Random Walk in a Random Multiplicative Environment

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We investigate the dynamics of a random walk in a random multiplicative medium. This results in a random, but correlated, multiplicative process for the spatial distribution of random walkers. We show how the details of these correlations determine the asymptotic properties of the walk, i.e., the central limit theorem does not apply to these multiplicative processes. We also study a periodic source–trap medium in which a unit cell contains one source, followed by L-1 traps. We calculate the asymptotic behavior of the number of particles, and determine the conditions for which there is growth or decay in this average number. Finally, we discuss the asymptotic behavior of a random walk in the presence of randomly distributed, partially-absoprbing traps. For this case, a temporal regime of purely exponential decay of the density can occur, before the asymptotic stretched exponential decay, $\exp(-at^{1/3})$, sets in.

KEY WORDS: Random walk; randcom multiplicative process; sources and traps.

1. INTRODUCTION

The problem of a random walk moving in an environment containing static traps has been extensively studied. (1-10) Situations such as a single trap, (1-3) a periodic, (4) or a random distribution of traps, (5-8) as well as a distribution of trap strengths, (9,10) have been considered. A relatively good understanding of the rate at which the density of random walkers decays in such media has now emerged.

In this paper, we study the dynamics of a discrete random walker on a one-dimensional lattice in which traps and sources are present. In our

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model, each time a random walk A visits a defect B (a trap or source), the reaction⁽³⁾

$$A + B \to (1 + \varepsilon)A + B \tag{1.1}$$

takes place. That is, the defect is unaltered, while the random walker is "multiplied" by a factor $1+\varepsilon$. For $\varepsilon>0$, the ε new walkers are spawned when a particle meets the source, while if $-1\leqslant \varepsilon<0$, the defect is a trap, and the incident walker is partially absorbed for $\varepsilon>-1$, or totally absorbed, when $\varepsilon=-1$. Equivalently, one can consider the *mass* of the particle, rather than the number of particles, being multiplied by a factor of $1+\varepsilon$ upon each visit to the defect. Then the relevant dynamical quantity is the mass of a *single* random walker as it through the medium. It is worth emphasizing that these two descriptions for the manifestation of the defect can be easily shown to be mathematically equivalent when one averages over all configurations of the random walk.

For even the simplest cases, such as one trap and one source, or for a periodic distribution of traps and sources, the walker visits each of the defects at random. Thus, the number of random walkers undergoes a multiplicative process, but one which is not entirely random because of the correlations between successive visits of the walker to the defects. We shall discuss the conditions that give rise to the growth or decay of the average number of particles and elucidate the role of correlations in determining the asymptotic behavior of this type of multiplicative process. Potential applications of our model include understanding the role of correlations in random multiplicative processes and also for providing an idealized description of the number of neutrons in a radioactive material, where radioactive nuclei (sources) produce additional neutrons, while the moderator (traps) absorb neutrons. Within a continuum description, the particle density obeys the reaction-diffusion equation

$$\frac{\partial \rho(x,t)}{\partial t} = D\nabla^2 \rho(x,t) + \eta(x) \,\rho(x,t) \tag{1.2}$$

where $\eta(x)$ represents a source or trap, respectively, when $\eta(x) \ge 0$.⁽¹¹⁻¹⁵⁾ This model is related to directed self-avoiding walks in random media⁽¹⁶⁾ and to interfaces in Ising spin systems in two dimensions,⁽¹⁷⁾ and by a particular nonlinear transformation can be mapped to the Burger's equation in the presence of a random force.⁽¹⁸⁾

This paper is organized as follows. In Section 2, we outline some basic facts about random multiplicative processes in order to motivate the correlated multiplicative process induced by a random walk moving in a source—trap environment. We present a generating function solution for

the distribution of random walkers in the presence of a single defect (source or trap) in Section 3. Explicit expressions for the number of random walkers and their spatial distribution are given. In Section 4, we consider a source-trap dipole, and derive the condition for the average particle number to diverge or converge. Some of these results have been given previously, but the present treatment is more complete. We also compare the dynamics of a random walk with a purely random multiplicative process to understand how correlations affect asymptotic properties. In Section 5, we study a random walk in a periodic distribution of defects. We derive a formal solution for the average number of particles, and write the general condition for the particle number to reach a steady state. We also provide a recipe for coarse-graining a periodic source-trap medium into an effective homogeneous medium. In Section 6, we exploit this recipe to obtain the survival probability of a random walk moving in a random distribution of partially-absorbing traps. We find pure exponential decay at short times, crossing over to stretched exponential decay asymptotically, with the crossover time depending on the trap strength. We conclude in Section 7.

2. RANDOM MULTIPLICATIVE PROCESS

To motivate studying a random walk in a multiplicative environment, consider first the problem of calculating the average of a product of random variables. (11,19,20) As a specific example, suppose that the numbers $1 + \varepsilon_1 = 2$ and $1 + \varepsilon_2 = 1/2$ appear with equal probability in a product of N factors. Typically there will appear an equal number of 2's and 1/2's, so that the most probable value of the product \mathcal{N}_{mp} equals 1. However, the average value $\langle \mathcal{N} \rangle_N$ is

$$\langle \mathcal{N} \rangle_{N} = \frac{1}{2^{N}} \sum_{m=0}^{N} {N \choose m} 2^{m} (1/2)^{N-m}$$

$$= \left(\frac{2+1/2}{2}\right)^{N} = \left(\frac{5}{4}\right)^{N} \tag{2.1}$$

Thus, the mean value and the typical value of the product are very different as $N \to \infty$. More generally, for a process in which the factors 1/2 and 2 occur with probabilities p and 1-p, respectively, then

$$\langle \mathcal{N} \rangle_N = \sum_{m=0}^N \binom{N}{m} 2^m (1/2)^{N-m} p^m (1-p)^{N-m}$$

= $[2p + (1-p)/2]^N$ (2.2)

The essential reason for the disparity between $\langle \mathcal{N} \rangle_N$ and \mathcal{N}_{mp} is the relatively important role played by rare events. For example, a sequence consisting entirely of 2's occurs with an exponentially small probability, but the value of this product is exponentially large. This extreme event makes a finite contribution to $\langle \mathcal{N} \rangle_N$ and a dominant contribution to the higher moments of the product. The predominance of rare events means that numerical simulations of random multiplicative processes will generally yield the most probable value of an observable. (19)

