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Diffusion and Survival in a Medium with Imperfect Traps

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This paper deals with independent particles diffusing on a line with traps at random positions. It is shown how the long-time decay of the survival probability is exhanced when particles do not necessarily disappear upon hitting a trap. The results are compared with predictions for a model where particles are either absorbed or reflected by traps.

KEY WORDS: Diffusion; trapping problem; survival probability; imperfect traps.

1. INTRODUCTION

Diffusion models, where independent particles may be absorbed by traps located at arbitrary positions, have been studied for many purposes. They may describe excitons in solids or interstitial hydrogen atoms in metals, as well as the diffusion-controlled reaction $A + B \rightarrow B$, where B is immobile.

Most studies have been done on infinite media with perfect traps. Perfect means that every diffusing particle will be absorbed when hitting a trap. Of particular interest is the behavior of the survival probability $\Psi(t)$ for long times. In a d-dimensional medium it has a stretched exponential decay, $\Psi(t) \sim \exp(-at^{d/(d+2)})$, for very long times. Particles vanish more slowly than exponentially because of the occurrence of arbitrarily large regions without traps, where they can survive for a long time. The stretched exponential decay was first derived by Balagurov and Vaks,[1] using a result of Lifshitz[2] on exponential band tails in the density of states in linear random problems. A strict mathematical proof was given by Donsker and Varadhan[3] and the subject was recently reviewed by Haus and Kehr.[4]

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Corrections to the above asymptotic result are important for practical applications. The general behavior is

$$\Psi(t) \sim \exp(-at^{d/(d+2)} - bt^{(d-1)/(d+2)} - ct^{(d-2)/(d+2)} + \cdots)$$

It is seen that in one dimension, subdominant corrections show up as an overall prefactor. The exact asymptotic behavior for $\Psi(t)$ in $d=1$ was derived by Anlauf,[5] who also calculated a number of correction terms. In three dimensions, the subleading terms have been resummed by field-theoretic methods in the limit of small concentration c of traps at times scaled with c.[6] It was found that the onset of stretched exponential decay occurs when only very few particles have survived.

The problem of imperfect traps, where particles may hit a trap but escape from it at the next time step, has been studied less intensively. Even in one dimension it cannot be solved exactly. However, the results of ref. 6 also apply to the case of imperfect trapping in three dimensions. In the present paper we shall study the one-dimensional situation with imperfect traps. We shall compare our results with a model introduced by Weiss and Havlin.[7] Here particles are either absorbed by traps or reflected. Hence, they never pass the two adjacent traps and, as for the case of perfect trapping, the problem is solvable exactly.

The setup of the paper is as follows. In Section 2 we define the model and point out the role of the density of states. In Section 3 we study the long-time behavior of the return and survival probabilities. In Section 4 we study the prefactor of this behavior for the case of identical, imperfect traps. In Section 5 we redo calculations of Weiss and Havlin;[7] in their model, particles will be trapped or reflected. Section 6 closes with a summary.

2. DEFINITION OF THE MODEL AND THE ROLE OF THE DENSITY OF STATES

We consider diffusion on a chain described by a symmetrical nearest-neighbor random walk. Trapping at site r is described by a probability w_r with which the particle disappears before the next time step. For $w_r = 0$ there is no trap at site r, for $w_r = 1$ the trap is perfect, and for $0 < w_r < 1$ it is imperfect. For each site r the value of w_r is drawn from a distribution which is independent of r and not correlated to different sites. The traps are quenched, i.e., the w_r do not vary in time.

For discrete-time dynamics the system obeys the master equation

$$p(r, t+\tau) = \tfrac{1}{2}(1 - w_r)[p(r+1, t) + p(r-1, t)] \tag{1}$$

where $p(r, t)$ is the probability that a particle is at site r at time t, and both hopping and trapping occur at half-integer time steps. The continuous version of (1) is obtained by setting

$$w_r = \frac{v_r \tau}{1 + v_r \tau} \tag{2}$$

and expanding to first order in τ

$$\dot{p}(r, t) = \frac{1}{2\tau} [p(r+1, t) + p(r-1, t) - 2p(r, t)] - v_r p(r, t) \tag{3}$$

where $v_r = 0$ if there is no trap and $v_r = +\infty$ for a perfect trap. Eigenmodes of this equation are defined by

$$p(r, t) = b(r) e^{-Et} \tag{4}$$

and satisfy

$$2(1 - E\tau + v_r \tau)\, b(r) = b(r+1) + b(r-1) \tag{5}$$

The eigenvalues E_j are determined by the requirement that $b(r)$ can be normalized.

For obtaining the return and survival probability it is usefull to define the average probability of displacement over a distance r in time t,

$$P(r, t) = \left\langle \sum_{r_0 = 1}^{N} p(r_0 + r, t \mid r_0, 0)\, p(r_0, 0) \right\rangle \tag{6}$$

It involves the conditional probability that a particle starts at site r_0 at $t = 0$ and is at site $r_0 + r$ at time t. We assume a uniform initial distribution $p(r, 0) = 1/N$, where N is the number of sites in the chain and is taken to infinity at an appropriate moment. The brackets in (6) denote the average over the distribution of traps. We may study this average, because the quantity within the brackets is already self-averaging in the limit $N \to \infty$. The return probability $R(t)$ is obviously

$$R(t) = P(0, t) \tag{7}$$

The survival probability $\Psi(t)$ is given by a sum over all sites

$$\Psi(t) = \sum_r P(r, t) \tag{8}$$

It is convenient to introduce the Fourier–Laplace transform of (6)

$$\hat{P}(q, s) = \int_0^{\infty} dt\, e^{-st} \sum_r e^{iqr} P(r, t) \tag{9}$$

The formal solution of the equation of motion (3) for the conditional probability is

$$p(r_0+r, t \mid r_0, 0) = (e^{-t(V+\Phi/2\tau)})_{r+r_0, r_0} \tag{10}$$

where we defined matrices

$$V_{r,r'} = \delta_{r,r'} v_r \qquad \text{and} \qquad \Phi_{r,r'} = 2\delta_{r,r'} - \delta_{r,r'+1} - \delta_{r,r'-1} \tag{11}$$

