Slowdown in the Annihilation of Two Species Diffusion-Limited Reaction on Fractal Scale-Free Networks

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Abstract. In the diffusion-limited reaction process $A + B \rightarrow \emptyset$ on random scale-free networks, particle density decays as $\rho(t) \sim t^{-\alpha}$ when $\rho_A(0) = \rho_B(0)$, where $\alpha > 1$ for the degree exponent $2 < \gamma < 3$ and $\alpha = 1$ for $\gamma \leq 3$. We investigate the reaction on fractal scale-free networks numerically, finding $\rho(t)$ decays slowly with the exponent $\alpha \approx d_s/4 < 1$, where d_s is the spectral dimension of the network.

Keywords: diffusion-limited reaction, fractal scale-free network, segregation.

1 Introduction

Diffusion-limited reaction kinetics has been studied for long time. It can be used for modeling chemical reactions, epidemic spreading, and so on. Here, we limit our interest to the two-species annihilation process $A + B \rightarrow \emptyset$.

It is known that if the initial densities of A and B particles are equal, the density decays as $\rho(t) \sim t^{-\alpha}$. In a mean-field approximation, α is 1. This approximation is valid for the processes in Euclidean space with $d > d_c = 4$. For $d < 4$, however, the mean-field approach is invalid, and α is d/d_c, which is less than 1. This behavior is caused by the segregation effect: A-rich or B-rich domains form, and reactions can take place only at the limited area, that is, the boundary between those domains [1,2,3]. And this argument can be extended to the fractal case, giving $\alpha = d_s/4$ when $d_s < 4$, where d_s is the spectral dimension. Although this value is in good agreement with many numerical results [15,16], this extension has been questioned [3] in some cases.

Recent studies show that in complex networks, particle density can decay faster, and α can be larger than 1 [4]. In random scale-free networks, α can be obtained analytically and is $1/(\gamma - 2)$ for $2 < \gamma < 3$ and 1 for $\gamma > 3$ where γ is the exponent of the degree distribution $P_d(k) \sim k^{-\gamma}$ [8]. This fast decay can be explained in terms of the existence of hubs and extremely small diameter. Particles tends to move towards hubs which are closely located. Distance between particles of different species are close because of small diameter. These two factors cause A and B particles to mix, accelerating the reactions.

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2 Two-Species Annihilation on Fractal Scale-Free Networks

We study two-species annihilation reaction on fractal scale-free networks. When a network is fractal, this network satisfies the scaling $N_B(l_B) \sim l_B^{-d_f}$, where l_B is the size of boxes and N_B is the number of boxes needed to cover the network. In a fractal scale-free network, hubs are located repulsively. Particles move towards the local hubs nearby, and reactions occur. As a result, it is likely to remain particles of the same species in the vicinity of the local hubs, forming domains. After forming domains, reactions take place at the boundaries between domains, causing particle density to decay slowly.

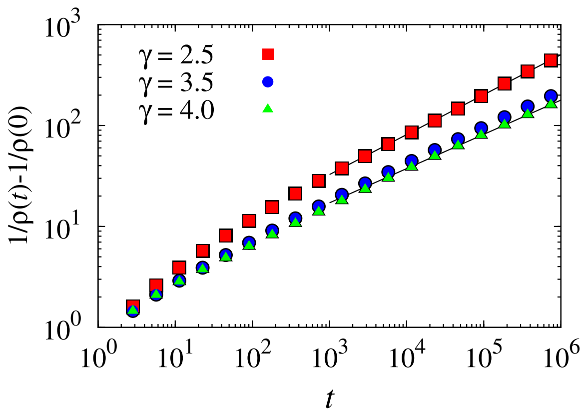

Fig. 1. The particle density as a function of time on the critical branching trees. Guidelines have slopes 0.40 (top) and 0.34 (bottom).

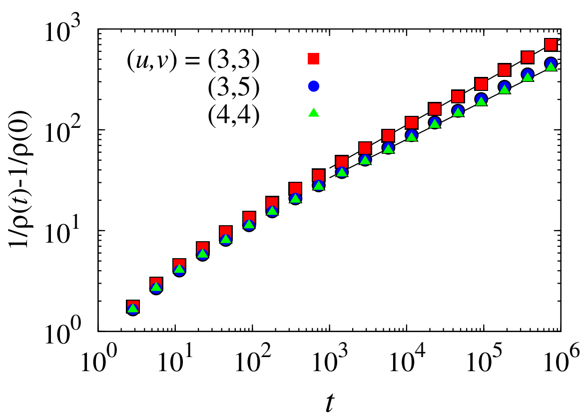

Fig. 2. The particle density as a function of time on the (u, v)-flower networks. Guidelines have slopes 0.43 (top) and 0.38 (bottom).