An intriguing feature of this random multiplicative process is the sensitivity of $\langle \mathcal{N} \rangle_N$ to short-range correlations in the sequence of variables that are being multiplied. As an example, suppose that there are "no immediate reversals" in the sequence of factors. That is, when a 2 first appears in the sequence, the next $\mathcal{L}-1$ elements must also be a 2. Only after the \mathcal{L} th appearance of a 2 does the sequences become uncorrelated again. This \mathcal{L} th-neighbor correlation is equivalent to replacing the sequence of N correlated variables, which may either 2 or 1/2, by a sequence of N/\mathcal{L} independent variables, which may be either $2^{\mathcal{L}}$ or $(1/2)^{\mathcal{L}}$. For this correlated sequence,

$$\langle \mathcal{N} \rangle_N = \left[\frac{2^{\mathcal{L}} + (1/2)^{\mathcal{L}}}{2} \right]^{N/\mathcal{L}} \geqslant \left(\frac{5}{4} \right)^N \quad \text{as} \quad N \to \infty$$
 (2.3)

The larger value of $\langle \mathcal{N} \rangle_N$ compared to the uncorrelated process arises because rare events play an increasingly larger role as \mathcal{L} increases. As $\mathcal{L} \to N$, the possibility of a product containing only 2's becomes increasingly likely, and this event will dominate in the average value. This simple result shows that there is no analog of a central limit theorem for this type of correlated multiplicative process.

For a diffusing particle moving in a medium containing sources of strength $\sigma=1+\varepsilon_1$ and traps of strength $\tau=1+\varepsilon_2$, the temporal sequence of σ 's and τ 's will be correlated, reflecting the propensity for the particle to revisit a particular defect before visiting other defects. These correlations in the first passage probability become stronger as the spatial dimension is decreased, and enhance the probability of rare events relative to the uncorrelated process. In the remainder of this paper, we will attempt to elucidate the role of these correlations in governing the asymptotic properties of a random walk in a source-trap environment.

3. RANDOM WALK IN THE PRESENCE OF A SINGLE DEFECT

We begin by deriving a generating function solution for the temporal behavior of a random walk moving on a one-dimensional chain with a single defect located at the origin. Following ref. 3, we define $P_n(r)$ to be the probability that a pure random walk is at position r on the nth step if it starts at the origin. Similarly, we define $Q_n(r)$ to be the expectation value for the total number of particles, or equivalently, the mass at position r on the nth step, when the particle starts at the origin. We also define the Fourier transforms and the corresponding generating functions,

$$Q(z,r) = \sum_{n=0}^{\infty} Q_n(r) z^n$$
(3.1a)

$$\widetilde{Q}_n(k) = \sum_{r = -\infty}^{\infty} Q_n(r)e^{ikr}$$
(3.1b)

$$\widetilde{Q}(z,k) = \sum_{r=-\infty}^{\infty} Q(z,r)e^{ikr}$$
(3.1c)

and similarly for $P_n(r)$. By the construction of the single source process, $Q_n(r)$ can be written in the convolution form⁽³⁾

$$Q_n(r) = P_n(r) + \alpha \sum_{j=0}^{n} Q_j(0) P_{n-j}(r)$$
(3.2)

where $\alpha \equiv \varepsilon/(1+\varepsilon)$. In terms of the generating functions, this may be solved for both Q(z, r) and Q(z, 0) to yield

$$Q(z, r) = \frac{P(z, r)}{1 - \alpha P(z, 0)}$$
(3.3a)

or, in terms of the Fourier transform,

$$\tilde{Q}(z,k) = \tilde{P}(z,k) \frac{(1-z^2)^{1/2}}{(1-z^2)^{1/2} - \alpha} \equiv \tilde{P}(z,k) F(z)$$
 (3.3b)

where $\tilde{P}(z, k) = (1 - z \cos k)^{-1}$ is the propagator for the one-dimensional symmetric random walk. Thus, for a defect at the origin, $\tilde{P}(z, k)$ is "dressed" by the function F(z).

The dependence of the average number of walkers on n can be computed by inverting the generating function $\tilde{Q}(z, k)$ at k = 0. To accomplish this, we denote the Taylor expansion of F(z) by

$$F(z) = \sum_{n=0}^{\infty} f_n z^n \tag{3.4}$$

and by straightforward expansion of the square root, we obtain

$$f_{2m} = \frac{\alpha(1+\alpha)}{(1-\alpha^2)^{m+1}} - \sum_{n=1}^{m} \frac{(2n-3)!!}{2^n n!} \frac{\alpha}{(1-\alpha^2)^{m-n+1}}, \qquad m \geqslant 1 \quad (3.5)$$

where we use $(-1)!! \equiv 1$, and $f_0 = 1 + \varepsilon$. Noticed that F(z) is an even function of z, corresponding to the fact that a random walk can visit the defect only every other step. Consequently, the average number of particles in the system at the 2mth step is $\mathcal{Q}_{2m} \equiv \sum_r Q_{2m}(r) = \mathcal{Q}_{2m+1}$, i.e., \mathcal{Q}_n changes only every second step.

To obtain the asymptotic behavior of the number of particles, we require the large-m behavior of f_{2m} . When the defect is a source, there is a simple pole in F(z) at $z_c = (1 - \alpha^2)^{1/2} < 1$, while if the defect is a trap, F(z) has a branch point singularity at $z_c = 1$. Exploiting a Tauberian theorem, f(z) we then find

$$\mathcal{Q}_{2n} = \sum_{m=0}^{n} f_{2m} \sim \begin{cases} \frac{2}{(1-\alpha^2)^{n+1}}, & \alpha > 0 \text{ (source)} \\ \frac{2}{|\alpha| (\pi n)^{1/2}}, & \alpha < 0 \text{ (trap)} \end{cases}$$
(3.6)

Therefore, in the presence of a single source, the average number of particles diverges exponentially with n, whereas it decays as $1/\sqrt{n}$ for a trap (Fig. 1). In this sense, the effect of a single source is "stronger" than that of a single trap on the time dependence of the total number of particles.

