

Variance of random walks on Cayley trees: application to the trapping problem

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1990 J. Phys. A: Math. Gen. 23 5611

(<http://iopscience.iop.org/0305-4470/23/23/031>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 01/06/2010 at 09:54

Please note that [terms and conditions apply](#).

Variance of random walks on Cayley trees: application to the trapping problem

G H Köhler and A Blumen

Physical Institute and BIMF, University of Bayreuth, D-8580 Bayreuth, Federal Republic of Germany

Received 2 August 1990

Abstract. We investigate the trapping of particles on regularly multifurcating Cayley trees by using random walk methods. In order to find a good approximation for the survival probability of the walker, we use a cumulant expansion, and obtain an exact expression for the variance of the range of nearest-neighbour random walks; the expressions are corroborated to high accuracy by simulation calculations. The method may turn out to be useful for more complex problems, such as walks on ultrametric spaces.

1. Introduction

The interest on random walks (RWs) on regular lattices (as for instance, simple cubic) is kindled by the possibility which it offers to the study of dynamic processes (such as energy transfer, charge transport and recombination, chemical reactions) in crystalline environments [1-3]. Thus it is possible to investigate reactions under diffusion-limited conditions, as for instance the annihilation of mobile charge carriers of opposite sign which react on encounter with each other. One example which has attracted considerable interest during the last few years is the trapping problem [1, 3, 4]. This describes the diffusion of a particle among immobile traps, which are randomly distributed over the lattice with density p . Here one is interested in the survival probability of the particle during n steps, Φ_n . However, the more the description of amorphous solids comes into general scrutiny [3, 4], the more one is tempted to carry over those ideas, gained for regular environments, to concepts which model *disorder*: prominent representatives for systems without translational symmetry are for instance fractals [5-8] or ultrametric spaces (UMSs) [9-12]. Here it is worthwhile to notice that a natural link between ordered and disordered systems is provided by regularly multifurcating Cayley trees (CTs): on the one hand these structures show similarities to high-dimensional regular lattices [13, 14], whereas on the other hand they are a special case of hierarchical systems such as UMSs [15, 16] (used to model energetic disorder). Thus the study of CTs may yield valuable insights and is a testing ground for methods for the investigation of disordered materials.

In this article we study trapping for nearest-neighbour RWs on CTs. As is usual for the trapping, a completely general analytical treatment is out of reach because of mathematical difficulties [1-3]. In the trapping problem the range R_n of the RW plays a crucial role [17]. R_n is a random variable which denotes the number of distinct sites visited in n steps. Apart from one-dimensional nearest-neighbour RWs, for which the whole distribution R_n is known analytically [1, 18], far less is known in general cases:

here one has either to resort to simulations for the range [1, 2, 19, 20] (for fractal or ultrametric structures see [7] and [21]), to rather elaborate analyses of *higher* moments of the range, such as the variance V_n [22–24] (of course, the *first* moment of R_n , denoted by S_n , is well known in the physical literature since the pioneering works of Montroll and Weiss [25]), or to limit theorems [26, 27] for large stepping number n . Similarly, much effort has been spent in establishing the leading term of $\tilde{\Phi}_n$ for large n . One finds [18, 28–35] on d -dimensional lattices $\log(\tilde{\Phi}_n) \approx -Cn^{d/(d+2)}$ (where C is a positive constant), i.e. a decay which is slower than exponential for all finite d . However, it turns out that this asymptotic form is valid only for very small survival probabilities [36, 37].

Hence we use a cumulant expansion [2] as an appropriate approach for analysing the decay of $\tilde{\Phi}_n$ on CTs for moderately large n . A central point here will be the derivation of an analytical expression for the second-order cumulant, the variance V_n , for which we use generating function techniques. As we show, our derivation also requires the knowledge of the first *two* terms in the expansion of S_n , the average of R_n . For both S_n and V_n we show by comparison to numerical studies that their asymptotic limits are reached quite fast: both quantities increase linearly with n , a result which agrees with the general findings of Jain and Orey for strongly transient RWs [22]. Moreover, the simulation shows that for ramified CT (branching ratio larger than three) the second-order cumulant expansion is sufficient to fit the exact decay $\tilde{\Phi}_n$ in all regimes of physical interest. $\tilde{\Phi}_n$ shows a pure exponential decay without significant deviations over several orders of magnitude. This again stresses the infinite effective dimension of CTs for large branching ratios.

The course of the paper is as follows: In the second section we outline the calculation of the survival probability of a particle diffusing among traps. In section 3 we establish the mathematical methods which allow us to express the variance of the range in terms of generating functions. In section 4 we apply the theory to regularly multifurcating CTs, for which we obtain exact, close analytical expressions. The analysis of these results for large n is given in section 5. Using Tauberian arguments, we find for CTs a linear asymptotic dependence of the variance V_n on the number of steps, n , in agreement with the prediction of Jain and Orey [22]. We also establish that the variance diminishes for increasing CT branching ratios. These analytical results are compared with numerical studies in section 6. Both for the mean and for the variance we find excellent agreement between the asymptotic form and the Monte Carlo simulation data. This allows us to give a good approximation for $\tilde{\Phi}_n$ which is corroborated by the simulation: for high CT-branching ratios $\tilde{\Phi}_n$ may be approximated to a very high accuracy by an exponential form. Section 7 is devoted to a summary; technical details are relegated to the appendix.