This can be inserted in (6) and integrated over t. It follows that $\hat{P}(q, s)$ is a Green's function

$$\begin{aligned} \hat{P}(q, s) &= \lim_{N \to \infty} \frac{1}{N} \sum_{r, r_0} e^{iqr} \left\langle \frac{1}{S + V + (1/2\tau)\Phi} \right\rangle_{r+r_0, r_0} \\ &= \left\langle \frac{1}{S + V + (1/2\tau)\Phi} \right\rangle_{q,q} \end{aligned} \tag{12}$$

where

$$S_{r,r'} = \delta_{r,r'} s \tag{13}$$

Since the distribution of disorder is independent of r, the average Green's function is translationally invariant in the thermodynamic limit $N \to \infty$. Hence it is diagonal in Fourier space.

The function $\hat{P}$ has a cut along the negative real axis

$$\operatorname{Im} \hat{P}(q, -E \pm i0) = \mp \pi \rho(q, E) \tag{14}$$

where $\rho(q, E)$ is the density of states at wavenumber q. It can also be expressed as a sum over the eigenmodes of (5),

$$\rho(q, E) = \lim_{N \to \infty} \frac{1}{N} \sum_{j=1}^{N} \sum_{r,r'=1}^{N} e^{iq(r-r')} \langle \delta(E - E_j)\, b_j(r)\, b_j(r') \rangle \tag{15}$$

This enables us to invert (9)

$$P(r, t) = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \int_0^\infty e^{-Et} e^{-iqr} \rho(q, E)\, dE \tag{16}$$

In particular, the survival probability is given by

$$\Psi(t) = \int_0^\infty e^{-Et} \rho(0, E)\, dE \tag{17}$$

where $\rho(0, E)$ is the density of states at zero wavenumber. The return probability is given by

$$R(t) = \int_0^\infty e^{-Et} \rho(E)\, dE \tag{18}$$

where

$$\rho(E) = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \rho(q, E)$$

is the *total* density of states.

3. LONG-TIME BEHAVIOR OF THE RETURN AND SURVIVAL PROBABILITY

From Eqs. (17) and (18) it is clear that the long-time decay of the return probability $R(t)$ and the survival probability $\Psi(t)$ is dominated by the small-energy singularity in $\rho(E)$ and $\rho(0, E)$. This behavior is known for arbitrary dimension from the work of Lifshitz,[2]

$$\rho(q, E) \sim \rho(E) \sim \exp(-k_d \lambda E^{-d/2}), \qquad \lambda = -\ln p \tag{19}$$

where p is the probability that a given site contains no trap, and k_d is a constant. The behavior (19) is called the *Lifshitz tail*. It has its origin in the occurrence of arbitrarily large regions without traps, as marked by the factor $p = e^{-\lambda}$. From (19) and (18) the return probability is found to have the leading asymptotic behavior

$$R(t) \sim \exp(-a_d \lambda^{2/(d+2)} t^{d/(d+2)}) \tag{20}$$

The precise behavior is determined by the corrections to (19). In the one-dimensional situation this can be done in great detail, as was shown in a series of papers by Nieuwenhuizen and Luck.[8–10] These authors studied harmonic chains with random masses, which are closely related to the system discussed here. In particular, a random mass in the harmonic system plays the role of a trapping strength in the present diffusion model. The equation of motion for a displacement $a(r) e^{i\omega t}$ in a harmonic chain with random masses m_r is

$$-m_r \omega^2 a(r) = K[a(r+1) + a(r-1) - 2a(r)] \tag{21}$$

where K is the force constant. We set $\omega^2 = (2K/m_-)(1 + \cos \varepsilon)$, where m_-

is the smallest value of the masses. Then (21) is equivalent to Eq. (5) under the mapping

$$b(r) \to (-1)^r a(r) \tag{22}$$

$$1 - E\tau \to \cos \varepsilon \tag{23}$$

$$v_r \tau \to (m_r - m_-) \frac{\omega^2}{2K} \tag{24}$$

This implies connections between the densities $\rho(E)$ and $\rho(q, E)$ of the trapping problem and the spectral densities $\rho_h(\omega^2)$ and $\rho_h(q, \omega^2)$ of the harmonic problem

$$\begin{aligned} \rho(q, E) &= \frac{\tau}{2} \omega_m^2 \rho_h \left[\pi + q, \omega_m^2 \left(1 - \frac{E\tau}{2} \right) \right] \\ \rho(E) &= \frac{\tau}{2} \omega_m^2 \rho_h \left[\omega_m^2 \left(1 - \frac{E\tau}{2} \right) \right] \end{aligned} \tag{25}$$

where $\omega_m = (4K/m_-)^{1/2}$ is the maximal frequency in the harmonic system. In particular, low energies correspond to high frequencies, and $q \simeq 0$ in the trapping problem corresponds to $q \simeq \pi$ in the harmonic system. From (24) it is seen that if the distribution of trapping rates v_r is independent of energy, the distribution of masses in the corresponding harmonic problem necessarily depends on frequency. However, for the low-energy results to be discussed below, the approximation $\omega^2 \simeq \omega_m^2$ in (24) will suffice.

