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Annihilation of two-species reaction–diffusion processes on fractal scale-free networks

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Abstract. In the reaction–diffusion process $A + B \rightarrow \varnothing$ on random scale-free (SF) networks with the degree exponent γ, the particle density decays with time in a power law with an exponent α when initial densities of each species are the same. The exponent α is known as $\alpha > 1$ for $2 < \gamma < 3$ and $\alpha = 1$ for $\gamma \geqslant 3$. Here, we examine the reaction process on fractal SF networks, finding that $\alpha < 1$ even for $2 < \gamma < 3$. This slowly decaying behavior originates from the segregation effect: fractal SF networks contain local hubs, which are repulsive to each other. Those hubs attract particles and accelerate the reaction, creating particle domains containing the same species of particles. Then, the reaction takes place at the non-hub boundaries between those domains, and the particle density decays slowly. Since many real SF networks are fractal, the segregation effect has to be taken into account in the reaction kinetics among heterogeneous particles.

Diffusion-limited reaction kinetics has been studied for a long time as an interdisciplinary subject. It can be a model of electron–hole recombination in semiconductors [1] and annihilation of primordial monopoles in the early universe [2, 3], etc. The annihilation process involving two species of particles A and B, $A + B \rightarrow \varnothing$ is studied here, particularly on fractal scale-free (SF) networks. When the densities of particles A and B are initially equal, the density of each species $\rho_A(t)$ or $\rho_B(t)$ decays as a power law, that is, $\rho_A(t) = \rho_B(t) \equiv \rho(t) \sim t^{-\alpha}$. In a mean-field (MF) approximation, the density of particles decays as $\rho(t) \sim t^{-1}$, which is valid when the reaction takes place in Euclidean space with the spatial dimension $d > d_c = 4$. For $d < d_c$, the exponent α is reduced to $\alpha = d/d_c$, which is less than 1. The slow decaying behavior of particle density

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originates from the formation of A-rich or B-rich domains, and the reaction takes place at the boundary of those domains in Euclidean space [4]–[6].

In complex networks, however, the particle density $\rho(t)$ can decay faster than the MF behavior $\rho(t) \sim t^{-1}$ in the long time limit [7]. This fast decay is caused by the existence of hubs, at which particles gather through the diffusion process and then reactions take place frequently. This phenomenon is related to the fact that the probability of finding a random walker at a node is proportional to the degree of that node [8, 9]. For the uncorrelated SF networks, the particle density $\rho(t)$ was derived analytically for $A + A \to \varnothing$ [10] and $A + B \to \varnothing$ [11] as

$$\frac{1}{\rho(t)} - \frac{1}{\rho(0)} = \begin{cases} t^{1/(\gamma-2)}, & \text{for } 2 < \gamma < 3, \\ t \ln t, & \text{for } \gamma = 3, \\ t, & \text{for } \gamma > 3, \end{cases} \tag{1}$$

where γ is the exponent of the degree distribution $P_d(k) \sim k^{-\gamma}$ of the SF networks.

In this paper, we point out that the result (1) can be misleading when SF networks are fractal [12, 13], where the particle density decays slowly with the exponent $\alpha \leqslant 1$, different from formula (1). The fractal SF network is a network satisfying the fractal scaling $N_B(\ell_B) \sim \ell_B^{-d_f}$, where N_B is the number of boxes needed to cover the entire network with boxes of size ℓ_B. The fractal scaling holds in the system where hubs are located separately from each other [14, 15]. Many SF networks observed in the real world are fractals. However, most artificial networks including the Barabási and Albert (BA) model [16] are not fractals [17]. In fractal networks, local hubs attract particles and accelerate the reaction. As a result, in the early time regime, the particle density decreases rapidly with highly effective values of α. During the process, the initial particle density fluctuation creates particle A-rich or particle B-rich domains. Then, the reaction takes place only at the boundary between those domains, which are not hubs. Thus the particle density decays slowly in the long time limit with $\alpha \leqslant 1$. Such a segregation behavior can also occur in modular SF networks, even if they are non-fractal. The structural feature of the modular network, being composed of a large number of links within modules but a small number of links between modules, hampers the diffusion of particles across modules.

