Absence of depletion zone effects for the trapping reaction in complex networks

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(Received 15 June 2009; published 16 October 2009)

In the present work we examine in detail the formation of a depletion zone in the trapping reaction in networks, with a single perfect trap. We monitor the particle density $\rho(r)$ with respect to the distance r from the trap. We show using Monte Carlo simulations that the depletion zone is absent in regular, Erdos-Renyi (ER), and scale-free (SF) networks. The density profiles show significant differences for these cases. The particles are homogeneously distributed in regular and ER networks with the depletion effect appearing in very sparse ER networks. In SF networks we reveal the important role of the hubs, which due to their high random walk centrality are critical in the trapping reaction. In addition, the degree distribution plays a significant role in the distribution of the particles recovering the depletion zone formation for high γ values. The mean connectivity of the network is found to play a significant role in both ER and SF networks.

DOI: 10.1103/PhysRevE.80.046111 PACS number(s): 82.40.Ck, 89.75.Hc, 02.70.−c

I. INTRODUCTION

In recent years there has been a considerable amount of interest in investigating diffusion using models of random walks [1–3]. The systems which have recently attracted interest for studying their properties are complex networks [4,5] particularly in the diffusion-reaction scheme [6–11]. These networks include communication networks such as the Internet, social networks, networks of collaboration between scientists, transport networks, gene regulatory networks, and many other examples in biology, sociology, economics, and even linguistics.

This interest has emerged because it became apparent that these properties are very different in comparison to lattices. For example, in the annihilation reaction of one-kind it was shown that the well known depletion zone in lattices does not appear in networks [8,12]. Similarly, for the two-kind reaction the formation of segregation of the two kinds of reactants does not appear in scale-free networks [8,13].

In the present work we examine in detail the formation of a depletion zone in the trapping reaction in networks. Since scale-free networks are thought of as systems of infinite dimensionality, it is also expected here that trapping behaves differently than the well known case in lattices. In graph theory, the Erdos-Renyi model [14] is used to generate random graphs by taking N nodes and introducing a link between them with a probability p. This yields (in the limit $N \to \infty$) a Poisson distribution (for $p<1$) of the degree k of the node: $P(k)=(\langle k\rangle^k/k!)e^{-\langle k\rangle}$ with $\langle k\rangle = p(N-1)$. When $p=1$, all possible links exist and this construction gives the complete graph, where each site is connected to all the other sites in the graph.

Scale-free (SF) networks have been widely studied during the recent years since they describe many real-world structures [4,5,15,16]. This class of networks is defined by having a degree distribution which follows a power law $P(k) \propto k^{-\gamma}$, where γ is a parameter which controls the broadness of the distribution and is characteristic of the structure of the network. Another important parameter in the construction of the network is m or $k_{\min}$, which indicates the minimum number of links a node can have and plays a large role in the connectivity of the network.

SF networks, termed after the absence of characteristic typical node connectivity, exhibit many unusual properties compared to simple lattice models, random graphs, or even small-world (Watts-Strogatz) networks [6]. This scale-free character results in the existence of a small number of superconnected nodes (termed hubs) which have been shown to have a central role in the interpretation of many of the network properties. A lot of work has been devoted in the literature to the study of static properties of the networks, while interest is growing for dynamical properties.

II. RANDOM WALKS AND TRAPPING

An important process related to random walk theory is trapping. Trapping reactions have been widely studied in the frame of physical chemistry as part of the general reaction-diffusion scheme. The trapping reaction can be formulated as $A+T \to T$, where T is a static trap and A is a diffusing species that may be annihilated upon collision with the trap depending on the trap strength. This corresponds to the original Smoluchowski work on coagulation, a process involving the trapping of mobile particles A by stationary aggregates B, which became the basis for classical reaction theory [17].

