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Trapping of Random Walks on the Line

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Several features of the trapping of random walks on a one-dimensional lattice are analyzed. The results of this investigation are as follows: (1) The correction term to the known asymptotic form for the survival probability to n steps is $O((\lambda^2 n)^{-1/3})$, where $\lambda = -\ln(1-c)$, and c is the trap concentration. (2) The short time form for the survival probability is found to be $\exp[-a(c)n^{1/2}]$, where $a(c)$ is given in Eq. (21). (3) The mean-square displacement of a surviving random walker is found to go like $n^{2/3}$ for large n. (4) When the distribution of trap-free regions is changed so that very large regions are much rarer than for ideally random trap placement the asymptotic survival probability changes its dependence on n. One such model is studied.

KEY WORDS: Random walks; trapping; diffusion; survival probabilities.

The subject of the motion of random walkers on a lattice with randomly placed traps has engaged the attention of many investigators recently. Many analyses of this problem are based on simulations, others rely on bounds or approximate arguments, and there are a very few rigorous results, mainly for the expected survival after a random walk of n steps. All of the rigorous results are asymptotic in nature, the most complete analysis of survival fraction being that of Donsker and Varadhan.(1) Several authors have studied the kinetics of one-dimensional random walks(2–8) since when steps are restricted to being to nearest neighbors only exact solutions of the resulting problem can be given. However, the structure of these solutions is quite difficult to analyze, and none of the investigators who have studied trapping problems in one dimension (1-D) have gone much beyond verifying the asymptotic results for the probability of survival after n steps. In this note we study several problems for which, hopefully, the solution in 1-D will suggest generalizations in higher dimensions.

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The first of these is important in the evaluation of simulated results. It is known from the work of Donsker and Varadhan[1] that the averaged survival of an n step walk is asymptotically proportional to $\exp(-\alpha n^{D/(D+2)})$ in D dimensions where α is a constant that depends on trap concentration. How large n must be for this asymptotic form to be valid is unanswered by Donsker and Varadhan's analysis. We will calculate a first correction term in 1-D to shed light on this problem. A second question that has not attracted much attention[9] is that of the short-time behavior of the average survival fraction. Klafter, Zumofen, and Blumen suggest that (in 1-D) this should be of the form $\exp(-\beta n^{1/2})$ and we show that this is indeed correct, and furnish a value for β. A third problem that lends itself to our analysis is that of the effect of allowing attraction or repulsion between traps, so that the distribution of spacing between adjacent traps differs from that implied by pure random placement. We will show that restricting the occurrence of large gaps between adjacent traps will change the asymptotic form of the survival fraction. This confirms the general argument given by several authors[10,11] that the large intertrap spacing governs the qualitatively important features of the asymptotic survival fraction. Finally, we will calculate the averaged mean-square displacement of a random walker which has survived n steps without being trapped. It will be shown that for the strictly random placement of traps (i.e., each lattice point a trap with probability c), this quantity goes like $n^{2/3}$ rather than the first power of n expected for the unrestricted random walk.

Our first result will be that for the averaged survival probability for a symmetric lattice random walk in 1-D with steps to nearest neighbors only. Let us first consider an interval $(0, l)$ for which the end points 0 and l, respectively, are traps and there are no traps interior to the interval. Feller[12] has shown that the probability that a random walker is at r in the interval, given that it started at r_0, is

$$p_n(r \mid r_0) = \frac{2}{l} \sum_{j=1}^{l} \cos^n\left(\frac{\pi j}{l}\right) \sin\left(\frac{\pi j r}{l}\right) \sin\left(\frac{\pi j r_0}{l}\right) \tag{1}$$

