is convenient to substitute $z = 1 - x$ and to consider small x. We have

$$P(0;x) = \left(\frac{1-p_f}{2p_f x}\right)^{1/2} + \frac{2p_f - 1}{2p_f} + O(x^{1/2}) \qquad (7)$$

and thus for small x,

$$\langle S \rangle(x) = \left(\frac{2p_f}{1-p_f}\right)^{1/2} x^{-3/2} - \frac{2p_f - 1}{1-p_f} x^{-1} + O(x^{-1/2}). \qquad (8)$$

Application of Tauberian theorems[19] yield

$$\langle S_n \rangle = (8fn/\pi)^{1/2} + 1 - f + O(n^{-1/2}), \qquad (9)$$

where we introduced the correlation factor for one-dimensional correlated random walk (5). The leading term of Eq. (9) was already obtained by Keller.[16]

In the case $p_f = 1/2$ or $f = 1$ one recovers the result of uncorrelated random walk.[1,5] Note that the constant correction term is absent in this case. The leading term in Eq. (9) is obtained from the uncorrelated case by rescaling the number of steps n by f. The correction term does not follow from this rescaling. For correlated walk $\langle S_n \rangle$ is given asymptotically as a series where the terms decrease only with $n^{-1/2}$, contrary to the uncorrelated case where these terms decrease[5] with n^{-1}.

B. Comparison with simulations

Figure 1 gives the result of simulations of the mean number of sites visited by correlated random walk for three different p_f values. One recognizes good agreement of the simulated values with the theoretical results of Sec. III A. There are small deviations, mainly downwards, which are within error estimates; hence we consider them as insignificant. It is obvious that the leading term of Eq. (9), which obeys scaling, does not yet represent the actual behavior of $\langle S_n \rangle$. We investigated various p_f values in the range $0.5 \leqslant p_f \leqslant 0.99$, with quite similar results to the ones selected for these figures.

Another way of comparing the behavior of $\langle S_n \rangle$ for correlated random walk with that of uncorrelated random walk is to define the efficiency E_n by

$$E_n = \frac{\langle S_n \rangle_{\text{corr}}}{\langle S_n \rangle_{\text{uc}}}. \qquad (10)$$

Figure 2 shows simulation results for E_n in $d = 1$, for various values of the correlation factor f. It is seen that the efficiency increases with the step number and reaches an asymptotic value for large n. The effect is most pronounced for large values of f and it is readily understood from the presence of the correction term $1 - f$ in the expression for $\langle S_n \rangle$. In fact, a simple expression for E_n can be obtained from Eq. (9):

$$E_n = f^{1/2} - (f-1)(\pi/8n)^{1/2} + O(n^{-1}). \qquad (11)$$

According to this equation, large values of f produce a strong variation of E_n with n, while values of f close to unity give a small dependence on n only. Equation (11) agrees quite well with the numerical results, except at smaller step numbers for the largest f values where further corrections should be taken into account.

