Novel behavior of biased correlated walks in one dimension

K. Kang and S. Redner
Center for Polymer Studies and Department of Physics, Boston University, Boston, Massachusetts 02215

(Received 29 August 1983; accepted 7 December 1983)

The asymptotic properties of a biased correlated walk model in one dimension are treated analytically. In this model, a weight factor p is associated with the walk each time it visits a new site, and different fugacities are assigned for steps to the left and to the right. The range $0 < p < 1$ corresponds to attractive correlations, and this case describes aspects of biased diffusion on a lattice with randomly distributed static traps. A generating function for the correlated walk model is defined which equals the configurational averaged survival probability for biased diffusion in the presence of traps. The quantity is found to decay exponentially with N, the number of steps in the walk. We find an interesting transition in the average number of visited sites. For weak bias, this quantity varies as $N^{1/3}$, suggesting a zero drift velocity; for strong bias it varies linearly with N, indicating a transition to a finite drift velocity.

I. INTRODUCTION

Recently, a correlated walk model was introduced[1] in which a single parameter may be varied to yield either attractive or repulsive correlations. In this model, a weight factor of p is associated with the walk each time it visits a new site, so that a walk which visits s distinct sites has a statistical weight of p^s. For $0 < p < 1$, a walk which returns to previously visited sites is more likely to occur, while for $p > 1$, a walk is more likely to visit new sites at each additional step. These two cases correspond to a self-attracting or a self-repelling walk, respectively, while the special case $p = 1$ is an uncorrelated random walk.

This correlated walk model is of interest because it describes aspects of self-interacting polymer chains and because it appears to exhibit some of the intriguing features of diffusion on a medium with randomly distributed static traps.[2–7] The correlation in our model can be thought of as the result of performing a configurational average over static disorder. This approach has the advantage of casting a diffusion problem on a random medium in terms of a correlated diffuison process on a homogeneous lattice.

A precise connection between correlated walks and diffusion in random media can be formulated in terms of the following generating function[1–3]:

$$\mathscr{Z}(N,p) = q^{-N} \sum_{s=2}^{N+1} C(N,s) p^s, \tag{1.1}$$

where $C(N,s)$ is the number of walks of N steps that visit s distinct sites, and it is convenient to include a normalization factor of q^{-N}, where q is the lattice coordination number. This generating function equals the *exact* probability, averaged over all possible configurations of traps, that a diffusing particle will survive until N steps when placed on a lattice containing static traps randomly distributed at density $1 - p$. This equivalence rests on the fact that for a walk to survive when traps are present, each visited site must be a nontrap, while the remaining lattice sites may be either traps or nontraps.[1,2] Consequently, a walk which has visited s distinct sites survives with probability p^s. Upon averaging over all walks of N steps, one arrives at Eq. (1.1). We recently derived an analytical solution of this model in one dimension for the case of spatial isotropy and a number of interesting properties were found.[3] For $\mathscr{Z}(N,p)$, we obtained

$$\begin{aligned} \mathscr{Z}(N,p) &= 1, && p = 1, \\ &\sim e^{aN}, && p > 1, \\ &\sim N^{-1/3} e^{-bN^{1/3}}, && p < 1 \end{aligned} \tag{1.2}$$

valid asymptotically in the limit $s, N \to \infty$. The last result agrees with previous approximate predictions for diffusion in the presence of static traps,[4–6] except that a power law prefactor is predicted as well. We also found that the mean number of sites visited after N steps $\langle s_N(p) \rangle$ plays a central role in characterizing correlated walks. We obtained

$$\begin{aligned} \langle s_N(p) \rangle &\sim N^{1/2}, && p = 1, \\ &\sim N, && p > 1, \\ &\sim N^{1/3}, && p < 1. \end{aligned} \tag{1.3}$$