There are distributions of masses for which $\rho_h(\omega^2)$ and $\rho_h(q, \omega^2)$ have been solved exactly.[11,12] In units where $K = m_- = 1$ the masses decompose as

$$m_r = 1 + Mx_r \tag{26}$$

where the x_r have the density

$$v(x) = \begin{cases} p\,\delta(x) + (1-p) e^{-x}, & x \geqslant 0 \\ 0, & x < 0 \end{cases} \tag{27}$$

From these exact solutions the Lifshitz tail of $\rho_h(\omega^2)$ and $\rho_h(q, \omega^2)$ have been derived in ref. 8. The first result reads, for ω^2 near $\omega_m^2 = 4$,

$$\begin{aligned} \rho_h(2 + 2\cos\varepsilon) = {} & \frac{\pi(1-p)^2}{2p\varepsilon^3} \sum_{n=-\infty}^{+\infty} p^{\pi/\varepsilon} e^{2\pi i n \pi/\varepsilon} \\ & \times f_n^2 [1 + A_n^{(1)} \varepsilon \ln \varepsilon + A_n^{(2)} \varepsilon + O(\varepsilon^2 \ln^2 \varepsilon)] \end{aligned} \tag{28}$$

In this expression one needs the solution of the differential equation

$$f''(x) = \frac{1-e^{-x}}{4Mx(1-pe^{-x})} f(x) \tag{29}$$

with boundary conditions $f(0)=1$, $f(+\infty)=0$. It has singularities at $x = x_n \equiv \ln p + 2\pi i n$, where f behaves as

$$f(x_n+\delta) = f_n + \varphi_n \, \delta \ln \delta + \psi_n \, \delta + O(\delta^2 \ln^2 \delta) \tag{30}$$

It follows that $\varphi_n = -(1-p) f_n/(4Mpx_n)$, whereas f_n and ψ_n can only be determined numerically. Further,

$$\begin{aligned} A_n^{(1)} &= \frac{2\varphi_n}{\pi f_n} \\ A_n^{(2)} &= \frac{1}{\pi f_n^2}\left[\frac{f_n - f_n^2}{x_n} + 2f_n(\varphi_n + \psi_n) - 2f_n\varphi_n(\ln \pi + \gamma_e)\right] \end{aligned} \tag{31}$$

where γ_e denotes Euler's constant. Equation (28) shows that the leading Lifshitz tail $p^{\pi/\varepsilon}$ is multiplied by a power and a periodic function, such that the integral

$$H_c(\omega^2) = \int_{\omega^2}^{\omega_m^2} \rho(x)\, dx$$

behaves as $p^{\pi/\varepsilon}$ times a periodic amplitude. The very same result was derived in ref. 9 by more physical considerations. In the latter paper the leading behavior of (28) was derived for arbitrary mass distributions. It was shown that the f_n in general result from a periodic amplitude in the Dyson–Schmidt function.[13] For the distribution (26)–(27) the problem can be reduced to the solution of (29). In Section 4 we calculate f_0 for the binary disorder.

The Lifshitz tail in the function $\rho_h(q, \omega^2)$ was calculated in ref. 8. We have checked the lengthy derivation.[3] In the present paper we are interested in low-energy and long-wavelength behavior of the trapping problem. For the harmonic system there exists a scaling behavior near $q = \pi$ and $\omega^2 = \omega_m^2 \equiv 4$.[8] Via the connections (25), this implies a scaling behavior near $q = 0$ and $E = 0$ in the trapping problem:

$$\rho(Q(2E\tau)^{1/2}, E) = \rho(E) \cdot S(Q) \qquad (E \to 0,\ Q \text{ fixed}) \tag{32}$$

[3] We find a discrepancy in the constituent $Q_{2,n}$ of $\rho(q, \omega^2)$: the terms linear in f_n in Eq. (3.29c) must have an additional factor (-1). Further, we find that also the first two terms multiplying f' in Eq. (3.22) should have a minus sign.

with scaling function

$$S(Q)=\frac{4}{\pi(2E\tau)^{1/2}}\frac{1+\cos\pi Q}{(1-Q^2)^2} \tag{33}$$

normalized to

$$\int_{-\pi}^{\pi}\frac{dq}{2\pi}S(Q)=1$$

With the above results we can calculate the long-time behavior of the quantities discussed in the previous section. From (18), (25), and (28), one gets by saddle point methods in the limit of long times the asymptotic behavior. The return and survival probability behave roughly as

$$\exp[-\tfrac{3}{2}(\pi\ln 1/p)^{2/3}(t/\tau)^{1/3}]$$

which confirms the prediction (20) for our case and includes the constants. This behavior involves a further power law and a numerical prefactor, depending on the concentration $c=1-p$. We also derive the first correction terms. The full result reads

$$\begin{aligned}R(t)=f_0^2\frac{(1-p)^2}{p\ln 1/p}\left(\frac{2}{3}\pi x\right)^{1/2}e^{-3x/2}\Bigg[&1+\left(\frac{5}{18}+\frac{(\pi\lambda)^2}{24}\right)\frac{1}{x}\\&+A_0^{(1)}\frac{\pi\lambda}{x}\ln\frac{\pi\lambda}{x}+A_0^{(2)}\frac{\pi\lambda}{x}+O(x^{-2}\ln^2 x)\Bigg]\end{aligned} \tag{34}$$

where

$$x=(\pi\lambda)^{2/3}\left(\frac{t}{\tau}\right)^{1/3},\qquad \lambda=-\ln p \tag{35}$$

and $A_n^{(1,2)}$ have been defined in (31). It is to be noted that terms with $n\neq 0$ in (28) give exponentially small corrections to (34), because for these terms the saddle point value has a larger real part.

