Target problem on small-world networks

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In this work we focus on reactions on small-world networks (SWN's), disordered graphs of much recent interest. We study the target problem, since it allows an exact solution on regular lattices. On SWN's we find that the decay of the targets (for which we extend the formalism to disordered lattices) is again related to $S(n)$, the mean number of distinct sites visited in n steps, although the $S(n)$ vs n dependence changes here drastically in going from regular linear chains to their SWN.

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I. INTRODUCTION

Small-world networks (SWN's) are structures of much recent interest [1–6]. One may construct such structures by adding, in a random way, links to an ordered lattice; the usual way consists in assuming that links between any pairs of sites are equiprobable [1,4,5].

In this way interesting structures arise, whose characteristic feature is that even at a very low density of additional links, the chemical distance (minimal distance between two points) drastically decreases from its original value on the underlying regular lattice. Realizations of SWN's range from social acquaintances to computer nets. Starting from a simple linear chain, SWN's are particularly interesting, because they may be seen as a precursor for the formation of networks, a subject of quite difficult treatment. Note that SWN's possess inherent loops and therefore display other properties than disordered treelike structures, such as hyperbranched polymers [6,10].

The statical properties of SWN's have attracted much interest. Also some studies have focused on SWNs' dynamical properties. These may be related in a chemical picture to monomolecular reactions. In this work we focus on bimolecular reactions on SWN's, by studying the (perhaps simplest) model, namely target annihilation [11–15]. The model [11,12] supposes that there exist static target molecules (denoted by T), randomly distributed on the lattice; the T's are annihilated by other molecules (the A's) that perform random walks on the lattice and destroy the T's at first encounter. As is well-known in the literature, the target decay is different from trapping [16–19], for which a general analytical solution in dimensions larger than 1 is not known [20]; for target annihilation the decay on regular lattices can be given in analytical form, in which only $S(n)$, the mean number of distinct sites visited in n steps, enters [11,12]. This is vastly different from trapping, which shows so-called Lifschitz anomalies [19], such that in low-dimensional systems the decay depends not only on $S(n)$ but on higher moments of the number of distinct sites visited [16–19]. The question is now whether the target decay stays a simple function of $S(n)$ in the presence of massive *disorder*, such as is found for SWN's.

As we will show in the following both analytically and numerically, for random SWN's the decay of the targets is still related in a simple manner to $S(n)$, although in going from a linear chain to the corresponding SWN the dependence of S on n changes from $S\sim\sqrt{n}$ to $S\sim n$.

The paper is structured as follows: In Sec. II we present the SWN. Furthermore, we derive the target decay for arbitrary networks, and reformulate the problem in order to comply with the disordered nature of the SWN. In Sec. III we present the results of our computer simulations for random-walks on SWN's; we determine both $S(n)$ and the target decay and compare the results with the analytical forms of Sec. II. Section IV summarizes our conclusions.

II. SMALL-WORLD NETWORK AND THE TARGET PROBLEM

A realization of the small-world network (SWN) we consider is obtained by starting from N sites on a ring, where each of the sites is connected by bonds to its two nearest neighbors. Then we consider all pairs (i,k) of sites, which are not in nearest-neighbor position, and connect with probability $2p/(N-3)$ the corresponding sites with a new bond. In this way we add on the average pN new bonds to the ring. This construction of the SWN does not delete bonds as in Ref. [1]; it follows the procedure outlined in Refs. [2] and [4], which we found to be better suited for analytical approaches. Noting that the SWN's so obtained are undirected graphs, we introduce as usual the corresponding symmetric connectivity matrix $\mathbf{C}$, whose coefficients C_{ik} give the numbers of bonds connecting sites i and k; the diagonal elements of $\mathbf{C}$ are zero.

Let us recall some basic definitions concerning random walks (RW) on general graphs. This will help us to generalize the target problem [11,12] from RW on regular [8,9,20] to random graphs [21–23]. A random walk on an arbitrary graph is constructed from the probabilities to jump from site i to k,

$$W_{ki}=\frac{C_{ki}}{D_i}=(\mathbf{CD^{-1}})_{ki}, \tag{1}$$

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where $D_i=\Sigma_j C_{ji}$ ensures the normalization of the probabilities; furthermore, in Eq. (1) the matrix **D** is defined by $D_{ki}=D_i\delta_{ki}$.