Over the years a lot of work has been devoted to the trapping problem which, even in its simplest form, was shown to yield a rich variety of results, with diverse behavior over different geometries, dimensions, and time regimes [1,2,18,19]. The quantity that is usually monitored for such a process is the survival probability $\Phi(n,c)$, which denotes the probability that a particle A survives after performing n steps in a space which includes traps with a concentration c. The problem was studied in regular lattices and in fractal spaces [1,18–21] and recently in small-world [9], Erdos-Renyi [11], and scale-free networks [6,11].

In the trapping reaction in low dimensions, the occurrence of A-T reactions creates a depletion zone around the trap,

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which is a form of self-segregation of reactants [22]. The growth of the depletion zone in the trapping reaction in low dimensions leads to anomalous kinetics for a variety of dynamic quantities. A number of studies have been devoted to the problem of the depletion zone in the vicinity of a single trap [22–30]. Among many possible quantities to characterize the dynamics of the depletion zone is the so-called θ distance (r_θ), which is defined as the distance from the trap T to the point where the concentration of the reactants A reaches a given arbitrary fraction $(0<\theta<1)$ of its initial value [22,23].

The θ distance has been shown, by theory [19,30] and experiment [25], to increase asymptotically as $t^{1/2}$ in one dimension (1D). The $t^{1/2}$ dependence in 1D is explained on the basis of diffusion of particles toward the trap. In three dimensions, the depletion zone stays localized in the asymptotic time limit and hence the θ distance is time independent. The two-dimensional (2D) case produces the most intriguing result of nonuniversality for the θ distance, which is theoretically predicted to scale as $t^{\theta/2}$ at the long-time limit, namely, it depends on the seemingly arbitrary choice of θ. Experimental work and computer simulations have verified this behavior [22–25].

The aim of this work is to study the problem of trapping in networks, which is an analog to the propagation of information in a network. This information is in the form of "packets," e.g., like the data packets used in communication networks in routers, which receive and transmit packets over a communication network. A trap acts as a node which is malfunctioning and where the information is lost, e.g., like a router which can receive but not transmit data due to a malfunction or an e-mail server unable to forward incoming mails. Furthermore, the model may be relevant to social systems, where some information may initially spread randomly, but in later stages it might be held by certain individuals.

The particle density $\rho(t)$, which represents the fraction of particles left on the network, has been studied in [11]. This, however, provides no information of how the particles are distributed on the network and in relation to the location of the trap. Here we study the distribution of the particles for various network types, connectivity patterns, and trap locations. We model the diffusion of particles with many random walkers and a single perfect trap placed on a random node or a node with a specific degree. We use Monte Carlo simulations.

III. MODEL

ER networks are generated in the following manner: given a finite set of N isolated nodes, all the $N(N-1)/2$ pairs of nodes are considered and a link between two nodes is added with probability p. The construction of an SF network follows the standard configuration model [31,32]. This model introduces correlations in the range $2<\gamma\leq 3$, which are, however, present in most real-world networks [33]. First, we fix the number of nodes N in the system and the γ parameter of the particular network and each node i is assigned a number of links k_i from the $k^{-\gamma}$ distribution. The value of k lies in the range from $k_{\min}$ or m (m being typically in the range of 1–3) to $k_{\max}=N-1$ (no upper cutoff value is used for k).

Initially no links are established in the system. Each node i extends k_i "hands" toward all other nodes. We randomly select two such hands (that do not belong in the same node) and connect them, thus creating a link. No double links are allowed, so if two nodes are already connected this link is rejected. We continue this process until all nodes have reached their preassigned connectivity. However, it is possible that in the last stages of the construction we will reach a dead end where no further links may be established according to the above rules. In this case we simply ignore the extending hands that cannot be connected, since their number is always very small and they generally do not influence the structure of the network. We use the same algorithm to construct regular random networks (networks in which nodes are connected randomly but have equal degree).

