Trapping of random walks on small-world networks

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We investigate the trapping of random walkers on small-world networks (SWN's), irregular graphs. We derive bounds for the survival probability Φ_n^{SWN} and display its analysis through cumulant expansions. Computer simulations are performed for large SWNs. We show that in the limit of infinite sizes, trapping on SWNs is equivalent to trapping on a certain class of random trees, which are grown during the random walk.

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I. INTRODUCTION

The trapping of random walkers by randomly distributed sinks is a rich problem that has been widely investigated in the last two decades [1–13]. Besides its intrinsic mathematical interest as an example of rare events statistics [1], the trapping problem is a central model for energy transfer and carrier recombination in ordered and disordered materials [4,5]. Trapping has been investigated using very different techniques, ranging from rigorous mathematical treatments [1] and field theory [6,7] to extensive simulations [3,4,9]. While the short- and medium-time decay are well reproduced by Smoluchowski-type approaches [3] and lead to exponential decays on regular D-dimensional lattices with $D>2$, at very long times, surprisingly, the decay law Φ_n is expected to tend towards [1,4–11]

$$\Phi_n \sim \exp[-cn^{D/(D+2)}], \tag{1}$$

where Φ_n is the probability that a random walker is still not trapped, c is a constant, and n is the number of steps. Even more complex aspects are revealed when monitoring Φ_n on structures such as fractals [11], Cayley trees [12], and ultrametric spaces (UMS) [13], which mimic disorder. When letting the trapping rates on the one-dimensional (1D) lattice be strongly correlated with the hopping probabilities [8] the asymptotic behavior Eq. (1) is changed by logarithmic corrections.

In this paper, we study the trapping problem on a particularly interesting class of random graphs, namely, on small-world networks (SWN's). Recently these structures have attracted much interest [14–20]. Thus, SWN's may be constructed by inserting in a random way additional links (AL) into a regular lattice. Examples for realizations of SWN's range from the net of social acquaintances to computer clusters [14].

We proceed with displaying the general properties of SWN's in Sec. II. In Sec. III we study trapping on SWN's and derive analytical results, which allow us to obtain a qualitative understanding of the problem. In Sec. IV we present the results of our computer simulations and contrast these with the insights gained in Sec. III. We end with our conclusions in Sec. V.

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II. THE SMALL-WORLD NETWORK

To envisage the construction of the SWN's considered here, we start from a ring with L sites, $i=1,...,L$, where each site i is connected by bonds to its two nearest neighbors $i-1$, $i+1$. Then we add with probability p from each lattice site i a bond (AL) to one of the other sites k, chosen randomly, with equal probability. In this way, we add on the average pL, additional AL to the ring. The parameter p measures the degree of disorder of the SWN, since it interpolates between a ring for $p=0$ and a nearly completely random graph for p large, say $p=1$. The probability $2rp/(L-1)$ of drawing an AL between the lattice points i, k whose mutual distance is less than a preassigned length r, i.e., $|i-k|\leq r$, tends to zero in the limit $L\to\infty$ and the same is true for loops of bounded length. This implies that in the limit of large L, a SWN can hardly be distinguished from a treelike structure, in as far as the local properties are concerned. This is very similar to the case of purely random lattices (where the weight of clusters with closed loops vanishes for $L\to\infty$ [21,22]), and we will make use of this fact later, when considering the $L\to\infty$ limit of Φ_n^{SWN}, the decay due to trapping on very large SWN's.

From the construction described above, it follows that the probability w_k for a lattice point i to have k AL attached to it amounts to

$$w_k = p\binom{L-1}{k-1}\left(1-\frac{p}{L-1}\right)^{L-k-2}\left(\frac{p}{L-1}\right)^{k-1} + (1-p) \times\binom{L-1}{k}\left(1-\frac{p}{L-1}\right)^{L-1-k}\left(\frac{p}{L-1}\right)^{k}. \tag{2}$$

The first term in Eq. (2) stems from having at i one outgoing and $k-1$ incoming AL, while the second term is due to having zero outgoing and k incoming AL [an outgoing AL has probability p, an incoming AL probability $p/(L-1)$].