To obtain the moments of the displacement distribution, we use the fact that for a pure random walk

$$\langle r(n)^{2m} \rangle = \frac{\partial^{2m} \tilde{P}_n(k)}{\partial (ik)^{2m}} \bigg|_{k=0} \xrightarrow{n \to \infty} \frac{(2m)!}{2^m m!} \langle r(n)^2 \rangle^m$$
$$= \frac{(2m)!}{2^m m!} n^m \tag{3.7}$$

Here $\langle r(n)^{2m} \rangle$ denotes the average of the 2mth power of the displacement after n steps. (Odd moments are zero, by symmetry.) For the single-defect problem, the convolution form of the generating function, Eq. (3.2), immediately leads to the following expression for the moments of the displacement:

$$\langle r(n)^{2m} \rangle = \frac{1}{\widetilde{Q}_n(k)} \frac{\partial^{2m} \widetilde{Q}_n(k)}{\partial (ik)^{2m}} \bigg|_{k=0} = \frac{\sum_{l=0}^n f_l \langle r(n-l)^{2m} \rangle}{\sum_{l=0}^n f_l}$$
(3.8)

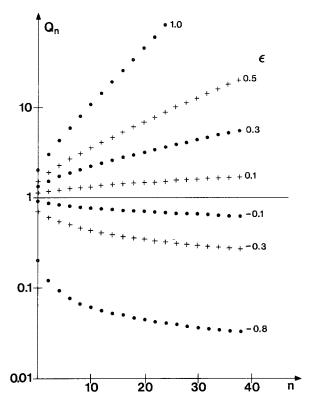


Fig. 1. Behavior of Q_{2n} as a function of the number of steps n for various values of the defect strength ε . The data are plotted on a semilogarithmic scale, for which Eq. (3.6) predicts a linear behavior for the case $\varepsilon > 0$.

Note that these moments are defined with respect to the walkers which survive. For the second moment, we exploit the properties of the \mathcal{Q}_n given in Eq. (3.6) to obtain the simpler form

$$\langle r(n)^2 \rangle = \frac{\sum_{m=0}^{n} Q_m}{Q_n} \sim \begin{cases} [2(1-\alpha^2)/\alpha^2][1-(1-\alpha^2)^{n/2}] & \text{source} \\ 2n & \text{trap} \end{cases}$$
 (3.9)

Thus, for a single source, the mean-square displacement converges exponentially to a finite limit whose value depends on the source strength. A random walk is localized about the source with a localization length that diverges when $\varepsilon \to 0^+$. For a trap, $\langle r(n)^2 \rangle$ grows linearly in n, but with an amplitude that is twice that of the pure random walk, *independent* of the strength of the trap (Fig. 2). The increased amplitude follows from the fact that walkers which wander further away from the origin are less likely to

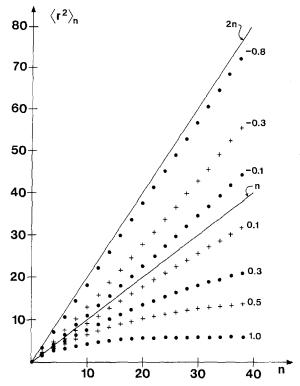


Fig. 2. Plot of the mean-square displacement $\langle r(n)^2 \rangle$ for a random walk which starts at the defect site, as a function of the number of steps n, for various values of ε . Notice that $\langle r(n)^2 \rangle$ saturates at a finite ε -dependent value when the defect is a source, and that $\langle r(n)^2 \rangle \sim 2n$, independent of ε , when the defect is a trap. As a guide to the eye, straight lines having slopes of 1 and 2 are also plotted.

be absorbed, but the independence on the trap strength follows from the recurrence of the random walk. If a walk hits the origin once, it will hit an infinite number of times and eventually be absorbed. Therefore the mean-square displacement is governed, asymptotically, by walks which never hit the origin. It is also worth noting that pure random walk behavior cannot be recovered by merely taking the limit of $\alpha \to 0$ in Eqs. (3.6) and (3.9).

4. RANDOM WALK IN THE PRESENCE OF A "DIPOLE"

To illustrate the competing effects of traps and sources, consider a random walker on a line containing two defects, with weights ε_1 and ε_2 , which are separated by a distance L (Fig. 3). The dynamics of the spatial

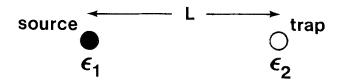


Fig. 3. A source-trap dipole.

distribution of random walks can be obtained by generating function methods. (3,22) A formal solution was given by Eq. (9) of ref, 3, and by explicitly writing out this formula, we obtain for the generating function for the average number of walkers $Q(z) = \sum_{r} Q(z, r)$,

$$Q(z) = \frac{1}{1-z} \left\{ 1 + \frac{(\alpha_1 + \alpha_2) \zeta^{L/2} / (1-z^2)^{1/2} + 2[\alpha_1 \alpha_2 / (1-z^2)](\zeta^{3L/2} - \zeta^{L/2})}{1 - (\alpha_1 + \alpha_2) / (1-z^2)^{1/2} + \alpha_1 \alpha_2 (1-\zeta^{2L}) / (1-z^2)} \right\}$$
(4.1)

where $\zeta = [1 - (1 - z^2)^{1/2}]/z$. If Q(z) has a simple pole at a value $z_c < 1$, then the average number of particles at the *n*th step, \mathcal{Q}_n , diverges as z_c^{-n} . The location of such a pole is determined by the condition

$$(1-z^2) - (\alpha_1 + \alpha_2)(1-z^2)^{1/2} + \alpha_1 \alpha_2(1-\zeta^{2L}) = 0$$
 (4.2)

To determine whether this equation has a solution, it is useful to write $\sin \theta = (1 - z^2)^{1/2}$, which then gives $\zeta = [(1 - \sin \theta)/(1 + \sin \theta)]^{1/2}$. Now Eq. (4.2) becomes

$$(\sin \theta - \alpha_1)(\sin \theta - \alpha_2) = \alpha_1 \alpha_2 \left(\frac{1 - \sin \theta}{1 + \sin \theta}\right)^L \tag{4.3}$$

and this can be solved graphically (Fig. 4).

Three cases arise. If both defects are traps, then $\alpha_i < 0$, so that Eq. (4.2) has no zeros in the interval (0, 1), and the square-root singularity in the numerator of Q(z) leads to the average number of particles decaying algebraically in n. A second case is that both defects are sources. Then $\alpha_i > 0$, and there always exists either one or two zeros of Eq. (4.2) in (0, 1). The smaller of the two zeros satisfies the condition $z_c < (1 - \max\{\alpha_1^2, \alpha_2^2\})^{1/2}$, so that the divergence of \mathcal{Q}_n is faster than that due to either of the two sources alone.