To study the two-species reaction $A + B \to \varnothing$ on fractal SF networks specifically, we first recall the previous studies [5, 6] of the reaction kinetics taking place on the fractal structure embedded in Euclidean space. In this case, the formula $\rho(t) \sim t^{-d/d_c}$ may be replaced with

$$\rho(t) \sim t^{-d_s/4}, \tag{2}$$

where d_s is the spectral dimension of the fractal structure. The variable d_s is related to the random walk dimension d_w and fractal dimension d_f as $d_s = 2d_f/d_w$. The random walk dimension is defined through the anomalous power-law relationship between the mean-square displacement $\langle \ell^2(t) \rangle$ of a diffusing particle and time t as $\langle \ell^2(t) \rangle \sim t^{2/d_w}$. Formula (2) has been questioned, however, because it does not take into account structural features in a given fractal structure such as the degree of ramification. Nevertheless, it appears that numerical results are essentially in agreement with the prediction (2) for many cases [18, 19]. In this paper, we show that in contrast to the standard random SF network cases, for the fractal SF networks we study here, even though they are SF, the particle density decays in the form given by (2).

Here, we first generate a fractal SF tree structure through the multiplicative branching process. At each branching step, a node creates its m branches (offsprings) with probability $p_m \sim m^{-\gamma}$ $(m \geqslant 1)$. It has to satisfy the criticality condition $\langle m \rangle = \sum_{m=0}^{\infty} m p_m = 1$ [13]. Then, the resulting tree structure is a SF tree with the degree exponent γ. Such a random

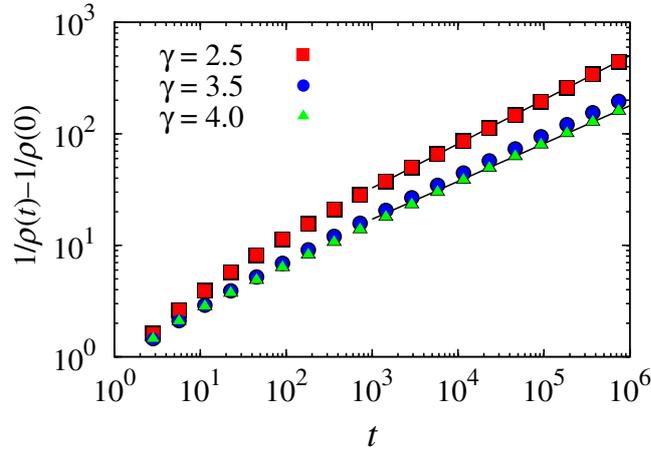**IOP** Institute of Physics ⏀ DEUTSCHE PHYSIKALISCHE GESELLSCHAFT

Figure 1. The particle density as a function of time on the CBT with various degree exponents. Guidelines have slopes 0.40 (top) and 0.34 (bottom).

Table 1. Comparison of the exponent α numerically obtained, denoted as α_{num}, with $d_s/4$ for various degree exponent γ's for the CBT. For comparison, we also list the MF value obtained from formula (1).

γ	α_{num}	$d_s/4$	MF value
2.5	0.4(1)	0.38	2.00
2.7	0.36(1)	0.35	1.43
3.5	0.35(1)	0.33	1.00
4.0	0.34(1)	0.33	1.00
4.5	0.34(1)	0.33	1.00

critical branching tree (CBT) structure is a fractal SF network with the fractal dimension $d_f = (\gamma - 1)/(\gamma - 2)$ for $2 < \gamma < 3$ and $d_f = 2$ for $\gamma > 3$. The spectral dimension is [20, 21]

$$d_s = \begin{cases} \dfrac{2(\gamma - 1)}{2\gamma - 3}, & \text{for } 2 < \gamma < 3, \\ \dfrac{4}{3}, & \text{for } \gamma > 3. \end{cases} \tag{3}$$

We measure particle density $\rho(t)$ as a function of time t in the form

$$\frac{1}{\rho(t)} - \frac{1}{\rho(0)} \sim t^\alpha. \tag{4}$$

We find that the particle density decays quickly in the short time regime, followed by a slow decay in the long time regime as shown in figure 1. Indeed, the numerically obtained values listed in table 1 are close to the ones obtained from the formula $d_s/4$, and are different from the ones obtained from formula (1).