In the limit $L\to\infty$, this distribution turns into a weighted sum of two Poisson distributions

$$w_k = p\frac{p^{k-1}}{(k-1)!}e^{-p} + (1-p)\frac{p^k}{k!}e^{-p}. \tag{3}$$

From Eq. (3), it follows that each lattice point has a mean number $\langle k\rangle = 2p$ of AL's and that the variance $\sqrt{\langle k^2\rangle - \langle k\rangle^2}$ of the connectivity distribution is given by $\sqrt{p(2-p)}$.

III. TRAPPING ON SWN

Given a particular SWN realization, we now consider a particular trap distribution over it; each site can, with probability q, be occupied by an immobile trap. In this way, the disorder is quenched. Random walkers are then placed on the SWN at the 0th step ($n=0$) and are trapped (annihilated) at the first encounter of a trap. We focus on the probability Φ_n^{SWN} that the walker has survived (is not yet trapped) at the nth step, averaged over all SWN realizations, over all possible placements of the traps and over all random-walk (RW) realizations.

Denoting by R_n the number of distinct sites visited in n steps, the walker survives n steps, if none of the R_n visited sites is a trap. This event has the probability [3]

$$P_n = (1-q)^{R_n - 1}, \tag{4}$$

taking into account only walkers that start from trap-free sites. Thus, we obtain the exact survival probability by performing the average over all RW and SWN realizations

$$\Phi_n^{\mathrm{SWN}} = \langle (1-q)^{R_n}\rangle = \sum_{R=1}^{\infty} p_n^{\mathrm{SWN}}(R)(1-q)^{R-1}, \tag{5}$$

where $p_n^{\mathrm{SWN}}(R)$ is the probability that a n step RW has visited exactly R distinct sites on lattices *devoid* of traps.

Since for SWN the R_n values are not smaller than for the underlying 1D chain and since $(1-q)^{R_n-1}$ is a monotonically decaying function of R, we obtain the inequality

$$\Phi_n^1 \geq \Phi_n^{\mathrm{SWN}}, \tag{6}$$

where Φ_n^1 is the survival probability on a regular lattice.

On the other hand, we obtain a lower bound by placing additional traps on each lattice site, to which at least one AL is connected. In this way, the AL's are completely screened by the traps and we are led to the trapping problem on a 1D chain with a different trap density $\tilde{q}$. From Eq. (3), the probability of having a trap-free site is given by $w_0(1-q)$; hence, the trap density $\tilde{q}$ equals

$$\tilde{q} = 1 - w_0(1-q) = 1 - e^{-p}(1-p)(1-q). \tag{7}$$

Thus, we have the inequality

$$\Phi_n^{\mathrm{SWN}}(q) \geq \Phi_n^1(\tilde{q}). \tag{8}$$

We stop to note that Eq. (8) makes sense only for $p<1$; otherwise, our construction of the lower bound assigns to each lattice site a trap, which renders $\Phi_n^1(\tilde{q})$ identically zero.

We infer that Φ_n^{SWN} is bounded from above and from below by the decay forms of trapping in 1D calculated for q and for $\tilde{q}$. As we will show in the next section, the relations Eqs. (6) and (8) are well fulfilled. Furthermore, we infer that given the asymptotic 1D behavior, which leads to the exponent $D/(D+2) = 1/3$ in Eq. (1), as analytically established in [2], Φ_n^{SWN} behaves in the same way.

The key feature that leads to this fact is that SWN's display extended chain-like portions. Of course, the general understanding is that most experiments are not able to reach the asymptotic limit [9,10]