Now **W** is a stochastic matrix, which defines a Markov chain [21–24], namely, the random walk on the SWN. Note, however, that since the SWN has randomly distributed bonds, the D_i are random; hence in general $D_i\neq D_k$ and thus $W_{ik}\neq W_{ki}$. From Eq. (1) the probability of reaching in n steps site j starting from site i is

$$P_{ji}=(\mathbf{W}^n)_{ji}. \tag{2}$$

Equation (2) gives rise to the generating function

$$\tilde{P}_{ki}(z)\equiv\sum_{n=0}^{\infty} z^n P_{ki}(n)=\left(\sum_{n=0}^{\infty}(z\mathbf{W})^n\right)_{ki}=[(1-z\mathbf{W})^{-1}]_{ki}. \tag{3}$$

Equation (3) is identical in structure to the expression valid for regular lattices [8,9]. In the same way it is possible to define a generating function $\tilde{F}_{ki}(z)$ through the probabilities $F_{ki}(n)$ of reaching for the first time site k starting from i after n steps. The basic relationship between $P_{ki}(n)$ and $F_{ki}(n)$ is given by

$$P_{ki}(n)=\sum_{m=0}^{n} F_{ki}(m)P_{kk}(n-m). \tag{4}$$

Multiplying Eq. (4) by z^n and summing over n leads to the connection

$$\tilde{F}_{ki}(z)=\frac{\tilde{P}_{ki}(z)-\delta_{ki}}{\tilde{P}_{kk}(z)} \tag{5}$$

between generating functions. One may note in all these expressions the explicit dependence on i. We stop to note that Eqs. (3) and (5) give an analytical expression in closed form for $\tilde{F}_{ki}(z)$. Expanding $\tilde{F}_{ki}(z)$ in a series in z leads to the $F_{ki}(n)$, which are fundamental quantities in the target decay; see Eqs. (8)ff below.

From the relation

$$(\mathbf{W}^n)^T=[(\mathbf{C}\mathbf{D}^{-1})^n]^T=(\mathbf{D}^{-1}\mathbf{C})^n=\mathbf{D}^{-1}\mathbf{W}^n\mathbf{D} \tag{6}$$

one deduces with the help of Eqs. (2) and (3) that $\tilde{P}_{ki}(z)=(D_k/D_i)\tilde{P}_{ik}(z)$, which in turn implies the property

$$\tilde{F}_{ki}(z)=\frac{\tilde{P}_{kk}(z)}{D_k}\frac{D_i}{\tilde{P}_{ii}(z)}\tilde{F}_{ik}(z) \tag{7}$$

of the generating function $\tilde{F}_{ki}(z)$.

Now we are placing with probability q walkers on the lattice sites and consider the decay behavior of resting targets that are annihilated if a walker is visiting their site [11,12]. The probability that a walker starting at i reaches the target at k during the first n steps is

$$H_{ki}(n)=\sum_{m=1}^{n} F_{ki}(m). \tag{8}$$

Hence the probability that the target at site k survives n time steps for a certain initial distribution κ_i of walkers is given by

$$\phi_k(n)=\prod_{i,i\neq k}[1-\kappa_i H_{ki}(n)], \tag{9}$$

and the distribution function κ_i is 1 if a walker is placed at site i for $n=0$ and 0 otherwise. Now it is straightforward to perform the average over the quenched disorder of the walker distributions, because the occupancy of each site is independent from the others:

$$\begin{aligned}\langle\phi_k(n)\rangle&=\sum_{\{\kappa_i=0,1\}}\prod_{i,i\neq k} q^{\kappa_i}(1-q)^{1-\kappa_i}[1-\kappa_i H_{ki}(n)]\\&=\prod_{i,i\neq k}\sum_{\kappa=0,1} q^{\kappa}(1-q)^{1-\kappa}[1-\kappa H_{ki}(n)]\\&=\prod_{i,i\neq k}[1-qH_{ki}(n)]\equiv\Phi_k(n).\end{aligned} \tag{10}$$

Hence $\Phi_k(n)$ in Eq. (10) is averaged over the initial placement of the walkers and their motion. However, $\Phi_k(n)$ depends on the particular SWN and on the site k of the target. Note also that via Eq. (8) the decay $\Phi_k(n)$ can be calculated exactly, when the $F_{ki}(n)$ are known.