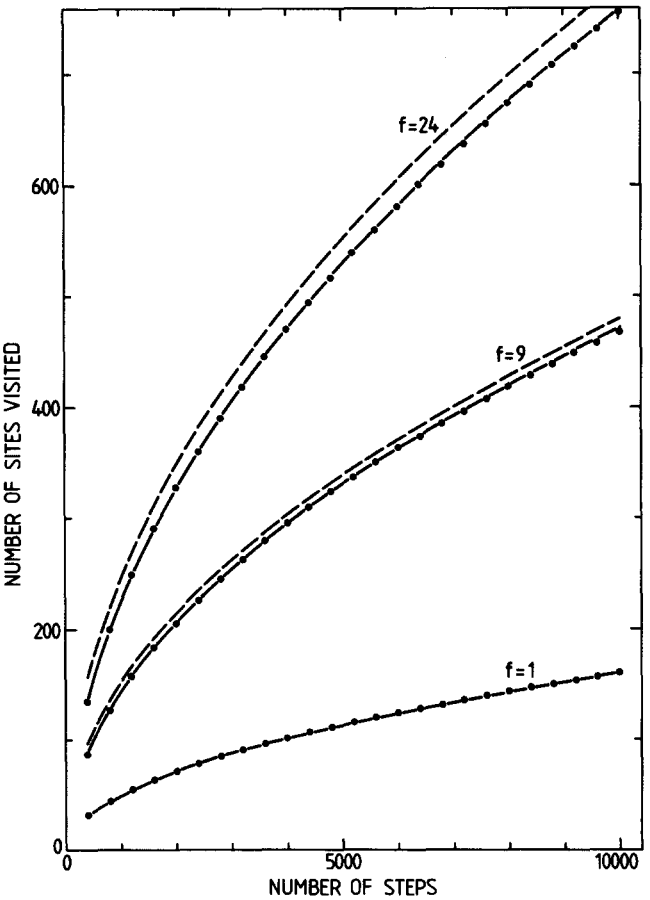

FIG. 1. Mean number of distinct sites visited by correlated random walk of a particle on a linear chain. The points are the results of simulations, the full lines represent the theory including the correction term, and the dashed lines the theory without correction term.

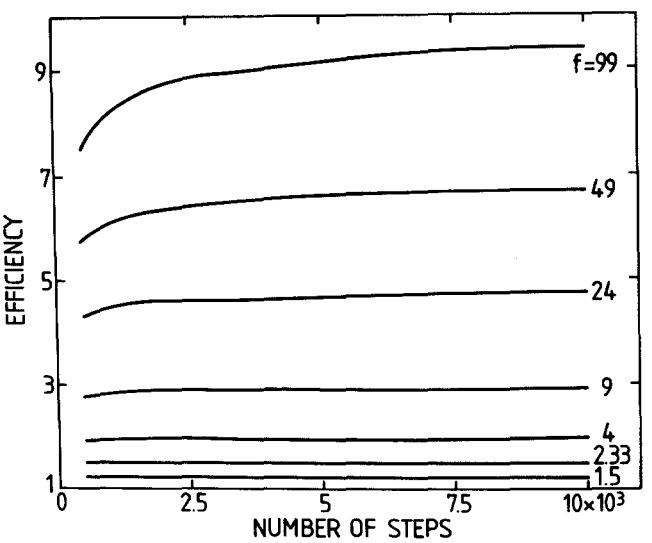

FIG. 2. Efficiency E_n of correlated walks in $d = 1$ as defined in Eq. (10). The simulation results are represented as continuous curves. The parameter correlation factor is indicated on the right.

IV. MODEL WITH REDUCED PROBABILITY OF REVERSAL

In this section we investigate the correlated-walk model with a reduced probability p_b for a step of the particle in the reversed direction of the preceding step. We require $p_b < 1/z$, where z is the coordination number of the lattice. The stepping probability in any other direction is given by $(1-p_b)/(z-1)$. The generating function for the mean number of distinct sites visited is related in arbitrary dimensions to the generating function of the return probability to the origin by Eq. (2). The generating function of random walk with restricted probability of reversal was derived in arbitrary dimensions by Domb and Fisher.[13] A direct derivation of the corresponding quantity in continuous-time random walk was given in Ref. 14. The result is in Fourier space:

$$P(\mathbf{k};z) = \frac{1-\delta z p(\mathbf{k})}{1-z(1+\delta)p(\mathbf{k})+\delta z^2}. \tag{12}$$

For the square, simple-cubic, and hypercubic lattices (lattice constant $a=1$)

$$p(\mathbf{k}) = \frac{1}{2d}\sum_{i=1}^{d}\cos(k_i). \tag{13}$$

The parameter δ measures the strength of the restriction of reversals. It also represents the average angle between two consecutive steps. The mean-square displacement following from Eq. (12) behaves asymptotically as fn where the correlation factor f is given by[13]

$$f = (1+\delta)/(1-\delta). \tag{14}$$

The advantage of Eq. (12) is that it allows a relatively simple derivation of $\langle S_n\rangle$ in the dimensionalities 2 and 3.