We identify the largest cluster of the network using a breadth-first search (BFS) algorithm as described in [34]. Breadth-first search is one of the simplest algorithms for searching a graph and the archetype for many important graph algorithms. Given a graph $G=(V,E)$ and a distinguished source vertex s, breadth-first search systematically explores the edges of G to record every vertex that is reachable from s. It computes the distance (smallest number of edges) from s to each reachable vertex. Breadth-first search is so named because it expands the frontier between discovered and undiscovered vertices uniformly across the breadth of the frontier. The algorithm discovers all vertices at distance r from s before discovering any vertices at distance $r+1$. We use the trap as a source when running BFS and discover the geodesic distance from the trap to every node in the network, i.e., the number of links in the shortest path from the trap to an arbitrary node.

Diffusion is modeled by random walks of particles, which are independent of each other. These particles are initially placed at random nodes on the network. We have performed simulations, both allowing and prohibiting multiple occupancy (i.e., the property of a node to be occupied by more than one particle). In the figures we present, multiple occupancy is not allowed unless explicitly mentioned in the figure caption. The initial particle density value was $\rho_0=0.25$. We distinguish two cases. In the first case we place a perfect trap either on a random node and in the second case we place it on the node with the maximum degree. We monitor the particle density $\rho(r)$ with respect to the distance r from the trap, i.e., the number of particles on all the nodes that span this distance from the trap.

The steps of the algorithm for particle diffusion on networks are described as follows:

(1) We select a particle.

(2) One of its neighboring (adjacent) nodes is randomly chosen.

(3) If multiple occupancy is not allowed and the particle lands on an occupied node, we select another particle.

(4) If the site we chose is the trap, then the particle is removed from the network, else it is allowed to land on the chosen node.

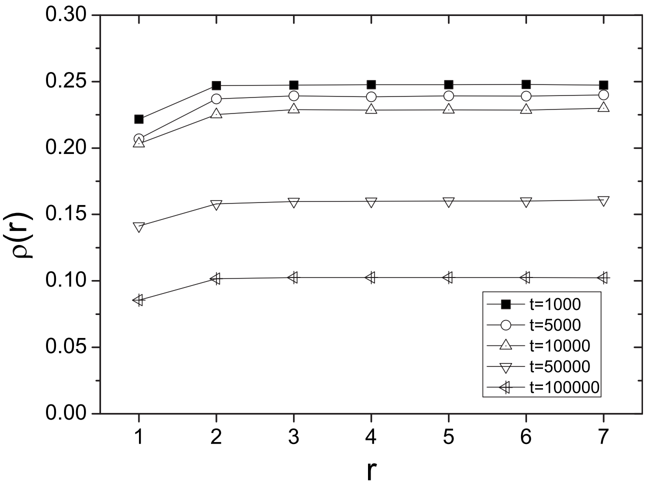

FIG. 1. Particle density $\rho(r)$ vs distance r for various times. Regular random networks of $N=10^5$ with $k=10$. The trap is placed on a random node.

(5) After each particle on the network at a given time has moved exactly once, one time step [Monte Carlo step (MCS)] has been accomplished.

We typically use networks of size $N=10^5$ or $N=10^4$ (where N is the number of nodes of the network). In the case of $N=10^5$ we have performed 10 runs on 100 different network configurations and in the case of $N=10^4$ we used 1000 different network configurations (totaling 1000 runs in both cases). For $N=10^5$ simulations are performed for 10^5 MCS while for $N=10^4$ the time is extended to 10^6 MCS.

IV. RESULTS

We examine the particle distribution for the trapping reaction by Monte Carlo simulations in regular random networks, in ER and in SF networks. The lines between the points which are the simulation results in all figures are provided as a visual guide. In Fig. 1 we show $\rho(r)$ in regular random networks of $N=10^5$ and $k=10$ with the trap placed on a random node. We observe here that $\rho(r)$ does not depend on r, the distance from the trap node. This means that the depletion zone is completely absent.

