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Absorption time by a random trap distribution

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The average trapping time and probability distribution of trapping times are calculated for a random walk on a D-dimensional lattice containing a random distribution of traps. Approximations suitable to the limits of high and low trap density are given. The anomalous case of one dimension is given special attention.

I. INTRODUCTION

Consider a simple cubic lattice in any number D of dimensions and infinite in extent, on which a particle is performing a random walk. If the lattice contains a fraction q of randomly located "trap" sites at which the walk is ended, what is the average time to trapping?

This problem was raised in a previous publication[1,2] and approximate answers for the limit of small q were given. Here the range of validity of these results will be extended to the limit of q close to unity. The main result of this paper is Fig. 1.

An expression for the time to trapping will be derived and criticized in Sec. II. Here too, the large-q case will be discussed. Section III will resolve an apparent discrepancy between various results that have been given for the $D = 1$ case. The $D = 3$ version of this problem has been discussed recently by Weiss.[3]

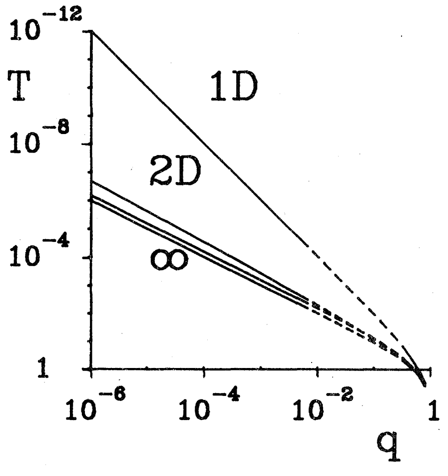

FIG. 1. Mean trapping times in one, two, three, and infinite dimensions. The 3D curve is unlabeled.

II. THEORY OF THE TRAPPING TIME

The theory that will be given here is a simple extension of that of Ref. 1; the derivation is given in an extended form that will make the generalization to all values of q simpler, and make clear which approximations are valid for which values of D and q.

First consider a trapless network of coordination number z (in the case of a cubic lattice, $z = 2D$), and construct the ensemble of all random walks of N steps starting at the origin of this network. Label the walks with an index i, where $1 \leq i \leq z^N$. For any particular walk, we will define $V_i(t)$ for $t \leq N$ to be the number of distinct sites visited in the first t steps of walk i, taking $V_i(0) = 1$ in all cases; and for any function $f_i(t)$ we let

$$\langle f(t) \rangle = z^{-N} \sum_{i=1}^{z^N} f_i(t) \tag{2.1}$$

be the average over the ensemble of walks. This average is independent of N (provided $N \geq t$) because $f_i(t)$ does not depend on which of the z^{N-t} future continuations of the walk are chosen. We also define the quantity

$$\phi_i(t) = V_i(t) - V_i(t-1) \quad , \tag{2.2}$$

which is unity if step t of walk i arrives at a site for the first time (and zero otherwise).

We are now ready to consider a network containing a random distribution of traps with density q. Then the probability that the walk ends on step t is

$$P_i(t) = q\,\phi_i(t)(1-q)^{V_i(t-1)} \tag{2.3}$$

since step t must bring the walker to a trap (probability q) and must do so for the first time (the factor ϕ_i), and the previous $(t-1)$ sites visited must not have been traps. In writing this expression we have implicitly assumed the traps to be randomly located, and taken the ensemble average over all arrangements of traps. To obtain the probability $P(t)$ that a walk ends at step t, we average this expression over the ensemble of walks

$$P(t)=\langle P_i(t)\rangle = q\sum_{v} Q(t,v)(1-q)^{v-1} \quad , \tag{2.4}$$

where

$$Q(t,v)=\langle \phi_i(t)\delta(v-V_i)\rangle \tag{2.5}$$

is the probability that a walker visits v sites in t steps and arrives at a new site on the last step. The expected duration T of a walk is given by

$$T=\sum_{t=0}^{\infty} tP(t) \quad . \tag{2.6}$$

We shall also define

$$R(t,v)=\langle \delta(v-V_i)\rangle \tag{2.7}$$

to be the probability that a walk of t steps visits v sites. This quantity is particularly useful because its behavior for large t has been studied previously.[4] It is related to $Q(t,v)$ in this way:

$$R(t,v)-R(t-1,v)=Q(t,v)-Q(t,v+1) \tag{2.8}$$

which says that on taking a step $(t-1\rightarrow t)$ the population of v-site walks decreases because some of the walks visit a new site, but also increases by promotion of $(v-1)$-site walks. Multiplying this expression by $(1-q)^v$ and summing over all $v\geqslant 0$ gives

$$\sum_{v=0}^{\infty}(1-q)^v[R(t,v)-R(t-1,v)] = -q\sum_{v=1}^{\infty} Q(t,v)(1-q)^{v-1} \tag{2.9}$$

[because $Q(t,0)=0$]. Comparison of the left-hand side with Eq. (2.4) shows that

$$P(t)=F(t-1)-F(t) \quad , \tag{2.10}$$

where

$$F(t)=\langle (1-q)^{V_i(t)}\rangle = \sum_{v=0}^{\infty}(1-q)^v R(t,v) \quad . \tag{2.11}$$

Let us first consider low trap densities. When q is small, most walks will last a large number of steps, and visit a large number of sites. In two or more dimensions, the probability distribution $R(t,v)$ becomes sharp[4] for large t,

$$R(t,v)\rightarrow \delta(v-\bar{V}(t)) \quad , \tag{2.12}$$

in the sense that

$$\langle [V_i-\bar{V}(t)]^2\rangle << \bar{V}(t)^2 \quad . \tag{2.13}$$

Then a binomial expansion gives

$$\langle (1-q)^{V_i(t)}\rangle = (1-q)^{\bar{V}(t)}\langle (1-q)^{V_i(t)-\bar{V}(t)}\rangle = (1-q)^{\bar{V}(t)}\{1-q\langle V_i(t)-\bar{V}(t)\rangle + \tfrac{1}{2}q^2\langle [V_i(t)-\bar{V}(t)]^2\rangle \cdots\} \quad . \tag{2.14}$$

The expression in curly brackets may be put to unity, since the second term vanishes identically, and the third is negligible if $q\bar{V}(t)$ is less than unity [according to Eq. (2.13)]. In the case where $q\bar{V}(t)$ is large, the prefactor $(1-q)^{\bar{V}(t)}$ is small. Then Eqs. (2.10), (2.11), and (2.14) combine to give an expression

$$\begin{aligned} P(t) &= (1-q)^{\bar{V}(t-1)}-(1-q)^{\bar{V}(t)} \\ &\cong -\frac{d}{dt}(1-q)^{\bar{V}(t)} \\ &\approx q(1-q)^{\bar{V}(t)}\frac{d\bar{V}}{dt} \quad . \end{aligned} \tag{2.15}$$

This result, together with Eq. (2.6) and the known asymptotic expressions[1,5] for $\bar{V}(t)$, provides estimates of the average time to trapping, as has been described in Ref. 1.

Now consider high trap densities, for which $(1-q)$ is small. In this case Eq. (2.4) can be used directly, because $Q(t,v)$ need be calculated only for small v, which can be done by direct enumeration of walks. The procedure is illustrated in Appendix A. The nonzero values for $v\leqslant 4$ are

$$\begin{aligned} &Q(0,1)=1 \quad , \\ &Q(1,2)=1 \quad , \\ &Q(t,3)=(z-1)z^{1-t} \text{ for } t\geqslant 2 \quad , \\ &Q(3,4)=(z-1)^2z^{-2} \quad , \\ &Q(t,4)=(z-1)(3z-4)2^{(t-3)/2}z^{1-t} \\ &\qquad -(z-1)(2z-3)z^{1-t} \text{ for odd } t\geqslant 5 \quad , \\ &Q(t,4)=(z-1)(2z-3) \\ &\qquad \times(2^{(t-2)/2}-1)z^{1-t} \text{ for even } t\geqslant 4 \quad . \end{aligned} \tag{2.16}$$

These terms, substituted into Eq. (2.4) give an approximation for $P(t)$; the value of T in this approximation is found from Eq. (2.6)

$$T=(1-q)+\frac{z}{z-1}(1-q)^2 + \frac{z(z+1)}{z^2-2}(1-q)^3+O(1-q)^4 \quad . \tag{2.17}$$

The probability that the random walker escapes from the first four sites is $(1-q)^4$ because the probability of escaping from any one of them is $(1-q)$. Thus the fraction of all cases that is described by our approximation (2.17) is $1-(1-q)^4$, which should be close to unity for the approximation to be valid. This limits us to q less than 0.5. More terms of the approximation could be found, but even with a large number of terms in the series this approach is limited to the study of the lower right-hand corner of Fig. 1, since it is an expansion in $(1-q)$.