To analyze the decay given by $\Phi_k(n)$ we consider the expansion of $\ln\Phi_k(n)$ in powers of q [11]:

$$\begin{aligned}\ln\Phi_k(n)&=\sum_{i,i\neq k}\ln[1-qH_{ik}(n)]\\&=-\sum_{j=0}^{\infty}(q^j/j)\sum_{i,i\neq k}[H_{ki}(n)]^j.\end{aligned} \tag{11}$$

Taking only the first term in this expansion leads to an upper bound of $\Phi_k(n)$, since only terms of negative sign are discarded. On the other hand, $H_{ki}(n)$ is the probability of reaching k starting from i in n steps and therefore the inequality $H_{ki}(n)<1$ always holds. Replacing powers of $H_{ki}(n)$ by $H_{ki}(n)$ itself leads to a lower bound [11]. Putting these expressions together we are led to

$$\exp\left(-\gamma\sum_{i,i\neq k}H_{ki}(n)\right)\leqslant\Phi_k(n)\leqslant\exp\left(-q\sum_{i,i\neq k}H_{ki}(n)\right), \tag{12}$$

where $\gamma=-\ln(1-q)$. Note that for small q, one has to first order $\gamma=q$, so that the bounds tend for small q to the same exact limit.

Let us turn now to the mean number of distinct sites $S_i(n)$, visited by a random walker starting at i in n steps. Conventionally [8,9] one takes $S_i(0)=1$. Now, one has for disordered lattices:

$$S_i(n)=\sum_{k,k\neq i}\sum_{m=1}^{n}F_{ki}(m)+1=\sum_{k,k\neq i}H_{ki}(n)+1. \tag{13}$$

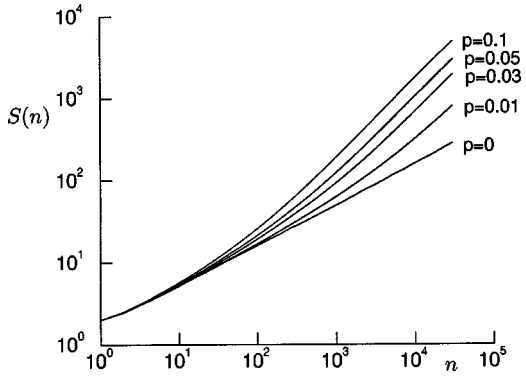

FIG. 1. The mean number $S(n)$ of distinct sites visited in n steps on SWN, plotted in double logarithmic scales. In these axes power-law behaviors $S(n)\sim n^{\alpha}$ are directly visible as straight lines of slope α. The underlying SWN belong to different p, as indicated.

In general, $S_i(n)$ depends explicitly on i; note that the sum in Eq. (12) differs from the sums in Eq. (13) by the fact that in Eq. (13) one sums over k. For regular lattices, of course, the situation simplifies, since, first $S_i(n)\equiv S(n)$ independent of i, and second, in Eq. (7) $\tilde{P}_{kk}(z)$ and D_k are also k independent, from which $\tilde{F}_{ki}(z)=\tilde{F}_{ik}(z)$ and $H_{ki}(n)=H_{ik}(n)$ follow; hence one can replace the sums in Eq. (12) simply by $S(n)-1$. In the limit of small q one recovers the former result for the target decay on *regular* lattices [11,12]:

$$\Phi(n)\simeq\exp\{-q[S(n)-1]\}\equiv\tilde{\Phi}(n). \tag{14}$$

It should be emphasized that translational invariance is sufficient but not necessary to imply Eq. (14), since the independence of P_{kk} and D_k of k also holds, for example, on deterministic Sierpinski gaskets. Having Eq. (14) as a good approximation for the target decay is extremely worthwhile, since, in general, $S(n)$ is much easier to determine than $\Phi(n)$. On the other hand, Eq. (14) does not have to hold; the complicated forms found in the *trapping* problem may serve as clear-cut counter examples [16–19].