2. The survival probability

Here we follow the ideas for treating trapping, as developed for regular lattices [2]. For a particular realization of the RW, we denote by R_n the number of distinct sites visited in n steps. Then the probability $\tilde{\Phi}_n$ that the RW is not trapped up to step n is given by

$$\tilde{\Phi}_n = \langle (1-p)^{R_n} \rangle \quad (1)$$

where p is the trap concentration, and the average $\langle \cdot \rangle$ is taken with respect to all

possible walk realizations. By introducing $\lambda = -\ln(1 - p)$, equation (1) can be recast into

$$\tilde{\Phi}_n = \langle e^{-\lambda R_n} \rangle = \exp \left(\sum_{j=1}^{\infty} \kappa_{j,n} (-\lambda)^j / j! \right) \tag{2}$$

where $\kappa_{j,n}$ is the j th cumulant of the n -step walk. The first two cumulants, for instance, are given by

$$\kappa_{1,n} = \langle R_n \rangle = S_n \tag{3}$$

and

$$\kappa_{2,n} = \langle R_n^2 \rangle - \langle R_n \rangle^2 = V_n \tag{4}$$

i.e. they are the mean S_n and the variance V_n of the distribution R_n .

Because, in general, higher cumulants are not known explicitly, one is tempted to approximate the full expansion of equation (2) by the first N terms:

$$\tilde{\Phi}_{N,n} = \exp \left(\sum_{j=1}^N \kappa_{j,n} (-\lambda)^j / j! \right). \tag{5}$$

Since it is possible that the neglected cumulants show a faster increase for large n than the first N ones, equation (5) may be a good approximation only in a regime of a small or medium number of steps. The restriction $N = 1$, the so-called Rosenstock approximation [38], is a good description of $\tilde{\Phi}_n$ only for a very restricted range of decay and for three-dimensional lattices [2]; deviations from this approximation are very pronounced for dimensions $d = 1$ and $d = 2$. Beyond $d = 1$, the second-order term $\tilde{\Phi}_{2,n}$ approximates $\tilde{\Phi}_n$ excellently over several orders of magnitude. We will find a similar behaviour on CTs, namely slight deviations of $\tilde{\Phi}_{1,n}$ from the numerically computed $\tilde{\Phi}_n$, and very good agreement between $\tilde{\Phi}_{2,n}$ and $\tilde{\Phi}_n$.

Remarkably, for general lattices the first cumulant S_n is easily amenable to an analytical investigation using generating functions. The determination of the second cumulant, the variance V_n , is considerably more involved. We thus devote the next sections to the derivation of an analytical expression for the variance V_n on CTs.

3. Calculation of the variance

In this section we give an expression for the variance V_n using well-established rw techniques [17, 25, 39]. For a quite general case, Jain and Orey [22] demonstrated that V_n depends linearly on the stepping number n , if the rws are strongly transient: $V_n \approx Cn$. (For a definition of the term *strongly transient* see [17], [22] or [23]. Examples are all rws on d -dimensional lattices for $d \geq 5$, but also rws on CTs.) In order to calculate the constant C we make use of generating functions. These methods are widely used on regular lattices [25, 39], but carry readily over to other homogeneous lattices, such as CTs.

The procedure is as follows: We first introduce the stochastic variable I_i , called the indicator. I_i equals unity if the rw hits a new site at step i and is zero otherwise. Then the range of the walk is given by

$$R_n = \sum_{i=0}^n I_i. \tag{6}$$

Now we define

$$Q_n \equiv \langle R_n(R_n - 1) \rangle = 2 \sum_{0 \leq i < j \leq n} \langle I_i I_j \rangle. \tag{7}$$

Since we have $V_n = \langle R_n^2 \rangle - \langle R_n \rangle^2$, equation (7) implies that

$$V_n = Q_n + S_n - S_n^2. \tag{8}$$

To evaluate V_n , since S_n is known for CTs [13, 40–42], it remains to calculate the term Q_n in equation (8). For that we mention that $I_i I_j = 1$, with $0 \leq i < j$, holds if and only if a walk visits a new site at step i and a new site later at step j . Obviously, setting ($I_0 = 1$), the expectation of this event can be written alternatively as

$$\langle I_i I_j \rangle = \sum_x \sum_{y \neq x} F_i^{(y)}(0, x) F_{j-i}(x, y) \tag{9}$$

where $F_i^{(y)}(0, x)$ is the probability that the walk starts in 0 and reaches x in the i th step for the first time without having been at y before. $F_n(x, y)$ is the probability that the walk reaches y for the first time in step n when it started at x . For computational convenience, we set $F_0(0, x) = \delta_{0x}$, $F_0^{(y)}(0, x) = \delta_{0x}$ and $F_n(x, x) = \delta_{0n}$, which is a slightly different notation from the one in [25]. Switching over to generating functions, from the last equations we obtain

$$Q(z) = \sum_{n=0}^{\infty} z^n Q_n = 2(1-z)^{-1} \left(\sum_x \sum_{y \neq x} F^{(y)}(0, x; z) F(x, y; z) \right) \tag{10}$$

where z denotes the generating variable.

