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Long-Time Asymptotics in the One-Dimensional Trapping Problem with Large Bias

A. Aldea,[1] M. Dulea,[1] and P. Gartner[1]

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The survival probability of a particle which moves according to a biased random walk in a one-dimensional lattice containing randomly distributed deep traps is studied at large times. Exact asymptotic expansions are deduced for fields exceeding a certain threshold, using the method of images. In order to cover the whole range of fields, we also derive the behavior of the survival probability below this threshold, using the eigenvalue expansion method. The connection with the continuous diffusion model is discussed.

KEY WORDS: Biased random walk; random traps; survival probability; method of images.

1. INTRODUCTION

In the last few years, diffusion in a medium containing randomly distributed traps has been the subject of considerable theoretical work. The general interest this problem generates is due to the wide range of its applications in the field of nonequilibrium phenomena, from chemical reactions to recombination processes in semiconductors.[1,2] The one-dimensional model with stationary random deep traps was studied intensively because its simplicity allows the deduction of exact solutions. Various results have been obtained in this case concerning some quantities of physical significance.[3-10] Among them, the survival probability of a particle which performs a random walk stands out by its importance for the characterization of the temporal evolution of the system. The results published so far regarding the dominant long-time behavior of this quantity can be summarized as follows.

[1] Institute of Physics and Technology of Materials, Bucharest, Rumania.

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1. In the case of free diffusion the probability of survival goes like $\exp(-\text{const} \cdot t^{1/3})$.[1,4,6,8,11]

2. If an external field is present, this behavior becomes exponential: $\exp(-Kt)$.[3,5,8–10]

3. There is a critical field strength which separates two different regimes: below this value, K is only field dependent, while above it, K depends also on the concentration of traps.[5,8,9] The above statements were proved for both continuous and discrete media. For the continuous diffusion model, a rigorous deduction of the dependence of K on the field and trap concentration was made for any values of these parameters, using the Brownian motion formalism.[9] On the other hand, the expression for K was obtained in the model of hopping on a lattice only for low fields and low concentration of traps.[4,5]

This paper provides the exact long-time solution for the survival probability in the case of the biased random walk on a lattice with infinitely deep traps. The results are valid for any bias and trap concentration. The main result is the following expression, which gives the coefficient K (which determines the dominant long-time behavior) as a continuous, nonanalytical function of the bias η, defined in (2.2), and the trap concentration c:

$$K(\eta, c) = \begin{cases} 2[1-(1-\eta^2)^{1/2}], & \eta < \eta_0 \\ \dfrac{c(2\eta - c - \eta c)}{1-c}, & \eta > \eta_0, \quad \eta_0 = \dfrac{1-(1-c)^2}{1+(1-c)^2} \end{cases} \tag{1.1}$$

At the same time, besides the leading asymptotic term, the next to leading corrections (of any order) are given in a way which permits the estimation of errors.

The next section contains the model and its subcritical behavior deduced by the use of the eigenvalue representation method. Section 3 is devoted to the derivation of the large-time asymptotics at supracritical fields, which is our main result. The conclusions and discussions are left for the last section.

2. SUBCRITICAL BEHAVIOR

The description of the biased random walk dynamics on a chain is made here in the framework of the rate equation formalism. The probabilities of finding the particle at the nth site at the time t, denoted by $P_n(t)$, satisfy the following set of equations:

$$dP_n/dt = -(W_+ + W_-)\, P_n + W_+ P_{n-1} + W_- P_{n+1}, \qquad n \in \mathbb{Z} \tag{2.1}$$

where $W_{\pm}$ are the transition rates between nearest neighbor sites in the right or left direction, respectively. We suppose also the fulfilment of the detailed balance condition, which relates the ratio of these quantities to the field strength E, the lattice spacing a, and the charge of the particle e:

$$\frac{W_+}{W_-} = \exp(2\varepsilon) = \frac{1+\eta}{1-\eta}, \qquad \varepsilon = \frac{eaE}{2k_B T}, \qquad 0 \leqslant \eta \leqslant 1 \tag{2.2}$$

If we rescale the time with the mean transition rate $W = (W_+ + W_-)/2$, Eq. (2.1) can be written as an expression containing only the bias η, which was defined above:

$$dP_n/dt = -2P_n + (1+\eta)\, P_{n-1} + (1-\eta)\, P_{n+1}, \qquad n \in \mathbb{Z} \tag{2.3}$$