Similarly, the survival probability has the asymptotic behavior

$$\begin{aligned}\Psi(t)=f_0^2\frac{(1-p)^2}{p\ln^2 p}\frac{8}{\pi}\left(\frac{2x^3}{3\pi}\right)^{1/2}e^{-3x/2}\Bigg[&1+\left(\frac{17}{18}+\frac{(\pi\lambda)^2}{24}\right)\frac{1}{x}\\&+A_0^{(1)}\frac{\pi\lambda}{x}\ln\frac{\pi\lambda}{x}+A_0^{(2)}\frac{\pi\lambda}{x}+O(x^{-2}\ln^2 x)\Bigg]\end{aligned} \tag{36}$$

This expression can be compared with the result of Anlauf.[5] He has studied the case of perfect traps, which can be solved by enumeration techniques. A closely related model will be studied in Section 5. For perfect traps, it holds that $f_0 = 1$, $A_0^{(1)} = A_0^{(2)} = 0$.[8] Inserting these values in (36), we recover the leading behavior derived by Anlauf. For the term within brackets in (36) he finds

$$\left[1 + \left(\frac{17}{18} - \frac{(\pi\lambda)^2}{12}\right)\frac{1}{x} + O(x^{-2})\right]$$

and calculates corrections up to the order x^{-4} included. The difference in the $1/x$ coefficient with regard to our result (36) can be traced back to the fact that (36) holds for a continuous-time process. Indeed, Laplace inversion brings a factor e^{-Et} for continuous times [cf. Eqs. (17), (18)]. For discrete times, on the other hand, there will be a factor $(1-E)^t \simeq \exp(-Et)\cdot(1-E^2t/2)$, which causes the above-mentioned difference.

The scaling behavior (32) for small wavelengths implies a scaling behavior for the probability that a particle has moved a large distance without being trapped:

$$P(r, t) \simeq R(t)\cdot F\left(\frac{r}{\xi(t)}\right) \tag{37}$$

with the scaling function

$$F(y) = \begin{cases} (1-|y|)\cos(\pi y) + \dfrac{1}{\pi}\sin(\pi\,|y|), & -1 \leqslant y \leqslant 1 \\ 0, & \text{else} \end{cases} \tag{38}$$

and correlation length

$$\xi(t) = \left(\frac{\pi^2 t}{\tau \ln 1/p}\right)^{1/3} \tag{39}$$

This scaling function is plotted in Fig. 1.

It shows that the probability of survival gets smaller if the particle has moved further from its starting point. As a consequence, particles which have escaped trapping have performed a random walk of characteristic range $\xi(t)$. Since $\xi(t) \sim t^{1/3} \ll t^{1/2}$, these are rather compact walks. The time dependence of ξ says that for longer and longer times, the dominant number of nontrapped particles is to be found in larger and larger trap-free regions. For $|r| < \xi(t)$, particles have diffused in such a region without

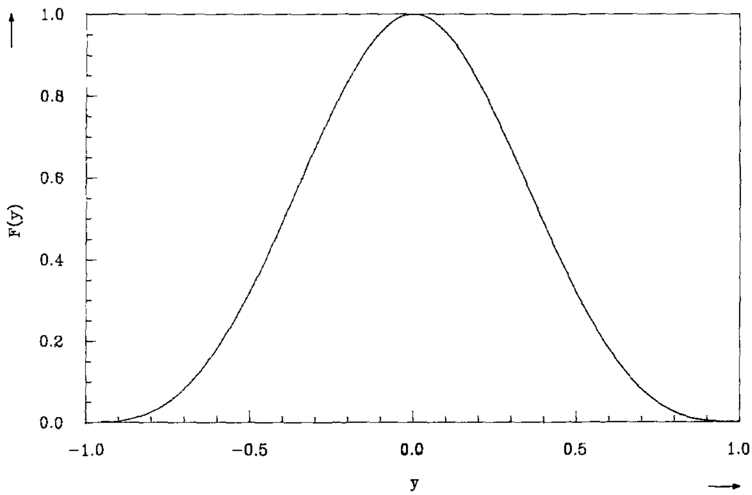

Fig. 1. The scaling function $F(y)$ entering the long-time and large-distance scaling form of $P(r, t)$ of Eq. (37).

reaching a trap; for $|r| > \xi(t)$, they must have passed a trap and the probability of survival is zero to leading order (it is exactly zero for perfect traps). By integrating (37), one recovers the survival probability (36), as one should, up to a factor $1-2/(3x)$. The origin of the discrepancy lies in our omission of subleading corrections to (37), (38).

4. PERFECT VERSUS IMPERFECT TRAPPING

From Eqs. (34) and (36) it is seen that the strength of traps only enters the dominant long-time decay through the factor f_0^2. Indeed, the only assumption made there is that with probability p a site contains no trap. In the exactly solvable case

$$v_r = \frac{2Mx_r}{\tau} \tag{40}$$

with x_r distributed according to (27), one studies a system where a fraction $1-p$ of the sites contains an imperfect trap, with strength drawn from an exponential distribution. For this system f_0 follows by solution of the second-order differential equation (29). A plot of f_0 as a function of M was given in Fig. 2 of ref. 8. In the limit $M \to \infty$ all traps become perfect, and $f(x) = 1$ solves (29), implying $f_0 = 1$ for perfect traps.