It remains to derive an expression for $F^{(y)}(0, x; z)$: one can decompose the probability $F_j(0, x)$ into two parts, namely to visit x with and without having been at y before. Thus for x and $y \neq x$ one gets

$$F_j(0, x) = F_j^{(y)}(0, x) + \sum_{i=0}^j F_i^{(x)}(0, y) F_{j-i}(y, x) \tag{11}$$

or, written in terms of generating functions

$$F(0, x; z) = F^{(y)}(0, x; z) + F^{(x)}(0, y; z) F(y, x; z) \tag{12}$$

from which one obtains the expression

$$F^{(y)}(0, x; z) = \frac{F(0, x; z) - F(0, y; z) F(y, x; z)}{1 - F(x, y; z) F(y, x; z)}. \tag{13}$$

With equations (10) and (13) we are able to express $Q(z)$ fully in terms of the first passage functions $F(x, y; z)$. Note that equation (13) is valid for RWs on arbitrary lattices. Moreover, the summation over pairs of points (x, y) can be simplified for RWs which obey further symmetries. Thus, firstly, if the RW is symmetric (as is the case here) one has $F(x, y; z) = F(y, x; z)$, for all pairs of points $\{x, y\}$. Therefore $Q(z)$ reads

$$Q(z) = 2(1-z)^{-1} \sum_x F(0, x; z) \sum_{y \neq x} F(x, y; z) [1 + F(x, y; z)]^{-1}. \tag{14}$$

We note furthermore that regular cubic lattices, UMSs and regular multifurcating CTs are homogeneous, which means that all points of the lattice are equivalent. For such homogeneous spaces many calculations simplify, paralleling the behaviour for translationally invariant d -dimensional Euclidean lattices. Here, by using the relation $F(x, y; z) = F(0, y - x; z)$, equation (14) may be rewritten as

$$Q(z) = 2(1-z)^{-1} \sum_x F(0, x; z) \sum_{y \neq 0} F(0, y; z) (1 + F(0, y; z))^{-1}. \tag{15}$$

One should remark that the last step leads to the decoupling of the twofold sum over (x, y) into two single sums. They furthermore depend only on $F(0, x; z)$, a classical quantity in the RW study. Note that we can express $Q(z)$ also in terms of $P(0, x; z)$, the generating function of $P_n(0, x)$, the probability of being at site x in step n : on homogeneous lattices [25] $F(0, x; z)$ and $P(0, x; z)$ are connected by $F(0, x; z) = P(0, x; z)/P(0, 0; z)$.

4. Regularly multifurcating Cayley trees

In this section we apply the obtained general results to regularly multifurcating CTs. The CTs are simply connected graphs with no loops. The CT branching ratio b is given by the number of bonds from each site (see figure 1). We consider next-neighbour hopping between sites; thereby each of the b neighbours of a site can be reached with equal probability $1/b$. This RW problem was investigated by a number of authors, recent references being [13, 40–43]. These works have obtained the probability of reaching site x in the n th step, $P_n(0, x)$, the mean number of visited sites, S_n , and also the first passage probabilities $F_n(x, y)$ in terms of generating functions. The result for $S(z)$ is

$$S(z) = \frac{b - 2 + [b^2 - 4z^2(b - 1)]^{1/2}}{2(b - 1)(1 - z)^2}. \tag{16}$$

For $F_n(x, y)$ it is convenient to introduce the CT distance d_{xy} , which is defined as being the minimal number of bonds which connect x and y . Because of symmetry one has

$$F(x, y; z) = [f(z)]^{d_{xy}} \tag{17}$$

where $f(z)$ is the generating function of the first passage probability to a neighbouring site of the origin:

$$f(z) \equiv \frac{2z}{b + [b^2 - 4z^2(b - 1)]^{1/2}}. \tag{18}$$

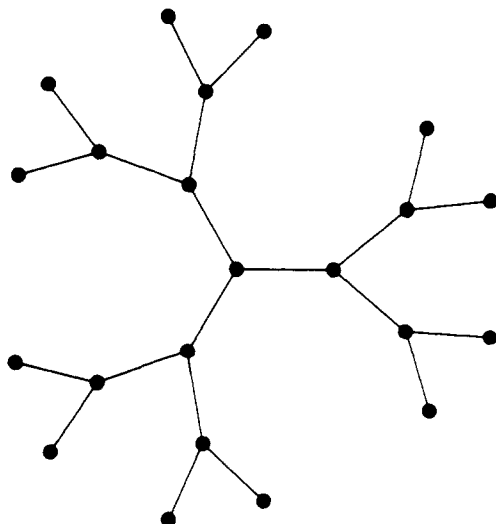


Figure 1. The regularly multifurcating Cayley tree with branching ratio $b = 3$.

We now calculate $Q(z)$ by summing in equation (15) over shells. For this we set $a \equiv b - 1$ and notice that the i th shell around the origin consists of the ba^{i-1} points which have distance i from 0. Hence we change the summation over *all* points into a summation over distances, weighted by the number of sites in each shell. Thus

$$\sum_x F(0, x; z) = 1 + \sum_{i=1}^{\infty} ba^{i-1}(f(z))^i = \frac{1+f(z)}{1-af(z)}. \tag{19}$$

This agrees with a standard RW result [25], in which $S(z)$ and $F(0, x; z)$ are connected by

$$S(z) = \frac{1}{1-z} \sum_x F(0, x; z) \tag{20}$$

as can be verified by comparing equations (16), (18) and (19). Furthermore

$$\begin{aligned} \sum_{y \neq 0} \frac{F(0, y; z)}{1+F(0, y; z)} &= \sum_{i=1}^{\infty} ba^{i-1} \frac{(f(z))^i}{1+(f(z))^i} \\ &= \frac{b}{a} \left(\frac{1}{1-af(z)} - \eta(a, f(z)) - \frac{1}{2} \right) \end{aligned} \tag{21}$$

where η is defined through the series

$$\eta(a, f) \equiv \sum_{n=0}^{\infty} (af)^n \frac{f^n}{1+f^n}. \tag{22}$$

From equations (15), (19) and (21) we obtain finally

$$Q(z) = \frac{2}{1-z} \left(\frac{b}{a} \frac{1+f(z)}{(1-af(z))^2} - \frac{b}{a} \frac{1+f(z)}{1-af(z)} \left[\eta(a, f(z)) + \frac{1}{2} \right] \right) \tag{23}$$

the sought-after, exact expression.