The interesting case is that of a "dipole" consisting of a source, with $\alpha_1 > 0$, and a trap, with $\alpha_2 < 0$. By comparing the slopes of each side of Eq. (4.3) at $\sin \theta = 0$, one finds that a solution exists in (0, 1) only for $L > L_c$, with

$$L_c = \frac{1}{2} \left(\frac{1}{\alpha_1} + \frac{1}{\alpha_2} \right) \tag{4.4}$$

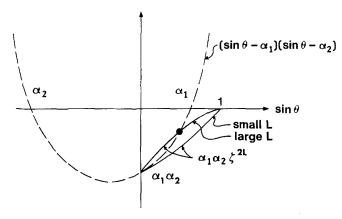


Fig. 4. Illustration of the graphical solution to Eq. (4.3), which describes the behavior of a random walk in the presence of a source-trap dipole. The dashed parabola $(\sin \theta - \alpha_1)(\sin \theta - \alpha_2)$ intersects the solid curve $\alpha_1 \alpha_2 \zeta^{2L}$ at the dot only for sufficiently large L.

This gives a "phase boundary" that delineates between trap-dominated and source-dominated dipoles (Fig. 5). Exponential growth of \mathcal{Q}_n occurs for $L > L_c$, and algebraic decay occurs in the opposite case. Notice that an infinitesimally weak source can dominate if L is sufficiently large, which stems from the recurrence of random walks.

We can now make contact with the random multiplicative process of Section 2. If the random walker is on the source, then it will take of the order of L^2 time steps to arrive for the first time at the trap, a distance L away. During this process, each of the L sites between the dipole, including the source, will be visited of the order of $L^2/L = L$ times. Thus, at a simpleminded level, the dynamics of a random walker in the presence of a dipole

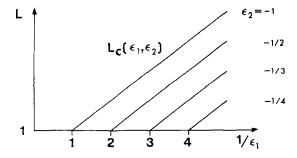


Fig. 5. "Phase diagram" of a random walk in the presence of a source-trap dipole for various values of ε_2 . For $L > L_c(\varepsilon_1, \varepsilon_2)$, the source dominates, and the number of random walkers diverges exponentially in time.

can be replaced by that of an uncorrelated random multiplicative process in which the factors in the product are the dipole and source strengths raised to the *L*th power. This defines the effective correlation range of the multiplicative process induced by the random walk as *L*.

For this L-correlated multiplicative process, the average value of the product of the factors $(1 + \varepsilon_1)$ or $(1 + \varepsilon_2)$ is, from Eq. (2.3),

$$\langle \mathcal{N} \rangle_N = \left\lceil \frac{(1+\varepsilon_1)^L + (1+\varepsilon_2)^L}{2} \right\rceil$$
 (4.5)

For fixed ε_1 and ε_2 , $\langle \mathcal{N} \rangle_N$ is an increasing function of N for sufficiently large L, even for ε_1 very close to zero, i.e., an infinitesimally weak source. Similar considerations suggest that the correlation range of the effective multiplicative process will be of order $\ln L$ for a dipole in two dimensions, and will be finite for higher dimensions.

5. PERIODIC DEFECT DISTRIBUTION

5.1. Generating Function Approach

Motivated by the fact that sources tend to dominate over traps, we now study a periodic system in which sources of strength ε_1 are located at r = nL, with $n = 0, \pm 1, \pm 2,...$, while traps of strength ε_2 occupy all of the remaining sites (Fig. 6). To obtain a formal solution for the distribution of particles, we start with the master equations for the evolution of the average number of particles at position r at the nth step

$$Q_n(r) = W(r-1 \to r) Q_{n-1}(r-1) + W(r+1 \to r) Q_{n-1}(r+1)$$
 (5.1)

For the period L system, the transition function, $W(r \pm 1 \rightarrow r)$, equals $(1 + \varepsilon_1)/2 \equiv \sigma/2$, or $(1 + \varepsilon_2)/2 \equiv \tau/2$, respectively, if r is at the location of a source or a trap. (The related problem of vibrations on this "generalized" diatomic chain was considered some time ago.⁽²³⁾)

It is convenient to classify sites according to their location in the period as sites (l), for r = l + mL, with m an arbitrary integer, and corre-



Fig. 6. The periodic distribution of sources and traps considered in the text. Shown is the case where L=4.

spondingly append the superscript (l) to $Q_n(r)$. The master equations then become

$$Q_{n}^{(0)}(r) = \frac{1}{2}\sigma[Q_{n-1}^{(L-1)}(r-1) + Q_{n-1}^{(1)}(r+1)]$$

$$Q_{n}^{(1)}(r) = \frac{1}{2}\tau[Q_{n-1}^{(0)}(r-1) + Q_{n-1}^{(2)}(r+1)]$$

$$\vdots$$

$$Q_{n}^{(L-1)}(r) = \frac{1}{2}\tau[Q_{n-1}^{(L-2)}(r-1) + Q_{n-1}^{(0)}(r+1)]$$
(5.2)

To solve these equations, we introduce the transform function

$$\tilde{Q}^{(l)}(z,k) = \sum_{n=0}^{\infty} \sum_{r \in (l)} Q_n^{(l)}(r) e^{ikr}$$
(5.3)

With the initial condition of a single particle located at the origin, $\tilde{Q}^{(l)}(z, k)$ is the solution of the matrix equation,

$$\widetilde{\mathbf{Q}} = (1 - \mathbf{M})^{-1} \begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix} \tag{5.4}$$

where $\tilde{\mathbf{Q}}$ is the column vector [omitting the arguments of $\tilde{\mathcal{Q}}^{(l)}(z,k)$]

$$\widetilde{\mathbf{Q}} = \begin{pmatrix} \widetilde{Q}^{(0)} \\ \widetilde{Q}^{(1)} \\ \vdots \\ \widetilde{O}^{(L-1)} \end{pmatrix}$$
 (5.5)

and M is the $L \times L$ matrix

$$\begin{pmatrix}
0 & \frac{1}{2}z\sigma e^{-ik} & 0 & \cdots & 0 & \frac{1}{2}z\sigma e^{ik} \\
\frac{1}{2}z\tau e^{ik} & 0 & \frac{1}{2}z\tau e^{-ik} & 0 & \cdots & 0 \\
0 & \frac{1}{2}z\tau e^{ik} & 0 & \frac{1}{2}z\tau e^{-ik} & \ddots & 0 \\
\vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & \frac{1}{2}z\tau e^{ik} & 0 & \frac{1}{2}z\tau e^{-ik} \\
\frac{1}{2}z\tau e^{-ik} & 0 & 0 & \cdots & \frac{1}{2}z\tau e^{ik} & 0
\end{pmatrix} (5.6)$$