Next, we study the reaction kinetics on deterministic fractal SF networks, the so-called (u, v)-flower and (u, v)-tree networks, introduced and modified in [22] and in [23], respectively. These networks are hierarchical networks, generated iteratively from a simple basic structure to higher level ones. Each link in the nth generation is replaced by two parallel paths that are
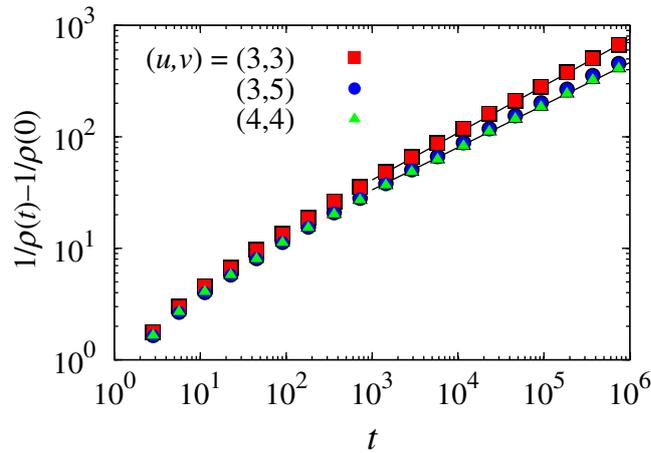
Figure 2. The particle density of A or B species as a function of time for the (u, v)-flower networks. Guidelines have slopes 0.43 (top) and 0.38 (bottom).

Table 2. Comparison of the exponent α numerically obtained, denoted as α_{num}, with $d_{\mathrm{s}}/4$ for various degree exponent γ's for the (u, v)-flower networks. For comparison, the MF value obtained from (1) is 1.0.

(u, v)	γ	α_{num}	$d_{\mathrm{s}}/4$
(2,2)	3	0.53(1)	0.5
(2,4)	3.58	0.45(1)	0.43
(3,3)	3.58	0.43(1)	0.41
(2,6)	4	0.43(1)	0.42
(4,4)	4	0.38(1)	0.38

Table 3. The same as table 2 but for the (u, v)-tree networks.

(u, v)	γ	α_{num}	$d_{\mathrm{s}}/4$
(2,2)	3	0.34(1)	0.33
(2,4)	3.58	0.37(1)	0.36
(3,3)	3.58	0.31(1)	0.31
(2,6)	4	0.38(1)	0.38
(4,4)	4	0.31(1)	0.30

u and v links long. The detailed rule can be found in [23]. Depending on the rule, constructed networks are either the flower structure, which contains loops, or trees. These networks are fractal SF networks with the degree exponent, $\gamma = 1 + \frac{\ln(u+v)}{\ln 2}$, the fractal dimension, $d_{\mathrm{f}} = \frac{\ln(u+v)}{\ln u}$, and the spectral dimension, $d_{\mathrm{s}} = \frac{2\ln(u+v)}{\ln uv}$ for flowers and $\frac{2\ln(u+v)}{\ln u(u+v)}$ for trees. Numerical values of the exponent α are close to those from $\alpha = d_{\mathrm{s}}/4$ as can be seen in tables 2 and 3 for the flower and tree structures, respectively. Some numerical data are shown in figure 2.
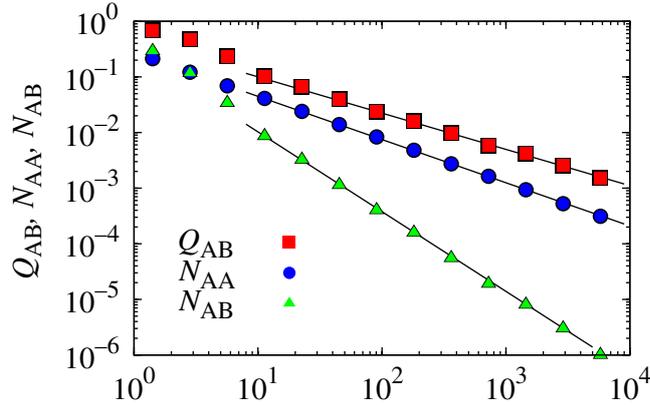
Figure 3. Plot of Q_{AB}, N_{AB} and N_{AA} versus time t for a (3,3)-flower network. The slopes of the guidelines are -0.65, -0.78 and -1.43 from the top.