5. The asymptotic form of S_n and V_n

As mentioned in section 3, the knowledge of $S(z)$, equation (16), and of $Q(z)$, equation (23), allows us to determine the variance V_n for arbitrary n ; one has only to perform a Taylor expansion in z , and to make use of equation (8). We will use this method in section 6, in order to obtain the values for V_n for n up to $n=20$ and for several branching ratios b . On the other hand, from the above equations it is also possible to obtain the asymptotic behaviour of V_n for large n , as we now proceed to show.

First of all we turn to the asymptotic behaviour of S_n , which follows from its generating function $S(z)$, equation (16). Standard arguments, obtained through Tauberian theorems, give as the leading term [13]:

$$S_n \approx \frac{b-2}{b-1} n + \dots \tag{24}$$

In our further analysis we also need the second term in this expansion; as derived in the appendix, one has a more accurate expression:

$$S_n \approx \frac{b-2}{b-1} n + \frac{b^2-2b+2}{b^2-3b+2} + \dots \tag{25}$$

from which it follows that

$$S_n^2 \approx \left(\frac{b-2}{b-1}\right)^2 n^2 + \frac{2(b^2-2b+2)}{(b-1)^2} n + \dots \tag{26}$$

The term $Q(z)$, equation (23), can be analysed along the same lines (see the appendix), and one has

$$Q_n \approx \left(\frac{b-2}{b-1}\right)^2 n^2 + \frac{1}{a^2} [2b^2 - 2b(b-2)\tau_a]n + \dots \tag{27}$$

Now, from equation (8) together with equations (25)-(27), the variance V_n for large n follows. Note that the quadratic terms drop out, so that we have finally

$$V_n \approx \frac{1}{a^2} [b^2 + b - 2 - 2b(b-2)\tau_a]n + \dots \tag{28}$$

where τ_a stands for the series

$$\tau_a \equiv \sum_{n=0}^{\infty} \frac{(1/a)^n}{1 + (1/a)^n} \tag{29}$$

The variance V_n thus depends linearly on the number of steps n [22]; moreover, τ_a is finite for all $a \geq 2$, since it is bounded by the geometric series $\sum_{n=0}^{\infty} (1/a)^n$. Furthermore, for large branching ratios, $a \rightarrow \infty$, τ_a tends to $\frac{1}{2}$, and from equation (28) we see that

$$V_n \rightarrow 0 \quad \text{as } b \rightarrow \infty. \tag{30}$$

Thus on CTs the distribution becomes very narrow when the branching ratio b gets large.

To close this section, we analyse the special case for which b takes the value 2. Then the CT shrinks to a linear chain, on which a one-dimensional nearest-neighbour RW takes place. The formulae for $Q(z)$, equation (23), and for $S(z)$, equation (16), yield the correct expressions even in this special case, and the derivation of V_n becomes equivalent to Torney's [24] resulting in

$$V_n \approx (4 \log 2 - 8/\pi)n + \dots \tag{31}$$

a well known fact in the RW literature [1].

6. Numerical results

In this section we give comparisons of computer data to the analytically obtained results of the last sections, and simulation results for $\tilde{\Phi}_n$ for different trap concentrations p and branching ratios b .

First of all we have performed explicit enumerations on CTs with branching ratio b between 3 and 9. We have obtained the exact values for S_n and V_n from $n = 18$ (for $b = 3$) maximum to $n = 10$ (for the larger b). Furthermore, we have also evaluated explicitly the generating functions for $S(z)$, equation (16), and $Q(z)$, equation (23),

using the computer program MACSYMA. The values of S_n and V_n evaluated by both methods are in complete agreement.

Secondly, to establish how quickly the asymptotic domain is reached we performed Monte Carlo simulations for CTs with branching ratios b between 3 and 20 and compared the results with those from equations (25) and (28). For several n values we used up to 50 000 realizations of the RW. Characteristic results for n between 100 and 1000, where 10 000 RW realizations were used, are shown in figures 2 and 3. We observe that

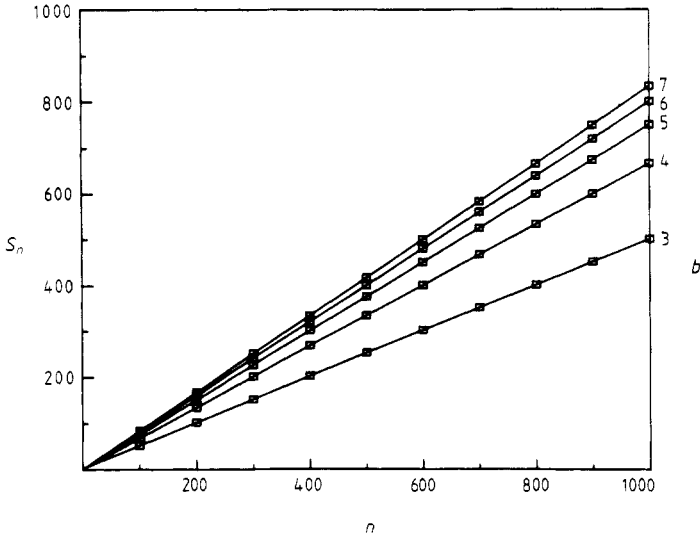


Figure 2. The mean number of visited sites, S_n , plotted as a function of the number of steps, n . The straight lines are the analytical data obtained from equation (25) for several values of b .