Inserting $\gamma = -\ln(1-q)$ into Eq. (5) leads to the following expansion [3]:

$$\Phi_n^{\mathrm{SWN}} = \langle \exp(-\gamma R_n)\rangle = \exp\left[\sum_{j=1}^{\infty} \kappa_{j,n}^{\mathrm{SWN}}(-\gamma)^j/j!\right], \tag{9}$$

where $\kappa_{j,n}^{\mathrm{SWN}}$ are the cumulants of the distribution of R_n on SWN lattices *devoid* of traps. For instance, the first two cumulants are

$$\kappa_{1,n}^{\mathrm{SWN}} = \langle R_n\rangle \equiv S_n^{\mathrm{SWN}} \quad \text{and} \quad \kappa_{2,n}^{\mathrm{SWN}} = \langle R_n^2\rangle - \langle R_n\rangle^2 \equiv (\sigma_n^{\mathrm{SWN}})^2, \tag{10}$$

with S_n^{SWN} and $(\sigma_n^{\mathrm{SWN}})^2$ being the mean and the variance of R_n. Taking only the first term in the sum of Eq. (9) into account is known as the Rosenstock approximation (RA); as in Ref. [3], we denote the approximations that are obtained by restricting the sum in Eq. (9) to the first N terms by $\Phi_{N,n}^{\mathrm{SWN}}$. According to the Jensen-Peierls inequality $\Phi_{1,n}^{\mathrm{SWN}} \leq \Phi_n^{\mathrm{SWN}}$ [23], i.e., RA is a lower bound to the true decay. We remark that RA leads to very good expressions for the target problem [17,24,25]; it is also very good in high-dimensional spaces and for small γ, for short and medium times. On the other hand RA is poor in low dimensions [3] and, of course, it does not lead to the asymptotic behavior of Eq. (1).

As a first approximation step for trapping on SWN, we first focus on $\Phi_{1,n}^{\mathrm{SWN}} = \exp(-\gamma S_n^{\mathrm{SWN}})$, and hence, on S_n^{SWN}. As shown in Ref. [17], S_n^{SWN} is closely described by the following scaling relation:

$$S_n^{\mathrm{SWN}} = n^{1/2} f(np^2), \quad \text{where } f(x) = \begin{cases} \sqrt{8/\pi}, & \text{for } x \to 0 \\ c'\sqrt{x}, c' \text{ constant}, & \text{for } x \to \infty \end{cases}. \tag{11}$$

We stop to note that the form of $f(x)$ may be specified in more detail, by considering that for small p, $p \ll 1$, a random walker moves mostly on the 1D structure. Now, each time the random walker makes a step along an AL, it starts to explore a 1D segment, for which S_n is given (for n not too small) by $S_n \simeq \sqrt{8n/\pi}$. Therefore, a walker that in n steps makes A_n steps along AL's, visits $A_n + 1$ different segments (if we neglect returns over the AL's), of average length $n/(A_n+1)$ each; on each segment on the average $\sqrt{8n/\pi(A_n+1)}$ sites are visited, hence,

$$S_n^{\mathrm{SWN}} = (A_n+1)\sqrt{\frac{8n}{\pi(A_n+1)}} = \sqrt{\frac{8n}{\pi}}(A_n+1)^{1/2}. \tag{12}$$

On the other hand, the probability that a step leads to crossing an AL instead of continuing over the segment is roughly

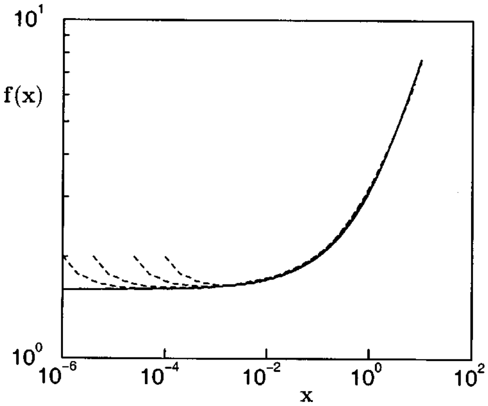

FIG. 1. The scaling function $f(x)$ Eq. (13), plotted as a solid line, compared with $S_n^{\mathrm{SWN}}/\sqrt{n}$, displayed as a function of $x=np^2$ through dashed lines. Here, $p=0.001$, 0.002, 0.005, and 0.01 from left to right.

