Reaction-diffusion processes in scale-free networks

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ABSTRACT

In this work we investigate the dynamics of reaction-diffusion processes on scale-free networks. Particles of two types, A and B, are randomly distributed on such a network and diffuse using random walk models by hopping to nearest neighbor nodes only. Here we treat the case where one species is immobile and the other is mobile. The immobile species acts as a trap, i.e. when particles of the other species encounter a trap node they are immediately annihilated. We numerically compute $\Phi(n, c)$, the survival probability of mobile species at time n, as a function of the concentration of trap nodes, c. We compare our results to the mean-field result (Rosenstock approximation), and the exact result for lattices of Donsker-Varadhan. We find that for high connectivity networks and high trap concentrations the mean-field result of a simple exponential decay is also valid here. But for low connectivity networks and low c the behavior is much more complicated. We explain these trends in terms of the number of sites visited, S_n, the system size, and the concentration of traps.

Keywords: Scale-free networks, reaction-diffusion, trapping

1. INTRODUCTION

Diffusion-limited reactions constitute one of the most important chapters in physical chemistry. The general scheme includes two different species A and B, which diffuse freely in a given space and upon proximity they react according to A+B→C. Many different variations describe a plethora of physical phenomena. The case where A particles are immobile and the reaction between A and B is A+B→A is known as the trapping problem. The simplest mean-field analytical treatment predicts an exponential decay in the density of B's, while the earlier contributions to the subject go back to Smoluchowski,[1] who was the first to attempt to relate the macroscopic behavior with the microscopic picture by taking into account local density fluctuations. However, over the years a lot of work[2,3] has been devoted to the trapping problem which, even in its simplest form, was shown to yield a rich diversity of results, with varying behavior over different geometries, dimensionalities and time regimes.

The main property monitored during such a process is the survival probability $\Phi(n, c)$, which denotes the probability that a particle B survives after performing n steps in a space which includes traps A with a concentration c. It is well-known that Φ behaves differently in different dimensions, as well as in different time-regimes. The problem was studied in regular lattices and in fractal spaces,[2,3] and, recently, in small-world networks by Blumen and collaborators.[4–6] A new structure that has attracted considerable interest lately, though, is that of a scale-free network.[7,8] These networks are made by nodes connected to each other via undirected links. The special feature that distinguishes this class of networks is the fact that the probability for a node to have k links to other nodes obeys a power law:

$$P(k) \sim k^{-\gamma}, \tag{1}$$

where γ is a parameter that measures how densely connected a network can be. There is a wide range of real-life networks[7,8] that have been shown to follow this power-law form in their connectivity, including networks in nature, such as the cell, metabolic networks and the food web, artificial networks such as the Internet, the WWW and power grids, or even social networks, such as sexual partnership networks.

The scale-free networks, termed after the absence of a characteristic typical node connectivity, exhibit many unusual properties as compared to simple lattice models, random graphs, or even small-world networks. In this work, we study trapping processes on scale-free networks with varying connectivities. Trapping has been considered in the past as a model for energy transfer, but also in a more general frame in the context of networks, as a model for the probability of reaching targets located on the network in a given concentration via random moves. It is of interest to study the mechanism, the effects of connectivity, concentration, size, etc on such structures that exhibit these unique properties.

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2. THE TRAPPING PROBLEM

The simplest treatment of the trapping problem on a lattice assumes that when a random walker has performed n steps and has visited S_n different lattice sites at least once, the probability that it has not yet been trapped is equal to $(1-c)^{S_n}$, where c is the trap concentration. When this quantity is averaged over all different possible walks the resulting survival probability will be equal to

$$\Phi(n,c) = \left\langle (1-c)^{S_n} \right\rangle = \left\langle e^{-\lambda S_n} \right\rangle , \qquad (2)$$

where $\lambda = -\ln(1-c)$. The simplest treatment of this equation was first proposed by Rosenstock[9] and simply substitutes this expression with the typical value of the distribution, i.e.

$$\Phi(n,c) = e^{-\lambda \langle S_n \rangle} . \qquad (3)$$

This approximation has the advantage that the mean value of the number of sites visited $\langle S_n \rangle$ is well known for practically all dimensionalities (including e.g. fractal ones).[10] The formula predicts exponential decay of the survival probability with the number of steps n for $d \geq 3$, and exponential dependence on $\sqrt{n}$ in $d = 1$. In 2 dimensions the predicted behavior is rather complex, with logarithmic corrections in the exponent. The applicability of equation (3) is limited to short-times and/or large trap concentrations, but when the survival probability becomes low enough, this expression deviates significantly from the correct behavior.