In the range in which Eq. (2.17) is valid—viz., small enough $(1-q)$—the duration T is, for given q, seen to be an increasing function of dimensionality D. The same was found to be true for small q in Eq. (17) of Ref. 1. Together, these two results suggest that T is an increasing function of D for any value of q. Accordingly, it seems likely that the puzzling crossover shown in Fig. 1 of Ref. 1 is consequence of extrapolating the small-q expressions beyond their range of validity.

The case of infinite D and z is of particular interest. The coefficients of $(1-q)^k$ shown in Eq. (2.17) all become unity, and the reader of Appendix A can easily verify that this will hold to all orders of $(1-q)$. (Observe that in a space of a high number of dimensions, backtracking becomes very unlikely, so that only the first diagram in Table I—and, indeed, only its first term—need be considered. This leads to $a_v = v-1$ and $b_v = 1$ for all v.) Equation (2.17) can then be replaced by

$$T = \sum_{k=1}^{\infty} (1-q)^k \ , \tag{2.18}$$

which can be summed, for any value of q, to give simply

$$T = q^{-1} - 1 \ . \tag{2.19}$$

This expression should be compared with Eq. (17c) of Ref. 1,

$$T = 1/(1-F)q \ , \tag{2.20}$$

which is valid in any number of dimensions but for small q only; the two are consistent because F, defined as the probability of eventual return to the origin in absence of traps, would be expected to approach zero as the dimensionality becomes large (again, because backtracking is very unlikely when D is large).

III. ANOMALOUS CASE $D = 1$

In one dimension three estimates of the average time to trapping have been given:

(1) In Ref. 1, the problem was solved exactly, with result

$$T = (1-q)/q^2 \quad \text{(exact random)} \ . \tag{3.1}$$

(2) Montroll[6] has solved the similar problem of a regular array of traps with spacing L. His result is

$$T = (1-q)(1+q)/6q^2 \quad \text{(exact periodic)} \ . \tag{3.2}$$

[Montroll's model did not allow traps to be starting points for walks, whereas the problem we discuss does. Since walks starting at traps have duration zero, a normalizing factor $(L-1)/L = (1-q)$ is all that is required. This factor has been incorporated in Eq. (3.2).] The large difference between these two results—nearly a factor of 6 for most values of q—is indeed surprising.

(3) The average number of sites visited in t steps by a random walker in one dimension is[5]

$$\bar{V}(t) = (8t/\pi)^{1/2} \ , \tag{3.3}$$

accurate to leading order in t. Substitution into Eqs. (2.5) and (2.6) gives

$$T = \tfrac{1}{4}\pi/q^2 \quad \text{(approximate random)} \ , \tag{3.4}$$

which does not quite agree with Eq. (3.1) either.

We shall dispose of this last discrepancy first. In Eq. (2.14) it was assumed that the second term in the curly brackets is negligible; however, this fails in one dimension because $\langle [V_i - \bar{V}(t)]^2 \rangle \sim \bar{V}(t)^2$; according to Eqs. (3.3) and (3.4) $\bar{V}(t) \sim q^{-1}$ is still the range of interest, and the bracket is not unity. The distribution $R(t, v)$ is insufficiently sharp, and walks that visit an anomalously small number of sites play a significant role. Thus we would expect Eq. (2.15) to be an underestimate in this special case.

The difference between Eqs. (3.1) and (3.2) is this: in one dimension, the traps dissect the lattice completely into separate "runs" of k ordinary sites bounded on each end by one trap. In Montroll's case, k is equal to $L-1$ always; in the random case, k is equal to $L-1$ on the average, but can vary from zero to infinity. Runs with large k may be few in number, but they contribute strongly to the duration of the walks—especially since their duration is proportional to k^2, according to Eq. (3.2). Therefore, the larger mean duration found in Eq. (3.1) can be attributed to the large contribution from the long "runs" of ordinary sites.

