Journal of Statistical Physics, Vol. 43, Nos. 3/4, 1986

Escape Times in Interacting Biased Random Walks

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Received August 26, 1985; final December 10, 1985

The dynamics of N particles with hard core exclusion performing biased random walks is studied on a one-dimensional lattice with a reflecting wall. The bias is toward the wall and the particles are placed initially on the N sites of the lattice closest to the wall. For $N=1$ the leading behavior of the first passage time T_{FP} to a distant site l is known to follow the Kramers escape time formula $T_{FP} \sim \lambda^l$ where λ is the ratio of hopping rates toward and away from the wall. For $N>1$ Monte Carlo and analytical results are presented to show that for the particle closest to the wall, the Kramers formula generalizes to $T_{FP} \sim \lambda^{lN}$. First passage times for the other particles are studied as well. A second question that is studied pertains to survival times T_S in the presence of an absorbing barrier placed at site l. In contrast to the first passage time, it is found that T_S follows the leading behavior λ^l independent of N.

KEY WORDS: Interacting random walks; bias; generalized Kramers escape problem; survival times.

1. INTRODUCTION

The problem of escape of a single particle from a one-dimensional potential well has been studied for a number of years, and the classical Kramers result[1,2] for the escape time has been rederived in various ways.[3] The single particle problem has been generalized relatively recently to allow for higher dimensional potentials.[4] However, it seems that escape times in the presence of interactions between particles have not been studied before. We address this problem in the present paper. We allow for hard core interactions between particles and confine our attention to a linear potential produced by a constant field on one side of a reflecting wall.

The motivation for considering such a system comes partly from studies of the infinite percolation cluster in an external field.[5-8] Particles

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0022-4715/86/0500-0561$05.00/0

which enter dead-end branches which point predominantly in the direction of the field have to be activated against the field to resume transport. In a system of noninteracting particles this leads to anomalous behavior such as a drift velocity which decreases as the field increases. However, in any application to real systems it is crucial to account for hard core exclusion; such interactions cause branches to fill up and cease to be effective as traps.[9] The present study is a preliminary attempt to understand the dynamics of deeply trapped interacting particles in branches.

We describe this problem as that of interacting random walkers with hard core exclusion on a one-dimensional lattice with a reflecting wall. (Particles can occupy sites with positive labels 1, 2, 3,...; site 0 plays the role of a wall). Quantities of interest are first passage and survival times, steady-state distributions and spreads. We study these using Monte Carlo simulations and also analytically. In the Monte Carlo study, the effect of the external field is incorporated by allowing the particles to perform a biased random walk, with steps along the field (toward the wall) being more likely than in the opposite direction. Steps onto already occupied sites are disallowed, which is consistent with hard core interactions.

Interacting random walks are of current interest[10,11] but it should be noted that the presence of bias makes analysis difficult as it renders the reflection principle invalid. Biased random walks with nearest-neighbor interactions, in addition to hard core exclusion, have been simulated using periodic boundary conditions[12] and phase transitions in the current-carrying steady state in two dimensions were investigated.

With a wall, the full time-dependent problem for a single walker on the one-dimensional lattice has been solved recently.[13] The mean first passage time $\tau(l)$ to reach a site a distance l lattice spacings from the wall is consistent with the Kramers formula

$$\tau(l) \sim [\lambda(g)]^{l-1} \tag{1}$$

where $\lambda(g) \equiv (1+g)/(1-g)$ is the ratio of backward to forward hopping rates. One of the principal results of the present work is that with N hard-core particles in the well, the first passage time T_{FP} for the particle that starts out closest to the wall to cross a distant site l is

$$T_{FP}(l, N) \sim [\lambda(g)]^{N(l-1)} \tag{2}$$

First passage times for the other particles are also studied. We also study survival times $T_S(l, N)$ for hard core particles when an absorbing boundary is placed at site l. We find that in contrast to first passage times, the survival time $T_S(l, N)$ follows (1). A detailed discussion of T_{FP} and T_S is given in Sections 3 and 4, respectively; in the next section we discuss the steady-state properties of the system.