In this article, we study the behavior of this correlated walk model in one dimension with the added influence of an external bias. We employ the recently introduced transfer matrix method,[3] exact enumeration, and steepest descents to obtain the physical quantities of interest in the model. We find that for any bias, $\mathscr{Z}(N,p)$ decays exponentially with N for all $p < 1$. Following the same line of reasoning as outlined for the isotropic case,[3] it may be readily verified that the generating function in the biased case equals the configurational averaged survival probability for a biased random walker to survive until N steps on a lattice with static traps at density $1 - p$. Due to this equivalence, we predict an exponential decay in the survival probability as a natural byproduct of our calculation. This is in agreement with the recent work of Grassberger and Procaccia[7] on diffusion and drift in a continuous medium with randomly distributed static traps. However, we also find a transition in $\langle s_N(p) \rangle$ from an $N^{1/3}$ behavior to a linear dependence on N as a function of the correlation parameter p. Alternatively, for a fixed value of p, the situation may be regarded as a transition from zero velocity ($\langle s_N(p) \rangle \sim N^{1/3}$) for sufficiently weak bias, to a finite velocity ($\langle s_N(p) \rangle \sim N$) for strong bias. There is also a corresponding change in the rate constant of the exponential decay law which was not predicted in Ref. 7.

In Sec. II, we calculate the distribution of visited sites

 0021-9606/84/062752-04$02.10

$C(N,s)$ for biased walks by using a transfer matrix method in combination with an exact enumeration approach. This distribution is the basic ingredient in our solution. It has been obtained previously for the unbiased case,[3,8–12] but the more formal solutions[8–12] are not suitable for extracting the asymptotic behavior required for our solution of correlated walks. In Sec. III, this asymptotic distribution and the steepest descent approach are used to calculate the generating funtion and the mean number of visited sites. We also compare our results with the predictions of Grassberger and Procaccia.[7] Finally in Sec. IV, we summarize the main results of our approach and calculation.

II. DISTRIBUTION OF VISITED SITES

We showed previously[3] that in one dimension, the asymptotic form of the distribution of visited sites $C(N,s)$ can be expressed as a product of the asymptotic forms for $C(N,s)$ in the two limits $s/N \to 0$ and $s/N \to 1$. This approach yielded

$$C(N,s) \cong A\,[2\cos(\pi/(s+1))]^N e^{-s^2/2N}, \tag{2.1}$$

where A is a normalization coefficient.

We now extend this result for $C(N,s)$ to biased walks. To introduce a bias, we associate a fugacity a for a step to the right, and a different fugacity b for a step to the left. A walk which contains r steps to the right after N total steps will now be weighted by a factor $a^r b^{N-r}$. For the biased case, the definition of $C(N,s)$ may now be generalized to account for the combinations of left- and right-hand steps that lead to s distinct sites being visited. We write

$$C(N,s) = \sum_{r=0}^{N} D(N,s,r) a^r b^{N-r}, \tag{2.2}$$

where $D(N,s,r)$ is the number of N step walks which visit s distinct sites and take r steps to the right.

To calculate the asymptotic form of $C(N,s)$ for $s/N \to 0$, we consider the $s \times s$ transfer matrix T_s:

$$T_s = \begin{pmatrix} 0 & a & & & & \\ b & 0 & a & & 0 & \\ & b & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & a \\ & 0 & & & b & 0 & a \\ & & & & & b & 0 \end{pmatrix}. \tag{2.3a}$$

The matrix T_s moves a random walker either one step to the left, with weight b, or one step to the right, with weight a, on a one-dimensional chain consisting of s sites. Therefore, the product

$$(1,1,\ldots,1) T_s^N \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \tag{2.3b}$$

generates all biased walks of N steps on this chain, and the largest eigenvalue of T_s determines the properties of $C(N,s)$ in the limit $s/N \to 0$.[3] To calculate this largest eigenvalue, note that the matrix elements of T_s depend on the row index i and the column index j simply through $i-j$. Therefore, we may Fourier transform[13] on the variable i–j, to find the eigenvalue spectrum

$$\lambda^{(k)} = 2\sqrt{ab}\,\cos(\pi k/(s+1)),\ \ k = 1,2,\ldots,s.$$

Therefore in the limit $s/N \to 0$, the asymptotic form of $C(N,s)$ can be written as

$$\lim_{s/N \to 0} C(N,s) \cong [2\sqrt{ab}\,\cos(\pi/(s+1))]^N, \tag{2.4}$$

where the symbol $\cong$ indicates that only the dominant behavior arising from the largest eigenvalue of T_s is being kept.