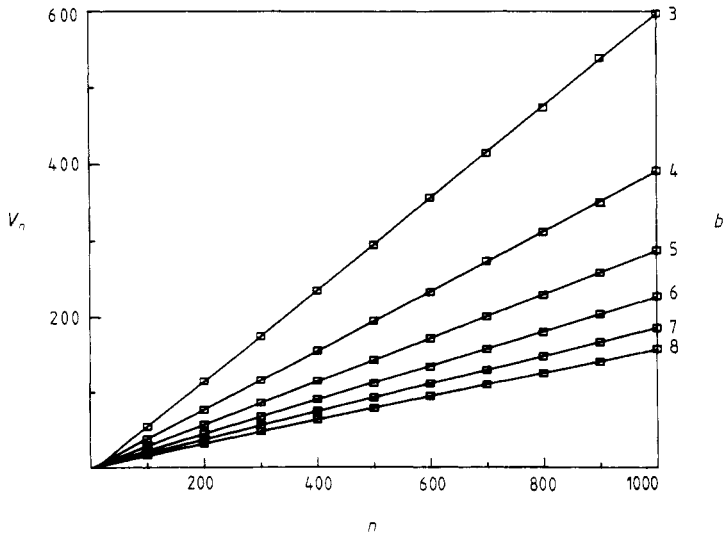


Figure 3. The variance V_n of the RW range plotted as a function of the number of steps, n . The straight lines are fits to the simulated data for several values of b .

the agreement between the simulations and analytical forms is excellent, even for rather small ($n \approx 100$) numbers of steps.

We find that the S_n extracted from the numerical data agree extremely well both with former simulations by Bleris *et al* [44], and also with the analytical result from equation (25). Table 1 summarizes results for several values of the branching parameter b . The variance V_n , equation (28), which we have derived analytically in the course of this article, shows a similar good agreement with the simulation results. In figure 3 the simulated data are fitted by straight lines, and the fit parameters are listed in table 2. They are compared with the slope of V_n which results from equation (28). As is to be seen, there is no significant difference between both results.

Now we turn to the trapping on CTs. We have performed numerical simulations for several branching ratios b . To obtain the decay function $\tilde{\Phi}_n$, we used equation (1) and provided the distribution of R_n by considering up to 500 000 realizations of the walk per stepping number n . The exact values in figures 4 and 5 are indicated by solid circles, connected by full lines. Furthermore, from the knowledge of the distribution we calculated the first five cumulants in order to compare the exact result from equation (1) with different orders of the expansion in equation (5). The values of $\tilde{\Phi}_{N,n}$ are indicated for $N = 1$ by triangles and for $N = 2$ by squares. Because the terms $\tilde{\Phi}_{N,n}$ for $N = 3, 4, 5$ coincide with $\tilde{\Phi}_{2,n}$, they are not shown in figures 4 and 5. Moreover, the

Table 1. Data for S_n for different branching ratios b . S_n is given in the form $S_n = \alpha n + \beta + \dots$. The index a refers to the analytical data, the index s to the simulated data.

b	α_a	β_a	α_s	β_s
3	0.500 00	2.500 00	0.500 00	2.497 00
4	0.666 67	1.666 67	0.666 70	1.673 00
5	0.750 00	1.416 67	0.750 00	1.423 00
6	0.800 00	1.300 00	0.800 00	1.278 00
7	0.833 33	1.233 33	0.833 30	1.240 00
8	0.857 14	1.190 48	0.857 20	1.167 00
9	0.875 00	1.160 71	0.875 00	1.160 00
10	0.888 89	1.138 89	0.889 00	1.122 00
15	0.928 57	1.082 42	0.928 60	1.082 00
20	0.947 37	1.058 48	0.947 40	1.059 00

Table 2. Data for V_n for different branching ratios b . V_n is given in the form $V_n = \gamma n + \delta$. The index a refers to the analytical data, the index s to the simulated data.

b	γ_a	γ_s	δ_s
3	0.603 25	0.602 60	-6.016
4	0.392 78	0.392 10	-1.473
5	0.288 63	0.288 70	-0.916
6	0.227 08	0.227 80	-1.002
7	0.186 69	0.186 60	-0.410
8	0.158 25	0.158 40	-0.389
9	0.137 20	0.137 30	-0.300
10	0.121 01	0.121 00	-0.195
15	0.075 85	0.075 59	-0.013
20	0.055 13	0.054 91	0.016