2. THE MODEL AND STEADY STATE

We study interacting biased random walks on the infinite half line $i = 1, 2, \ldots$. Initially the N particles occupy the sites $i = 1, 2, \ldots, N$. At each subsequent time step, these N particles are moved at random, with the restriction that a particle can move onto a neighboring site only if it is vacant (Kawasaki dynamics). The probability for attempting to move right (left) is $(1-g)/2$ [respectively, $(1+g)/2$]. The site $i=0$ is a reflecting boundary; no particle is allowed on or to the left of this site.

Due to the presence of bias, the system is expected to reach steady state eventually. The time required to do so depends strongly on the bias g as do various characteristics of the steady state (see below). In contrast to the situation with periodic boundary conditions,[12] the steady state for the system with a wall can be described by a Hamiltonian $\mathscr{H}$. If $n_l = 0$ or 1 is the occupation number of site l, we have

$$\mathscr{H} = \sum_{l=1}^{\infty} \varepsilon_l n_l \tag{3}$$

where $\varepsilon_l = El$ is the potential energy corresponding to a constant field $-E$. The bias g of the random walk is connected to E and the inverse temperature β by

$$\lambda(g) \equiv \frac{1+g}{1-g} = e^{\beta E} \tag{4}$$

Starting with (3) we can find either the canonical partition function $Q(N, g)$ or the grand partition function $Z(\beta\mu, g)$ where μ is the chemical potential. We find

$$Z(\beta\mu, g) = \prod_l [1 + \exp \beta(\mu - \varepsilon_l)] \tag{5}$$

while the mean number of particles on site l is given by

$$\langle n_l \rangle = [1 + \exp \beta(\varepsilon_l - \mu)]^{-1} \tag{6}$$

Monte Carlo results obtained using a fixed number N of particles can be compared with the consequences of this formula for the density profile. Some results are shown in Fig. 1. Besides $\langle n_l \rangle$, we have plotted the ratio

$$R_l = \frac{\langle n_{l+1} \rangle / (1 - \langle n_{l+1} \rangle)}{\langle n_l \rangle / (1 - \langle n_l \rangle)} \tag{7}$$

as it follows from (6) that R_l should be equal to $\lambda(g)$ for all l.

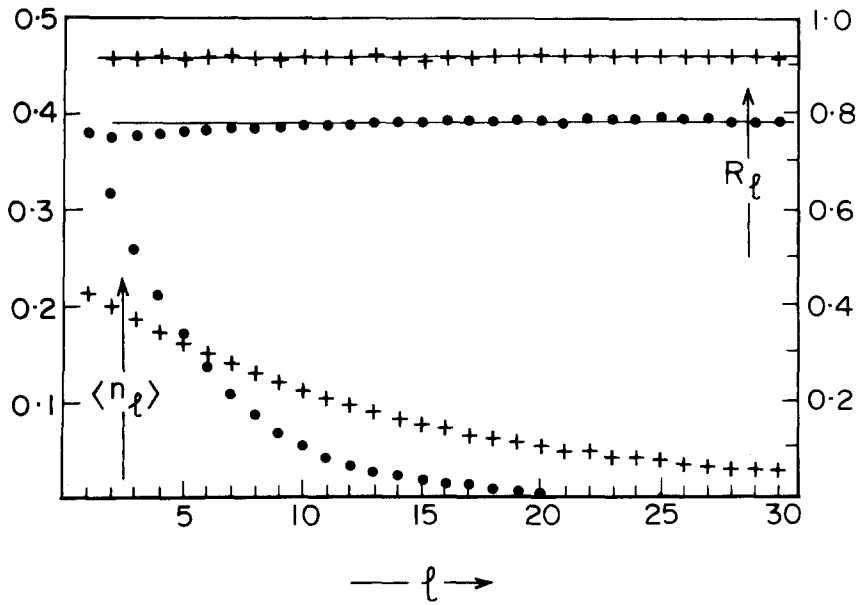

Fig. 1. Monte Carlo results for the steady-state density of particles $\langle n_l \rangle$ on site l are shown. Each point is the average over 10,000 random walks in each of which 5000 Monte Carlo steps were averaged over after equilibriation. Circles (crosses) represent results for $N=3$ and $g=0.12$ (respectively, $N=2$, $g=0.04$). The ratio R_l defined in (7) is compared against the expected value $1-g/1+g$.