On the assumption that the starting points, r_0, are uniformly distributed over $(1, l-1)$ one finds for the survival probability after n steps

$$\begin{aligned} F_n(l) &= \frac{1}{l-1} \sum_{r=1}^{l-1} \sum_{r_0=1}^{l-1} p_n(r \mid r_0) \\ &= \frac{2}{l(l-1)} \sum_{j=0}^{[(l-1)/2]} \cos^n\left(\frac{\pi(2j+1)}{l}\right) \cot^2\left(\frac{\pi(2j+1)}{2l}\right) \end{aligned} \tag{2}$$

where the square brackets denote "the largest integer contained in." This, by itself, is not an interesting result, but its average over all intertrap intervals is. Let us suppose that the probability that an arbitrary intertrap interval is equal to l is q_l, $l = 1, 2,...$. For example, for strictly random trap placement $q_l = c(1-c)^{l-1}$, where c is the probability that a given site is a trap. The correct set of probability to be used in the averaging process is not the q_l but the length-biased estimate,[13] p_l, defined by

$$p_l = lq_l \Big/ \sum_{j=1}^{\infty} jq_j, \qquad l = 1, 2,... \tag{3}$$

so that, for example, for random traps $p_l = c^2 l(1-c)^{l-1}$. The intuitive reason for using p_l rather than q_l is that the random walker is more likely to have its starting point on a large trap-free interval than on a small one. Thus, for the strictly random trap one finds that

$$\langle F_n \rangle = c^2 \delta_{n,0} + 2c^2 \sum_{l=2}^{\infty} \frac{(1-c)^{l-1}}{l-1} \sum_{j=0}^{[(l-1)/2]} \cos^n \left(\frac{\pi(2j+1)}{l} \right) \cot^2 \left(\frac{\pi(2j+1)}{2l} \right) \tag{4}$$

which may be regarded as a power series in $1-c$. This equation is convenient for computation when c is close to 1. To lowest order in $1-c$ when $c \approx 1$ and $n > 0$, $\langle F_n \rangle$ can be written

$$\langle F_n \rangle = 3c^2(1-c)^2(1/2)^n + O((1-c)^3) \tag{5}$$

When c is close to zero we can examine the analytic behavior of $\langle F_n \rangle$ by observing that the divergence of $\langle F_n \rangle$ at $c = 0$ is governed by the behavior of the coefficient of the term $c^2(1-c)^{l-1}$ in Eq. (4):

$$a_l(n) = \frac{2}{l-1} \sum_{j=0}^{[(l-1)/2]} \cos^n \left(\frac{\pi(2j+1)}{l} \right) \cot^2 \left(\frac{\pi(2j+1)}{2l} \right) \tag{6}$$

in the large-l limit. To find this behavior we have the estimates

$$\begin{aligned} \cos^n \left[\frac{\pi(2j+1)}{l} \right] &\sim \exp\left[-\frac{n\pi^2(2j+1)^2}{2l^2} \right] \\ \cot^2 \left[\frac{\pi(2j+1)}{2l} \right] &\sim \frac{4l^2}{\pi^2} \frac{1}{(2j+1)^2} \end{aligned} \tag{7}$$

which implies that

$$a_l(n) \sim \frac{8l^2}{\pi^2} \sum_{j=0}^{\infty} \frac{\exp[-n\pi^2(2j+1)^2/(2l^2)]}{(2j+1)^2} \tag{8}$$

This expression for $a_l(n)$, together with an easily justified interchange of orders of summation, allows us to write the following approximation for $\langle F_n \rangle$:

$$\langle F_n \rangle \sim \frac{8c^2}{\pi^2} \sum_{j=0}^{\infty} \frac{1}{(2j+1)^2} \sum_{j=1}^{\infty} l(1-c)^{l-1} \exp\left[-\frac{n\pi^2(2j+1)^2}{2l^2}\right]$$
$$= \frac{8c^2}{\pi^2} \sum_{j=0}^{\infty} \frac{1}{(2j+1)^2} U\left(\pi^2(2j+1)^2 \frac{n}{2}\right) \tag{9}$$

in which $U(m)$ is the infinite sum

$$U(m) = \sum_{l=1}^{\infty} l(1-c)^{l-1} \exp\left(-\frac{m}{l^2}\right) \tag{10}$$