A. Dimension $d=2$

In $d=2$ the following integral has to be evaluated:

$$P(\mathbf{0};z) = \pi^{-2}\iint_0^{\pi} d^2k\, P(\mathbf{k};z), \tag{15}$$

where Eq. (12) is inserted. The integral can be decomposed, in arbitrary dimensions,

$$P(\mathbf{0};z) = \frac{1-\delta z A(z)}{(1+\delta)z} I_d + \frac{\delta}{1+\delta}, \tag{16}$$

where

$$A(z) = \frac{1+z^2\delta}{z(1+\delta)} \tag{17}$$

and for $d=2$,

$$I_2 = \pi^{-2}\iint_0^{\pi} d^2k\,[A-p(\mathbf{k})]^{-1}.$$

The integral I_2 leads to a complete elliptic integral of the first kind[20] for the square lattice:

$$I_2 = (2/\pi A)K(A^{-1}). \tag{18}$$

We investigate all quantities near $z=1$ and substitute $z=1-x$. The quantity A behaves as

$$A(x) = 1 + x/f + O(x^2). \tag{19}$$

The modulus $k = A^{-1}$ of the elliptic integral K approaches 1; hence an expansion in terms of the complementary modulus must be made (see Ref. 20). The resulting expansion of I_2 is

$$I_2(x) = \pi^{-1}\ln(8f/x) + O(x) \tag{20}$$

and that of $P(\mathbf{0};z)$, with $z=1-x$,

$$P(\mathbf{0};x) = (\pi f)^{-1}\ln(8f/x) + (f-1)/2f + O(x). \tag{21}$$

The ensuing generating function $\langle S\rangle(x)$ follows from Eq. (2). The backtransformation from $\langle S\rangle(x)$ to $\langle S_n\rangle$ was studied in detail by Henyey and Seshadri[5] for the case that $P(\mathbf{0};x)$ contains a logarithmic term. Henyey and Seshadri discuss the form

$$\langle S\rangle(x) = \frac{-\alpha}{x^2\ln(x/\beta)}[1+O(x)]. \tag{22}$$

The expression for $\langle S\rangle(x)$ derived here is of this form with $\alpha = \pi f$ and

$$\beta = 8f\exp[\pi(f-1)/2]. \tag{23}$$

Henyey and Seshadri then deduce the series

$$\langle S_n\rangle \sim \frac{\alpha n}{\ln(\beta n)}\sum_{j=0}^{\infty} c_j(\ln\beta n)^j[1+O(1/n)], \tag{24}$$

where the coefficients c_j are given by derivatives of gamma functions. Reference 5 contains a table with explicit c_j up to $j=20$. Since $c_0=1$ the leading term has the form, appropriate for the square lattice,

$$\langle S_n\rangle \sim \frac{\pi f n}{\ln(8fn)+\pi(f-1)/2}. \tag{25}$$

When $f=1$ the previous results for uncorrelated random walk are recovered.[5] The representation (25) of the leading term of the series for $\langle S_n\rangle$ makes it explicit that the result for correlated walk is obtained by rescaling the step number with f, but there appear corrections that do not obey scaling. Note that the denominator of Eq. (25) appears also in the series (24). The corrections are especially important for smaller and intermediate step numbers.

Figure 3 gives a comparison of the theory described above with simulations. One recognizes an excellent agreement between the simulations and the result (24) where Eq. (23) was used. We notice that $f=2$ is the largest possible value of the correlation factor, resulting from $p_b=0$. It is also seen from the figure that the scaling prediction (dashed line) for $\langle S_n\rangle$ produced by correlated random walk does not describe the data. The curves representing the scaling prediction were obtained by using $\beta = 8f$, i.e., by omitting the correction term in the denominator of Eq. (25) and in the terms of the series (24).