Due to presence of infinitely deep traps, we have to solve (2.3) for a finite chain, free of traps, but with absorbing boundary conditions. Denoting by $P_N(n, m, t)$ the probability of finding the particle at the site n at time t if it started from the site m at $t=0$ inside a chain of length $a(N-2)$, the survival probability is obtained by averaging over all the configurations of traps:

$$S(\eta, c, t) = c^2 \sum_{N=2}^{\infty} (1-c)^{N-2} \sum_{n,m=1}^{N-1} P_N(n, m, t) \tag{2.4}$$

Explicit expressions for P_N can be obtained in two ways: (1) representing them in terms of the eigenvalues of the evolution operator for the finite-chain problem with perfectly absorbing ends, or (2) using the method of images. It will be shown in Section 3 that the second method gives good results at long times for supracritical fields. In this section we adopt the eigenvalue representation.

Let us consider a chain containing $N-1$ sites, bounded by two infinite traps. The particle dynamics is described by Eq. (2.3) with perfectly absorbing boundary conditions. The Jacobi-type matrix which describes the rhs of this equation is non-Hermitic and has the eigenvalues

$$\gamma_k = 2[1-(1-\eta^2)^{1/2}\cos\theta_k], \qquad \theta_k = k\pi/N, \quad k = 1,\ldots, N-1 \tag{2.5}$$

The corresponding normalized right (left) eigenvectors have the components

$$(2/N)^{1/2}\, z^{\pm(n-1)} \sin n\theta_k, \qquad n = 1,\ldots, N-1 \tag{2.6}$$

where

$$z = [(1+\eta)/(1-\eta)]^{1/2}, \qquad z \geqslant 1$$

If we write the solution $P_N(n, m, t)$ using the spectral decomposition of the above matrix, we obtain

$$P_N(n, m, t) = \frac{2}{N} \sum_{k=1}^{N-1} e^{-\gamma_k t} z^{n-m} \sin m\theta_k \sin n\theta_k \tag{2.7}$$

One expects the long-time behavior of the survival probability to be governed by the lowest eigenvalue $k=1$ and by long chains (large N), so that Eq. (2.4) may be approximated as follows:

$$S(\eta, c, t) \sim \frac{\pi^2(1-\eta^2)^{1/2}}{[1-(1-\eta^2)^{1/2}]} \left(\frac{c}{1-c}\right)^2 \exp\{-2[1-(1-\eta^2)^{1/2}]t\} \times \sum_{N=2}^{\infty} \frac{1}{N^3} \exp\left\{N \ln[(1-c)z] - \frac{\pi^2(1-\eta^2)^{1/2}}{N^2} t\right\} \tag{2.8}$$

Provided that $(1-c)z < 1$, the sum in (2.8) can be evaluated by the saddle point method[6] and after some trivial algebra one gets the following time decay of the survival probability[10]:

$$S(\eta, c, t) \sim \exp(-Ct - C_1 t^{1/3}), \qquad C = 2[1-(1-\eta^2)^{1/2}]$$
$$C_1 = \tfrac{3}{2}\{2\pi^2(1-\eta^2)^{1/2} \ln^2[(1-c)z]\}^{1/3} \tag{2.9}$$

It is obvious from (2.8) that the equation $(1-c)z = 0$ defines a critical bias

$$\eta_0(c) = [1-(1-c)^2]/[1+(1-c)^2] \tag{2.10}$$

above which the saddle point method breaks down and the summation over N does not even converge. This means that the lowest eigenvalue approximation used for the deduction of (2.8) fails. As we shall see in the next section, at $\eta = \eta_0$ the qualitative behavior of the coefficient K changes, too.

3. SUPRACRITICAL FIELDS

The supracritical regime is defined by $(1-c)z > 1$ $(\eta > \eta_0)$. Returning to the general expression (2.7), let us use the well-known expansion

$$\exp(t \cos \alpha) = \sum_{p=-\infty}^{\infty} J_p(t) \cos p\alpha$$

where J_p is the modified Bessel function of integer order p and in our case $\alpha = k\pi/N$. Then the summation over k, which indexes the eigenvalues, can be carried out easily and one gets

$$P_N(n, m, t) = (\exp\{-2t[1-(1-\eta^2)^{1/2}]\})\, z^{n-m}$$
$$\times \sum_{p=-\infty}^{\infty} [P(n-m-2pN, (1-\eta^2)^{1/2}\, t)$$
$$- P(n+m-2pN, (1-\eta^2)^{1/2}\, t)] \tag{3.1}$$

In the above expression $P(n, t)$ is nothing else but the solution for the free random walk problem, without field and traps, i.e.,

$$P(n, t) = e^{-2t} J_n(2t), \qquad P(n, 0) = \delta_{n,0} \tag{3.2}$$

This formulation allows a straightforward parallel to the method of images (see, for instance, ref. 8). Indeed, the positive term with $p = 0$ represents the source (i.e., the solution of the problem in the absence of traps), while all the other terms represent its images needed to enforce the absorbing boundary conditions.