As an illustrative example, consider the case L=3. Then the solution to Eqs. (5.4)–(5.6) yields

$$\tilde{Q}^{(0)} = \frac{1 - \frac{1}{4}z^{2}\tau^{2}}{1 - \frac{1}{2}z^{2}\sigma\tau - \frac{1}{2}z^{2}r^{2} - \frac{1}{4}z^{3}\sigma\tau^{2}\cos 3k}$$

$$\tilde{Q}^{(1)} = \tilde{Q}^{(2)} = \frac{\frac{1}{2}z\tau\cos k + \frac{1}{2}z^{2}\tau^{2}\cos 2k}{1 - \frac{1}{2}z^{2}\sigma\tau - \frac{1}{4}z^{2}\tau^{2} - \frac{1}{4}z^{3}\sigma\tau^{2}\cos 3k}$$
(5.7)

In particular, by setting k = 0 and $\sigma = \tau = 1$, these expressions reduce to the generating functions for the probability that a pure random walk occupies the set of (l) sites. Specifically, for the (0) sites, we find

$$\tilde{Q}^{(0)}(z, k=0; \sigma=\tau=1) = \frac{1-z^2/4}{1-3z^2/4-z^3/4}$$
 (5.8)

and the *n*th term in the power series representation of the right-hand side yields the probability that a pure random walk, starting at the origin, occupies the set of sites r = 3j, with j an arbitrary integer, at the nth step.

While the complete solution for arbitrary period is unwieldy, the condition for the average number of particles to reach a steady state can be analyzed in detail. A steady state occurs when the generating function is singular at $z_c = 1$, and this, in turn, is equivalent to the vanishing of the following determinant, when $\lambda = 1$ and k = 0:

$$\mathcal{D}_{L}(\lambda) = \begin{vmatrix} -\lambda & a' & 0 & \cdots & 0 & a \\ b & -\lambda & b' & 0 & \cdots & 0 \\ 0 & b & -\lambda & b' & \cdots & 0 \\ \vdots & \vdots & & \ddots & \ddots & \vdots \\ \vdots & \vdots & & b & -\lambda & b' \\ b' & 0 & 0 & \cdots & b & -\lambda \end{vmatrix}_{L \times L}$$
(5.9)

where a, $a' = \frac{1}{2}\sigma e^{\pm ik}$ and b, $b' = \frac{1}{2}\tau e^{\pm ik}$. To solve this, define

$$D_{L}(\lambda) = \begin{vmatrix} -\lambda & b' & 0 & \cdots & 0 & 0 \\ b & -\lambda & b' & 0 & \cdots & 0 \\ 0 & b & -\lambda & b' & \cdots & 0 \\ \vdots & \vdots & & \ddots & \ddots & \vdots \\ \vdots & \vdots & & b & -\lambda & b' \\ 0 & 0 & 0 & \cdots & b & -\lambda \end{vmatrix}_{L \times L}$$
(5.10)

The determinant $\mathcal{D}_L(\lambda)$ obeys the recursion relation

$$\mathcal{D}_{L}(\lambda) = -\lambda D_{L-1}(\lambda) - (a'b + ab') D_{L-2}(\lambda) + (-1)^{n-1} (a'b'^{n-1} + ab^{n-1})$$
(5.11)

while $D_L(\lambda)$ has the explicit solution (see, e.g., ref. 24)

$$D_L(\lambda) = c_1 \gamma_1^{n-1} + c_2 \gamma_2^{n-1}$$
 (5.12a)

where

$$\gamma_{1,2} = \frac{-\lambda \pm (\lambda^2 - 4bb')^{1/2}}{2}, \qquad c_{1,2} = -\frac{\lambda}{2} \pm \frac{\lambda^2 - 2b^2}{2(\lambda^2 - 4bb')^{1/2}}$$
 (5.12b)

The results for $c_{1,2}$ are based on the initial conditions $D_1(\lambda) = -\lambda$ and $D_2(\lambda) = \lambda^2 - bb'$. Using this result for $D_L(\lambda)$, the condition for a steady state, $\mathcal{D}_L(\lambda = 1) = 0$, gives the "balance" condition

$$\begin{split} \sigma_{\text{balance}}(L) &= \left\{ \left[1 + (1 - \tau^2)^{1/2} \right]^L - \left[1 - (1 - \tau^2)^{1/2} \right]^L \right\} \\ &\quad \times \left(\tau \left\{ \left[1 + (1 - \tau^2)^{1/2} \right]^{L-1} - \left[1 - (1 - \tau^2)^{1/2} \right]^{L-1} \right. \\ &\quad + 2\tau^{L-2} (1 - \tau^2)^{1/2} \right\} \right)^{-1} \end{split} \tag{5.13}$$

Thus, when $\sigma = \sigma_{\text{balance}}(L)$, the average number of particles in the system remains constant at long times.

Equation (5.13) can be simplified by substituting $\cos 2\theta = (1 - \tau^2)^{1/2}$ to yield

$$\sigma_{\text{balance}}(L) = \frac{1 + x^L}{x(1 + x^{L-2})}$$
 (5.14)

where $x = \tan \theta = [1 - (1 - \tau^2)^{1/2}]/\tau$. The qualitative behavior of the

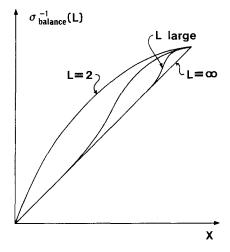


Fig. 7. A plot of the "balance" condition $\sigma_{\text{balance}}^{-1}(L)$ versus x for various values of L. Notice that $\sigma_{\text{balance}}^{-1}(L)$ converges to $\sigma_{\text{balance}}^{-1}(\infty)$ nonuniformly in L.

balance condition is shown in Fig. 7. We see that $\sigma_{\text{balance}}(L)$ converges non-uniformly to $\sigma_{\text{balance}}(\infty)$, where

$$\sigma_{\text{balance}}(\infty) = \frac{1}{x} = \frac{\tau}{1 - (1 - \tau^2)^{1/2}}$$
 (5.15)

Thus, a *single* source can dominate over a uniform background of traps provided that $\sigma > \sigma_{\rm balance}(\infty)$. On the other hand, for weak traps, $\tau = 1 - \delta$ (with $\delta L \ll 1$), the balance condition reduces to $\sigma \simeq 1 + (L-1)\delta$. This corresponds to writing the balance condition in terms of the typical event in which each site is equiprobably occupied, namely, $\sigma \tau^{L-1} = 1$.