B. Dimension $d=3$

To derive $\langle S_n\rangle$ for correlated walk on a three-dimensional lattice, we evaluate

$$P(\mathbf{0};z) = \pi^{-3}\iiint_0^{\pi} d^3k\, P(\mathbf{k};z) \tag{26}$$

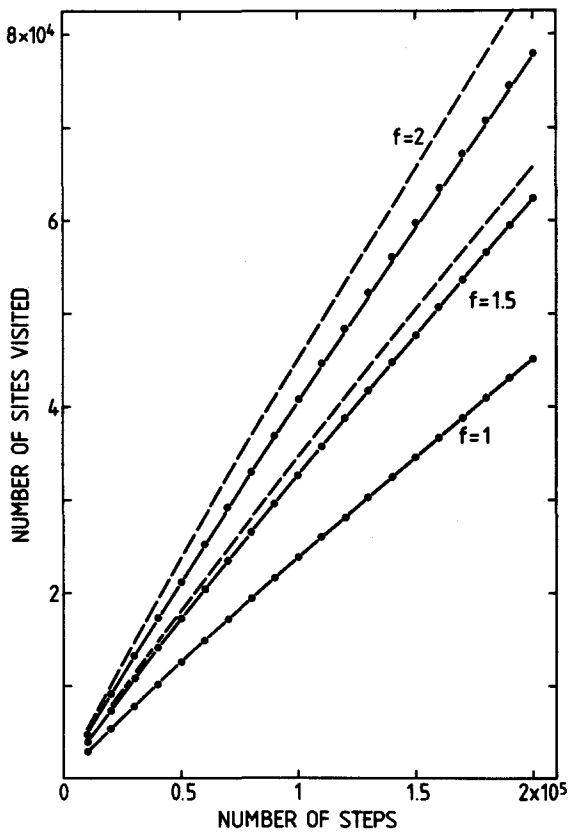

FIG. 3. Mean number of distinct sites visited by correlated walk in $d = 2$ according to model of reduced reversals. Points results of simulations, full lines theory described in the text, dashed lines theory without correction terms.

with $P(\mathbf{k}; z)$ given by Eq. (12), where $p(\mathbf{k})$ for $d = 3$ is used. $P(\mathbf{0};z)$ is decomposed according to Eq. (16) with

$$I_3 = \pi^{-3} \int_0^{\pi}\int\int d^3k\, [A(z) - p(\mathbf{k})]^{-1}. \tag{27}$$

The quantity $A(z)$ is given by Eq. (17). We are again interested in the behavior near $z = 1$ or $x = 0$ when $x = 1 - z$ is introduced. The expansion of $A(x)$ is given in Eq. (19). The resulting expansion of I_3 is

$$I_3 = P_{\rm uc}(\mathbf{0};1) + O(x^{1/2}), \tag{28}$$

where $P_{\rm uc}(\mathbf{0};1)$ is related to the return probability p_r for uncorrelated random walk,

$$P_{\rm uc}(\mathbf{0};1) = (1 - p_r)^{-1}. \tag{29}$$

We content ourselves with the leading terms in the expansions of I_3 and $P(\mathbf{0};z)$. The expansion of $P(0;x)$ is given by

$$P(\mathbf{0};x) = P_{\rm uc}(\mathbf{0};1)/f + (f-1)/2f + O(x^{1/2}). \tag{30}$$

This expression is inserted into the formula (2) relating $\langle S\rangle(x)$ to $P(\mathbf{0};x)$. The ensuing asymptotic behavior is

$$\langle S_n\rangle = \frac{(1-p_r)fn}{1+\frac{1}{2}(f-1)(1-p_r)} + O(n^{1/2}). \tag{31}$$

The main point we wish to make here is that the result (31) violates scaling already in the leading-order term proportional to n. On the other hand, a correction term should be present for the following reason. The quantity $1 - p_f = 0.659\,426\,7\ldots$ in the simple-cubic lattice.[2] The maximal f for walk with excluded reversal ($p_b = 0$) is 1.5 in $d = 3$. If no correction term were present, $\langle S_n\rangle \approx 0.989n$—a too large value for the walk considered. Equation (31) predicts that $\langle S_n\rangle \approx 0.849n$ for $f = 1.5$.

Figure 4 contains the results of the above derivations (31) as full lines and the scaling prediction $\langle S_n\rangle \sim (1 - p_r)\,fn$ as dashed lines. One notices very good agreement between theory and the data points obtained by numerical simulations. Hence also in $d = 3$ the theory must include correction terms that do not obey scaling.