$2p/3$, so that $A_n=S_n^{\mathrm{SWN}}2p/3$. Thus, $S_n^{\mathrm{SWN}}=\sqrt{8n/\pi(S_n^{\mathrm{SWN}}2p/3+1)}$, and solving this equation for S_n^{SWN} leads to

$$f(x)=\frac{8}{\pi}\left(\sqrt{\frac{x}{9}}+\sqrt{\frac{x}{9}+\frac{\pi}{8}}\right). \tag{13}$$

This result is confirmed by our numerical investigations, see Fig. 1, the details of which are presented in the next section.

IV. SIMULATION RESULTS

In our numerical calculations, we start from Eq. (5), since it offers the great advantage of being, in fact, a q-independent procedure: as stressed in [3], q appears only through γ, a parameter. Numerically, one has only to evaluate the R_n distribution on lattices *devoid* of traps.

We start our procedure as follows: For a given q, we construct ten different SWN's of size $L=9\times10^5$ each. On these, we simulate a total of 10^5RW's with randomly chosen starting points, and determine the R_n values for each walk. By choosing the starting points randomly we sample, in fact, a very large class of local SWN geometries, much larger than the ten SWN realizations would indicate at first glance. The so determined R_n allow us then to compute S_n, see Fig. 1 and also via Eq. (5), to evaluate numerically for different q values both Φ_n^{SWN}, and also the corresponding $\Phi_{N,n}^{\mathrm{SWN}}$. The results of these calculations are presented in Figs. 2(a) and 2(b). To emphasize the regions of stretched exponential decay

$$\Phi_n^{\mathrm{WMN}}\sim\exp(-cn^{\alpha}), \tag{14}$$

and to be able to highlight the exponent α, we plotted $\log_{10}(-\ln\Phi_n^{\mathrm{SWN}})$ versus $\log_{10}n$; then the exponent α is given directly by the slope of the curves.

As we proceed to discuss, we obtain (depending on the values of p, q, and n) different regimes that follow Eq. (14). We start by considering the range of small and medium large n, a region of much experimental interest. If the term $\lambda^2(\sigma_n^{\mathrm{SWN}})^2/2$ in Eq. (9) is small, we expect the RA

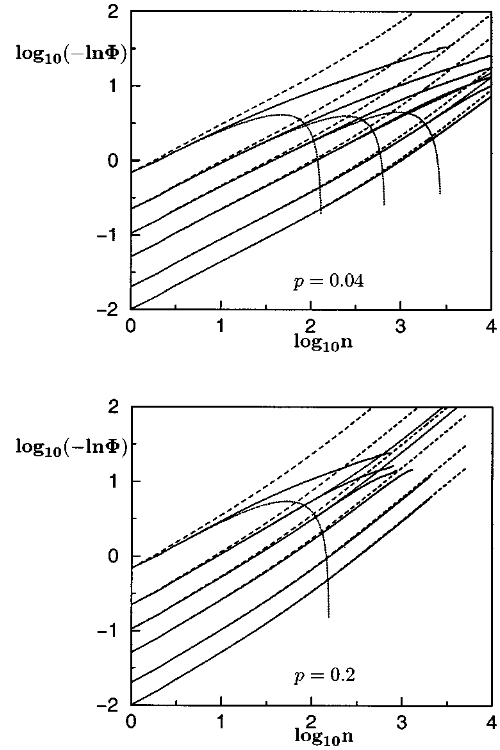

FIG. 2. (a) Survival probabilities Φ_n^{SWN} given as full lines, as a function of n, the number of steps for $p=0.04$. We display the dimensionless quantities $\log_{10}(-\ln\Phi_n^{\mathrm{SWN}})$ versus $\log_{10}n$ for the trap densities $q=0.5$, 0.2, 0.1, 0.05, 0.02, and 0.01 from above to below. In addition, the first and second cumulant approximations, Eqs. (9) and (10) are shown as dashed and dotted lines, respectively. (b). Same as (a) for $p=0.08$.