The asymptotic behavior of $\langle F_n \rangle$ can be obtained if we can evaluate the sum $U(m)$ for large m. This can be done by using the method of steepest descents modified for sums, or more succinctly by converting the sum to an integral with the Euler–Maclaurin formula. In this way we find that

$$U(m) \sim \int_0^{\infty} x e^{-\lambda x - m/x^2}\, dx$$
$$= (m/\lambda)^{2/3} \int_0^{\infty} v \exp\left[-(m\lambda^2)^{1/3}\left(v + \frac{1}{v^2}\right)\right] dv \tag{11}$$

in which $\lambda = \ln[1/(1-c)]$. The steepest descents approximation to the integral yields

$$U(m) \sim \frac{2}{\lambda}\left(\frac{\pi}{3}\right)^{1/2} m^{1/2} \exp[-(m\lambda^2)^{1/3}] \tag{12}$$

which is to be substituted into Eq. (9). Since we are interested in large n the main contribution to the sum will come from the $j=0$ term. In this way we find the approximation

$$\langle F_n \rangle \sim \frac{8c^2}{\pi^2} U\left(\frac{\pi^2 n}{2}\right) \sim \frac{16c^2}{\lambda}\left(\frac{n}{6\pi}\right)^{1/2} \exp\left[-\left(\frac{\pi^2 n\lambda^2}{2}\right)^{1/3}\right] \tag{13}$$

The exponent is in agreement with that calculated by Donsker and Varadhan.[1] A rough idea of the value of n required for Eq. (13) to be a useful approximation can be obtained by calculating a correction term to the value of $U(m)$. If we call $U_0(m)$ the approximation given in Eq. (12), then one can show using higher terms in the expansion of Eq. (11) that

$$U(m) = U_0(m)\left[1 + O\left(\frac{1}{(m\lambda^2)^{1/3}}\right)\right] \tag{14}$$

which indicates that the number of steps required to effectively cause the correction term to be negligible can be rather large. For example, when $c = 0.1$ the correction term is 0.26 for $n = 10^3$, 0.12 for $n = 10^4$, and 0.06 for $n = 10^5$. The correction terms increase in absolute magnitude as the trap concentration decreases. The $n^{-1/3}$ dependence of the correction term has been checked against accurate numerical calculations reported in Ref. 8, and found to be in agreement with them. These results are relevant to simulation studies in which one might want to study further properties of the asymptotic regime. It is tempting to conjecture that in $D > 1$ dimensions the correction term to the Donsker–Varadhan result is $O((m\lambda^2)^{-D/(D+2)})$ but our present calculations can only suggest but not verify this result.

A calculation of the transient behavior of $\langle F_n \rangle$ for $c \to 0$ and moderate n starts by expanding the exponential appearing in the definition of $U(m)$ in Eq. (10),

$$\begin{aligned} U(m) &\sim \sum_{l=1}^{\infty} l(1-c)^{l-1}\left(1 - \frac{m}{l^2}\right) \\ &= \frac{1}{c^2} - \frac{m}{1-c}\ln\frac{1}{c} \\ &\sim \frac{1}{c^2}\exp\left[-\frac{mc^2\ln(1/c)}{1-c}\right] \end{aligned} \tag{15}$$

This, in turn implies the approximation

$$\langle F_n \rangle \sim \frac{8}{\pi^2}\sum_{j=0}^{\infty}\frac{1}{(2j+1)^2}\exp\left[-\frac{\pi^2 nc^3\ln(1/c)}{2(1-c)}(2j+1)^2\right] \tag{16}$$

Therefore, in the indicated limit we must find the behavior of the function

$$h(\eta) = \frac{8}{\pi^2}\sum_{j=0}^{\infty}\frac{1}{(2j+1)^2}\exp[-\eta(2j+1)^2] \tag{17}$$

in the limit $\eta = 0$. It is evident that $h(0) = 1$. On differentiating this last formula with respect to η we find

$$h'(\eta) = -\frac{8}{\pi^2}\sum_{j=0}^{\infty}\exp[-\eta(2j+1)^2] \tag{18}$$

The small η form can be obtained either exactly by using a Poisson transformation, or to lowest order using the Euler–Maclaurin sum formula. The latter gives

$$h'(\eta) \sim -\frac{4}{\pi^2}\int_0^\infty e^{-\eta x^2}\,dx = -\frac{2}{(\pi^2\eta)^{1/2}} \tag{19}$$