V. FORWARD STEPPING MODEL

The forward stepping model is characterized by a larger-than-average probability that a step of the particle in one direction is followed by a step in the same direction. The probability for forward steps is called p_f, we require $1/z < p_f < 1$. The probability for a step in any other directions is given by $(1 - p_f)/(z - 1)$. Although it includes only a memory to the preceding step, the forward stepping model is apparently more difficult to treat analytically than the model with restricted reversals.

The generating function of this model is no more of the simple form (12), and we could not derive analytical expres-

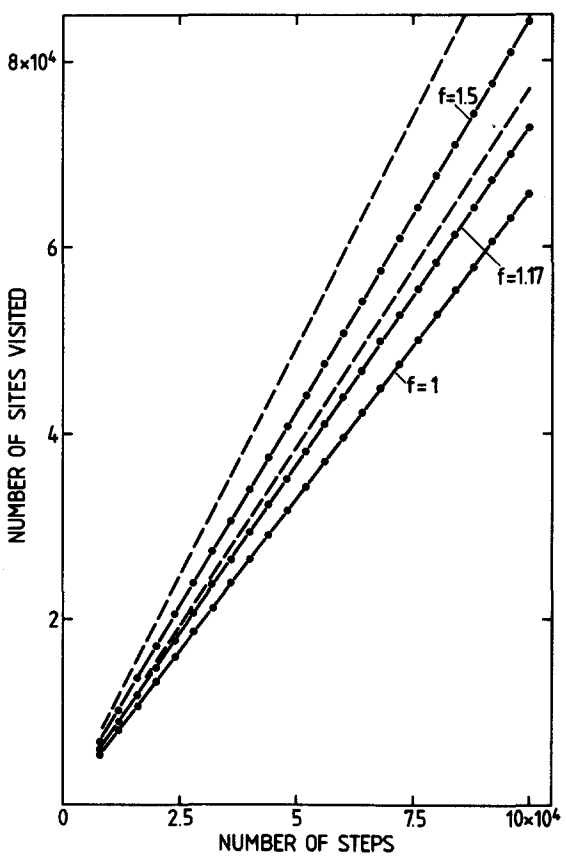

FIG. 4. Mean number of distinct sites visited by correlated walk in $d = 3$ according to model with reduced reversals. Points results of simulations, full lines theory described in the text, dashed lines theory without correction terms.

sions for the mean number of distinct sites visited according to the forward stepping model.

We suppose that $\langle S_n \rangle$ for the forward stepping model has the same *form*, in each dimension, as for the model with reduced reversals. Hence we assume that $\langle S_n \rangle$ has the following form in $d = 2$:

$$\langle S_n \rangle = \frac{\pi f n}{\ln(\beta n)} \sum_{j=0}^{\infty} c_j (\ln \beta n)^{-j}, \tag{24}$$

where we set

$$\beta = 8 f e^B \tag{32}$$

and consider B as a fitting parameter. The particular form (32) is taken to have explicit scaling of the ln term, e.g., $\ln \beta n = \ln 8 f n + B$.

We fitted the numerical results for $\langle S_n \rangle$ for various values of p_f with Eqs. (24) and (32). The resulting parameters B are given in Table I. We included six coefficients c_j of the series (24), more than sufficient for all our step numbers used. Figure 5 gives the numerical results for three values of $p_f > 1/4$, together with the fit of the data. The fit is quite good, as expected. The results for uncorrelated walk are included for comparison.

Table I shows that the parameter B becomes large for larger values of the correlation factor f. The influence of the correction term becomes then large compared to the term $\ln(8fn)$, for the step numbers and values of f investigated. As a consequence, the ln term does not have much influence in $\langle S_n \rangle$, i.e., $\langle S_n \rangle$ is almost a straight line. This is seen in Fig. 5 for the two larger values of f. The ln term would become important only for extremely large step numbers. That the correction term B, which does not obey scaling, is necessary can also be seen from the following argument. The values that f can take are unrestricted in the forward stepping model. The scaling form of $\langle S_n \rangle$ with $B = 0$ and large f would yield values $\langle S_n \rangle > n$ except for extremely large step numbers. This is unreasonable.

