Asymptotic Solution of Interacting Walks in One Dimension

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An asymptotic solution to interacting walks in one dimension is presented. For repulsive and attractive interactions, respectively, the model describes aspects of uncorrelated diffusion on a lattice with sources or with randomly distributed traps. In the latter case, the average number of sites visited varies with the number of steps in the walk as $N^{1/3}$, while the survival probability decays as $N^{-1/3}\exp(-bN^{1/3})$, improving on previous predictions for diffusion with traps.

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Consider a discrete random walk on a lattice in which each new site visited has a weight p, so that a walk which visits s distinct sites has a statistical weight p^s . This model was recently introduced in order to describe various aspects of diffusion in randomly porous media and self-interacting polymer chains. For p>1, a walk is more likely to visit new sites at each step and the walk is self-repelling. Alternatively, when a new site is visited, the additional weight factor of p is equivalent to p-1 new copies of the original walk being "born" and included in a statistical ensemble. This may be thought of as uncorrelated diffusion in a medium consisting of uniform sources.

For p < 1, walks which return to previously visited sites are more likely to occur and the walk is self-attracting. Equivalently, as each new site is visited the weight factor of p less than unity may be regarded as a nonzero probability that the walk will "die" and disappear from the ensemble. In fact, it has been demonstrated that there is an exact correspondence between the total statistical weight of an ensemble of self-attracting walks of N steps, and the quenched average probability that a diffusing particle will survive until N steps in a medium with randomly distributed traps present with probability 1-p, a problem of classical importance as well as the focus of recent interest. $^{2-10}$

In this Letter, we present an asymptotic solution for this interacting walk model in one dimension. For the self-repelling case, we find that for all p>1, the mean number of sites visited after N steps, $\langle s_N \rangle$, scales linearly in N, while the number of walks present in a statistical ensemble after N steps grows as e^{aN} . For the attracting case, we find that for all $0 , <math>\langle s_N \rangle \sim N^{1/3}$ while the survival probability varies as $N^{-1/3} \exp(-bN^{1/3})$. The latter result lies between the lower and up-

per bounds given recently by Grassberger and Procaccia⁹ and by Kayser and Hubbard, ¹⁰ respectively.

Our solution is based on calculating the distribution of visited sites in a one-dimensional random walk. This problem has received considerable attention in the past, and a number of exact solutions have been published. 11 The resulting expression is rather complicated, however, and it is not clear how to extract an asymptotic form for the distribution which is suitable for application for interacting walks. Our T-matrix approach has the advantage that the asymptotic form of the distribution can be calculated in a simple manner. Furthermore, we can also calculate the *exact* expression for the distribution and the average number of visited sites much more simply than the earlier approaches. 12 In addition to solving the problem at hand, the T matrix can be applied to treat interacting walks with an external bias as well. 13

To begin, define $P_N(s)$ as the number of N-step random walks that visit s sites on an infinite one-dimensional chain (Fig. 1). The minimum value of s is 2 corresponding to a walk which reverses direction at each step, while the maximum value of s is N+1 corresponding to a completely

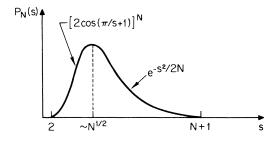


FIG. 1. Schematic picture of the distribution function $P_N(s)$ for unrestricted random walks in one dimension.

stretched walk. It is possible to enumerate the number of N-step walks that visit s sites when $s \cong N$, by an application of the reflection method. For s > N/2, a relatively simple expression may thereby be derived in terms of binomial coefficients. Finally, employing Stirling's approximation, we find the asymptotic form,

$$\lim_{s \to N} P_N(s) \sim \exp(-s^2/2N). \tag{1}$$

To find the asymptotic form of $P_N(s)$ in the limit $s/N \to 0$, let us represent the one-dimensional chain as the (1+1)-dimensional space-time lattice indicated in Fig. 2. The trajectory of a random walk on the chain then maps to a directed random walk on the two-dimensional strip. In terms of the $s \times s$ transfer matrix

one may readily verify that the number of directed random walks of N steps on a strip containing s sites per row equals

$$(1 \ 1 \ 1 \dots 1)T_s^N \begin{bmatrix} 1\\1\\1\\\vdots\\1 \end{bmatrix} \equiv \langle T_s^N \rangle. \tag{2b}$$

To see this result, note that the matrix T_s trans-

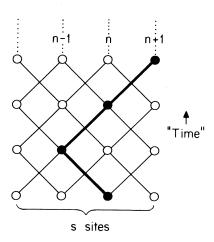


FIG. 2. Representation of a one-dimensional chain of s sites as a (1+1)-dimensional strip. A sample random walk is indicated.

fers a particle up by one row in a strip of s sites by moving the particle from column n to column n+1 or n-1. Therefore the Nth power, T_s^N , transfers a walk N rows, and the column and row vectors consisting of all ones performs a summation over all starting and terminal points of the walk. By a Fourier transformation, one readily finds the eigenvalue spectrum $\lambda^{(k)} = 2\cos[\pi k/(s+1)]$, $k=1,2,\ldots,s$, and eigenvectors $e_n^{(k)} \sim \sin[\pi nk/(s+1)]$, where $n=1,2,\ldots,s$ refers to the nth component of the eigenvector.