so that

$$h(\eta) \sim 1 - \left(\frac{\eta}{\pi^3}\right)^{1/2} \sim \exp\left[-\left(\frac{\eta}{\pi^2}\right)^{1/2}\right] \tag{20}$$

which yields, as the short-time low concentration limiting form for $\langle F_n \rangle$

$$\langle F_n \rangle \sim \exp\left\{-c\left[\frac{\ln(1/c)n}{2\pi(1-c)}\right]^{1/2}\right\} \tag{21}$$

in which the exponent is proportional to $n^{1/2}$.

As we have noted, when traps are randomly assigned to lattice points with a concentration equal to c then the probability that l lattice points separate two adjacent traps is $q_l = c(1-c)^{l-1}$, $l = 1, 2, \ldots$. Let us now suppose that an effective attraction between traps is introduced so that the probability that really large gaps occur is decreased. One way the attraction can be introduced is to choose

$$q_l = e^{-\beta l^2} \Big/ \sum_{j=2}^{\infty} e^{-\beta j^2}, \qquad l = 2, 3, \ldots \tag{22}$$

for which the effective concentration is

$$c = \sum_{l=2}^{\infty} e^{-\beta l^2} \Big/ \sum_{l=2}^{\infty} l e^{-\beta l^2} = 1/\langle l \rangle \tag{23}$$

The exact formula for the survival function is, from Eq. (2),

$$\langle F_n \rangle = \sum_{l=2}^{\infty} a_l(n) e^{-\beta l^2} \Big/ \sum_{l=2}^{\infty} e^{-\beta l^2} \tag{24}$$

where the expression for $a_l(n)$ is that shown in Eq. (6). From this one finds that in the small c limit

$$\langle F_n \rangle \sim \frac{8}{\pi^2}\sum_{j=0}^{\infty}\frac{1}{(2j+1)^2}\, V\left(\frac{n\pi^2(2j+1)^2}{2}\right) \tag{25}$$

where, now,

$$V(m) = \sum_{l=2}^{\infty} l \exp\left(-\beta l^2 - \frac{m}{l^2}\right) \Big/ \sum_{l=2}^{\infty} l \exp(-\beta l^2) \tag{26}$$

Remembering now that we are working in the small c range we can convert the summations to integrations using the Euler–Maclaurin formula, finding that

$$\begin{aligned} V(m) &\sim \int_0^{\infty} x e^{-(\beta x^2 + m/x^2)}\, dx \Big/ \int_0^{\infty} x e^{-\beta x^2}\, dx \\ &= 2(m\beta)^{1/2} K_1(2(m\beta)^{1/2}) \end{aligned} \tag{27}$$

where $K_1(v)$ is a Bessel function of the second kind of imaginary argument. Using the known asymptotic forms of such Bessel functions we have as the large-n approximation for $\langle F_n \rangle$,

$$\langle F_n \rangle \sim \frac{8}{\pi^2} V\left(\frac{n\pi^2}{2}\right) \sim \frac{8}{\pi}\left(\frac{n\beta}{2}\right)^{1/4} \exp[-\pi(2n\beta)^{1/2}] \tag{28}$$

in terms of the parameter β. At low trap concentrations one can solve Eq. (24) for β in terms of c. To lowest order in c one has

$$\beta \sim (c/\pi)^2 \tag{29}$$

from which it follows that the large-n form for $\langle F_n \rangle$ is

$$\langle F_n \rangle \sim \frac{8}{\pi}\left(\frac{nc^2}{2\pi^2}\right)^{1/4} \exp[-c(2n)^{1/2}] \tag{30}$$

which differs from the purely random trap case. Of course this is to be expected since the longest survivals are for those random walkers who initially find themselves in the largest trap-free intervals. This property is expected to persist in $D > 1$ dimensions when similar attraction between trapping sites is introduced.[10,11] It would be interesting to develop the analog of the Donsker–Varadhan analysis for such cases.