For three-dimensional lattices we should assume that $\langle S_n \rangle$ has a form analogous to Eq. (31). For numerical convenience we have made a least-square fit of simulation data with a constant correction term D,

$$\langle S_n \rangle = \frac{(1 - p_r) f n}{1 + C} + D. \tag{33}$$

The parameters C, D resulting from the fit of the numerical data are given in Table II. Figure 6 shows the results of the simulations for three different $p_f > 1/6$, together with the fit by Eq. (33). Also the results for uncorrelated walk are given for comparison. The parameter D is small in all cases and the corresponding ordinates are scarcely noticed in the figure. The most prominent feature which emerges from this figure is the rather small increase of $\langle S_n \rangle$ by the introduction of

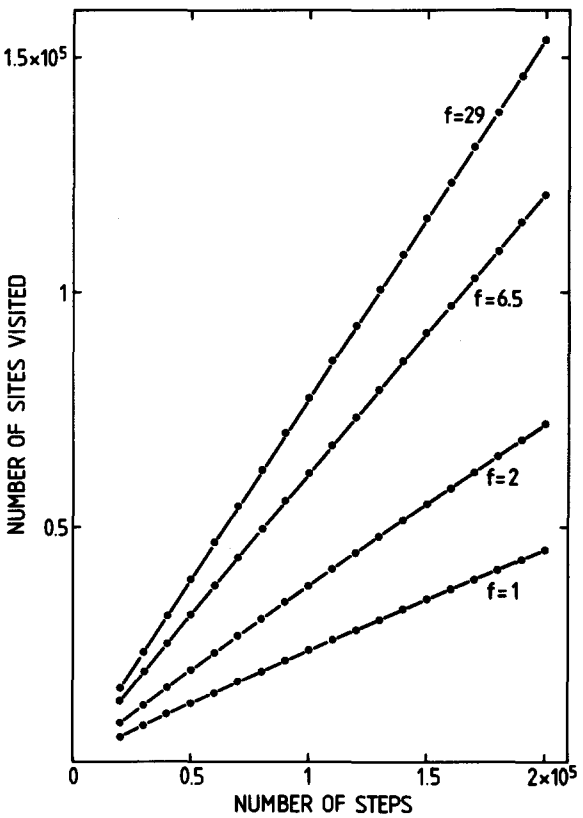

FIG. 5. Mean number of distinct sites visited by correlated walk in $d = 2$ according to forward stepping model. Points results of simulations, lines results of fit by Eqs. (24) and (32). Results for uncorrelated walk ($f = 1$) are shown for comparison.

correlations in the random walk. This is easily understood from the transient nature of random walks in $d = 3$. Since an uncorrelated random walk is visiting, asymptotically, already $\langle S_n \rangle \approx 0.659n$ new sites with n steps, the introduction of correlations cannot much increase $\langle S_n \rangle$ until the limit $\langle S_n \rangle = n$ is reached, corresponding to $f \to \infty$. It is also clear that $\langle S_n \rangle$ cannot be of the asymptotic scaling form $\langle S_n \rangle = (1 - p_r) fn$, since then $\langle S_n \rangle > n$ for larger f.

It is instructive to consider the efficiency E_n of correlated walks according to the forward stepping model in $d = 2$ and 3; cf. the definition (10). The results of the simulations for various values of the correlation factor f are represented in Fig. 7 for $d = 2$ and in Fig. 8 for $d = 3$. We observe that in $d = 2$ the efficiency increases with increasing step number, for large values of f, while in $d = 3$ the efficiency remains practically constant, except at the beginning. This behavior is explained by the different influence of correlations on $\langle S_n \rangle$ in $d = 2$ and 3. In $d = 2$ the number of visited sites by uncorrelated walk increases less strongly than the step num-

TABLE I. Parameter B determined by fit of two-dimensional numerical data with Eqs. (24) and (32).

p_f	0.4	0.5	0.6	0.7	0.8	0.9	0.95
f	1.5	2	2.75	4	6.5	14	29
B	1.491	2.872	5.233	9.452	18.14	45.21	101.2