The matrix product in Eq. (2a) counts walks which span the strip horizontally (i.e., visit every site of the projected one-dimensional chain), as well as walks which visit fewer sites. To find $P_N(s)$, only the spanning walks are relevant while the nonspanning walks must be subtracted off. It may be verified that

$$\langle T_s^N \rangle = P_N(s) + 2P_N(s-1) + 3P_N(s-2) + \dots + (s-1)P_N(2).$$
 (3)

By writing equations similar to (3) for $\langle T_{s-k}{}^N \rangle$, $k=1,2,\ldots,s-1$, one may then write $P_N(s)$ in terms of a sum over the expectation value of transfer matrices. It is then straightforward to calculate these expectation values in a basis where the matrices are diagonal, and we have thereby obtained the *exact* expression for $P_N(s)$. Notice also that Eq. (3) can be simply manipulated to yield the following formal expression for $\langle s_N \rangle$, for an unrestricted random walk in one dimension:

$$\langle s_N \rangle = \sum_{s=2}^{N+1} s P_N(s) = (N+2) - \frac{\langle T_s^N \rangle}{2^N}$$
 (4)

and by evaluating $\langle T_s^N \rangle$ in a basis where T_s is diagonal, one then finds $\langle s_N \rangle \simeq (8N/\pi)^{1/2}$, in agreement with well-known results.¹¹

For interacting walks, we require a simpler asymptotic form for $P_N(s)$. Since the largest eigenvalue of the lower-rank T matrices is smaller than that of T_s , we may write

$$\lim_{s/N\to 0} P_N(s) \sim \{2\cos[\pi/(s+1)]\}^N.$$
 (5)

As a rough approximation, we postulate that the full distribution for $P_N(s)$ can be adequately described by the product of the asymptotic forms for $s/N \to 0$ and $s \to N$. Thus

$$P_N(s) \cong A \{ 2 \cos[\pi/(s+1)] \}^N \exp(-s^2/2N),$$
 (6)

with A a normalization coefficient which we obtain approximately by steepest descents. We

write $P_N(s) = A \exp[f(s)]$, with

$$f(s) = N \ln \left\{ 2 \cos \left[\pi / (s+1) \right] \right\} - s^2 / 2N. \tag{7}$$

To find the maximum value of the distribution function, we calculate f'(s) and set it equal to zero. In the limit $s, N \rightarrow \infty$, we find for this maximizing value of s

$$s_{\max} \cong (N\pi)^{1/2} \tag{8}$$

in agreement with well-known results for the one-dimensional random-walk problem. This also suggests that the assumption made in Eq. (6) for $P_N(s)$ is valid asymptotically. Finally, by writing

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

we than perform a simple Gaussian integral to find that $A \sim N^{-1/2}$.

We now calculate the physical quantities of interest for $p \neq 1$. The distribution of visited sites now has the form

$$P_N(s,p) \equiv P_N(s)p^s \simeq N^{-1/2} \exp[g(s)],$$

with

$$g(s) = N \ln \left\{ 2 \cos \left[\frac{\pi}{(s+1)} \right] \right\} - \frac{s^2}{2N + s \ln p}.$$
 (9)

Setting g'(s) equal to zero yields, in the limit $s \rightarrow \infty$

$$N\pi^2/s^3 - s/N + \ln b = 0 \tag{10}$$

and the value of $s_{\rm max}$ now depends on p. For all p>1, if we assume that $s_{\rm max}$ grows more rapidly than $N^{1/2}$, we may neglect the first term in Eq. (10) to obtain

$$s_{\max} \sim N \ln p. \tag{11a}$$

This result indicates that for any p>1, the asymptotic behavior is governed by the self-avoiding walk limit, where $\langle s_N \rangle = N+1$. For $0 , we assume that <math>s_{\max}$ grows more slowly than $N^{1/2}$ so that the second term in Eq. (10) may be neglected. This gives

$$s_{\text{max}} \sim [N\pi^2/(-\ln p)]^{1/3}$$
. (11b)

We expect that in one dimension, the root mean square displacement should also scale as $s_{\rm max}$ so that a new type of transport law is predicted.

Notice that by setting $s_{\rm max}$ in Eq. (8) equal to that in Eq. (11a), we find a crossover value, $N_x \sim (\ln p)^{-2}$, below which random-walk behavior should occur, and above which self-avoiding-walk-like behavior should occur. Similarly for the attracting case, we find a crossover value of $N_x \sim (-\ln p)^{-2}$, beyond which the new $\langle s_N \rangle \sim N^{1/3}$

behavior should be observable.