A significant improvement was possible by the use of averaged quantities, known as cumulants, where the averaged quantity of equation (2) can be written as a function of the cumulant generating function:[11]

$$K(\lambda,n) = \sum_{j=1}^{\infty} (-1)^j \frac{\lambda^j}{j!} k_j(n) \quad . \qquad (4)$$

where $k_j(n)$ are the cumulants, which are associated to the moments of S_n, e.g. $k_1(n) = \langle S_n \rangle$, $k_2(n) = \langle S_n^2 \rangle - \langle S_n \rangle^2$, etc. Expression (2) then simply becomes

$$\Phi(n,c) = \exp(K(\lambda,n)) \quad . \qquad (5)$$

The use of (4) requires the knowledge of all the moments for the S_n distribution. This is possible only in one-dimensional lattices, while for $d > 1$ usually the first 2-4 moments are used.

A detailed analytical treatment of the problem was performed by Donsker and Varadhan,[12] who were able to predict the asymptotic behavior of the survival probability as

$$\lim_{n \to \infty} \Phi(n,c) = \exp(-K_d \lambda^{\frac{2}{2+d}} n^{\frac{d}{d+2}}) . \qquad (6)$$

The positive constant K_d depends only on the dimensionality and the structure of the lattice. This asymptotic expression does not provide any information on when the asymptotic limit is reached. Since it has been observed that the Rosenstock approximation describes quite well the high-Φ regime, it is obvious that a crossover to the Donsker-Varadhan behavior will take place. The location of this crossover has been studied in detail,[13–15] and it was shown that only with indirect methods it is possible to reach the asymptotic limit.

This asymptotic behavior has also been explained via heuristic arguments. The slow relaxation of Φ at long times is due to an interplay of two different factors. First, the mean-field treatment assumes a uniform trap distribution over the entire space. This is not strictly true, though, and for large enough sizes it is possible to find very extended trap-free regions. A random walker in such a region will survive for extremely long times compared to walkers in normal regions and will thus determine the asymptotic behavior. The second factor is due to unusually 'compact' random walks, which revisit many times the same sites, and thus result to a very small value of S_n, even at longer times.

Recently, a number of papers were published concerning trapping on small-world networks.[4–6] These networks, first proposed as a model by Watts and Strogatz,[16] are one-dimensional rings where additional links are inserted between two random sites with a given probability. It was shown that the results represent a fine interplay between

pure order and pure disorder statistics. Initially, the walkers feel only the presence of the one-dimensional lattice, but at longer times the behavior of the survival probability follows that of an open tree structure. The decays of the survival probability were clearly not exponential, and the cumulants description did not yield accurate coincidence with the numerical results in all of the studied cases.

In this work, we extend the trapping problem in the case where the underlying structure is a scale-free network, obeying a power-law in the nodes connectivity distribution. In this model certain nodes are designated as traps, having a concentration c, and the random walkers can only move along the nodes of this network. We present computer simulations results for different network connectivities and compare them to the known lattice Φ-behavior.

3. THE MODEL

The construction of a scale-free network takes place as follows: First, we fix the number of nodes N in the system and the γ parameter, characteristic of the particular network. By using the transformation method we select random numbers from the $k^{-\gamma}$ distribution. The formula that gives the number k of bonds that each node is going to have is derived by using the transformation as follows:

$$k = [a + r(b - a)]^{1/(1-\gamma)} \tag{7}$$

where r is a uniformly distributed random number in the range [0:1), $a = m^{1-\gamma}$, $b = M^{1-\gamma}$, while m and M denote the smallest possible (lower cutoff) and largest possible (upper cutoff) value that k can assume. In this work, we do not use any upper cutoff, thus each node is assigned a value of k in the range 1 to N.