TABLE II. Parameters C, D determined by fit of three-dimensional numerical data with Eq. (33).

p_f	0.4	0.5	0.6	0.7	0.8	0.9
f	1.778	2.333	3.167	4.555	7.333	15.667
C	0.5529	0.9532	1.562	2.5918	4.666	10.92
D	644	695	742	786	816	793

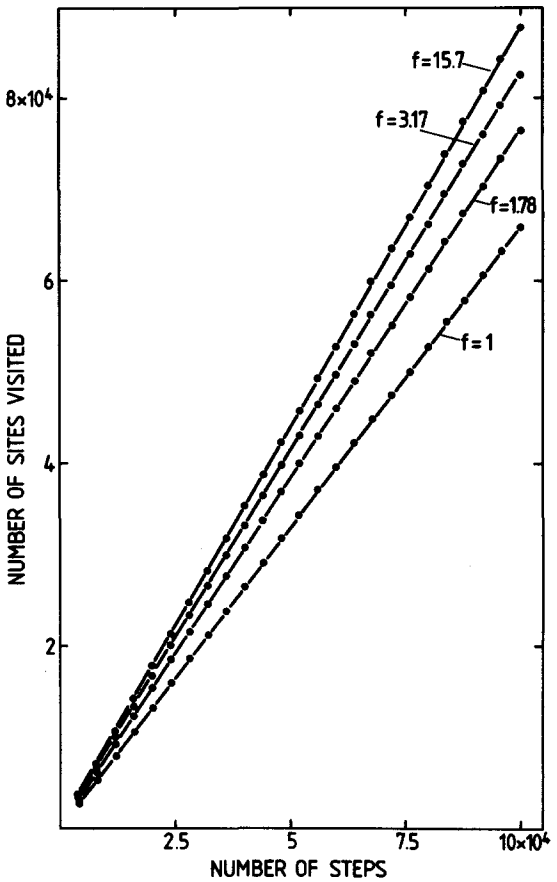

FIG. 6. Mean number of distinct sites visited by correlated walk in $d = 3$ according to forward stepping model. Points results of simulations, lines results of fit by Eq. (33). Results for uncorrelated walk ($f = 1$) are shown for comparison.

ber, due to the logarithmic correction in the denominator. For correlated walk, a constant correction appears in the denominator, resulting in an effective proportionality of $\langle S_n \rangle$ with n when f is large. Consequently the quotient of both quantities increases with increasing step number, and this effect is most pronounced for large f values. In $d = 3$ the number of distinct sites visited is linear in the step number, apart from small correction terms, both for uncorrelated and correlated walks. Hence the quotient of $\langle S_n \rangle$ for correlated and for uncorrelated walks is practically constant. The correlation factor only determines the magnitude of this quotient. Thus the qualitative behavior of E_n in $d = 2$ and 3 is understood, although analytical expressions are lacking for the forward stepping model considered here.

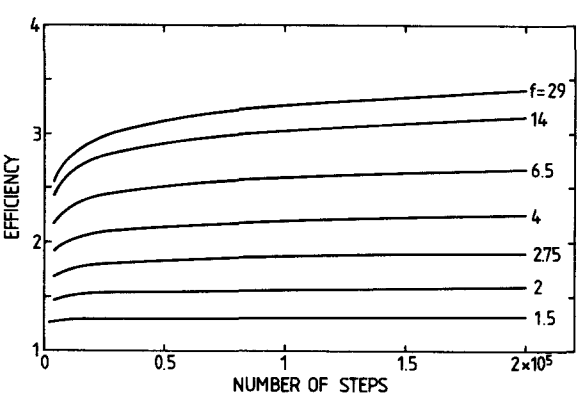

FIG. 7. Efficiency of correlated walks in $d = 2$. See Fig. 2 for details.