III. NUMERICAL RESULTS AND COMPARISON TO ANALYTICAL FORMS

To check the situation on SWN's, given that in general Eq. (14) does not have to hold exactly for the target decay on disordered graphs, we performed numerical simulations. We started by first investigating the behavior of $S_i(n)$, the mean number of distinct sites visited during n steps of a walk on a SWN starting from site i. We determine $S(n)\equiv\langle S_i(n)\rangle$ by averaging over 500 random walks and afterwards over 100 SWN realizations for each given probability p. As underlying lattice we have chosen a ring of size $N=50\,000$. The result for $S(n)$ is displayed in Fig. 1 in double logarithmic scales. This display stresses the power-law regimes, $S(n)\sim n^{\alpha}$, for which the curves show up as straight lines of slope α. As is evident from the figure, $S(n)$ follows first a power law behavior, $S(n)\sim n^{1/2}$, typical for a $1d$ lattice. After an intermediate regime $S(n)$ turns to the behavior for large n, for which we find $S(n)\sim n$. This dependence is typical for random walks on regular, infinite lattices of dimensions $d>2$.

Hence in what dynamical properties are concerned, the SWN construction pushes here the ''effective'' dimension from $d=1$ to d values larger than 2; in fact similar dynamical features have been observed in other contexts [5,6].

We note that the linear dependence of $S(n)$ on n for $n\gg 1$ holds for all values of $p>0$, On the other hand, for $p=0$ we recover exactly the $S(n)\sim n^{1/2}$ long-time behavior of $1d$ lattices. Thus the problem is different, depending on whether $p=0$ or $p>0$. A similar finding was observed for SWN concerning the quantity $\mathcal{L}=\langle l\rangle/N$ (with $\langle l\rangle$ being the mean distance between sites): $\mathcal{L}$ is found for $p\to 0$ to undergo a discontinuity in the thermodynamic limit which is called the small-world transition [2,3,7]. Qualitatively we understand the transition for $p>0$ to $S(n)\sim n$ by noticing that in SWN the $1d$ structure of the ring is interrupted on the average every $1/(2p)$ sites by bifurcations. This topological feature allows the walker to visit new regions on the ring.

Hence we have $\xi_{SWN}=1/p$ as a basic length scale of the SWN [2]. For $1\ll n\sim p^{-2}$ the random walker explores a linear region of $\xi_{reg}\sim n^{1/2}$ and visits on the average $S(n)\sim\sqrt{n}$ new sites in n steps. For $1\ll p^{-2}\ll n$ the walker spends around $\xi_{SWN}^2=p^{-2}$ steps inside each linear segment; $S(n)\sim n$ and the mean number of long-range links the walker visits in n steps is np^2.

Putting these aspects together we therefore assume that on the SWN $S(n)$ obeys a scaling law:

$$S(n)=n^{1/2}f(n/\xi_{SWN}^{\alpha})=n^{1/2}f(np^{\alpha}) \tag{15}$$

(we left now α to be an adjustable parameter), where $f(x)$ is a universal scaling function with the limiting forms

$$f(x)\sim\begin{cases}\text{const} & \text{for } x\ll 1\\ \sqrt{x} & \text{for } x\gg 1.\end{cases} \tag{16}$$

The upper relation holds because for small np^{α} most of the walkers do not yet encounter any long-range links, so that the walks proceed along linear segments.

Plotting $f(np^{\alpha})\equiv S(n,p)/\sqrt{n}$ against np^{α} we found out (for $n\gg 1$ and $p\ll 1$) that in the range investigated we bring our curves better into coincidence if we take in Eq. (15) $\alpha=1.85$ instead of $\alpha=2$. Figure 2 displays the best master curve behavior which we could achieve and shows that scaling is correct. Evidently the number of decay curves in Fig. 2 is limited; nonetheless, should our finding persist for much larger lattices, it would be extremely interesting, since it leads to a nontrivial scaling exponent α.