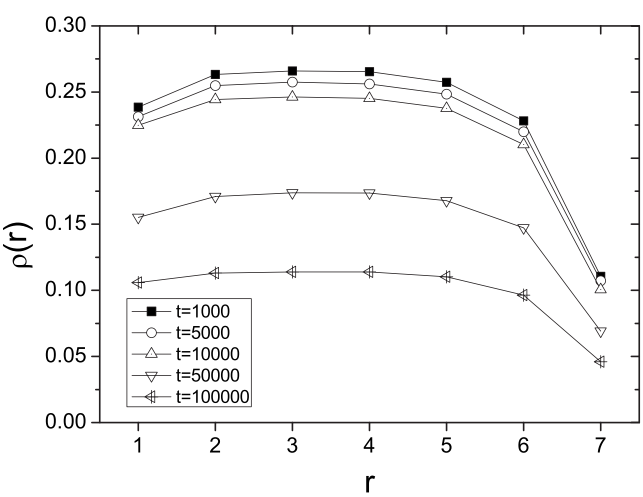

FIG. 2. Particle density $\rho(r)$ vs distance r for various times. ER networks of $N=10^5$ with $\langle k\rangle=10$. The trap is placed on a random node.

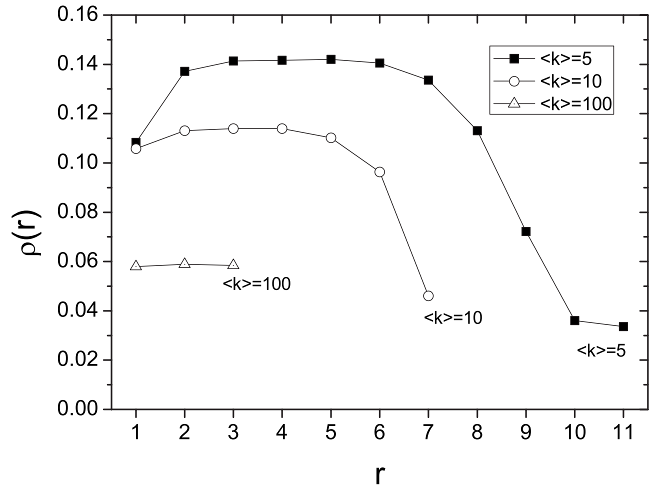

FIG. 3. Particle density $\rho(r)$ vs distance r for $t=10^5$ MCS. ER networks of $N=10^5$ with the trap placed on a random node. Comparison of networks with different values of $\langle k\rangle$.

This is a significant difference over lattices, where the depletion zone (an area with reduced particle density) is formed relatively fast near the trap and is existent in both 1D, 2D, and 3D lattices [19,22–25]. In regular random networks (Fig. 1), however, all particles are homogeneously distributed in the network with the particle density remaining constant for different distances and the picture remains the same for longer times as well. In this case it is evident that the trap has no effect in forming a density gradient in its immediate vicinity as is the case with lattices. Here, the particle distribution is different for lattices and regular networks, while the particle density $\rho(t)$, which represents the quantity of the particles, is an exponential function of time in both cases [1,2,11,18].

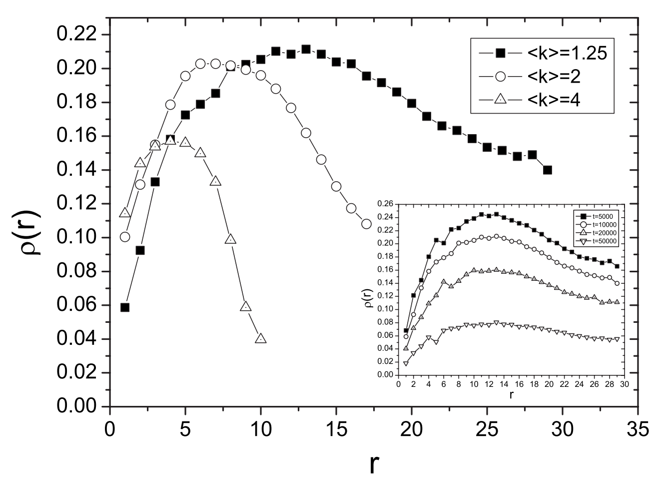

FIG. 4. Particle density $\rho(r)$ vs distance r for $t=10^4$ MCS. ER networks of $N=10^4$ with the trap placed on a random node. Comparison of networks with different values of $\langle k\rangle$ (very sparse networks). Inset: $\rho(r)$ vs r for an ER network of $\langle k\rangle=1.25$ for various times.