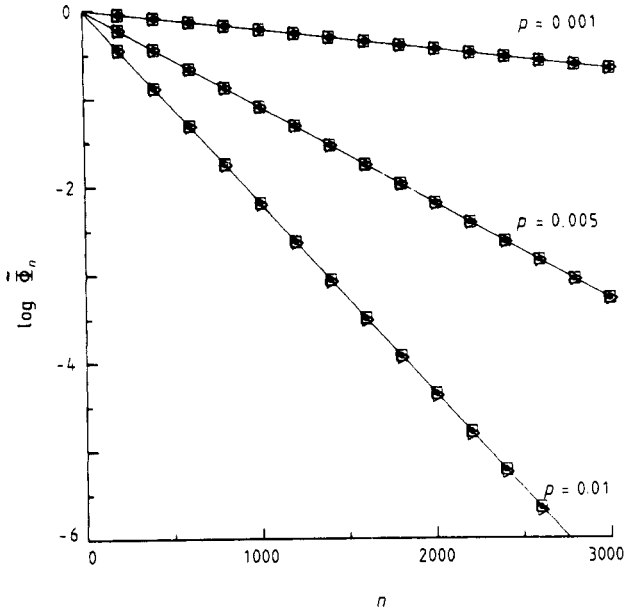


Figure 4. The logarithm of the survival probability Φ_n is plotted as a function of the number of steps, n , for three different trap concentrations. The branching ratio is $b = 3$. The symbols are explained in the text.

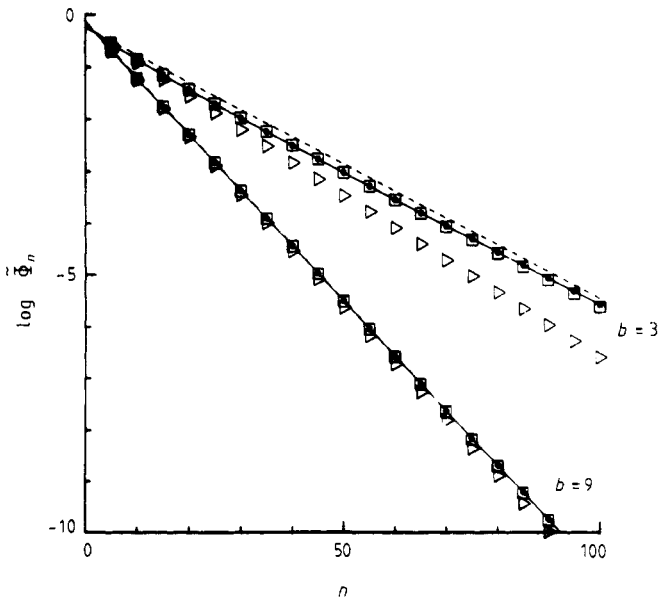


Figure 5. The same situation as in figure 4 but for a fixed trap concentration $p = 0.25$, and for two different branching ratios $b = 3$ and $b = 9$.

dotted line gives the values for $\tilde{\Phi}_{2,n}$ by using the *analytical* forms of S_n and V_n , i.e.

$$\tilde{\Phi}_{2,n}^a \equiv \exp(-\lambda S_n + \lambda^2 V_n/2) \tag{32}$$

with S_n and V_n taken from equations (25) and (28).

Figure 4 shows the decadic logarithm of the decay function, $\log \tilde{\Phi}_n$, plotted against the number of steps, n , for three realistic trap concentrations $p = 0.001, 0.005$ and 0.01 , and for branching ratio $b = 3$. One notices the pure exponential decay over the whole range without any significant deviations. All $\tilde{\Phi}_{N,n}$ and $\tilde{\Phi}_{2,n}^a$ coincide fully with the exact data. This is a situation similar to the higher-dimensional lattice ($d = 3$) in [2], where the first approximate terms also fit the exact decay very well. In one dimension, on the other hand, these approximations are rather poor, and one has to go up to $\tilde{\Phi}_{4,n}$ in order to fit $\tilde{\Phi}_n$ reasonably over an order of magnitude in the decay.

Figure 5 shows the influence of higher trap concentrations ($p = 25\%$) for different branching ratios $b = 3$ and $b = 9$. As before, the decay stays nicely exponential even at such high trap densities. However, one notices that for $b = 3$ a deviation from the Rosenstock approximation $\tilde{\Phi}_{1,n}$ is clearly visible. For increasing branching ratio the difference to the simulated decay becomes smaller: the CT looses any resemblance to the linear chain ($b = 2$), for which the low-order terms $\tilde{\Phi}_{N,n}$ are no good approximations. Moreover one notices that in figure 5, $\tilde{\Phi}_{2,n}$ fits the real decay very well. The analytical form $\tilde{\Phi}_{2,n}^a$ displays the correct slope, but is slightly shifted; this is due to the fact that we have obtained only the first term of V_n in equation (28), and have neglected the corrections in $\tilde{\Phi}_{2,n}^a$.

Concluding this section we note that the very good agreement between $\tilde{\Phi}_n$ and $\tilde{\Phi}_{2,n}$ is impaired only for small branching ratios ($b = 3$) and for very large trap densities (beyond $p = 50\%$): even for such high concentrations, for $b = 9$ the term $\tilde{\Phi}_{2,n}$ describes the real decay very well. Thus $\tilde{\Phi}_{2,n}$ (and also $\tilde{\Phi}_{2,n}^a$) is an excellent approximation for the decay due to trapping for all realistic trap concentrations, covering many orders of magnitude of the decay. All simulation results point to, for large n , a purely exponential decay of $\tilde{\Phi}_n$, as would also follow from the relation $\tilde{\Phi}_n \approx \exp(-Cn^{d/(d+2)})$ for $d \rightarrow \infty$. If this is the case, this would impose a (at most) linear increase on the absolute value of all cumulants (see equation (2)). We extracted the behaviour of the first five cumulants from our numerical data and found indeed a well defined linear decrease for the third cumulant. For the higher cumulants, however, the error bars become too large to permit a definite conclusion. Finally, we cannot decide based on simulations alone whether the exponential decay also remains valid for very large stepping numbers, or whether one has a cross-over to a slower decay.