Introducing (3.1) in (2.4), the survival probability can be written as the sum over the contributions of all images:

$$S(\eta, c, t) = \sum_{p=-\infty}^{\infty} (-1)^p\, S_p(\eta, c, t) \tag{3.3}$$

with

$$S_p(\eta, c, t) = \frac{c^2}{v^2} e^{-2(t-\tau)} \sum_{N=2}^{\infty} v^N \sum_{n,m=1}^{N-1} z^{n-m} P(n - x_{N,m}^p, \tau) \tag{3.4}$$

where

$$x_{N,m}^p = \begin{cases} Np + m, & p = \text{even} \\ Np + N - m, & p = \text{odd} \end{cases}$$

is the center of the image number p and $\tau = (1-\eta^2)^{1/2}\, t$, $v = 1 - c$.

The large-time behavior of (3.4) is much more easily estimated if we extend the summations over m and n in the following way:

$$e^{2(t-\tau)} S_p(\eta, c, t) \sim \frac{c^2}{v^2} \sum_{N=2}^{\infty} v^N \sum_{n=-\infty}^{N-1} \sum_{m=1}^{\infty} z^{n-m} P(n - x_{N,m}^p, \tau) \tag{3.5}$$

The supplementary terms introduced in this way do not change the asymptotic behavior because, using the obvious inequality $P(n, \tau) \leqslant 1$, they become dominated by convergent geometric series which do not depend on t. They are negligible in the $t \to \infty$ limit since, as we shall see later, the dominant term in Eq. (3.5) is exponentially increasing. Replacing n by $N-n$, we can cast Eq. (3.5) in the following form:

$$e^{2(t-\tau)}S_p(\eta, c, t) \sim \frac{c^2}{v^2} \sum_{n,m=1}^{\infty} \frac{1}{z^{n+m}} \sum_{N=2}^{\infty} (vz)^N P(N-n-x^p_{N,m}, \tau) \quad (3.6)$$

In the above formula the summation over N can be now extended to $-\infty$, using the same type of upper bounds, and taking into account that $vz > 1$.

For definiteness we consider here the case $p = \text{even}$. Then Eq. (3.6) reads

$$e^{2(t-\tau)}S_p(\eta, c, t) \sim \frac{c^2}{v^2} \sum_{n,m=1}^{\infty} \frac{1}{z^{n+m}} \sum_{N=-\infty}^{\infty} \lambda^{(p-1)N} \times P[(p-1)N+n+m, \tau], \qquad \lambda = (vz)^{1/(p-1)} \quad (3.7)$$

The summation over N is readily performed using

$$\sum_{n=-\infty}^{\infty} \lambda^n P(n, \tau) = \exp\left[\left(\lambda + \frac{1}{\lambda} - 2\right)\tau\right] \quad (3.8a)$$

and

$$\frac{1}{p}\sum_{s=0}^{p-1} \exp\left[i\frac{2s\pi}{p}(n-l)\right] = \sum_{N=-\infty}^{\infty} \delta_{n,pN+l} \quad (3.8b)$$

Equation (3.8a) is nothing but the generating function formula for the modified Bessel functions[13] written in terms of $P(n, \tau)$ [see Eq. (3.2)]. Combining (3.8a) and (3.8b), one gets

$$\sum_{N=-\infty}^{\infty} \lambda^{pN} P(pN+l, \tau) = \frac{1}{p}\sum_{s=0}^{p-1} (\bar{\lambda}_{p,s})^{-l} \exp\left[\left(\bar{\lambda}_{p,s} + \frac{1}{\bar{\lambda}_{p,s}} - 2\right)\tau\right], \qquad \bar{\lambda}_{p,s} = \lambda e^{i(2s\pi/p)} \quad (3.9)$$