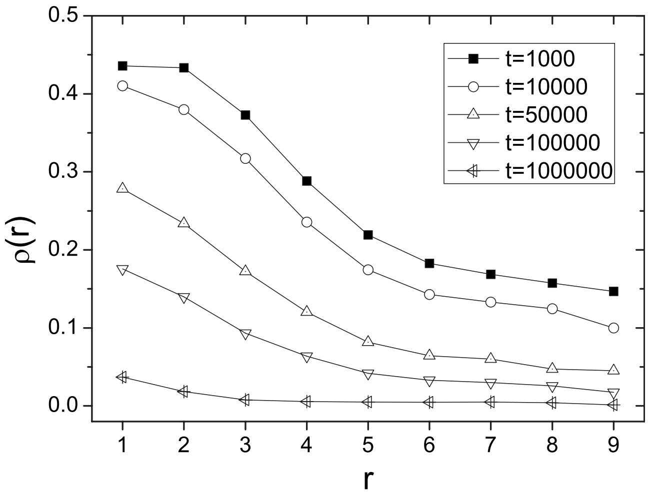

FIG. 5. Particle density $\rho(r)$ vs distance r for various times. SF networks of $N=10^4$ with $\gamma=2.5$ and $m=1$. The trap placed on a random node.

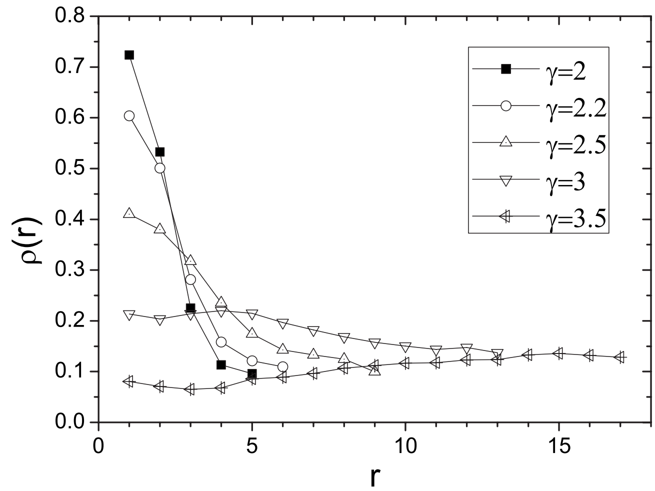

FIG. 7. Particle density $\rho(r)$ vs distance r for $t=10^4$ MCS. SF networks of $N=10^4$ and $m=1$ with the trap placed on a random node. Comparison of networks with different values of γ.

In ER networks (Fig. 2) the picture is quite similar. Here we perform simulations in ER networks of $N=10^5$ and $\langle k\rangle=10$, placing the trap on a random node. The main difference here is the reduced particle density in nodes that are far from the trap. These can be nodes with low degree, low betweenness centrality, or both, since shortest path betweenness is known to be strongly correlated with vertex degree in most networks [10,35–37]. Particle density in these nodes is reduced because the particles are attracted toward the center of the network, which includes nodes with relatively high random walk centrality [10].

The decrease in density far from the trap is not an effect of the trapping but of the central nodes which attract the particles. This, however, includes a large portion of the network so the density stays fairly constant in this section. The effect becomes more pronounced for lower values of $\langle k\rangle$, but is diminished for high values (Fig. 3), approaching the behavior of regular random networks (Fig. 1). However, for very low values of $\langle k\rangle$ (i.e., close to 1), the depletion zone effect is recovered (Fig. 4). We have also performed simulations allowing multiple occupancy and the results are almost the same in both cases.