In Fig. 3 we present the decay laws for the targets (solid lines). In the numerical simulations the walkers are placed randomly with probability $q=0.004$ on a one-dimensional small-world lattice with $N=50\,000$. All sites not occupied by walkers are viewed as targets. It turns out that a configurational average over 100 SWN realizations, over each of which target annihilation is simulated 500 times, is sufficient to lead to smooth decays. These are given in Fig. 3 through solid lines. Note that, based on the structure of the problem,

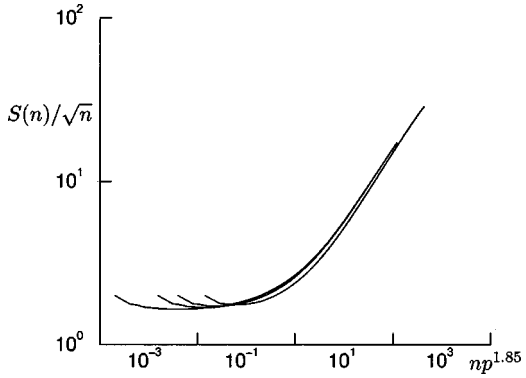

FIG. 2. Replot of the data of Fig. 1 for $p=0.01$, 0.03, 0.05, and 0.1 in the form $S(n)/\sqrt{n}$ as a function of $np^{1.85}$, in order to display the scaling discussed in the text, Eqs. (15) and (16). The curves for the smaller p begin more to the left.

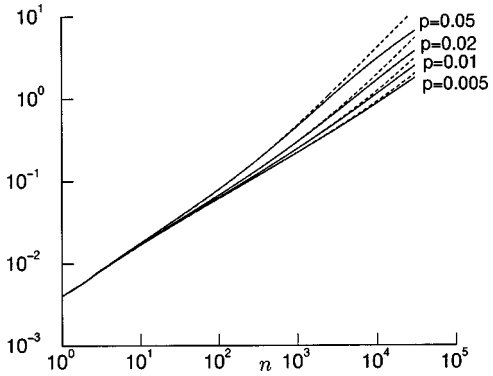

FIG. 3. Survival probabilities $\Phi(n)$ of the targets as a function of n, the number of steps. We display in double logarithmic axes $-\log_{10}\Phi(n)$ vs n for different SWN ensembles, whose p values are as given. The density of the walkers is $q=0.004$. The solid lines give the results of the simulations, and the dashed lines are the approximate form for $\Phi(n)$; see text for details.

e.g., Eq. (10), it is unnecessary to perform an additional configurational average over the target positions.

We compare now the decay $\Phi(n)$ obtained numerically, with Eq. (14), computed for $q=0.004$, where $S(n)$ was determined as in the beginning of Sec. III. The results for $\tilde{\Phi}(n)$ are given through dashed lines in Fig. 3. Comparing the two decays we find for short and intermediate times a very good agreement for all SWN considered ($p=0.005$, 0.01, 0.02, and 0.05). Only at large n does $\Phi(n)$ decay slower than $\tilde{\Phi}(n)$, a fact which we attribute in part to the large fluctuations of $S_i(n)$. Overall, however, we find a quite reasonable picture for the decay of the targets.

IV. CONCLUSIONS

In this work we have studied the target problem on SWN's. We have first determined analytically (extending thus the formalism of Refs. [11] and [12]) the changes which the problem encounters when studying disordered lattices. The important finding here was that the basic structure of the equations stays the same as for regular lattices, but that there appears an asymmetry in the sums involved in determining $S_i(n)$ and the decay $\Phi_k(n)$, where $i(k)$ denotes the initial position of the walker (target). To check in how far the approximating form Eq. (14) stays very good we performed computer simulations of $S(n)=\langle S_i(n)\rangle$, the mean number of distinct sites visited and of $\Phi(n)=\langle\Phi_k(n)\rangle$ the survival probability of the targets on the SWN.

In what $S(n)$ is concerned we find for SWN's that as soon as there appear long-range bonds, the large n behavior of $S(n)$ changes from $n^{1/2}$ to n. As a special aspect (dependence on p) we find, furthermore, that $S(n)$ obeys a scaling law of the form $S(n)=n^{1/2}f(np^{\alpha})$; from our numerical investigations here we infer for α a value around 1.85. With respect to the targets' decay Eq. (14) reproduces at short and intermediate times the numerically determined behavior very closely; marked deviations show up only at quite long times.

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