$$\Phi_n^{\mathrm{SWN}}\simeq\Phi_{1,n}^{\mathrm{SWN}}=\exp(-\gamma S_n^{\mathrm{SWN}}) \tag{15}$$

to hold very well [remember that for small q, one has $\gamma=-\ln(1-q)\simeq q$]; furthermore, if $(\sigma_n^{\mathrm{SWN}})^2\sim n$, this approximation becomes exact in the limit $n\ll q^{-2}$. Then the value of α is determined in this range by the behavior of S_n^{SWN}, which has two different regimes, see also [17]: For $n\ll p^{-2}$, Eq. (13) implies $S_n^{\mathrm{SWN}}\sim\sqrt{n}$, which leads to $\alpha=1/2$, while for $n\gg p^{-2}$, one has $S_n^{\mathrm{SWN}}\sim n$ leading to $\alpha=1$. On the other hand, for $n\to\infty$, we recalled in the Introduction that Φ_n^1 obeys Eq. (14), with $\alpha=1/3$, see Eq. (1). Furthermore, we showed in Sec. II (using upper and lower bounds for Φ_n^{SWN} based on Φ_n^1) that for $n\to\infty$ Φ_n^{SWN} also obeys Eq. (14) with $\alpha=1/3$. In Figs. 2(a) and 2(b), we show the numerically determined Φ_n^{SWN}. The scales chosen in Figs. 2(a) and 2(b) (see caption) allow us to monitor the change in the exponent α of Eq. (14). As is evident from the figures, for $p\ll1$, the Φ_n^{SWN} display a turning point for $q\simeq p$ (say, for $p=0.04$ and $q=0.05$), which we associate with a transition from $\alpha\simeq1/2$ to $\alpha\simeq1$. In Figs. 2(a) and 2(b) we also compare Φ_n^{SWN} with $\Phi_{1,n}^{\mathrm{SWN}}$ and with $\Phi_{2,n}^{\mathrm{SWN}}$. It turns out that for small values of q, the RA holds well as far as $n=10^4$. Interestingly, the RA gets better for

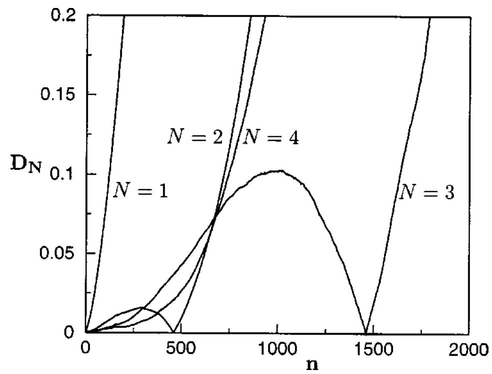

FIG. 3. The function $D_N = |\ln(\Phi_{N,n}^{\mathrm{SWN}}/\Phi_n^{\mathrm{SWN}})|$ for $N=1$, 2, 3, and 4, shown for $p=0.08$ and $q=0.05$.

larger values of p. This shows that for larger p, SWN's behave more and more like higher-dimensional lattices; as a reminder, on regular D-dimensional lattices, the RA, Eq. (15), gets better with higher D [3].

Including the second cumulants improves the quality of the approximation of Φ_n^{SWN} in the short and medium step ranges. On regular lattices, we found that the $\Phi_{N,n}^{\mathrm{SWN}}$ approximate in turn from above and from below, depending on whether N was even or odd [3]; this, however, does not seem to hold for $\Phi_{N,n}^{\mathrm{SWN}}$.

To investigate this, we plotted in Fig. 3, $D_N = |\ln(\Phi_{N,n}^{\mathrm{SWN}}/\Phi_n^{\mathrm{SWN}})|$ for $N=1$, 2, 3, and 4. We see that for small n, the approximations are getting better with increasing N, but this is not true any more for larger values of n; evidently, there is a crossover towards a regime where the long-time behavior of Eq. (1) begins to be felt.

In Figs. 4(a) and 4(b) we compare Φ_n^{SWN} with the lower bound Eq. (8) and the upper bound Eq. (6) the latter being given by the survival probability Φ_n^1 on a regular chain. Now, Φ_n^{SWN} equals Φ_n^1 for n of the order unity, since the influence of AL's may be neglected at the first steps. On the other hand, for $p \ll 1$ the lower bound Eq. (8) gets to approximate Φ_n^{SWN} very well in the limit of large n; the quality of the approximation increases with increasing trap density q. For intermediate step numbers, the true Φ_n^{SWN} decay lies between the two bounds. If the trap density q is large, walks over many AL's are of low probability; in this case, the upper and lower bounds get to be very near, so that Φ_n^{SWN} resembles Φ_n^1 closely.