As discussed in refs. 8 and 9, the factor f_0 can be defined for arbitrary distributions of disorder. Of particular interest is the case where the traps are identical

$$\rho(v) = p\,\delta(v) + (1-p)\,\delta\left(v - \frac{a}{2\tau}\right) \tag{41}$$

This distribution says that the trapping strength at a given site equals zero with probability p, and with probability $1-p$ it equals $a/(2\tau)$. The philosophy of ref. 9 was to solve the Dyson–Schmidt equation[13] at the band edge. For our case we need the Schmidt function

$$Z(u) = \lim_{r\to\infty} \left\{\text{Prob}\left(\frac{b(r)}{b(r+1)} > u\right)\right\} \tag{42}$$

at $E=0$. From Eq. (5) for $b(r)$ it follows that at $E=0$ the function $Z(u)$ satisfies the Dyson–Schmidt equation

$$Z(u) = pZ\left(2-\frac{1}{u}\right) + (1-p)\,Z\left(2+a-\frac{1}{u}\right) + \Theta(-u) \tag{43}$$

where Θ is a Heaviside step function. With the substitution

$$u = 1 - \frac{1}{v} \tag{44}$$

the handier form

$$Z\left(1-\frac{1}{v}\right) - pZ\left(1-\frac{1}{v-1}\right) = (1-p)\,\Theta\left(1+\frac{1}{a}-v\right) Z\left(1+a-\frac{1}{v-1}\right) \tag{45}$$

can be derived for $v>1$. In the region $v > 1 + 1/a$ the solution of this equation has the form

$$\begin{aligned} Z\left(1-\frac{1}{v}\right) &= p^{v} P(v) \\ &\equiv p^{v}\,\frac{1-p}{p} \sum_{n=-\infty}^{\infty} \frac{-1}{\ln p + 2\pi i n} f_n e^{2\pi i n v} \end{aligned} \tag{46}$$

where $P(v)$ is a periodic function with unit period. The second equality defines the coefficients f_n of the Lifshitz band tail.[8] Since Eq. (45) cannot be solved exactly, we study the physically interesting case $p \simeq 1$ of a small amount of traps. For $p=1$ one has the solution

$$Z^{(0)}\left(1-\frac{1}{v}\right) = \Theta(v) \tag{47}$$

This says that for $p=1$ there is only one chain in the ensemble, for which $b(r)/b(r+1)=1$ at $E=0$. For small concentrations $1-p$ of traps, Eq. (47) may be inserted in the rhs of (45). Solving this equation, we obtain

$$Z^{(1)}\left(1-\frac{1}{v}\right)=\begin{cases}1, & 0<v<1+1/a \\ p^{[v-1/a]}, & v\geqslant 1+1/a\end{cases} \tag{48}$$

where $[x]$ denotes the integer part of x. From (48) and (46) we obtain

$$f_0^{(1)}=p^{-1/a} \tag{49}$$

For perfect traps ($a=\infty$) this reduces to $f_0=1$, as it should. For finite a, $f_0^{(1)}$ is larger than unity, indicating that imperfect trapping leads to a larger survival probability than perfect trapping. Furthermore, also in the limit $p\to 1$ of small trap concentrations, $f_0^{(1)}$ goes to unity. This is to be expected too: on the time scales considered, repeated visits to imperfect traps let them look perfect. In the limit of vanishing trap strengths ($a\to 0$) the expression (49) diverges. This indicates that the stretched exponential decay becomes meaningless. Indeed, no particle gets trapped in this limit.

A better approximation for f_0 is obtained by inserting (48) in the rhs of (45) and iterating again. The result is

$$Z^{(2)}\left(1-\frac{1}{v}\right)=(1-p)\sum_k{}' p^{k+[x_k]}+p^{[v-1/2a]} \tag{50}$$

where

$$x_k=a^{-2}\left(1+\frac{1}{a}+k-v\right)^{-1}-\frac{1}{a}$$

The prime indicates that the sum is limited to the range

$$0<v-\frac{1}{a}-1<k\leqslant v-\frac{1}{2a}-1$$

From Eq. (50) one gets the approximation

$$f_0^{(2)}=p^{-1/a}(1-p)\sum_{n=0}^{\infty} p^{n+B_n} \tag{51}$$

with

$$B_n=a^{-2}\left(n+1+\frac{2}{a}\right)^{-1}$$

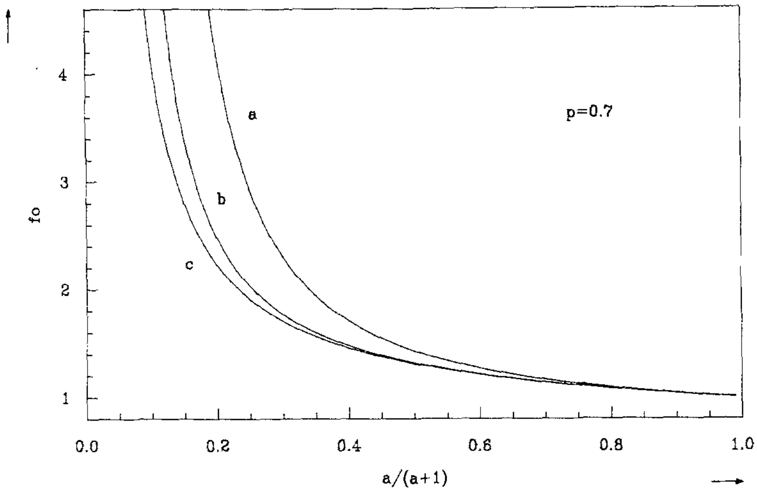

Fig. 2. Convergence of our iteration procedure for calculating f_0: (a) $f_0^{(1)}$; (b) $f_0^{(2)}$; (c) $f_0^{(7)} \simeq f_0^{(\infty)}$.