This identity holds for $p < 0$, too, if we change p into $|p|$ on the rhs. Using (3.9) in (3.7), one immediately gets

$$S_p(\eta, c, t) \sim \frac{c^2}{v^2} e^{-2(t-\tau)} \frac{1}{|p-1|} \sum_{s=0}^{|p-1|-1} \frac{1}{(z\bar{\lambda}_{|p-1|,s} - 1)^2} \times \exp\left[\left(\bar{\lambda}_{|p-1|,s} + \frac{1}{\bar{\lambda}_{|p-1|,s}} - 2\right)\tau\right] \quad (3.10a)$$

The calculation for $p=\text{odd}$ proceeds in the same way, giving

$$S_p(\eta, c, t) \sim \frac{c^2}{v^2} e^{-2(t-\tau)} \frac{1}{|p|} \sum_{s=0}^{|p|-1} \frac{1}{z^2 - z(\tilde{\lambda}_{|p|,s} + 1/\tilde{\lambda}_{|p|,s}) + 1} \times \exp\left[\left(\tilde{\lambda}_{|p|,s} + \frac{1}{\tilde{\lambda}_{|p|,s}} - 2\right)\tau\right] \tag{3.10b}$$

For each p, the dominant term is that corresponding to $s=0$. It behaves like

$$\exp\left\{-\left[2-(1-\eta^2)^{1/2}\left(\lambda+\frac{1}{\lambda}\right)\right]t\right\}, \qquad \lambda = \begin{cases} (vz)^{1/(p-1)}, & p=\text{even} \\ (vz)^{1/p}, & p=\text{odd} \end{cases} \tag{3.11}$$

It is obvious that the dominant asymptotic terms in the survival probability function $S(\eta, c, t)$ are those corresponding to the images $p=-1, 0, 1, 2$. Their total contribution is

$$\left(\frac{z^2v^2-1}{z^2v^2-v}\right)^2 \exp\left\{-\left[2-(1-\eta^2)^{1/2}\left(vz+\frac{1}{vz}\right)\right]t\right\} \tag{3.12}$$

The exponent in (3.12) coincides with (1.1) for $\eta > \eta_0$. Equations (3.10) also give as many successive terms as one desires in the asymptotic expansion of $S(\eta, c, t)$ by adding the contribution of more and more remote images to those already considered in (3.12). Moreover, the image expansion is very convenient for the control of errors. Indeed, if we split (3.3) into left ($p<0$) and right ($p \geqslant 0$) series, it is obvious that both are made up of monotonically decreasing terms with alternating signs. For such series it is well known that the first neglected term dominates the rest of the series.

4. CONCLUSIONS AND DISCUSSIONS

The problem of the long-time asymptotics of the survival probability $S(\eta, c, t)$ for a particle which performs a random walk i a one-dimensional lattice in presence of deep traps and external bias has been investigated. Its dominant behavior is described by the decay rate $K(\eta, c)$ given in Eq. (1.1), which turns out to be a nonanalytic function of η. There is a critical bias $\eta_0(c)$ where the second derivative of $K(\eta, c)$ is discontinuous. The preexponential factor is also calculated [see Eq. (3.12)]. Actually, Eqs. (3.10) give explicitly all the terms of the asymptotic series of $S(\eta, c, t)$.

The same problem can be approached for the continuous model described by a Fokker–Planck equation,[3,7,8] using exactly the same techniques. One obtains an asymptotic series whose leading term has the same exponent as given by Eisele and Lang.[9] The series can be also recovered from its discrete counterpart given in this paper by applying a scaling limit procedure consisting in taking the limit of small lattice spacing ($a \to 0$) and large time ($t \to \infty$) along with a corresponding scaling of η and c. More precisely,

$$S^{\text{cont}}(\eta, c, t) = \lim_{a \to 0} S(a\eta, ac, a^2 t) \tag{4.1}$$

This correspondence between the two models explains why Movaghar *et al.*,[5] although working on a discrete model (but in the approximation of small η and c) ended up with the leading term of the continuous case.

The present results have been obtained by the use of the eigenvalue expansion in the subcritical regime and by the image method in the supracritical one. Since the image expansion is well known for its poor convergence for large times,[8] it is worth pointing out why it works in this problem. This occurs because the width of any image increases as $t^{1/2}$, while the main contribution to the survival probability arises from chains with lengths $N \sim t$, so that at large times the spacing between the images is much greater than their width.

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