The usual procedure now is to choose randomly two open links that belong to different nodes and connect them. Thus, a link is established between these two nodes and the process continues until all nodes have reached their preassigned connectivity. However, it turns out that this method is not very general because for small γ values there are many links that remain unpaired. Thus, we modify it in the following way: Instead of choosing random links between nodes, we first sort all nodes according to their k value and proceed to complete the highest connectivity node first, then the second, etc. This may create a biased network. We remove this possible bias by 'thermalizing' the network, i.e. we cut a random link between, say, sites A and B. We then choose a random node (say C) and create a link between B and C. We cut one link between C and one of its neighbors, rewire it to another random node, and repeat this procedure a certain number of times until the network has lost any memory of the initial bias.

The largest cluster in the network is identified via the use of a spreading algorithm. We start with a random node and mark it with a label, say X. We then mark all the nodes connected to this node by X, and proceed iteratively by labeling their neighbors, etc, until the whole cluster has been labeled. We then choose another random node that has not been labeled by X, which means that it belongs to a different cluster. We mark it by Y and again spread this labeling throughout this cluster. When the entire network has been labeled we can easily identify the largest cluster from its size.

After a network has been created, we randomly choose a percentage c of its nodes and designate them as traps. A random walker is placed on a random non-trap node i, which has a connectivity k_i, and belongs to the largest cluster. At each Monte-Carlo step the walker makes a jump towards a node connected to i (i.e. nearest neighbor) with probability $1/k_i$. This process gives a Markovian walk, since each step is independent of all previous steps. When the walker meets a trap it is annihilated and the time n to trapping is recorded. We repeat the same process for many independent random walkers and different networks. Thus, we construct a histogram $H(n, c)$ of the number of walks that lasted exactly n steps. Then, the survival probability is simply given by

$$\Phi(n, c) = 1 - \frac{1}{R} \sum_{m=1}^{n} H(m, c), \tag{8}$$

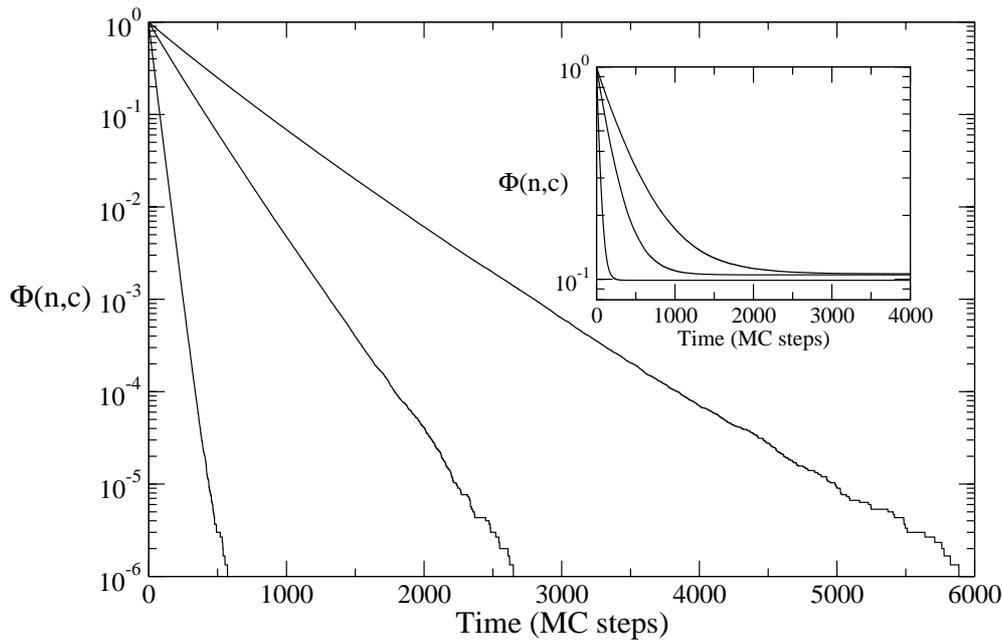where R is the total number of independent random walks sampled.