Finally, we calculate the quantity

$$f_N = \left\{ \sum_s P_N(s) p^s \right\} / 2^N. \tag{12}$$

This is the total statistical weight of all N-step interacting walks divided by the total number of N-step random walks. For p>1, f_N gives the growth rate for the number of N-step walks, while for p<1, f_N gives the probability for a random walk to "survive" to N steps on a lattice with randomly distributed traps. We have

$$f_N \sim N^{-1/2} \int_0^\infty \exp[g(s)] ds.$$
 (13)

By expanding g(s) in a Taylor series about s_{\max} and performing the Gaussian integral, we find for the repelling case, where $s_{\max} \sim N \ln p$,

$$f_N \sim \exp[N(\ln p)^2] \sim \exp(N/N_x), \tag{14a}$$

while for the attracting case, we use $s_{\text{max}} \sim [N/(-\ln p)]^{1/3}$ to obtain

$$f_N \sim (N/N_r)^{-1/3} \exp[-(N/N_r)^{1/3}].$$
 (14b)

Our result for f_N lies between the bounds given in Refs. 9 and 10. There the time dependence of the particle density at the origin was calculated, whereas we find the total particle density. However, our approach suggests that the exponential time dependence of these two quantities will be the same (see also Ref. 8). In addition to obtaining the dominant $\exp(-N^{1/3})$ behavior, we also find an $N^{-1/3}$ power-law correction not predicted by the approximate bounds. This power-law correction disagrees, however, with the result of Ref. 8. Also noteworthy is a $(\ln p)^{2/3}$ dependence in the exponential. This differs from the p dependence of $(1-p)^{2/3}$ given in Refs. 8-10, except in the limit $p \rightarrow 1$. However, for p not very close to 1, the methods of Refs. 8-10 appear to have some difficulties, suggesting that a power-law dependence on p is not an adequate description for all p.

In conclusion, we have presented a simple approach to solving an interacting-walk model in one dimension. For the self-repelling case, or equivalently walks which may self-replicate upon visiting new sites, we find that $\langle s_N \rangle \sim N$ and that the number of walks grows as e^{aN} . For the self-attracting case, we find that $\langle s_N \rangle \sim N^{1/3}$, and that the number of surviving walks varies as $N^{-1/3} \times \exp(-bN^{1/3})$. This latter result improves on earlier predictions for the time dependence of the density of diffusing particles on a lattice with randomly distributed static traps.

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Note added: After this paper was completed, we learned that M. D. Donsker and S. R. S. Varadhan [Commun. Pure Appl. Math. 28, 525 (1975)] have proved the existence of a nonexponential decay law in all dimensions; our results agree with theirs in one dimension. We thank Y. Oono and Y. Shapir for bringing this work to our attention.

- U. M. Titulaer, J. Chem. Phys. 76, 4178 (1982).
- 4 J. R. Lebenhaft and R. Kapral, J. Stat. Phys. $\underline{20}$, 25 (1979).
- ⁵M. Bixon and R. Zwanzig, J. Chem. Phys. <u>75</u>, 2354 (1981).
- ⁶T. R. Kirkpatrick, J. Chem. Phys. 76, 4255 (1982). ⁷M. Muthukumar and R. Cukier, J. Stat. Phys. 26,
- ⁸B. Movaghar, G. W. Sauer, and D. Würtz, J. Stat. Phys. 27, 472 (1982).
- ⁹P. Grassberger and I. Procaccia, J. Chem. Phys.
- 77, 6281 (1982).
 10R. F. Kayser and J. B. Hubbard, Phys. Rev. Lett. 51, 79 (1983).

 11 H. E. Daniels, Proc. Cambridge Philos. Soc. 37,
- 244 (1941); H. Kuhn, Helv. Chim. Acta 31, 1677 (1948): W. Feller, Ann. Math. Stat. 22, 427 (1951); R. J. Rubin, J. Chem. Phys. 56, 5747 (1972); B. Preziosi, to be published; for a review, see, e.g., G. H. Weiss and R. J. Rubin, Adv. Chem. Phys. 52, 363 (1982).
- ¹²K. Kang and S. Redner, unpublished.
- ¹³K. Kang and S. Redner, to be published.
- ¹⁴J. K. Percus, Combinatorial Methods (Springer-Verlag, Berlin, 1971), p. 81.

¹H. E. Stanley, K. Kang, S. Redner, and R. L. Blumberg, Phys. Rev. Lett. 51, 1223 (1983).

²M. v. Smoluchowski, Phys. Z. 17, 557 (1916).

³B. U. Felderhof and J. M. Deutch, J. Chem. Phys. 64, 4551 (1976); B. U. Felderhof, J. M. Deutch, and