This second approximation has the same qualitative behavior as $f_0^{(1)}$. Further approximants can be evaluated numerically. In Fig. 2 we compare $f_0^{(1)}$, $f_0^{(2)}$, and $f_0^{(7)} \simeq f_0^{(\infty)}$ for $p = 0.7$ as functions of the variable $a/(a+1)$. The convergence of the algorithm has also been checked by comparing with data for f_0 obtained by enumerating all possible random chains with length 16. This very precise method was used earlier[8] for harmonic systems. In the present case it fully confirms the results described above. In Fig. 3 we finally present plots of the quantity $f_0/p^{\bar{v}}$ as a function of the parameter $a/(a+1)$ for various values of p, where $\bar{v}(a)$ is defined in Eq. (79).

5. ABSORPTION AND REFLECTION

Weiss and Havlin[7] have introduced an interesting variant of the trapping problem. Particles are assumed to move at discrete times. If they hit a trap, they disappear with probability α $(0 \leqslant \alpha \leqslant 1)$ and are reflected to their position with the probability $1-\alpha$. For $\alpha = 1$ this reduces to the model of perfect trapping. The main interest in the model is that it can be solved exactly. The reason is that particles will never leave the trap-free interval where they start. Our motivation to redo the calculations of Weiss and Havlin comes from the fact that these authors find no change in the long-time survival probability when traps become imperfect. We shall show that this unphysical prediction is incorrect.

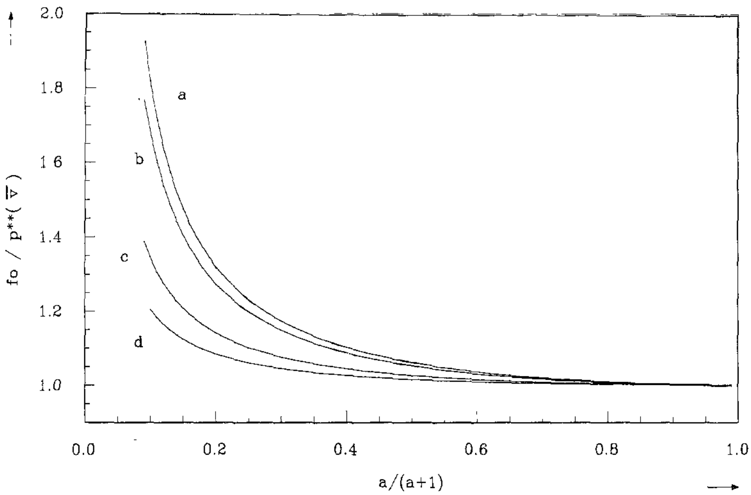

Fig. 3. The coefficient f_0 for (a) $p=0.5$; (b) $p=0.7$; (c) $p=0.9$; (d) $p=0.95$. A division by $p^{\bar{v}}$ has been made for reasons of graphical presentation.

Away from the traps the random walk satisfies the master equation

$$p_{n+1}(r \mid r_0) = \tfrac{1}{2} p_n(r+1 \mid r_0) + \tfrac{1}{2} p_n(r-1 \mid r_0) \tag{52}$$

Here we have taken units in which $\tau = 1$. We first consider an interval having traps at sites $r=0$ and $r=L$ and having no traps for $1 \leqslant r \leqslant L-1$. This interval occurs with probability $(1-p)^2\, p^{L-1}$ $(L \geqslant 2)$. The solution of (52) vanishing at $r=0$ and $r=L$ and satisfying $p_0(r \mid r_0) = \delta_{r,r_0}$ is

$$p_n(r \mid r_0) = \frac{2}{L} \sum_{j=1}^{L} \cos^n\left(\frac{\pi j}{L}\right) \sin\left(\frac{\pi j r}{L}\right) \sin\left(\frac{\pi j r_0}{L}\right) \tag{53}$$

Weiss and Havlin assume that the starting points are divided uniformly along the chain, but do not allow particles to start at trapping sites. The probability that in our interval a given particle has not hit a trap after n steps is

$$\begin{aligned} S_n &= \frac{1}{L-1} \sum_{r_0=1}^{L-1} \sum_{r=1}^{L-1} p_n(r \mid r_0), \qquad S_0 = 1 \\ &= \frac{2}{L(L-1)} \sum_{j=0}^{[L/2-1]} \cos^n \frac{\pi(2j+1)}{L} \cot^2 \frac{\pi(2j+1)}{2L} \end{aligned} \tag{54}$$

where again $[x]$ denotes the integer part of x. From S_n follows the probability s_n that a given particle hits a trap at the nth step as

$$\begin{aligned} s_n &= \frac{1}{2(L-1)} \sum_{r_0=1}^{L-1} \{p_{n-1}(1 \mid r_0) + p_{n-1}(L-1 \mid r_0)\} \\ &= S_{n-1} - S_n \end{aligned} \tag{55}$$

for $n \geqslant 1$ and we define $s_0 = 0$. The second equality follows from (52). We also need the probability T_n that a particle which starts next to a trap (that is, at $r=1$ or $r=L-1$) did not hit a trap after n steps:

$$\begin{aligned} T_n &= \frac{1}{2} \sum_{r=1}^{L-1} [p_n(r \mid 1) + p_n(r \mid L-1)] = \sum_{r=1}^{L-1} p_n(r \mid 1) \\ &= \frac{4}{L} \sum_{j=0}^{[L/2-1]} \cos^n \frac{\pi(2j+1)}{L} \cos^2 \frac{\pi(2j+1)}{2L} \end{aligned} \tag{56}$$