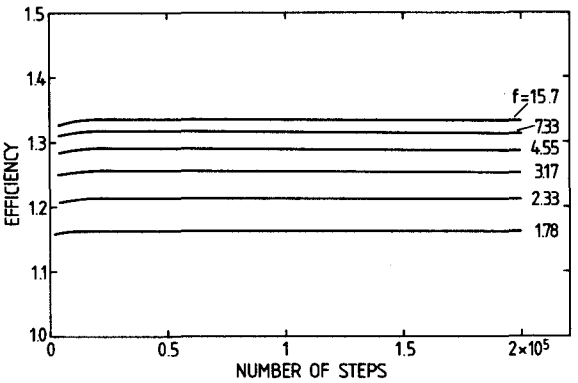

FIG. 8. Efficiency of correlated walks in $d = 3$. See Fig. 2 for details.

VI. CONCLUSION

In this article we investigated the mean number of distinct sites visited by correlated walks of a particle on one-, two-, and three-dimensional lattices. A memory to the preceding step was taken into account. While in $d = 1$ there is just one model of correlated walk with a one-step memory, there are several variants in $d \geqslant 2$. We studied two variants of such models, (i) the model with reduced reversals, and (ii) the model with a larger-than-average forward stepping probability. In the first case we could provide analytical solutions in $d = 2$, 3 which describe the numerical data quite well, in the second case we were restricted to numerical simulations and data analysis. The results obtained are extensions of previous results for uncorrelated walk. The common feature of the results for correlated walk is the appearance of corrections to scaling, i.e., the results cannot be simply obtained by rescaling the step numbers with the correlation factor f; there are additional correction terms.

Our results show that the original formulas of Montroll and Weiss[2] are modified as pointed out above. For the convenience of the reader we list the asymptotic results for $\langle S_n \rangle$ of the model (i) with reduced reversals in all dimensions.

$$\langle S_n \rangle = (8fn/\pi)^{1/2} + 1 - f + \cdots, \quad d = 1,$$

$$\langle S_n \rangle = \frac{\pi f n}{\ln(8fn) + \pi(f-1)/2} + \cdots, \quad d = 2,$$

$$\langle S_n \rangle = \frac{(1-p_r)fn}{1 + \frac{1}{2}(f-1)(1-p_r)} + \cdots, \quad d = 3. \qquad (34)$$

The order of the terms neglected in Eq. (34) was indicated in the main text.

An obvious extension of the present study is the investigation of correlated walks in lattices with inaccessible sites. The results of such an investigation will be reported in a future publication. There are also other models of correlated walk possible than the ones considered here. We wish to point out in the remainder of this section the relation of our models to a previously studied model of coherent energy

transfer.[6] The common point to both is that correlation (coherence) appears as an increased "mean free path" of the particle, caused by the retention of memory of a particular direction of motion over a certain number of lattice sites. In the previous model[6] the average length of such a path was specified by a parameter l, which was the mean value of a Gaussian distribution with a standard deviation σ. Thus the lengths of the mean free paths were chosen at random from a Gaussian-distributed random-number generator. But *all* individual sites belonging to these long paths were considered as visited one-at-a-time in the duration of the paths, they were tested for visitation, etc., in a similar way as in the present model. We can establish a relation between the previous model[6] and the forward stepping model by comparing the probability of scattering in a different direction. Since $1-p_f$ is the total probability of scattering in the forward model, the distribution of the lengths of paths in one direction is approximately Poissonian for p_f approaching 1,

$$P_l \approx (1-p_f)\exp[-(1-p_f)l]. \tag{35}$$

The average length of a mean free path in the forward model is $\langle l \rangle = (1-p_f)^{-1}$. Hence both models should give similar results when l in the previous model equals $(1-p_f)^{-1}$ in the present model. This is indeed borne out by the numerical simulations. From the experimental point of view, the previous model[6] seems to be quite appropriate to describe coherent energy transfer. From the theoretical point of view, the present model is preferable since it requires only one parameter (p_f) instead of 2 (l, σ), and is more easily amenable to analytical methods.

Note added in proof: Meanwhile two articles on the mean number of distinct sites visited were published. In the first one [J. B. T. M. Roerdink and K. E. Shuler, J. Stat. Phys. **40**, 205 (1985)] the leading asymptotic terms were derived for multistate random walks in $d = 1$ and 2, in the second one [J. B. T. M. Roerdink, J. Appl. Prob. **22**, 951 (1985)] the same was done for correlated walks.

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