It is also of interest to ask for the behavior of the spread S of the particles defined as the difference of location of the Nth (rightmost) and first (leftmost) particles. The spread starts out with its minimum allowed value $N-1$ at time $t=0$ and evolves to a characteristic steady-state value. The mean spread $\langle S \rangle$ in steady state is found to be inversely proportional to the bias g for small g. This result can be understood as follows. A length $L(g)=1/\ln \lambda(g)$ is associated with a value g of the bias. This length describes the exponential decay of probability density away from the wall when there is only one particle in the system. As long as $L(g) \gg N$, this is the underlying length scale in the problem. In particular, the locations of the first and Nth particles and, therefore, the spread, would each be expected to be proportional to $L(g)$, which in turn varies as g^{-1} as $g \to 0$. For a single particle, the time taken to approach steady state varies as g^{-2} as $g \to 0$[2] and we might have expected the same behavior even for $N=2$ or 3 particles. However, our Monte Carlo data for $N=2, 3$ for the time dependence of the spread seems more consistent with $g^{-1.6}$ than with g^{-2}. But we are not certain that this discrepancy is not caused by systematic errors due to nonequilibriation for very small g.

3. FIRST PASSAGE TIMES

Starting out at $t = 0$ with the particles in the N leftmost sites, what is the *first* time $t_{FP}(n, l; N)$ that the nth particle from the left crosses site l? The answer depends on the four parameters g, N, n, and l. In our Monte Carlo simulations we have not studied the full four-parameter space, but only relatively small values of the bias g and number of particles N. In particular, in all of our studies N is less than the bias-induced length $L(g)$ defined in the previous section.

First let us address the question for $n = 1$, the particle closest to the wall. An idea of what to expect is obtained by observing that the first particle crossing a distant site l is an extremely unlikely event, and that $t_{FP}(1, l; N)$ is consequently essentially given by the reciprocal of the probability of that event. This probability can be estimated as the ratio of a constrained partition function $Q_l(N, g)$ defined below, to the full partition function $Q(N, g)$. The appropriate constrained partition function is

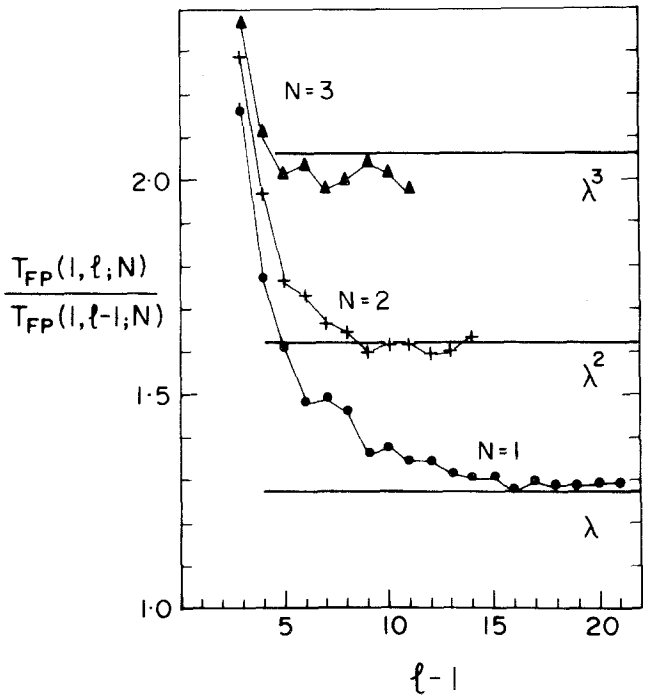

Fig. 2. The behavior of the first passage time of the particle closest to the wall ($n = 1$) is shown for systems of $N = 1$, 2, and 3 particles with $g = 0.12$. Here T_{FP} is the median first passage time over $M = 10{,}000$ distinct random walks. The results are consistent with $T_{FP}(1, l; N) \sim \lambda^{Nl}$.

obtained by summing over only those N-particle configurations in which all particles lie to the right of, or on, site l.