Of course $T_0 = 1$. Finally, the probability that a particle hits for the first time a trap at the nth step, given that it was next to a trap at time $n=0$, is

$$\begin{aligned} t_n &= \tfrac{1}{2} p_{n-1}(1 \mid 1) + \tfrac{1}{2} p_{n-1}(L-1 \mid 1) \\ &= T_{n-1} - T_n; \qquad t_0 = 0 \end{aligned} \tag{57}$$

The probability for surviving j visits to a trap is

$$F_j = (1-\alpha)^j \tag{58}$$

With these quantities the probability for survival after having made the nth step can be expressed as

$$\begin{aligned} \Omega_n = S_n &+ F_1 \sum_{j=0}^{n} s_j T_{n-j} + F_2 \sum_{l=0}^{n} \sum_{j=0}^{l} s_j t_{l-j} T_{n-l} + F_3 \\ &\times \sum_{k=0}^{n} \sum_{l=0}^{k} \sum_{j=0}^{l} s_j t_{l-j} t_{k-l} T_{n-k} + \cdots \end{aligned} \tag{59}$$

The first term describes particles which did not hit a trap; the second describes random walkers which hit a trap on the jth step without being absorbed; in the third term two visits to a trap have been made, etc. Further terms describe random walks which have made repeated visits to the traps without being absorbed. We introduce the generating function

$\Omega(z)=\sum_{n=0}^{\infty}\Omega_n z^n$ and similarly for $S(z)$, $s(z)$, $T(z)$, and $t(z)$. Further, we define

$$F(z)=\sum_{n=1}^{\infty} F_n z^{n-1} \tag{60}$$

From this it follows that

$$\Omega(z)=S(z)+s(z)\cdot T(z)\cdot F(t(z)) \tag{61}$$

Equations (55) and (57) become

$$\begin{aligned} s(z)&=1-(1-z)\,S(z)\\ t(z)&=1-(1-z)\,T(z) \end{aligned} \tag{62}$$

and

$$F(t(z))=\frac{\gamma}{1+\gamma(1-z)\,T(z)} \qquad \left(\gamma=\frac{1-\alpha}{\alpha}\right) \tag{63}$$

Inserting this into (61), one gets the final result for the generating function of the survival probability for a particle in an interval with $L-1$ trap-free sites,

$$\Omega(z)=\frac{S(z)+\gamma T(z)}{1+\gamma(1-z)\,T(z)} \tag{64}$$

We are interested in the dominant long-time behavior of Ω_n. Hence we can set $j=0$ in (54) and (56). The dominant behavior is

$$S(z)=\frac{8L}{\pi^2(L-1)}\frac{1}{1-z\rho}, \qquad T(z)=\frac{4}{L}\frac{1}{1-z\rho} \tag{65}$$

where

$$\rho=\cos\frac{\pi}{L} \tag{66}$$

The leading singularity of $\Omega(z)$ is found to be

$$\Omega(z)=\left(\frac{8}{\pi^2}\frac{L}{L-1}+\frac{4\gamma}{L}\right)\left[\left(1+\frac{4\gamma}{L}\right)(1-z\rho')\right]^{-1} \tag{67}$$

where

$$\rho'=\left(\rho+\frac{4\gamma}{L}\right)\left(1+\frac{4\gamma}{L}\right)^{-1} \tag{68}$$

Hence the leading long-time survival probability for a particle starting in the interval under consideration is

$$\Omega_n = (\rho')^n \left(\frac{8}{\pi^2}\frac{L}{L-1} + \frac{4\gamma}{L}\right)\left(1 + \frac{4\gamma}{L}\right)^{-1} \tag{69}$$

This result has to be averaged over the interval lengths L with weight $(1-p)^2 p^{L-1}$. At time zero each nontrapping site contains a particle. Hence our interval initially has $L-1$ particles and the survival probability is given by

$$\Psi_n = \sum_{L=2}^{\infty} (1-p)^2 p^{L-1}(L-1)\Omega_n(L) \Big/ \sum_{L=2}^{\infty} (1-p)^2 p^{L-1}(L-1) \tag{70}$$

Apart from exponentially small terms in n (generated, e.g., by the Euler–Maclaurin summation formula), the sum in the nominator may be replaced by an integral. One needs the asymptotic behavior for large L and n,

$$\Omega_n \simeq \frac{1}{L-1}\left[\frac{8}{\pi^2} L + 4\gamma\left(1 - \frac{8}{\pi^2}\right) + O(L^{-1})\right] \exp\left[-\frac{\pi^2 n}{2L^2} + h(L)\right] \tag{71}$$

where

$$h(L) = 2\gamma\pi^2 \frac{n}{L^3} - \left(\frac{\pi^4}{12} + 8\gamma^2\pi^2\right)\frac{n}{L^4} + O(nL^{-5}) \tag{72}$$

This results in the expression

$$\Psi_n \simeq \frac{(1-p)^2}{p^2}\int_0^{\infty} dL\left[\frac{8}{\pi^2} L + 4\gamma\left(1 - \frac{8}{\pi^2}\right)\right] \times \exp\left[-\lambda L - \frac{\pi^2 n}{2L^2} + h(L)\right] \tag{73}$$