To calculate the asymptotic form of $C(N,s)$ for $s/N \to 1$, we use an exact enumeration approach. When $s = N+1$, there are only two possible walks as shown in Fig. 1(a). Thus, $C(N,N+1)$ equals $(a^N + b^N)$. When $s = N$, there are four possible walks as shown in Fig. 1(b), and $C(N,N)$ is simply

$$2(a^{N-1}b + ab^{N-1}).$$

By continuing this procedure for a range of values of $s \lesssim N$, we find the dominant contribution to $C(N,s)$ in the $s \to N$ limit,

$$C(N,s) \cong \binom{N}{k} [a^{N-k-1} b^{k+1} + a^{k+1} b^{N-k-1}] + \cdots, \tag{2.5}$$

where the correction terms are lower-order in N, and $k = (N-s)/2$ for even $N-s$, and $k = (N-s-1)/2$ for odd $N-s$. By changing variables from k to s and neglecting the constant coefficient, we then find

$$C(N,s) \cong \binom{N}{(N-s)/2} [a^{(N+s)/2} b^{(N-s)/2} + a^{(N-s)/2} b^{(N+s)/2}]. \tag{2.6}$$

For an asymptotic analysis, the even–odd oscillation in $C(N,s)$ is not important, and we therefore consider only the

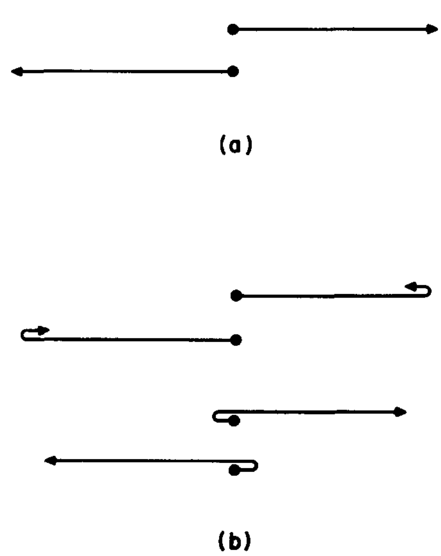

FIG. 1. Configurations of walks of N steps which (a) visit $s = N+1$ sites, and (b) visit $s = N$ sites. The symbol ● denotes the origin of the walk, and → the endpoint of the walk. For simplicity, intermediate sites are not shown.

even terms. Using Stirling's approximation, we have

$$\lim_{N\to\infty}\binom{N}{(N-s)/2}\cong 2^N\sqrt{\frac{2}{\pi N}}e^{-s^2/2N}. \tag{2.7}$$

Therefore, we write the following expression for $C(N,s)$ under the assumption that it is the product of the two asymptotic forms in the limits $s/N\to 0$, and $s/N\to 1$:

$$C(N,s)\cong A\,[2\sqrt{ab}\cos(\pi/(s+1))]^N e^{-s^2/2N} \times [a^{(N+s)/2}b^{(N-s)/2}+a^{(N-s)/2}b^{(N+s)/2}], \tag{2.8}$$

where A is the normalization factor which will be determined from the condition

$$\sum_{s=2}^{N+1} C(N,s)=(a+b)^N.$$

III. STEEPEST DESCENT APPROACH

Without loss of generality, we may set $a+b=2$ and also assume $a>b$. To find the normalization constant A in Eq. (2.8), we require

$$\int_2^{N+1} C(N,s)ds, \tag{3.1}$$

where

$$C(N,s)\cong A\,\{\exp[f(s)]+\exp[g(s)]\} \tag{3.2}$$

with

$$f(s)=N\ln\sqrt{ab}+N\ln[2\cos(\pi/(s+1))]+\frac{s}{2}\ln a/b \tag{3.3a}$$

and

$$g(s)=N\ln\sqrt{ab}+N\ln[2\cos(\pi/(s+1))]+\frac{s}{2}\ln b/a. \tag{3.3b}$$

If $a>b$ and s is sufficiently large, the second exponential in Eq. (3.2) may be neglected. Then by setting the derivative $f'(s)$ equal to zero, we find the following value of $s_{\max}$ which gives the maximum value of the distribution, $C(N,s)$, in the limit $s,N\to\infty$:

$$s_{\max}\cong\frac{N}{2}\ln a/b. \tag{3.4}$$

By expanding $f(s)$ about $s_{\max}$,

$$f(s)\cong f(s_{\max})+1/2(s-s_{\max})^2 f''(s_{\max})+\dots,$$

one may write Eq. (3.1) as a simple Gaussian integral, and we find

$$A\cong\sqrt{\frac{1}{2\pi N}}\exp\left\{-N\left[\frac{1}{8}(\ln a/b)^2+\ln ab\right]\right\} \tag{3.5}$$

We now calculate the normalized generating function for $p\neq 1$ by evaluating

$$\mathscr{Z}(N,p)\cong A\,2^{-N}\int_0^\infty \exp[f(s)+s\ln p]ds \tag{3.6}$$

by steepest descents. The value of s which maximizes the integrand now depends on the value of p, and it is found from the condition $f'(s)+\ln p=0$. The competition between attraction and bias plays a crucial role in determining asymptotic behavior. For $0<p<\sqrt{b/a}$ (strong attraction or weak bias limit) we obtain

$$s_{\max}\cong[-\pi N/(\tfrac{1}{2}\ln a/b+\ln p)]^{1/3}. \tag{3.7}$$

Thus, the effect of the bias can be suppressed by a sufficiently strong attractive interaction and $s_{\max}$ has essentially the same behavior as when no bias is present.[3] For $p>\sqrt{b/a}$ (weak attraction or strong bias limit), we find

$$s_{\max}\cong N(\tfrac{1}{2}\ln a/b+\ln p). \tag{3.8}$$

Thus, for sufficiently strong bias, the number of visited sites scales linearly with N, indicating that there is a superimposed drift on the diffusion. Finally, for $p=\sqrt{b/a}$,

$$s_{\max}\cong(\pi N)^{1/2}. \tag{3.9}$$

At this value of p, the effect of the attractive interaction and the bias balance to yield a diffusion process where $s_{\max}$ varies with N as in the uncorrelated random walk.

We may also calculate the generating function in Eq. (3.6) by writing the integrand as a Gaussian, and following the steps that led to Eq. (3.5). For $0<p<\sqrt{b/a}$, we find

$$\mathscr{Z}(N,p)\cong N^{-1/3}\exp\left[-\frac{N}{8}(\ln a/b)^2-\alpha N^{1/3}\right] \tag{3.10}$$

where

$$\alpha=[-(\tfrac{1}{2}\ln a/b+\ln p)]^{2/3}(1+\pi^{4/3}/2).$$

Surprisingly, the decay remains exponential even though $s_{\max}$ is proportional to $N^{1/3}$. For $p>\sqrt{b/a}$ we find

$$\mathscr{Z}(N,p)\cong\exp\left[\frac{N}{2}\ln p(\ln a/b+\ln p)\right]. \tag{3.11}$$

Thus, exponential decay is also predicted for $\sqrt{b/a}<p<1$, and exponential growth for $p>1$. At $p=\sqrt{b/a}$, we find an exponential decay with a different power law prefactor than in Eq. (3.10),

$$\mathscr{Z}(N,p)\cong N^{-1/2}\exp\left[-\frac{N}{8}(\ln a/b)^2\right]. \tag{3.12}$$

Due to the connection with diffusion in the presence of traps, we predict that in one dimension the survival probability for biased diffusion decays exponentially,[7]

$$\mathscr{Z}(N,p)\sim\exp(-kN),$$

for all values of p. However, the rate constant k undergoes a sharp transition. We have

$$\begin{aligned} k&\sim-\tfrac{1}{2}\ln p(\ln a/b+\ln p), && \sqrt{b/a}<p<1,\\ &\sim+\tfrac{1}{8}(\ln a/b)^2, && 0<p<\sqrt{b/a}\end{aligned}. \tag{3.13}$$

For small bias, one may interpret the quantity $\ln a/b$ as the drift velocity in biased diffusion. This then gives $k\sim v_{\rm drift}^2$ for small bias, and $k\sim v_{\rm drift}$ for large bias. This transition for the rate constant was predicted by Grassberger and Procaccia[7] in their investigation of a continuum model, but only for dimensions greater than one. It would therefore be of interest to test our predictions for one dimension by numerical simulations.