In SF networks we perform simulations placing the trap either on a random node or on the node with maximum degree. The role of high connectivity nodes is evident in both cases. The high random walk centrality of the hub is critical to its role in the trapping reaction and the degree distribution plays a significant role in the distribution of the particles in the networks, recovering the depletion zone formation for high γ values, as we see below. Figures 5–8 show $\rho(r)$ for networks with $N=10^4$, with the trap placed on a random node. Not only there is no depletion zone, but in this case we see that the particle density is increased in the immediate vicinity of the trap. Again, the particle distribution is different for lattices and SF networks, while the particle density $\rho(t)$ is exponential decay in lattices and very close to exponential decay in SF networks [6,11]. This is an important

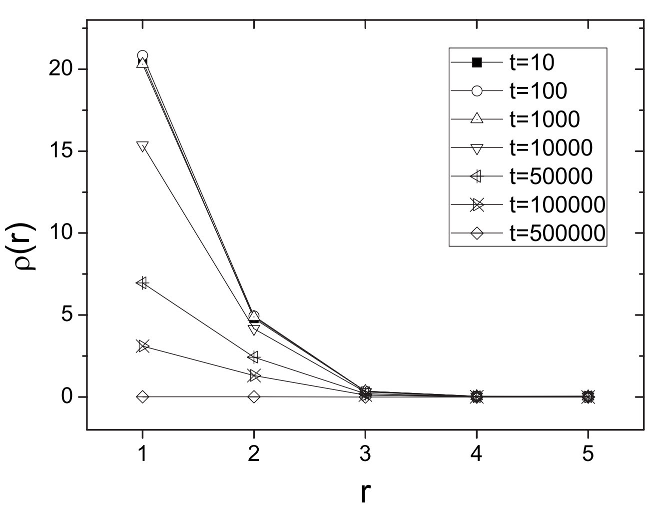

FIG. 6. Particle density $\rho(r)$ vs distance r for various times. SF networks of $N=10^4$ with $\gamma=2.5$ and $m=1$. The trap placed on a random node. Multiple occupancy is allowed.

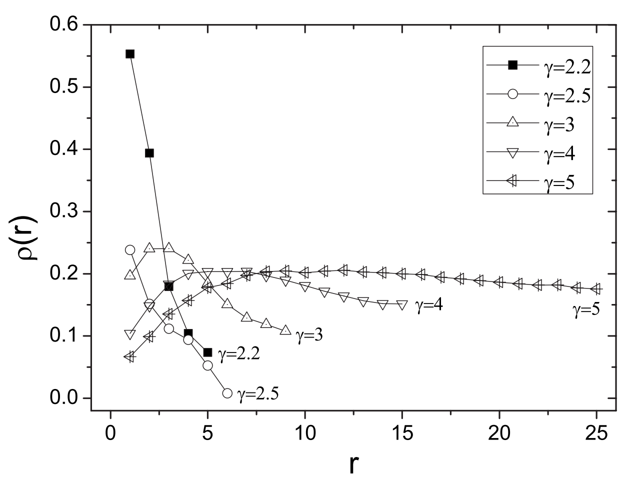

FIG. 8. Particle density $\rho(r)$ vs distance r for $t=10^4$ MCS. SF networks of $N=10^4$ and $m=2$ with the trap placed on a random node. Comparison of networks with different values of γ.

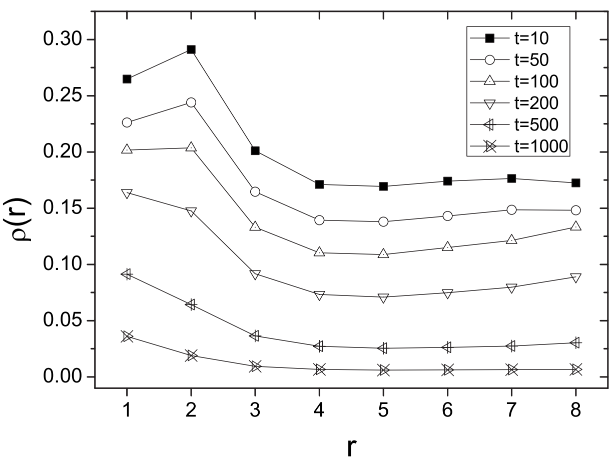

FIG. 9. Particle density $\rho(r)$ vs distance r for various times. SF networks of $N=10^5$, $\gamma=2.5$, and $m=1$. The trap placed on the node with the maximum degree.