5.2. Coarse-Graining Solution

Further insight into the periodic distribution can be gained by a coarse-graining approach, wherein the original random walk process is mapped onto a random walk only on the sublattice r=mL. In jumping between these sites, the average number of particles (or the mass of the walker) increases by a factor $\frac{1}{2}\langle \mathcal{N} \rangle_L$, and each jump requires an average time $\langle t \rangle_L$, where the average is taken over all walks in the ensemble. In this fashion the original problem is reformulated as a random walk in a uniform medium with defects of strength $\langle \mathcal{N} \rangle_L$ and a time rescaling factor of $\langle t \rangle_L$.

To calculate these quantities, we require the probability of getting from r=0 to r=L for the first time in n steps, Q(n;L), and the corresponding generating function

$$Q(z; L) = \sum_{n=0}^{\infty} Q(n; L) z^{n}$$
 (5.16)

In this section, we employ a slightly different notation for the Q's than what was used previously, to explicitly denote that we define the Q's for the interval 0 to L. In terms of this generating function,

$$\langle \mathcal{N} \rangle_L = 2 \sum_{n=0}^{\infty} Q(n; L) = 2Q(z; L) \Big|_{z=1}$$
 (5.17)

and

$$\langle t \rangle_L = \frac{\sum_{n=0}^{\infty} nQ(n;L)}{\sum_{n=0}^{\infty} Q(n;L)} = \frac{1}{Q(z;L)} \frac{\partial Q(z;L)}{\partial z} \bigg|_{z=1}$$
(5.18)

so that the initial terms in the power series for Q(z; L) can be represented as

$$Q(z;L) = \frac{1}{2} \langle \mathcal{N} \rangle_L \left[1 - \langle t \rangle_L (1-z) \right] + \mathcal{O}((1-z)^2)$$
 (5.19)

We now follow the approach of Goldhirsch and Gefen⁽²⁵⁾ and compute the generating function Q(z; L) in terms of

- (1) T(z; L), the generating function for leaving r = 0 and arriving at r = L, for the first time, without ever having returned to r = 0; and
- (2) R(z; L), the generating function for leaving r = 0 and returning to it for the first time, without having visited r = L. (The first step is assumed to have been taken to the right.) Our analysis is greatly simplified if T and R are defined on a lattice uniformly populated by defects of strength ε_2 .

Using the generating functions defined above and their usual property of transforming convolutions of the probability densities into simple multiplication, we obtain (omitting the arguments z and L, for simplicity)

$$Q = \left[1 + \left(2\frac{\sigma_1}{\sigma_2}R\right) + \left(2\frac{\sigma_1}{\sigma_2}R\right)^2 + \cdots\right]\frac{\sigma_1}{\sigma_2}T = \frac{\sigma_1T}{\sigma_2 - 2\sigma_1R}$$
 (5.20)

where $\sigma_{1,2} \equiv 1 + \varepsilon_{1,2}$. The term $[2(\sigma_1/\sigma_2)R]^n$ accounts for n returns to the origin, while the final transition to the point r = L is represented by $(\sigma_1/\sigma_2)T$. The prefactor σ_1/σ_2 accounts for the fact that Q(z;L) is defined on the period L chain of Fig. 6, while R(z;L) and T(z;L) are defined on the uniform chain of ε_2 defects.

In close analogy with ref. 24, the generating functions R(z; L) and T(z; L) obey the recursion relations

$$R(z; L) = \frac{(\frac{1}{2}\sigma_2 z)^2}{1 - R(z; L - 1)}$$
 (5.21a)

$$T(z; L)^{2} = \lceil R(z; L+1) - R(z; L) \rceil \lceil 1 - R(z; L) \rceil$$
 (5.21b)

Equation (5.21a) has the solution

$$R(z; L) = \left(\frac{1}{2}\sigma_2 z\right)^2 \frac{\lambda_1^{L-1} - \lambda_2^{L-1}}{\lambda_1^L - \lambda_2^L}$$
 (5.22a)

with

$$\lambda_{1,2} = \frac{1}{2} \left\{ 1 \pm \left[1 - (\sigma_2 z)^2 \right]^{1/2} \right\} \tag{5.22b}$$

Expanding Eqs. (5.20)–(5.22) about z = 1, one can now derive $\langle \mathcal{N} \rangle_L$ and $\langle t \rangle_L$.

We first specialize to the case of $\varepsilon_2 = 0$, that is, a chain with periodic defects of strength ε_1 placed a distance L apart. We then find

$$R(z;L) = \frac{L-1}{2L} - \frac{L^2 - 1}{3L} (1-z) + \mathcal{O}((1-z)^2)$$
 (5.23a)

$$T(z; L) = \frac{1}{2L} - \frac{L^2 + 2}{6L} (1 - z) + \mathcal{O}((1 - z)^2)$$
 (5.23b)

$$Q(z; L) = \frac{1}{2(1 - \alpha_1 L)} \times \left\{ 1 - \left[\frac{L^2 + 2}{3} + \frac{L^2 - 1}{3} \frac{2}{1 - \alpha_1 L} \right] (1 - z) \right\} + \mathcal{O}((1 - z)^2)$$
 (5.23c)

Using Eq. (5.19), the expressions for $\langle \mathcal{N} \rangle_L$ and $\langle t \rangle_L$ can now be immediately read off from (5.23c). Several cases are of interest:

- (a) Period L=1 (uniform chain of ε_1 defects). Substituting L=1 in Eq. (5.23c) correctly gives $\langle t \rangle_1 = 1$ and $\langle \mathcal{N} \rangle_1 = 1/(1-\alpha_1) = 1+\varepsilon_1$. This serves as a useful consistency check.
- (b) $\varepsilon_1 = 0$. This corresponds to a pure random walk, sampled at $\{r = mL \mid m = 0, \pm 1, \pm 2,...\}$. We find, as expected, $\langle \mathcal{N} \rangle_L = 1$, so that the number of walkers is constant, and $\langle t \rangle_L = L^2$, which is the first passage time between two sites a distance L apart.
- (c) $\varepsilon_1 > 0$ (periodic source distribution). We find $\langle \mathcal{N} \rangle_L = 1/(1-\alpha_1 L)$, which diverges for $L_c = 1/\alpha_1 = (1+\varepsilon_1)/\varepsilon_1$. Clearly, the expected number of particles increases between visits to adjacent sources, since a random walk recurs to a given source several times before reaching neighboring sources. The number of recurrences increases with separation L, until at $L = L_c$ the walker becomes infinitely multiplied and localized about the original source. Correspondingly, the first passage time for a jump to an adjacent source is larger than for the pure random walk model. For $L \ll L_c$, $\langle t \rangle_L \sim L^2 + \frac{2}{3}L(L^2-1)\alpha_1$, and $\langle t \rangle_L$ diverges when $L \to L_c^-$. These conclusions complement the results for a single source given in Section 3.
- (d) $\varepsilon_1 < 0$ (periodic distribution of traps). The expected number of particles between successive visits to adjacent traps decreases as $\langle \mathcal{N} \rangle_L = 1/(1+|\alpha_1|L)$. Also, $\langle t \rangle_L$ is decreased with respect to pure random walks, since walks that avoid recurring to the origin are not absorbed and outweigh slower recurring walks. From Eq. (5.23c), one has the asymptotic forms $\langle t \rangle_L \sim L^2 \frac{2}{3}L(L^2-1)|\alpha_1|$ for $L \leqslant 1/|\alpha_1|$, and $\langle t \rangle_L \sim \frac{1}{3}L^2$ for $L \gg 1/|\alpha_1|$.

We now turn to the general case of $\varepsilon_2 < 0$. A full analysis of Eqs. (5.20)–(5.22) becomes very tedious and unenlightening. However, in the limit $L \to \infty$ the analysis simplifies, and we find

$$\langle \mathcal{N} \rangle_L = \frac{2\sigma (1 - \tau^2)^{1/2}}{\tau - \sigma [1 - (1 - \tau^2)^{1/2}]} \left(\frac{\tau}{1 + (1 - \tau^2)^{1/2}} \right)^L$$
 (5.24)

Notice that by demanding $\langle \mathcal{N} \rangle_L = 1$, we recover the steady-state condition on $\sigma(\tau)$ given in Eq. (5.15).

We apply now these general conclusions in order to determine how to coarse grain a periodic chain of traps. That is, for chain A, with traps τ at sites $\{r = mL \mid m = 0, \pm 1, \pm 2,...\}$, we wish to find an equivalent uniform chain B with traps τ' on every site (Fig. 8). By the equivalence of A and B we mean that $\langle \mathcal{N} \rangle_L^{(A)} = \langle \mathcal{N} \rangle_L^{(B)}$, so that in the asymptotic limit the particle densities on the two chains decay at the same rate. For chain A we have [see case (d) of Eq. (5.23c)]

$$\langle \mathcal{N} \rangle_L^{(A)} = \frac{1}{1 + |(\tau - 1)/\tau|L} \tag{5.25}$$

For chain B, we first use the fact that $\langle \mathcal{N} \rangle_L = 2Q(1; L)$ from Eq. (5.19). Then from Eq. (5.20), we compute Q(1; L) for the case where $\sigma_1 = \sigma_2 = \tau'$. Finally, we substitute the expressions given in (5.21) and (5.22) for T(1; L) and R(1; L) to arrive at

$$\langle \mathcal{N} \rangle_L^{(B)} = 2 \frac{{\tau'}^L}{\Gamma 1 + (1 - {\tau'}^2)^{1/2} \Gamma^L + \Gamma 1 - (1 - {\tau'}^2)^{1/2} \Gamma^L}$$
 (5.26)

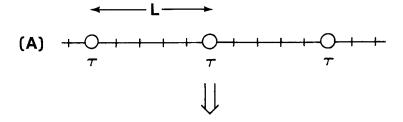




Fig. 8. Coarse graining of (A) a periodic chain of traps τ , which period L, into (B) a uniform chain of traps τ' .

Equating the two for the case of weak traps, we find the coarse-graining condition

$$\varepsilon' = \varepsilon/L + \mathcal{O}(L^{-3}) \tag{5.27}$$

This coarse-graining relation is used in the next section.

6. APPLICATION: RANDOMLY DISTRIBUTED, PARTIALLY ABSORBING TRAPS

As an application of coarse-graining, consider a random distribution of partially absorbing traps $(-1 < \varepsilon < 0)$ on a one-dimensional chain. The corresponding problem of perfect traps is exactly soluble, and the average number of particles decays as (5-8)

$$\langle \mathcal{N}(t) \rangle \sim \exp\left[-a(c^2t)^{1/3}\right]$$
 (6.1)

where a is a constant and c is the (small) trap concentration. The stretched exponential decay arises because of very large (but rare) trap-free regions that occur in a random distribution, in contrast with the purely exponential decay that occurs when the traps are *homogeneously* distributed.

For partially absorbing traps³ we develop an approximation which is based on properly averaging over rare events, together with the coarse-graining procedure of the previous section. Consider the trap-free interval (-L/2, L/2). When L is large, the random walk probability density $\rho(x, t)$ can be described by

$$\frac{\partial \rho(x,t)}{\partial t} = \frac{\partial^2 \rho(x,t)}{\partial x^2}, \qquad |x| < \frac{L}{2}$$
 (6.2a)

$$\frac{\partial \rho(x,t)}{\partial t} = \frac{\partial^2 \rho(x,t)}{\partial x^2} - \lambda^2 \rho(x,t), \qquad |x| > \frac{L}{2}$$
 (6.2b)

The term $-\lambda^2 \rho(x, t)$ in Eq. (6.2b) accounts for the absorption of the walker by the traps within a continuum description. We can estimate the value of λ^2 corresponding to partially absorbing traps by first approximating the region |x| > L/2 by a periodic chain of traps of strength ε and period L = 1/c. This region can then be coarse-grained using Eq. (5.27) to obtain a corresponding uniformly absorbing chain filled with traps of strength τ' . In the continuum limit $\tau' = \exp(-\lambda^2)$, so that

$$\lambda = \left[(1 - t)c \right]^{1/2} \tag{6.3}$$

³ See, however, ref. 26 for a derivation of the asymptotic behavior of the particle density for partially absorbing traps.