7. Summary

In this article we have investigated the trapping problem on regularly multifurcating CTs. A cumulant expansion allowed us to deal with small to medium numbers of steps. We were able to derive an exact analytical expression for the second cumulant of the range, the variance V_n . We thus found that V_n increases linearly with n when the number of steps is large. This is in agreement with rigorous mathematical predictions. Moreover, the range distribution peaks more and more around S_n when the CT branching ratio increases. Numerical simulations show that for CTs with large branching ratios the second-order cumulant expansion for the decay due to trapping agrees very well with the exact survival probability $\tilde{\Phi}_n$, a result which holds even for high trap densities.

We expect that elements of our analysis could be used for the determination of higher-order cumulants of R_n on CTs and also for the study of more complex structures, such as UMSs. This is a fact which would help towards understanding the dynamics on systems without translational invariance.

Acknowledgments

We gratefully acknowledge discussions (made possible by the Greek-German collaboration grant ‘Materialforschung’ Internationales Büro der KFA Jülich) with Professor K Kehr, and with Professor P Argyrakis, whose work with Dr G L Bleris and Dr N Pitsianis focused our interest on Cayley trees. Furthermore, we thank Dr G Zumofen for helpful advice concerning numerical problems. Our work was supported by the Deutsche Forschungsgemeinschaft (SFB 213), and by the Fonds der Chemischen Industrie (grant of an IRIS workstation).

Appendix

Here we extract the asymptotic behaviour of S_n , equation (25), for large n from the generating function $S(z)$, equation (16). Our basic assumption is that S_n can be written in the form

$$S_n = \alpha n^\beta + \gamma n^\delta + o(n^\delta) \tag{A1}$$

with $\beta > \delta$. This assumption is necessary since we want to apply Tauberian arguments *twice*: the monotonicity of the leading term is guaranteed from the monotonous increase of S_n , but for the second term we lack such information. Therefore the validity of equation (A1) must be confirmed by numerical results (see table 1).

Now we switch over to generating functions, and establish first the *pure n-dependences*:

$$r_0^{(n)} \equiv 1 \qquad r_1^{(n)} \equiv n \qquad r_2^{(n)} \equiv n^2.$$

Thus we have

$$r_0(z) \equiv \sum_{n=0}^{\infty} z^n = \frac{1}{1-z} \tag{A2}$$

$$r_1(z) \equiv \sum_{n=0}^{\infty} n z^n = \frac{z}{(1-z)^2} \tag{A3}$$

$$r_2(z) \equiv \sum_{n=0}^{\infty} n^2 z^n = \frac{z(1+z)}{(1-z)^3}. \tag{A4}$$

These series converge for all $|z| < 1$, but they diverge for $z \rightarrow 1^-$. Writing $x = 1 - z$, we have

$$r_0(x) = \frac{1}{x} \tag{A5}$$

$$r_1(x) = \frac{1}{x^2} - \frac{1}{x} \tag{A6}$$

$$r_2(x) = \frac{2}{x^3} - \frac{3}{x^2} + \frac{1}{x} \tag{A7}$$

and in general for $x \rightarrow 0^+$,

$$r_\alpha(x) \approx \frac{\Gamma(\alpha + 1)}{x^{\alpha+1}} \tag{A8}$$

for all $\alpha > -1$.

Now we can determine both coefficients and exponents in equation (A1). Starting from equation (16),

$$S(z) = \frac{b - 2 + [b^2 - 4z^2(b - 1)]^{1/2}}{2(b - 1)(1 - z)^2} \tag{A9}$$

we set $z = 1 - x$ and obtain

$$S(x) \approx \frac{1}{x^2} \frac{b - 2}{b - 1} + O(1/x) \tag{A10}$$

which diverges in the limit $x \rightarrow 0^+$. Thus from this asymptotic behaviour and from equation (A6) we have

$$S_n \approx \frac{b - 2}{b - 1} n + \gamma n^\delta + \dots \tag{A11}$$

which is just the result found in the literature [13, 42], equation (24).

To obtain the next term of the expansion, we simply subtract $(b - 2)r_1(z)/(b - 1)$ from equation (A9); thus the linear n dependence of the generating function drops out, and we repeat our analysis for $S(z) - (b - 2)r_1(z)/(b - 1)$. Substituting again $z = 1 - x$, and taking $x \rightarrow 0^+$, we find

$$S(x) - \frac{b - 2}{b - 1} r_1(x) \approx \frac{1}{x} \frac{b^2 - 2b + 2}{b^2 - 3b + 2} + O(1) \tag{A12}$$

which yields, from equation (A5), a constant contribution to S_n . Hence, we obtain equation (25):

$$S_n \approx \frac{b - 2}{b - 1} n + \frac{b^2 - 2b + 2}{b^2 - 3b + 2} + \dots \tag{A13}$$

The analysis of $Q(z)$ runs along the same lines. Again, the monotonous increase of the first term of Q_n follows from equation (7), but that of the second term must be assumed. We first have

$$Q(z) = \frac{2}{1 - z} \left(\frac{b}{a} \frac{1 + f(z)}{(1 - af(z))^2} - \frac{b}{a} \frac{1 + f(z)}{1 - af(z)} \left[\eta(a, f(z)) + \frac{1}{2} \right] \right) \tag{A14}$$

which is equation (23). For small $x = 1 - z$, we have two contributions to the divergence: firstly, of course, the factor $1/(1 - z)$, which yields $1/x$, and, secondly, the term $1/[1 - af(z)]$, which contributes $(b - 2)/(xb)$. This is due to the expansion of $f(z = 1 - x)$, equation (18), whose first terms are

$$f(x) \approx \frac{1}{a} - \frac{b}{a(a - 1)} x + \frac{b(3a - 1)}{a(a - 1)^3} x^2 + \dots \tag{A15}$$

All other terms in equation (A14) remain bounded. The exact analysis, paralleling that of S_n , finally yields equation (27).