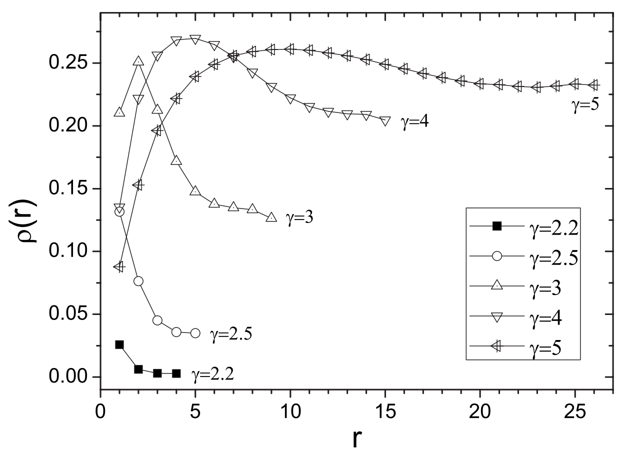

FIG. 11. Particle density $\rho(r)$ vs distance r for $t=200$ MCS. SF networks of $N=10^5$ and $m=2$, with the trap placed on the node with the maximum degree. Comparison of networks with different values of γ.

difference between lattices and SF networks, namely, that while $\rho(t)$ is the same function of time in both cases, the particle distribution in the system is drastically different.

The increased density is a direct result of the hub attracting the particles. The hub in this case plays a more important role than the trap in the process as far as particle distribution in the network is concerned. The effect becomes significantly more pronounced if multiple occupancy is allowed (Fig. 6). The contribution of the hub is increased, the hub attracting large number of particles, while in the case of excluded volume the particles are blocked in the hub, still allowing, however, an increased density in the immediate vicinity of the trap.

Figure 7 shows $\rho(r)$ for a fixed time for different network connectivities. As the value of γ parameter is increased the effect of the hub is diminished, reaching a nearly homogeneous distribution for larger values. This may be relevant to the fact that the largest component of the network is significantly small for these values. To keep the network fully connected we set $m=2$ (Fig. 8). Here it is evident that as the network becomes sparser (high γ values, i.e., lower values of $\langle k\rangle$), we begin to recover the depletion zone formation. In this case the importance of the trap in the process is increased and the contribution of the hub is diminished, therefore, approaching the behavior of the trapping reaction in regular lattices.

Figures 9–11 show the trapping reaction in networks with the trap placed on the node with maximum connectivity in SF networks of $N=10^5$. In this case, $\rho(t)$ has been found to yield a scaling with the system size drastically different than lattices [11] and the particle distribution is also different as revealed by our results (Fig. 12). Again, no depletion zone is formed near the trap and particle density is increased in the vicinity of the trap (Fig. 9). The increased density is not, however, as high as in case of the trap placed randomly. This happens because now the hub plays two roles: it both attracts and traps the particles, so particles are being drawn toward the trap but are removed from the system in the subsequent time steps.