Figure 1. Survival probability as a function of time, for a network of size $N = 10^4$ and $\gamma = 2.5$, for random walkers moving on the largest cluster only. From left to right, the trap concentration $c = 0.05$, 0.01, and 0.005 . Inset: Survival probability for random walkers moving on all clusters of the system.

4. RESULTS

In figure 1 we present the survival probability on the largest cluster as a function of time for a network with $\gamma = 2.5$, and for different trap concentrations. For a relatively high trap concentration, e.g. $c = 0.05$, we can see that Φ falls very rapidly and during the first 100 steps only a small percentage of the walkers has survived. The decay retains for the largest part an exponential character. As we have mentioned above, the simple exponential decay emerges when mean-field features are present. The scale-free networks have been shown to have a very small diameter, of the order $\ln(\ln N)$.[17] This means, effectively, that one node can be reached from all other nodes in the network within only a few steps. Thus, a high trap concentration implies that there will be no large trap-free regions, since a walker can easily escape any part of the system. However, as we gradually move towards lower concentrations the survival probability can no longer be described by a simple exponential law. The exponential character disappears at higher Φ values as we decrease c, and for $c = 0.005$ there does not exist any exponential regime in the curve. The walkers, of course, survive for longer times.

In the inset of figure 1 we also present the survival probability when the walkers can originate on any cluster, and not necessarily the largest one. A common feature of the curves in the inset is the non-zero asymptotic value of the survival probability. The walkers that have not been trapped will survive for infinitely long time. This is a reflection of the fact that the network is not fully connected, but there exist isolated islands which are not linked to the main body of the network.

The results were also found to depend on the system size N. As it can be seen in figure 2 for $\gamma = 2.5$, larger networks yield a significantly lower survival probability. This is due to the higher probability of finding a node with very high connectivity, which is linked directly with the largest part of the network. Due to the power-law dependence the appearance of these nodes increases as we increase the network size. However, we can see that the Φ-curves for the two largest networks presented ($N = 50000$ and $N = 100000$) practically coincide. Moreover, this N-dependence is much weaker for networks with higher γ values. As we can see in the plot, the asymptotic behavior is very close to an exponential decay, while smaller networks deviate from this behavior.

The decay of the survival probability is also greatly influenced by γ. In figure 3 we can see that as γ increases
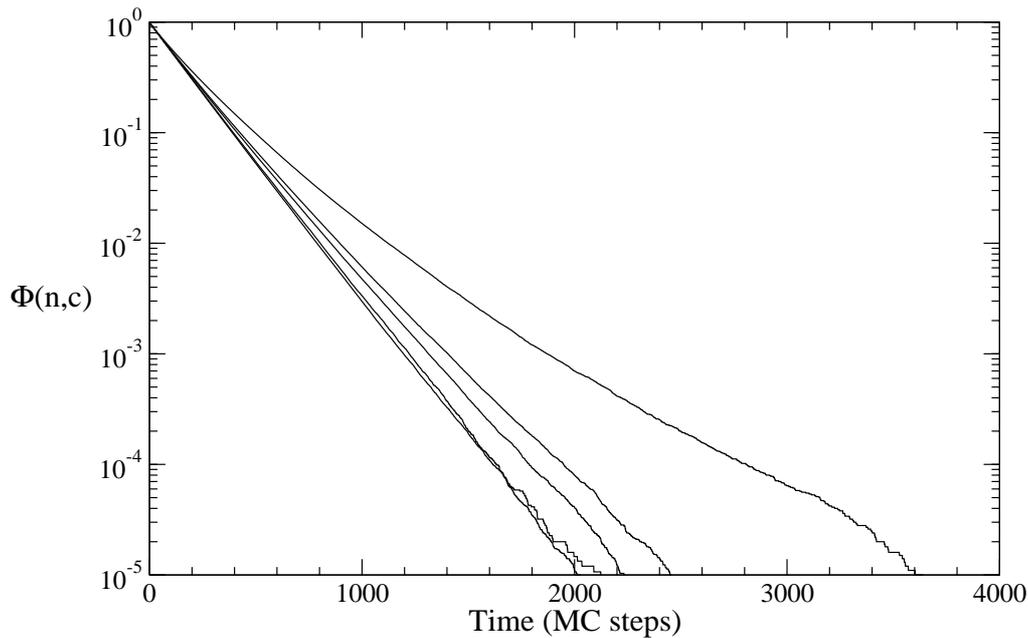
Figure 2. Survival probability as a function of time, for a network of $\gamma = 2.5$ and trap concentration $c = 0.01$. From top to bottom, the number of nodes in the network is $N =$ 1000, 5000, 10000, 50000 and 100000.