We may show the connection explicitly as follows: if a walk of t steps visits v sites and arrives on a new site for the first time on the last step, there is a probability $1/L$ that this is a trap site (regarding the origin of the walk to be random), and thus a probability $1/L$ that the particle is trapped on this step. Other locations of the trap site are divided among cases in which the particle has already been trapped or will be trapped in the future, but this is of no concern to us. Of course the particle is inevitably trapped when $v = L$. Thus

$$P(t) = \sum_{v=1}^{L} \frac{Q(t,v)}{L} \ .$$

If we now assume (not quite correctly) that Eq. (3.3) implies $Q(t,v) \sim \delta(t-\pi v^2/8)$ [the normalization is chosen so that $\sum_t Q(t,v)=1$] then

$$T=\sum_t tP(t)=\sum_{v=1}^{L}\frac{\pi v^2}{8}$$

$$=\frac{\pi}{48}(2L^2+3L+1)$$

$$\sim\frac{\pi}{4}\frac{1}{6q^2}\quad\text{(approximate periodic)}\ ,$$

where in the last step we have replaced L by $1/q$ and only kept the leading term. This result is clearly related to Eq. (3.2) in the same way that Eq. (3.4) is related to Eq. (3.1).

The anomalies noted here do not occur in higher dimensionality. The distribution $R(t,v)$ is indeed sharp in all other cases, and the periodic array (also discussed by Montroll) gives the same result as the random array (discussed in Ref. 1). Randomizing the location of the traps has a smaller effect in higher dimensionality because the walker is not confined into "runs" of ordinary sites. Each walker can be absorbed by any trap; moving one trap away from the starting point of one particular walker reduces the probability that the walker reaches that particular trap but leaves the probability of its being absorbed by any of the other traps only slightly affected. Therefore moving the position of one trap will have only a small effect, and so will randomizing the positions of all of them.

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APPENDIX A: EVALUATION OF $Q(t,v)$ IN ANY NUMBER OF DIMENSIONS

Here we show that as long as v is not too large, $Q(t,v)$ can be evaluated rather directly and without too much labor, for any number of dimensions. The procedure is to count up the number of walks $N(t,v)$ that visit v distinct sites in t steps, and arrive at a new site on the last step. $Q(t,v)$ is then given by $N(t,v)/z^t$.

$v=1$. A walk can visit a total of one point (which must necessarily be the origin) only before the walking actually starts. So $N(t,1)=1$ if $t=0$, and zero otherwise.

$v=2$. This is almost as easy: two points will have been visited by the time $t=1$ (viz., the origin and one of its nearest neighbors), and in D dimensions there are $z=2D$ such nearest neighbors. So $N(1,2)=z$. For all $t>1$, we have $N(t,2)=0$, because $N(t,2)$ was defined to count, among the walks that visit 2 sites in t steps, only those that do not visit the second site before the final step. There are no such walks.

$v=3$. You cannot visit three sites in fewer than two steps, so $N(0,3)$ and $N(1,3)$ vanish. For $t\geqslant 2$, $N(t,3)$ counts the walks that visit two sites during the first $t-1$ steps and a third site on step t. This leads to $N(t,3)=z(z-1)$ for all $t\geqslant 2$, because such walks can be realized only as follows: step onto one of the z nearest neighbors on step 1, return to the origin on step 2, move back and forth between these two points for the next $t-3$ steps, and finally step onto one of the $z-1$ accessible new sites on the last step.

$v=4$. Again we note that the last site visited is special, and that up to the last step the walk was confined to three sites. There can only be one path leading to the last site, corresponding to the last step. The contribution to $N(t,4)$ also depends on the starting point of the walk. Then there are five possible topologies for the cluster of sites visited, as shown in Table I.

The reason for considering the topological connectedness is that it is only the multiplicity of each of the five diagrams that depends on the dimensionality of the space; the number of allowed walks on any particular diagram is independent of dimensionality. Both the topological multiplicity of each diagram and the number of possible walks on it are given in Table I.