We stop to note that as long as $n \ll L$ one has, evidently, that all $R_n \ll L$. Now, Φ_n probes mainly the small R wing of the R_n distribution $p_n(R)$. Under these conditions, we expect that Φ_n does not distinguish between a SWN and a related, treelike structure. To demonstrate this, we perform simulations on random trees. We obtain these by opening branches. In Fig. 5, we show a small region containing several AL's to exemplify the fact that on SWN's the local structure is determined by branching. We hence grow the trees corresponding to a given SWN class by allowing each site to sprout new branches, with probabilities that follow from the distribution given by Eq. (3). The absence of closed loops simplifies the simulations, since we do not have to determine a particular

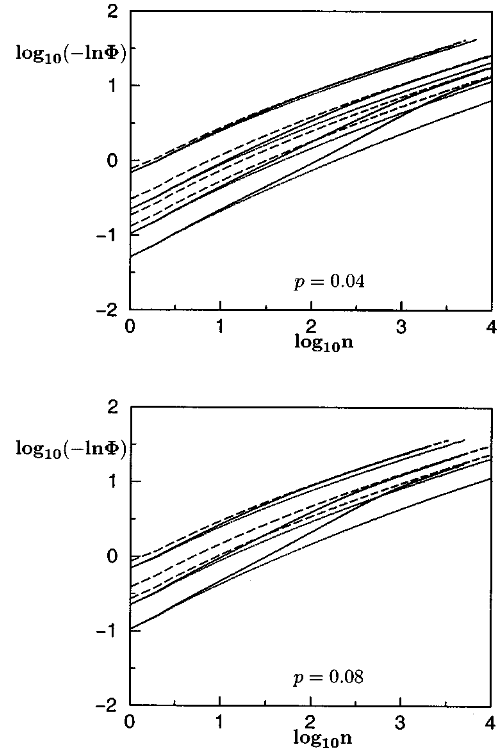

FIG. 4. (a) Data of Fig. 2(a) in the same scales, compared to the upper bound Φ_n^1 Eq. (6) (dotted lines), and to the lower-bound Eq. (8) (dashed lines). Here, $p=0.04$ and the trap densities are $q=0.5$, 0.2, 0.1, and 0.05 from above to below. (b). Same as (a) for the data of Fig. 2(b) and $p=0.08$.

realization of the SWN before we start performing the random walks to determine R_n. Instead, we let the tree grow during the random walk process, and we view the random walker as an "activator:" It diffuses on the already grown part of the tree, until making a step on a bond to the periphery, by which it triggers the addition of a new site; to this site, we assign one additional regular bond (solid line in Fig. 5) and (with probability w_k) k AL's (dashed lines) if the new site is reached via a regular bond, or two additional regular

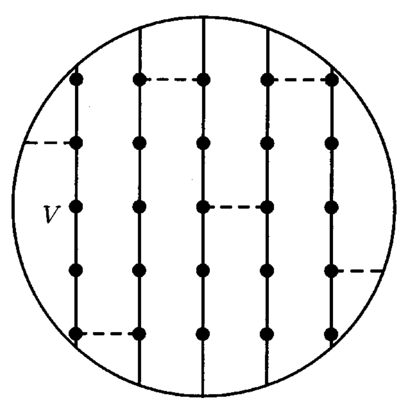

FIG. 5. The local tree structure of the SWN in the limit $L \to \infty$. The full lines indicate segments belonging to the original 1D chain and the dashed lines denote additional links AL. The circle gives the boundary of the local volume V. The segments are connected through loops, which, however extend far outside V.