the survival probability becomes higher. Since the number of connections between the nodes decreases with γ, we expect that the average value of the number of sites visited will also decrease and the walkers will spend more time in smaller network regions. This has a dramatic influence on Φ and as we can see in the figure the difference in the survival probability between networks of $\gamma = 2$ and $\gamma = 3.5$ can be two orders of magnitude, even only after a few hundred steps. The shape of the different curves is also different, since the exponential character of the lowest γ values is no longer retained for $\gamma > 3$. This change in the decay, along with the much slower relaxation is a manifestation of the network structure, which for $\gamma > 3$ corresponds to a loosely connected network where the number of nodes with extremely high connectivity has diminished.

Scale-free networks have been considered heuristically to behave as infinite-dimensional lattices. This assumption ($d \rightarrow \infty$), however, implies that the Donsker and Varadhan law (equation 6) would yield a single exponential decay $\exp(-n)$ with the number of steps n. As we have seen, though, this result can be verified by the simulations for networks with $2 < \gamma < 3$, but not for $\gamma > 3$. The reason is that in $d \rightarrow \infty$ the probability for a walker to revisit a site is vanishingly small, since at every step the walker has an infinite number of possible sites to jump to. Thus, the revisitation probability tends to zero and the number of sites visited is equal to the number of steps performed ($\langle S_n \rangle \sim n$). Equation (3) then predicts the same behavior as (6), i.e. $\Phi(n) \sim \exp(-n)$. For scale-free networks the situation is somewhat different, though. Although there are a few highly connected nodes in the system (hubs), from where a walker can be directed to previously unsampled areas of the network, the largest percentage of the nodes has a very small number of links, e.g. $k = 1$ or $k = 2$. A walker that reaches such a node will return at the next step to its former position. Thus, the character of a scale-free network cannot be described as purely infinite-dimensional. Depending on the value of γ, the area sampled depends on how connected a system can be and how easy it is for a random walker to visit new nodes. For sparse networks, for example, the revisitation probability increases (together with the network diameter) and leads to larger deviations of the above law.

Numerical results of $\langle S_n \rangle$ on scale-free networks are presented in figure 4. As we can see, initially the number of sites visited increases with a slow rate, but after a crossover value the increase is almost linear. This asymptotic linearity is observed in all γ values, but the crossover point shifts towards longer times with increasing γ. The early time slope means that the walkers initially spend some time exploring the neighborhood they were created
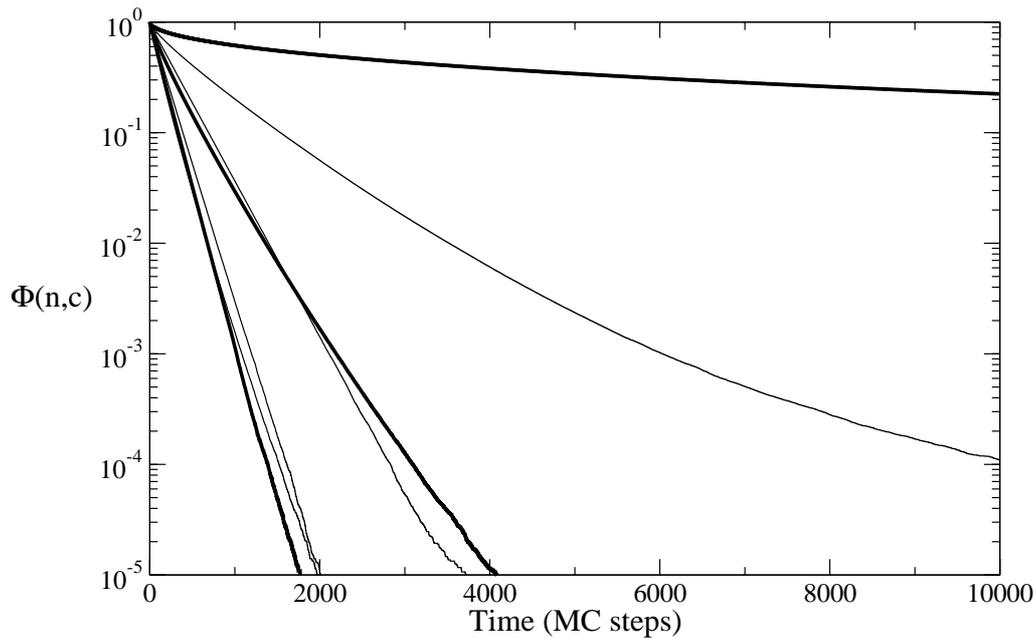
Figure 3. Survival probability as a function of time, for networks of size $N = 10000$ and trap concentration $c = 0.01$. From left to right, the network connectivity is (thin lines) $\gamma = 2.0, 2.5, 3.0$ and 3.5 . We also present the survival probability for regular networks (thick lines) in (top to bottom) $d = 1, 2$ and 3 dimensions.