$$Q_l(N, g) = \sum_{\{n_k\}}{}' \exp\left(-\beta \sum_{k=1}^{\infty} \varepsilon_{k+l-1} n_{k+l-1}\right) \tag{8}$$

$$= \exp[-\beta EN(l-1)] \sum_{\{n_k\}}{}' \exp\left(-\beta \sum_{k=1}^{\infty} \varepsilon_k n_{k+l-1}\right) \tag{9}$$

The prime on the summations in (8) and (9) indicates that only those states with $\sum_k n_k = N$ particles are included. With minor relabeling, the

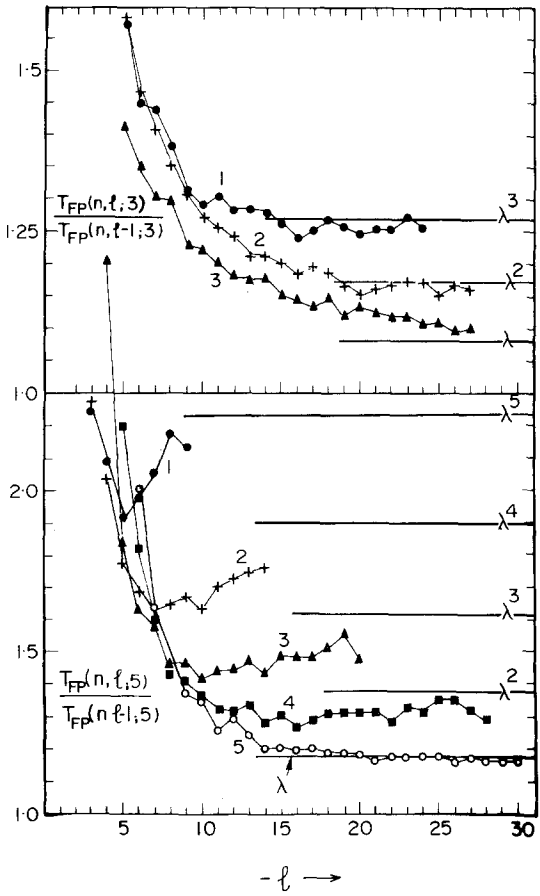

Fig. 3. Monte Carlo results for the dependence of T_{FP} on l for various particles $n = 1,..., N$. Each curve is labeled by the appropriate value of n. Top: $N = 3$, $g = 0.04$, $M = 10{,}000$. Bottom: $N = 5$, $g = 0.04$, $M = 5{,}000$. Here M is the number of random walks from which the median value T_{FP} is extracted.

sum in (9) can be recognized as the partition function $Q(N, g)$. The resulting estimate of the first passage time is

$$t_{\mathrm{FP}}^{-1} \sim \frac{Q_l(N, g)}{Q(N, g)} \sim \exp[-\beta EN(l-1)] \tag{10}$$

Equation (2) then follows from (10) and (4).

In the Monte Carlo simulations to determine $t_{\mathrm{FP}}(1, l; N)$, it proved expedient to extract the median $T_{\mathrm{FP}}(1, l; N)$ of the first passage time distribution (rather than the mean) as the distribution has a substantial tail. Instead of displaying the median first passage times $T_{\mathrm{FP}}(1, l; N)$, we have plotted in Fig. 2 the successive ratios $T_{\mathrm{FP}}(1, l; N)/T_{\mathrm{FP}}(1, l-1; N)$ versus l for various values of N and g. With increasing l, the ratio is seen to converge to $\lambda^N(g)$, thus providing evidence for (2).

We have also studied the median first passage times $T_{\mathrm{FP}}(n, l; N)$ for the nth particle to reach site l. Monte Carlo results are shown in Fig. 3. For different values of n, the ratios $T_{\mathrm{FP}}(n, l-1; N)/T_{\mathrm{FP}}(n, l; N)$ are seen to approach distinct values in the limit of large l. The data seem to be con-