In the large-time limit, only the lowest eigenvalue solution of Eq. (6.2) is relevant. This is

$$\rho(x,t) = \begin{cases} A\cos(\omega^{1/2}x)e^{-\omega t}, & |x| < L/2\\ B\exp[-(\lambda^2 - \omega)^{1/2}|x|]e^{-\omega t}, & |x| > L/2 \end{cases}$$
(6.4)

where ω , the lowest eigenvalue, and A/B are determined from the continuity of ρ and $\partial \rho/\partial x$ at $x = \pm L/2$. We thus find the following condition for the lowest eigenvalue:

$$\cot \xi = \frac{\xi}{(\bar{\lambda}^2 - \xi^2)^{1/2}} \tag{6.5}$$

where $\xi \equiv \omega^{1/2} L/2$, and $\bar{\lambda} \equiv \lambda L/2$. Equation (6.5) can be solved graphically, and a zeroth-order estimate for the lowest eigenvalue ξ_0 is (Fig. 9)

$$\xi_0 \simeq \begin{cases} \bar{\lambda}, & \bar{\lambda} \ll 1\\ \pi/2, & \bar{\lambda} \gg 1 \end{cases} \tag{6.6}$$

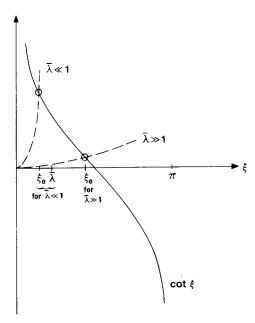


Fig. 9. Illustration of the graphical solution to Eq. (6.5). The right-hand side of this equation and the corresponding solutions to the equation are shown dashed for the two cases of $\bar{\lambda} \ll 1$ and $\bar{\lambda} \gg 1$.

The crossover between these two limits occurs for $\bar{\lambda} \simeq 1$, or $\lambda \simeq 1/L$. Thus, the time dependence of the particle density is

$$\rho(t) \simeq \begin{cases} e^{-\lambda^2 t}, & \lambda L \leqslant 1\\ e^{-\pi^2 t/L^2}, & \lambda L \gg 1 \end{cases}$$
(6.7)

Having found the survival probability of a particle in a trap-free interval of size L, the expected number of particles for a random trap distribution can be calculated by averaging $\rho_L(t)$ over all possible interval sizes. For a Poisson distribution, the probability of having a trap-free region of size L is $\rho(L) \propto e^{-cL}$. Then, by steepest descents, we find

$$\langle \mathcal{N}(t) \rangle \sim \int_0^\infty \rho_L(t) \ p(L) \ dL \sim \begin{cases} e^{-\lambda^2 t}, & \lambda L^* \leqslant 1 \\ e^{-\text{const.}(c^2 t)^{1/3}}, & \lambda L^* \geqslant 1 \end{cases}$$
 (6.8)

Here $L^* \sim (t/c)^{1/3}$ is the value of L at which the integrand achieves its maximum. Therefore, we find two regimes for the decay of $\langle \mathcal{N}(t) \rangle$. For early times, $t < t^*$, the decay is a pure exponential, as for a homogeneous distribution of traps, while for later times, $t > t^*$, the decay has the same functional form as for perfect traps, independent of the trap strength. The crossover time t^* depend on the trap strength and on concentration as

$$t^* = c/\lambda^3 \sim c^{-1/2} (1 - \tau)^{-3/2} \tag{6.9}$$

It should be emphasized that t^* gives the time scale beyond which partial traps appear to behave as perfect traps. This has no connection with the characteristic time that separates the $\exp(-t^{1/2})$ early time decay of the particle density from the asymptotic $\exp(-t^{1/3})$ decay in the case of randomly distributed *perfect* traps. Notice also that we have only given results for weak traps, i.e., $(1-\tau)/c^{1/2} \le 1$, since it is only in this case that there are two distinct times regimes, as expressed by Eq. (6.8).

7. DISCUSSION

We have studied the dynamics of a random walk moving in a onedimensional medium containing traps and sources. For a single source, the number of walkers (or the mass of a single walker) grows exponentially with time and the mean square displacement converges to a constant. For a single trap, the number of walkers decays as $n^{-1/2}$ and the mean square displacement grows asymptotically as 2n, twice as fast as for a random walker in a free environment.

For a source-trap "dipole," there may be either a trap-dominated algebraic decay or a source-dominated exponential growth of the number

of walkers, depending on the distance L between the two defects. In particular, a very weak source ultimately dominates over an arbitrarily strong trap if L is large enough. The dipole was also useful for elucidating the role of correlations in the multiplicative process governing the number of walkers induced by the successive visits of the walker to the same defect. We have shown that there is an equivalence between a random walker in the presence of a dipole of span L consisting of a source σ and a trap τ , and a random multiplication of the equiprobable factors σ^L and τ^L .

The role of rare events in determining the dynamics of a random walker was seen from our treatment of a periodic source-trap distribution. For a period-L chain consisting of a source followed by L-1 traps, the most probable number of random walks grows as $\sigma \tau^{(L-1)}$. Hence, we would expect that for $\sigma \sim 1/\tau^L$ there would be no change in the mass of the walker. However, from Eqs. (5.14)–(5.15) the condition for a stationary average number of walkers is $\sigma \sim 1/x \sim 1/\tau$ as $L \to \infty$. This shows that the very rare walks which visit the source L times as frequently as any of the traps dominate the average. Likewise, for a single source in a homogeneous background of traps, the walks which stay confined to the source dominate the average, so that a single source may win over the traps. In most practical situations, such as in Monte Carlo simulations, the sample of random walks available is much smaller than the complete ensemble of possible walks, and one observes most probable values rather than true averages. Thus, in a random distribution of traps and sources, we expect sources to dominate because of very rare events in which the sources are visited an anomalously large number of times. However, in a practical realization we would observe the most probable outcome and the sources will not necessarily dominate.

The analysis of periodic distributions provides an effective coarse-grained homogeneous trapping medium to account for systems containing a random distribution of traps at low concentration. In Section 6, we used this coarse graining to study the trapping of random walkers on a linear chain with a random distribution of partially absorbing traps. For short times, there is a simple exponential decay in the number of walkers which depends on the strength and concentration of traps, as in the case of a homogeneous absorbing medium. For later times, large trap-free regions favor the longer survival of particles and we find the same anomalous decay as for the case of perfect traps. This early-time regime of exponential decay is special to partial traps.

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