in and initially visit the same sites. After the first few steps (the exact number depends on the connectivity of the network) they escape their initial territory and diffuse around the entire network. Thus, it is possible to continuously visit new sites, which results in the linear increase of S_n. The size of the network used ($N = 100000$) was one order of magnitude larger than the number of steps performed, in order to avoid finite size effects. Despite of this precaution, the curve of $\gamma = 2$ seems to deviate from linearity at longer times. This phenomenon means that revisitation already starts to exhibit itself for the finite network we study.

This linear growth of S_n is similar to the behavior exhibited in dendrimer structures, modeled by Cayley trees. These are open structures, with every node having a fixed number k of connected nodes which are always directed away from the central core. It was also shown in that case[18] that S_n had a linear increase after a short early-time sublinear regime, due to the same reasons as here.

In order to test the validity of the Rosenstock approximation for scale-free networks, we used the numerical data presented in figure 4 and computed the survival probability Φ using equation (3). The results in figure 5 show that there is almost complete coincidence between the data. This figure validates the assumption that the mean-field approximation is true for the case of scale-free networks, as we discussed above.

5. SUMMARY

In this work we presented numerical results on trapping in scale-free networks, which is a well-studied process in many other systems. A comparison between the survival probability Φ in these networks and regular lattice systems is shown in figure 3. It is obvious that trapping in the most connected networks ($\gamma = 2 - 2.5$) behaves in a similar manner as in 3-dimensional lattices. This is due to the fact that S_n grows linearly in both cases, so that new territories are sampled continuously, which results in an exponential decay of Φ. For higher γ values, the survival probability remains for the largest part (and for the trap concentrations considered here) exponential, although this is not the case for trapping in lattices with $d \geq 2$. The case of two dimensions represents the borderline dimension for recurrent random walks in lattices, and the relaxation of Φ is not exponential, while for
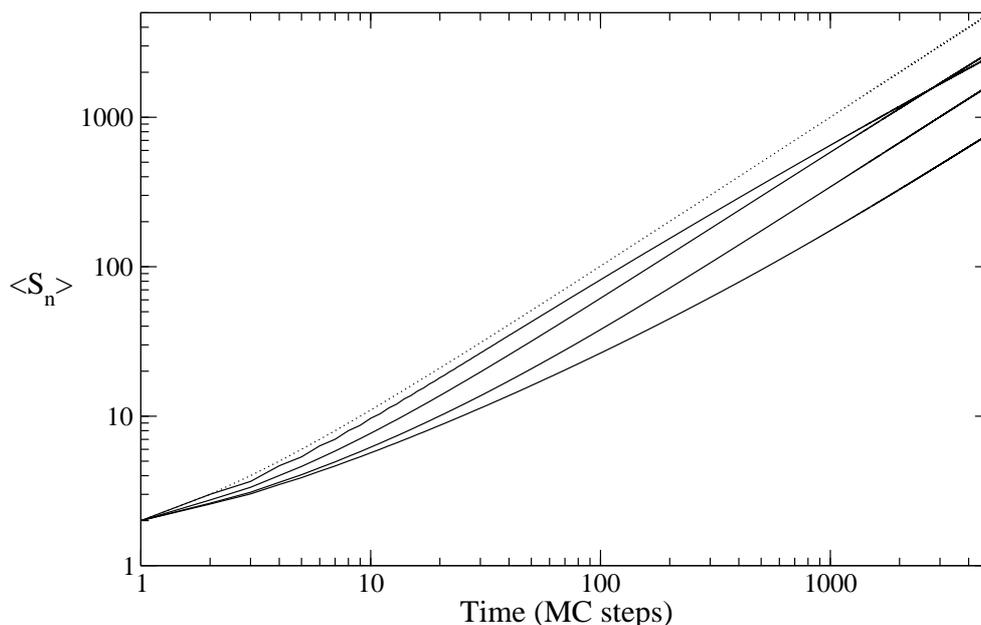
Figure 4. Number of distinct sites visited $\langle S_n \rangle$ after n steps for scale-free networks with (solid lines, top to bottom) γ=2.0, 2.5, 3.0 and 3.5. The dashed line is the infinite-dimensional case of $\langle S_n \rangle = n+1$. The network size was $N = 100000$.