References

- [1] Weiss G H and Rubin R J 1983 *Adv. Chem. Phys.* **52** 363
- [2] Zumofen G and Blumen A 1982 *Chem. Phys. Lett.* **88** 63
- [3] Blumen A, Klafter J and Zumofen G 1986 *Optical Spectroscopy of Glasses* ed I Zschokke (Dordrecht: Reidel)
- [4] Havlin S and Ben-Avraham D 1987 *Adv. Phys.* **36** 695
- [5] Mandelbrot B B 1982 *The Fractal Geometry of Nature* (San Francisco: Freeman)
- [6] Alexander S and Orbach R 1982 *J. Physique Lett.* **43** L625
- [7] Angles d'Auriac J C, Benoit A and Rammal R 1983 *J. Phys. A: Math. Gen.* **16** 4039
- [8] Blumen A, Klafter J, White B S and Zumofen G 1984 *Phys. Rev. Lett.* **53** 1301
- [9] Ogielski A T and Stein D L 1985 *Phys. Rev. Lett.* **55** 1634
- [10] Bachas C P and Huberman B A 1986 *Phys. Rev. Lett.* **57** 1965
- [11] Rammal R, Toulouse G and Virasoro M A 1986 *Rev. Mod. Phys.* **58** 765
- [12] Köhler G and Blumen A 1987 *J. Phys. A: Math. Gen.* **20** 5627
- [13] Hughes B D and Sahimi M 1982 *J. Stat. Phys.* **29** 781
- [14] Stauffer D 1985 *Introduction to Percolation Theory* (London: Taylor and Francis)
- [15] Grossmann S, Wegner F and Hoffmann K H 1985 *J. Physique Lett.* **46** L575
- [16] Engel A, Grossmann S and Mikhailov A S 1988 *Z. Phys. B* **70** 101
- [17] Spitzer F 1976 *Principles of Random Walk* 2nd edn (New York: Springer)
- [18] Anlauf J K 1984 *Phys. Rev. Lett.* **52** 1845
- [19] Zumofen G, Blumen A and Klafter J 1984 *J. Phys. A: Math. Gen.* **17** L479
- [20] Havlin S, Weiss G H, Kiefer J E and Dishon M 1984 *J. Phys. A: Math. Gen.* **17** L347
- [21] Blumen A, Klafter J and Zumofen G 1986 *J. Phys. A: Math. Gen.* **19** L77
- [22] Jain N C and Orey S 1968 *Israel J. Math.* **6** 373
- [23] Jain N C and Pruitt W E 1973 *Proc. 6th Berkeley Symp. on Math. Statistics and Probability* vol 3 (Berkeley: University of California Press) pp 31-50
- [24] Torney D C 1986 *J. Stat. Phys.* **44** 49
- [25] Montroll E W and Weiss G H 1965 *J. Math. Phys.* **6** 167
- [26] Jain N C and Pruitt W E 1971 *J. Analyse Math.* **24** 369
- [27] Weiss G H 1980 *Proc. Natl Acad. Sci. USA* **77** 4391
- [28] Balagurov B Ya and Vaks V G 1973 *Zh. Eksp. Teor. Fiz.* **65** 1939 (English translation 1974 *Sov. Phys.-JETP* **38** 968)
- [29] Movaghar B, Sauer G W, Würtz D and Huber D L 1982 *J. Stat. Phys.* **27** 473
- [30] Donsker M D and Varadhan S R S 1975 *Commun. Pure Appl. Math.* **28** 525
- [31] Donsker M D and Varadhan S R S 1979 *Commun. Pure Appl. Math.* **32** 721
- [32] Weiss G H and Havlin S 1984 *J. Stat. Phys.* **37** 17
- [33] Redner S and Kang K 1983 *Phys. Rev. Lett.* **51** 1729
- [34] Grassberger P and Procaccia I 1982 *J. Chem. Phys.* **77** 6281
- [35] Kayser R F and Hubbard J B 1983 *Phys. Rev. Lett.* **51** 79
- [36] Klafter J, Zumofen G and Blumen A 1984 *J. Physique Lett.* **45** L49
- [37] Havlin S, Dishon M, Kiefer J E and Weiss G H 1984 *Phys. Rev. Lett.* **53** 407
- [38] Rosenstock H B 1969 *Phys. Rev.* **187** 1166; 1974 *SIAM J. Appl. Math.* **27** 457
- [39] Rubin R J and Weiss G H 1982 *J. Math. Phys.* **23** 250
- [40] Kesten H 1959 *Trans. Amer. Math. Soc.* **92** 336
- [41] Kasteleyn P W 1983 *Lect. N. Phys.* **180** 499
- [42] Cassi D 1989 *Europhys. Lett.* **9** 627
- [43] Wada K 1978 *Prog. Theor. Phys.* **59** 313
- [44] Bleris G L, Pitsianis N and Argyrakis P unpublished