Finally, the mean number of visited sites $\langle s_N(p)\rangle$ can be calculated directly from the generating function by using[1]

$$\langle s_N(p)\rangle=\partial\ln Z(N,p)/\partial\ln p. \tag{3.14}$$

We find $\langle s_N(p)\rangle \sim N$ for $p>\sqrt{b/a}$, $\langle s_N(p)\rangle \sim N^{1/2}$ at $p=\sqrt{b/a}$, and $\langle s_N(p)\rangle \sim N^{1/3}$ for $0<p<\sqrt{b/a}$, thereby reflecting the properties of $s_{\max}$ found in Eqs. (3.7)–(3.9). We also expect that in one dimension, the rms displacement should also scale as $\langle s_N(p)\rangle$. Thus, for a weak bias, a diffusing particle is effectively localized, while for a strong bias, the particle has a finite drift velocity.

IV. CONCLUSIONS

We have found interesting behavior for biased, correlated diffusion in one dimension by calculating the distribution of visited sites $C(N,s)$. In our approach, the competition between the attractive interaction and the bias determines the long-time properties of the walk. A transition occurs when the decay length associated with the attraction, $(-\ln p)^{-1}$, equals the "barometric" length $(\frac{1}{2}\ln a/b)^{-1}$ associated with the biased chain. We find an exponential decay for the generating function for all $p<1$, although the rate constant of the decay changes at the transition. Due to the exact correspondence between the generating function of our model and the survival probability for diffusion in the presence of static traps, our approach also predicts an exponential decay for the particle density in the latter process. We also found that considerable insight on the nature of the transition is gained by studying the behavior of the mean number of visited sites $\langle s_N(p)\rangle$. We found $\langle s_N(p)\rangle \sim N^{1/3}$ for weak bias, while $\langle s_N(p)\rangle \sim N$ for strong bias. This indicates a transition from zero drift velocity to a finite drift velocity as a function of the bias.

Our approach has the advantage of casting a diffusion problem on a random medium in terms of a correlated diffusion process on a homogeneous lattice. Transition phenomena are then found simply in terms of the strength and sign of the correlation. It will be of great interest to try to extend the present approach to higher dimensions in order to gain a better understanding of the nonexponential decay processes recently predicted[3–6] for diffusion in the presence of randomly distributed traps.

ACKNOWLEDGMENTS

This work is supported in part by grants from the ARO, NSF, and ONR. We thank Professor H. E. Stanley for helpful discussions during this work.

[1]H. E. Stanley, K. Kang, S. Redner, and R. L. Blumberg, Phys. Rev. Lett. **51**, 1223 (1983).
[2]K. Kang (unpublished).
[3]S. Redner and K. Kang, Phys. Rev. Lett. **51**, 1729 (1983).
[4]P. Grassberger and I. Procaccia, J. Chem. Phys. **77**, 6281 (1982).
[5]B. Movaghar, G. W. Sauer, and D. Würtz, J. Stat. Phys. **27**, 473 (1982).
[6]R. F. Kayser and J. B. Hubbard, Phys. Rev. Lett. **51**, 79 (1983).
[7]P. Grassberger and I. Procaccia, Phys. Rev. A **26**, 3686 (1982).
[8]H. E. Daniels, Proc. Cambridge Philos. Soc. **37**, 244 (1941).
[9]H. Kuhn, Helv. Chim. Acta **31**, 1677 (1948).
[10]W. Feller, Ann. Math. Stat. **22**, 427 (1951).
[11]R. J. Rubin, J. Chem. Phys. **56**, 5747 (1972); For a review, see for example, G. H. Weiss and R. J. Rubin, Adv. Chem. Phys. **52**, 363 (1982).
[12]B. Preziosi (preprint).
[13]See, for example, R. Bellman, *Introduction to Matrix Analysis* (McGraw–Hill, New York, 1970), p. 222.