$d = 1$ the survival probability is considerably higher, since the walkers are confined between two trapping sites and perform a random walk in this region.

We also note that similar to the behavior of Φ in scale-free networks with small γ values is the case of dendrimer structures, an open structure as described above, contrary to the compact networks studied here. Because in these systems the number of sites visited grows linearly an exponential decay of Φ was also observed.[18] Thus, we see that the structure itself does not necessarily determine the behavior of Φ, but the important common feature in all these systems (e.g. 3-dimensional lattice, scale-free network, dendrimer) is the way that the number of sites visited S_n increases with time.

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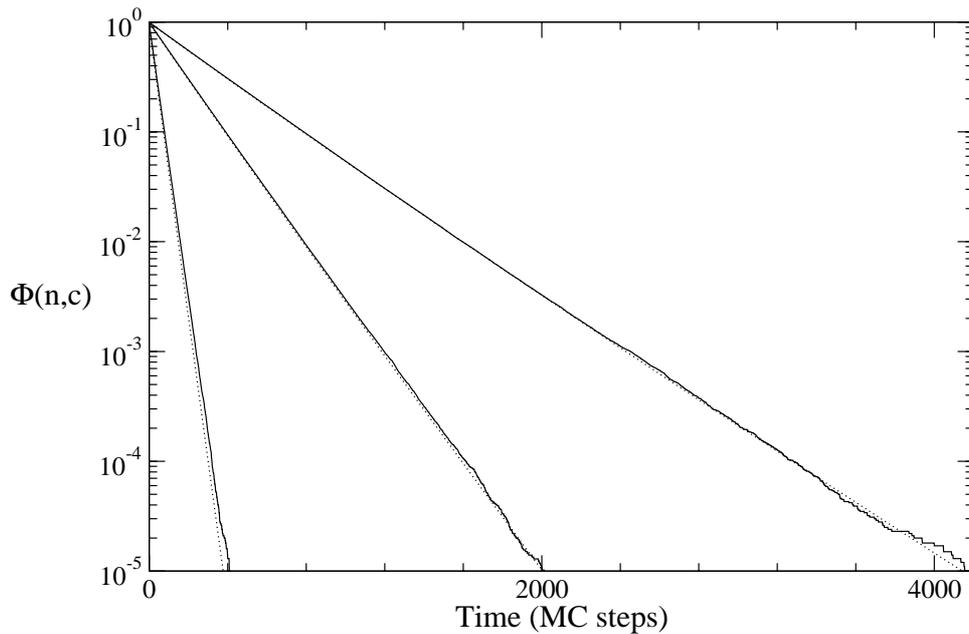
Figure 5. Comparison of the directly calculated survival probability (solid lines) and the Rosenstock approximation (dashed lines), based on the numerical data of figure 4, for a network with $\gamma = 2.5$ and $N = 100000$. From left to right: $c = 0.05, 0.01, 0.005$.

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