Performing the integral by saddle point methods, we obtain the final expression

$$\Psi_n \simeq p^{-2\gamma}\left(\frac{1-p}{p \ln p}\right)^2 \frac{8}{\pi}\left(\frac{2x^3}{3\pi}\right)^{1/2} e^{-3x/2} \times \left\{1 + \left[\frac{17}{18} - \frac{(\pi\gamma)^2}{12} - \gamma\lambda\left(10 - \frac{\pi^2}{2} + 8\gamma\lambda\right)\right]\frac{1}{x} + O(x^{-2})\right\} \tag{74}$$

where

$$\gamma = \frac{1-\alpha}{\alpha}, \qquad \lambda = -\ln p \tag{75}$$

This result can be compared with the expression (36) for the case where traps do not reflect particles. First, (74) has an extra factor $1/p$. This increase of survival probability is due to different initial conditions. Indeed, in Section 3 we allow particles to start at trapping sites. However, these particles surely get trapped on the time scale considered. Hence they do not contribute to the *number* of surviving particles, and their initial presence lowers the *probability* of survival by the factor p. Second, the role of f_0 in (36) is played by

$$f_0 = p^{-(1-\alpha)/\alpha} \tag{76}$$

As expected from previous section, f_0 goes to unity in the limit $\alpha \to 1$ or perfect trapping and in the limit $p \to 1$ of a small fraction of traps. We can also check (76) in the limit $p \to 0$. The idea is to consider the system of previous sections with imperfect, nonreflecting traps. For small p, a large, trap-free region will mainly lie in a sea of trapping sites. Particles which enter the left or the right trapping region will either be absorbed by a trap or escape and come back to the same trap-free region. On the time scale that we are interested in, this mechanism can be described by effective traps at the endpoints of the trap-free regions that either absorb or reflect particles. In order to calculate the effective reflection rate, we have to solve the master equation (3) for the case $v_r = a/(2\tau)$ for $-\infty \leqslant r \leqslant 0$ and $v_r = 0$ else. For $r \leqslant 0$ we can set the time derivative equal to zero, and find

$$p(r) = p(1) e^{-\mu(1-r)} \qquad (r \leqslant 0) \tag{77}$$

where

$$e^{-\mu} = 1 + \frac{a}{2} - \left(a + \frac{a^2}{4}\right)^{1/2} \tag{78}$$

In particular, it follows that $p(0) = p(1) e^{-\mu}$. This has to be inserted in Eq. (3) for $r = 1$, from which it is seen that $e^{-\mu}$ plays the role of the reflection coefficient $1 - \alpha$. Combining (78) and (76), we find

$$f_0 = p^{\bar{v}}, \qquad \bar{v} = \frac{1}{2}\left[1 - \left(\frac{a+4}{a}\right)^{1/2}\right] \qquad (p \to 0) \tag{79}$$

The very same result was derived in refs. 8 and 9 for binary harmonic chains with masses taking the values 1 or M; according to (24), M should be identified with $1 + a/4$. The approach in refs. 8 and 9 involved analysis of the Dyson–Schmidt equation. We conclude that (76) is confirmed in the limit $p \to 0$ through an analogy with results for nonreflecting imperfect traps.

We can now compare our calculations with those of Weiss and Havlin.[7] First, they inserted a factor L instead of $L-1$ in Eq. (70). Second, the asymptotic expressions for $S(z)$ and $T(z)$ deviate from (65). However, these effects do not change the leading behavior of Ψ_n. Weiss and Havlin made a continuum approximation, where it is assumed that p is close to unity, and changed the sum over L into an integral in a way different from ours. This replaces our prefactor $[(1-p)/(p \ln p)]^2$ in (74) by unity, which is exact for $p=1$. The main point, however, is that the correction $h(L)$ of (71) was omitted. Indeed, its leading saddle point value $2\gamma\pi^2 n/L^3$ equals $2\gamma\lambda$ and brings the prefactor $f_0^2 = p^{-2\gamma}$ when traps are not perfect. Weiss and Havlin made the approximation $\rho' = \rho$ in (68) and therefore missed this factor. This led them to the conclusion that the long-time survival probability remains unchanged when traps become imperfect. Our result (74), however, has a large prefactor $p^{2-2/\alpha}$ when α is small. Since the survival probability cannot exceed unity, this means that for smaller and smaller trapping rate α the stretched exponential decay sets in at later and later times.

6. SUMMARY

In the present paper we have performed a detailed analysis of a system where particles perform a random walk on discrete sites of a line, where a fraction $1-p$ of sites contains an imperfect trap. Our main interest is the long-time behavior of the return and survival probability. To obtain these quantities, we used results by Nieuwenhuizen and Luck[8,9] on Lifshitz tails in the spectral density of harmonic chains with random masses. This leads, e.g., to a scaling form for the probability of displacement over a long distance for long times. It is shown that, if traps are not perfect, there is an enhancement factor f_0^2 in the long-time survival and return probability. This factor has been calculated for the case that trapping strengths are drawn from an exponential distribution (see ref. 8, Fig. 2). In the present work it is determined for identical imperfect traps.

We also consider a model where particles are either absorbed or reflected by traps. It was introduced by Weiss and Havlin[7] and is exactly solvable. In contradiction to these authors, we again find an enhancement of the survival probability when traps are not perfect. We argue that for a small fraction of trap-free sites, the long-time survival probability of this and of the previous system should become equivalent. This is indeed confirmed by our calculations.

We wish to stress that only in the one-dimensional situation does the effect of imperfect trapping on the long-time survival probability show up as a simple prefactor. In dimensions larger than two, particles may never return to a trap that has been visited. Indeed, the escape probability enters the result derived for a three-dimensional simple cubic lattice with a small concentration with imperfect traps.[6] It seems that the two-dimensional case is the most subtle one; results on this problem would be most welcome.

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