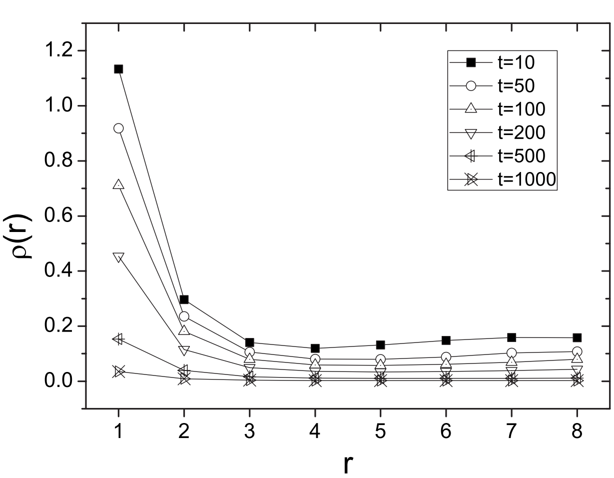

FIG. 10. Particle density $\rho(r)$ vs distance r for various times. SF networks of $N=10^5$, $\gamma=2.5$, and $m=1$. The trap placed on the node with the maximum degree. Multiple occupancy is allowed.

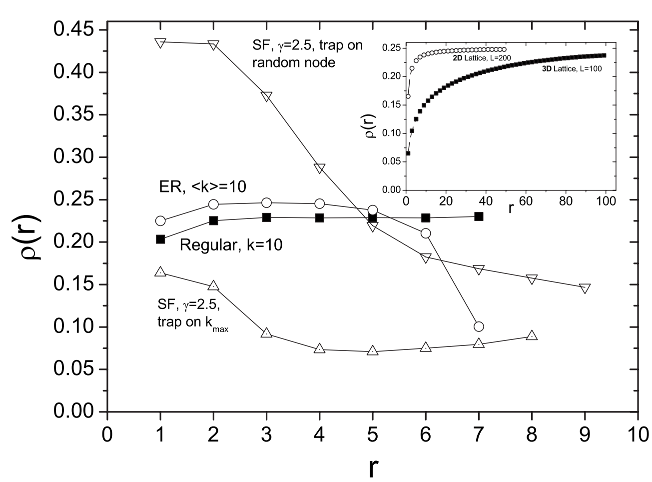

FIG. 12. Comparison of depletion zone dynamics in various systems. 2D lattice, 3D lattice, regular random network with $N=10^5$ and $k=10$, ER network with $N=10^5$ and $\langle k\rangle=10$, SF network with $N=10^5$ and $\gamma=2.5$ with the trap placed (i) on a random node or (ii) on the node with maximum degree.

The ability of the hub to attract particles is increased if multiple occupancy is allowed (Fig. 10) but the difference is not as pronounced as in the case of a random placement of the trap, because of its double role. Particles, however, do reach the area of the hub easier and remain in its immediate vicinity. If multiple occupancy is not allowed, the particles near the hub block some of the particles trying to reach it and the density does not fall as sharply (Fig. 9 compared with Fig. 10). As the network becomes sparser we begin to recover the depletion zone formation, which is evident in networks of high γ (Fig. 11), increasing the role of the hub as a trap and decreasing its ability to attract the particles. The mean node degree is therefore shown to play an important role in the depletion zone formation for the trapping process in networks.

V. CONCLUSIONS

We have investigated the trapping reaction of a density of particles in the presence of a single trap in complex networks using Monte Carlo simulations for particles performing random walks. The depletion zone near the trap, which is characteristic of lattices, is absent in complex networks, while the particle density $\rho(t)$ is an exponential decay function of time in both cases. We find that in contrast to lattices, the particles in regular and ER networks are homogeneously distributed, with a deviation for small values of $\langle k \rangle$ in ER networks, the trap having no effect in forming a density gradient in its immediate vicinity. In SF networks we reveal the important role of high degree nodes and show that there is significant difference if multiple occupancy is allowed. The high random walk centrality of the hubs has a pronounced effect in the distribution of the particles in the network. It is also evident that connectivity of the network plays a significant role in the distribution of the particles in both ER and SF networks, recovering the depletion zone formation for very sparse networks in both cases. This work complements previous results of diffusion-reaction systems where it was also observed that the lattice effects disappear in networks, i.e., the absence of depletion zone and the segregation effects [8,12,13].

ACKNOWLEDGMENTS

We would like to thank Professor Shlomo Havlin for helpful discussions.

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