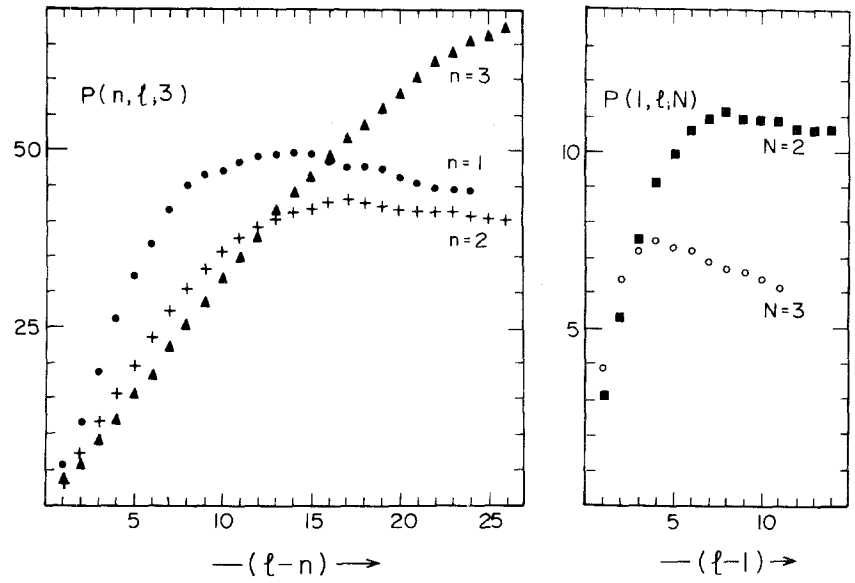

Fig. 4. Prefactors for the first passage problem [defined in (13)] are plotted against l for various n and N. Left: $N=3$, $g=0.04$, $M=10{,}000$. Right: $n=1$, $g=0.12$, $M=10{,}000$. Here M is the number of random walks that were sampled.

sistent with asymptotic values $[\lambda(g)]^{N-n+1}$, which would imply the leading behavior

$$T_{\mathrm{FP}}(n, l; N) \sim [\lambda(g)]^{(N-n+1)l} \tag{11}$$

Let us define a prefactor P by

$$T_{\mathrm{FP}}(n, l; N) = P(n, l; N)[\lambda(g)]^{(N-n+1)l} \tag{12}$$

Figure 4 shows the dependence of $P(n, l; N)$ on l, both as n varies with N fixed and as N varies with n fixed. We find P displays a smooth maximum as a function of l, the location of which moves to larger values of l as n is increased (with N held constant) or as N is increased (with n held fixed). It would be useful to have a theory which would account for this behavior.

4. ABSORBING BOUNDARY

For a single particle, the first passage time to a certain site l is clearly the same as the survival time of the particle in the presence of an absorbing barrier at l. Once there are two or more interacting particles, this identity breaks down for all but the outermost particle. It is interesting to ask for median survival times $T_{\mathrm{S}}(n, l; N)$ of particles $n = 1, 2, \ldots, N-1$ when there is an absorbing barrier at site l. The rightmost particle ($n = N$) will be the first to reach, followed by particle number $n = N-1$, etc., all the way to the leftmost particle $n = 1$. For the same distance of the absorbing boundary from the wall, the median survival times $T_{\mathrm{S}}(n, l; N)$ are found to vary by substantial factors as n varies from N to 1. However, successive ratios $T_{\mathrm{S}}(n, l; N)/T_{\mathrm{S}}(n, l-1; N)$ show much less variation and are plotted versus l in Fig. 5. In contrast to the first passage problem where the ratios separate out as functions of l and approach distinct asymptotic values (Fig. 3), we see from Fig. 5 that ratios in the survival problem seem to approach the same asymptotic value $\lambda(g) \equiv (1+g)/(1-g)$ for all $n = 1, 2, \ldots, N$. This indicates that the survival time for biased random walkers in the presence of an absorbing boundary follow the leading behavior

$$T_{\mathrm{S}}(n, l; N) \sim [\lambda(g)]^{l} \tag{13}$$

independent of n. A simple argument leading to this result is given in the next section.