The final result for $N(t,4)$ is obtained by multiplying the numbers in columns 2 and 3 of each line of Table I, and then adding the contributions from each line. The expressions for the probabilities $Q(t,v)$ given in Eq. (2.16) are then obtained by dividing by the total number of walks of t steps, z^t.

An expression for the expected duration of the walk is obtainable by substituting Eq. (2.4) into Eq. (2.6)

$$T=q\sum_{v=1}^{\infty}a_v(1-q)^{v-1}\ ,$$

where

$$a_v=\sum_{t-1}^{\infty}tQ(t,v)\ , \tag{A1}$$

or, writing q as $1-(1-q)$,

$$T=a_1+\sum_{v=1}^{\infty}b_v(1-q)^2\ , \tag{A2}$$

with

$$b_v=a_{v+1}-a_v\ . \tag{A3}$$

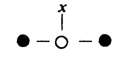
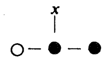
Substituting the expressions (2.16) into (A1) gives

$$a_1=0,\ a_2=1,\ a_3=(2z-1)/(z-1)\ ,$$

$$a_4=(3z^3-z^2-5z+2)/(z^2-2)(z-1)\ ,$$

and Eq. (A2) therefore takes on the form (2.17).

TABLE I. Configurations which contribute to a_4.

Configuration	Topological multiplicity	Number of t-step walks starting at ○ and ending at x	
○−●−●−x	$z(z-1)^2$	$2^{1/2(t-3)}$	if t is odd and ≥ 3
		0	otherwise
●−●−○−x	$z(z-1)^2$	$2^{1/2(t-3)}-1$	if t is odd and >3
		0	otherwise
●−○−●−x	$z(z-1)^2$	$2^{1/2(t-2)}-1$	if t is even and >3
		0	otherwise
	$\frac{1}{2}z(z-1)(z-2)$	$2(2^{1/2(t-3)}-1)$	if t is odd and >3
		0	otherwise
	$z(z-1)(z-2)$	$2^{1/2(t-2)}-1$	if t is even and >3
		0	otherwise

APPENDIX B: HOW THE FIGURE WAS DRAWN

In Ref. 1 it was shown[7] how to derive a function $T(q)$ which gives the dependence of the trapping time on the trap density q, accurate for small q. Of course the expansion of this function in powers of $(1-q)$ does not agree with the small-$(1-q)$ series derived in Sec. II (except in infinite dimensionality). Therefore in drawing Fig. 1 we interpolated by subtracting the leading terms in the $(1-q)$ expansion of $T(q)$ from that function and replacing them by the correct terms.

The two-dimensional curve is slightly different from what was given in Ref. 1: it was based on the expression for the number of distinct sites visited in t steps of an unrestricted random walk, as given in reference 1: $N(t)=\pi t/\ln t$. However, consideration of the correction terms to this expression (which can be derived by the methods of that work) show that a better result is $N(t)=\pi t/\ln(8t)$, which (using the methods of Ref. 1) implies $T(q)=(\pi q)^{-1}[1-C-\ln(\frac{1}{8}\pi)q]$.

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[1] H. B. Rosenstock, J. Math. Phys. 21, 1643 (1980).

[2] Some of the results of Ref. 1 were given earlier by R. P. Hemenger, R. M. Pearlstein, and K. Lakatos-Lindenberg, J. Math. Phys. 13, 1056 (1972).

[3] G. H. Weiss, Proc. Nat. Acad. Sci. U.S.A. 77, 4391 (1980).

[4] N. C. Jain and W. E. Pruitt, in *Proceedings of the 6th Berkeley Symposium on Mathematical Statistics and Probability* (University of California, Berkeley, 1972), Vol. III, p. 31; F. Spitzer, *Principles of Random Walk,* 2nd ed. (Springer-Verlag, New York, 1976), pp. 35− 39.

[5] E. W. Montroll and G. H. Weiss, J. Math. Phys. 6, 167 (1965).

[6] E. W. Montroll, J. Math. Phys. 10, 753 (1969).

[7] Erratum: In Ref. 1, Eq. (1): x_i should be changed to t_i.