As our final calculation for $D = 1$ we calculate the asymptotic form of the mean-squared displacement of a random walker in the presence of traps. It is most convenient to make this calculation for the case of a diffusing particle, although one can also evaluate the requisite sums for the lattice case with somewhat more complicated-looking final formulas. However, the diffusion limit can be shown to be equivalent to the very low trap concentration limit, so that we choose the most convenient framework for the calculation to follow. The probability density for the position of a particle diffusing between two traps at 0 and L is

$$p(x, t \mid x_0, 0) = \frac{2}{L} \sum_{j=0}^{\infty} \exp\left(-\frac{\pi^2 j^2 Dt}{L^2}\right) \sin\left(\frac{\pi j x}{L}\right) \sin\left(\frac{\pi j x_0}{L}\right) \tag{31}$$

where D is now a diffusion constant. In order to have results comparable to the random walk in discrete time we must replace Dt appearing in the exponent of this last equation by $n/2$, where n is the number of (discrete) steps. The mean-squared displacement at time t for all random walkers in a trap-free interval equal to L is defined by

$$\langle r^2(t) \mid L \rangle \equiv \frac{1}{L} \int_0^L dx_0 \int_0^L dx\, (x - x_0)^2\, p(x, t \mid x_0, 0) \tag{32}$$

For large Dt/L^2 we need only retain the $j = 1$ term in Eq. (31) to find the appropriate expression for $\langle r^2(t) \mid L \rangle$. This procedure yields

$$\langle r^2(t) \mid L \rangle \sim \frac{4L^2}{\pi^2} \left(1 - \frac{8}{\pi^2}\right) \exp\left(-\frac{Dt}{L^2}\right) \tag{33}$$

This must be averaged over the appropriate density for L, which in the present case is

$$g(L) = (L/\bar{L}^2) \exp(-L/\bar{L}) \tag{34}$$

where $\bar{L}$ is a function of c to be specified below. The asymptotic survival function is

$$\langle F(t) \rangle \sim \frac{8}{\pi^2 \bar{L}^2} \int_0^{\infty} L \exp\left(-\frac{L}{\bar{L}} - \frac{\pi^2 Dt}{L^2}\right) dL \tag{35}$$

We see that can be put exactly in the form of $\langle F_n \rangle$ in Eq. (13) provided that we replace Dt by $n/2$ and set

$$\bar{L} = 1/\lambda = 1\Big/\ln\left(\frac{1}{1-c}\right) \sim \frac{1}{c} \tag{36}$$

Furthermore the value of $\langle r^2(t) \mid L \rangle$ averaged over configurations and expressed in terms of n is

$$\langle r^2(n) \rangle \sim \frac{4}{\pi^2} \left(1 - \frac{8}{\pi^2}\right) \frac{1}{\lambda^2} \left(\frac{\pi^2 n \lambda^2}{2}\right)^{4/3} \int_0^{\infty} v^3 \exp\left[-\left(\frac{\pi^2 n \lambda^2}{2}\right)\left(v + \frac{1}{v^2}\right)\right] dv \tag{37}$$

Consequently the mean-squared displacement of those random walkers that survive to n steps for n large is

$$\frac{\langle r^2(n)\rangle}{\langle F_n\rangle} \sim 2^{-1/3}\left(1-\frac{8}{\pi^2}\right)\left(\frac{\pi^2 n}{2\lambda}\right)^{2/3} \tag{38}$$

i.e., it is proportional to $n^{2/3}$ rather than to the first power of n as would be the case for the unrestricted random walk. That this should be the case is intuitively reasonable since only those random walks which do not make too large excursions from their starting point will survive. For the model with attracting traps specified by Eq. (22) the comparable power of n is $1/2$ rather than $2/3$. In D dimensions we conjecture that the comparable n dependence is $n^{(D+1)/(D+2)}$.

When the transition probabilities of the random walk are asymmetric the survival probabilities decay exponentially because the expected number of distinct sites visited is asymptotically proportional to n. It would be of great value to be able to solve the 1-D problem with longer-range jumps to ascertain the effects of long-range jumps on the approach to the asymptotic decay form of the survival probability. Even in the very simplest of cases this seems beyond the reach of present analytical methods.

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