5. CONCLUSION

We have studied the manner in which the Kramers formula for first passage/survival times of a single particle generalizes when there are several

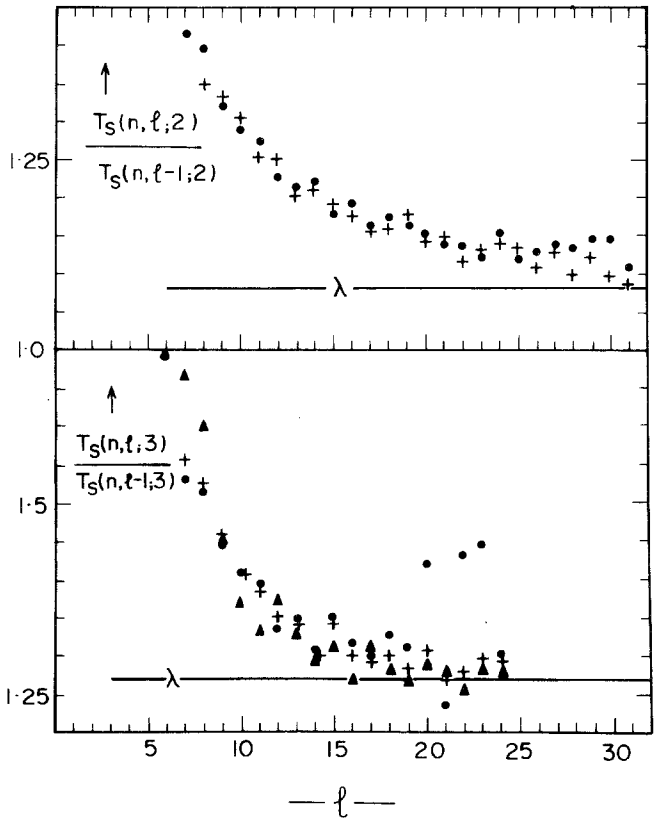

Fig. 5. Evidence is presented that the survival time T_S follows $T_S \sim \lambda^l$ independent of n in the presence of an absorbing barrier at site l. Circles, crosses, and triangles stand for $n=1, 2, 3$, respectively. Top: $N=2$, $g=0.04$, $M=10{,}000$; bottom: $N=3$, $g=0.12$, $M=10{,}000$. Despite relatively large scatter (especially for the innermost particle) the data is consistent with the approach of the ratios of survival times to an n-independent value, in contrast to the behavior of the ratios of first pasage times (Fig. 3).

interacting particles with hard core exclusion. The principal results, (11) for the first passage time T_{FP} and (13) for the survival time T_S in the presence of an absorbing barrier, can be rationalized in rather simple terms. In order that the rth particle from the right ($r=N-n+1$) be able to reach a distant site l for the first time, each of the $N-r$ particles on its right must have crossed site l earlier. In the survival problem, particles are absorbed and do not return once they reach site l. The time T_S taken by the rth particle to reach site l is thus the product of an r-dependent factor and the time $\sim[\lambda(g)]^l$ taken by a single particle to be absorbed, consistent with (13). In the first passage problem, on the other hand, particles keep coming back toward the wall under the influence of the bias. The probability that the rth

particle from the right reaches site l is then the product of r (approximately) independent probabilities, each given by $\sim[\lambda(g)]^{-l}$. Hence the probability for the compound event is given by λ^{-lr}, and the time T_{FP} is given by its inverse. However a complete theory which predicts prefactors as well is lacking for both T_{FP} and T_S and is clearly desirable.

There are some related open problems. First, we have addressed only situations in which the bias-induced length $L(g)$ is larger than the spread of the initial configuration, namely $(N-1)$ lattice spacings. What happens if the reverse is true?

Second, we have dealt only with a fixed number N of particles. In certain physical situations it may be more appropriate to let N fluctuate but with some other condition specified. For instance, in the case of a branch in the percolation problem discussed in the introduction one may fix only the mean density of particles at the point the branch is attached to the rest of the infinite cluster. A theory analogous to that presented at the beginning of Section 2 (but involving grand partition functions) can be worked out, with the result that the time required for all particles in a branch of length $l \gg L(g)$ to empty out grows as $\sim\exp[l^2/2L(g)]$. A verification of this formula would be valuable.

ACKNOWLEDGMENT

We thank Dr. D. Dhar for helpful discussions, and the referee for suggesting a simpler route to our results.

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