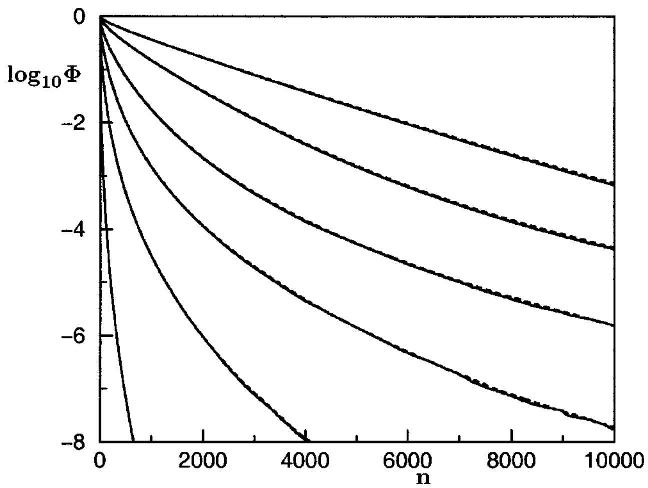

FIG. 6. The survival probability Φ_n^{tree} for trapping on trees grown as discussed in Sec. IV, compared to the Φ_n^{SWN} obtained on SWN's of size $L=9\times10^5$ (solid lines) for $p=0.04$. The trap densities q are the same (but in reverse order) as in Fig. 2(a).

bonds and $k-1$ AL's (with probability $w_k/(1-w_0),k\neq 0$) if the new site is reached via an AL. In this way, the desired number R_n of distinct visited sites in each realization is nothing else but the number of sites of the already grown tree.

In Fig. 6, we compare the numerical data for Φ_n^{tree} obtained from 3×10^6 growing processes with the Φ_n^{SWN} obtained for the simulations of Figs. 2(a) and 2(b). The agreement is very good, as can be readily checked by inspection.

We close this section with some remarks on the precision of our numerical approach. We calculated Φ_n from Eq. (5) with the help of the $p_n(R)$ distribution, which does not depend on the traps' placement. Determining $p_n(R)$ is in principle exact, because it involves only an enumeration. Thus, for example, on a 1D chain of size $2N,p_n(R)$ does not depend on the system's size, as far as $n<N$. This should be contrasted to direct simulations of Φ_n, performed on lattices with fixed trap distributions: There, one finds [10] a crossover time $t_\times$ from a stretched exponential to an exponential decay, and $t_\times$ depends logarithmically on the system's size N. This logarithmic dependence makes it impossible to see the asymptotic behavior of Φ_n, since it is hidden by the exponential decay of the finite lattice [10]. A proof that these two procedures to determine Φ_n differ is provided by our Figs. 2(a) and 2(b) where (distinct from Ref. [10]) no crossover to an exponential decay appears. In our case, the main limitation is that we cannot determine the full $p_n(R)$ distribution, but only a sample of it; we may miss some very rare events.

V. CONCLUSIONS

In this paper, we have studied the trapping problem on SWN's. We derived bounds for the survival probability Φ_n^{SWN} of walkers over SWN's with traps. We studied several approximations for Φ_n^{SWN}, and focused particularly on the Rosenstock approximation and on upper and lower bounds. These bounds are such that $\Phi_n^{\text{SWN}}\sim\Phi_n^1$ which lets us expect that asymptotically also $\Phi_n^{\text{SWN}}\sim\exp(-cn^{1/3})$ holds. The relation $\Phi_n^{\text{SWN}}\sim\Phi_n^1$ results from the existence of large 1D-like regions on SWN with low p. We verified these results by numerical simulations on SWN's of finite but large size L. In addition, we also investigated an approach to the trapping problem for $L\to\infty$. In this limit, short closed loops of the SWN's (of less than a preassigned length) have a vanishing probability; this renders the SWN's behavior (in what local quantities are concerned) equivalent to that of a certain kind of random trees. We demonstrated the correctness of this idea by performing simulations over such trees and comparing the obtained Φ_n^{tree} with the Φ_n^{SWN} found for SWN's. On such random trees, the simulations are simpler than on SWN's and the number R_n of distinct sites visited in n steps is given by the number of sites of the random tree grown during the walk.

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