Table 1. Comparison of the numerically obtained exponent $\alpha_{\rm num}$ with $d_s/4$

CBT			(u,v)-flower				(u,v)-tree			
γ	$\alpha_{\rm num}$	$d_s/4$	(u,v)	γ	$\alpha_{\rm num}$	$d_s/4$	(u,v)	γ	$\alpha_{\rm num}$	$d_s/4$
2.5	0.40	0.38	(2,2)	3	0.53	0.5	(2,2)	3	0.34	0.33
2.7	0.37	0.35	(2,4)	3.58	0.45	0.43	(2,4)	3.58	0.37	0.36
3.5	0.36	0.33	(3,3)	3.58	0.43	0.41	(3,3)	3.58	0.31	0.31
4.0	0.34	0.33	(2,6)	4	0.43	0.42	(2,6)	4	0.40	0.38
4.5	0.34	0.33	(4,4)	4	0.38	0.38	(4,4)	4	0.31	0.30

We use the critical branching tree [10], (u,v)-flower and (u,v)-tree [19] as substrates. Simulation results show that the particle density decays slowly as shown Figs. 1, 2. Numerical values of α are less than 1 and close to $d_s/4$ as can be seen in Table 1 for the critical branching tree, (u,v)-flower, and (u,v)-tree.

3 Role of Local Hubs in Fractal SF Networks

To confirm the role of local hubs, we measure the particle density on the networks generated by rewiring the links of $(3,3)$-flower under the conservation of the degree distribution. Fig. 3 shows the results. As we rewire the links, the density of particle decays faster and α increases from 0.43 to 1, which is the value on scale-free network with the same degree exponent γ.

Next, we measure a quantity introduced in Ref. [20],

$$Q_{AB} = \frac{N_{AB}}{N_{AA}+N_{BB}}, \tag{1}$$

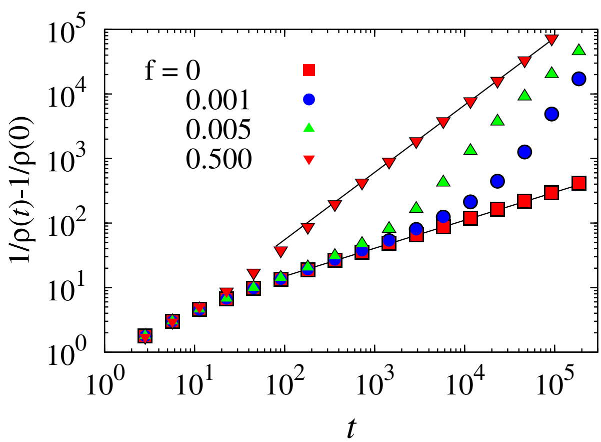

Fig. 3. The particle density on a (3,3)-flower($f=0$) and its rewired networks. f is the fraction of rewired links. Guidelines have slopes 0.43 (bottom) and 1.0 (top).

where N_{AB} is the the number of contacts between A and B particles, N_{AA} and N_{BB} are defined similarly. Q_{AB} close to 0 indicates that segregation occurs, and the value close to 1 means A and B particles are mixed completely. Fig. 4 is the plot of Q_{AB} as a function of time. From the figure, we confirm strong segregation on a fractal network. And as more links are rewired and the distance between hubs are closer, the segregation effect decreases.

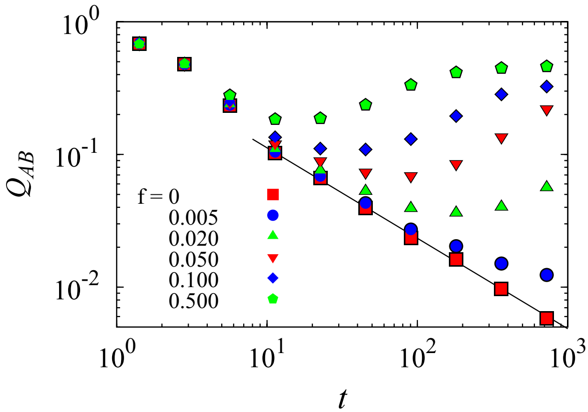

Fig. 4. Plot of Q_{AB} for the networks in Fig. 3

4 Summary

To sum up, in the two-species annihilation process $A + B \to \emptyset$ on fractal SF networks, segregation forms originated from the existence of local hubs, causing the particle density to decay slowly with the exponent $\alpha < 1$. More detailed results can be found in our recent paper [22].

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