To check whether the segregation of A-rich or B-rich domains occurs, we examine a quantity,

$$Q_{AB}(t) = \frac{N_{AB}}{N_{AA} + N_{BB}}, \tag{5}$$

where $N_{AB}(t)$ is the number of (A, B) pairs located as nearest neighbors averaged over different initial configurations. N_{AA} and N_{BB} are similarly defined [24]. If there are a few pairs of different species at neighbor nodes $Q_{AB} \to 0$, whereas $Q_{AB} \to 1$ when particles are mixed randomly. Since the particle density decreases in time, their separation becomes large and two particles are hardly found as nearest neighbors. We examine N_{AB} and N_{AA} independently as a function of time. Interestingly, they decrease with time in a power-law manner as shown in figure 3, which can be explained as follows:

Firstly, we examine N_{AA}. The linear size ℓ_d of a domain containing a species grows with time as $\sim t^{1/d_w}$. A typical closest distance ℓ_{AA} between two particles of the same species scales as $\sim (1/\rho)^{1/d_f}$. Assuming that $\rho(t) \sim t^{-d_s/4}$, one can obtain that $\ell_{AA} \sim t^{1/(2d_w)}$ [5]. When $d_s \leqslant 2$, the case in which we are interested in this paper, random walks are compact within the diffusion volume $\ell_d^{d_f}$, and thus that is also valid within the volume $\ell_{AA}^{d_f}$. The probability of finding two such particles as nearest neighbors is $1/\ell_{AA}^{d_f}$. Thus N_{AA} scales as $(1/\ell_{AA}^{d_f})\rho(t)$. That is,

$$N_{AA}(t) \sim t^{-d_s/2}. \tag{6}$$

Secondly, we examine $N_{AB}(t)$. When two particles of different species come to be nearest neighbors in the diffusion process, they can annihilate at the next step with a finite probability. Thus, we may set $N_{AB}(t) \propto d\rho/dt$, and obtain that

$$N_{AB}(t) \sim t^{-d_s/4-1}. \tag{7}$$

Next, Q_{AB} is obtained as $\sim t^{d_s/4-1}$ using equations (6) and (7). In table 4 the results obtained from simple arguments are compared with numerical ones.

To confirm that the segregation is caused by local hubs in the fractal structures, we destroy the local hubs by rewiring the links in the (3,3)-flower network while conserving the degree

Table 4. Comparison of the exponents N_{AA} and N_{AB} between theoretical and numerical values for various embedded spaces, one-dimensional regular lattice (1 dim), two-dimensional square lattice (2 dim), CBT with $\gamma = 2.5$ and $\gamma = 4.0$ and (3,3)-flower hierarchical network. The discrepancy for the case CBT ($\gamma = 2.5$) is probably caused by the disassortative mixing in the degree–degree correlation [25].

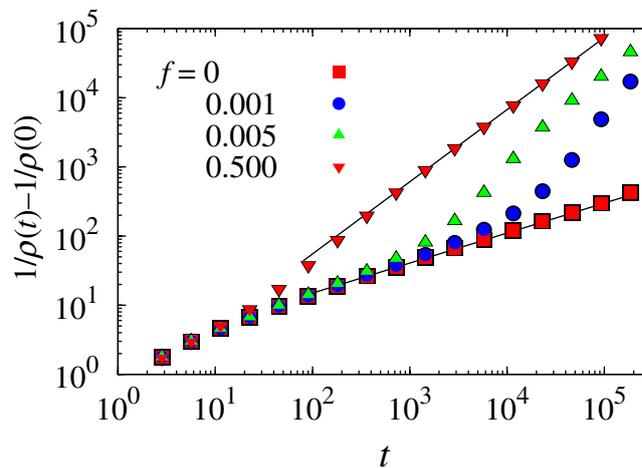| Space	N_{AA}		N_{AB}	
	$d_s/2$	Num.	$(d_s/4) + 1$	Num.
1 dim	0.5	0.49(1)	1.25	1.28(2)
2 dim	1.0	0.99(1)	1.50	1.59(1)
CBT ($\gamma = 2.5$)	0.75	0.58(1)	1.38	1.28(1)
CBT ($\gamma = 4.0$)	0.67	0.66(1)	1.33	1.32(2)
(3,3)-flower	0.82	0.78(1)	1.41	1.43(2)

Figure 4. The particle density versus time on rewired networks from a (3,3)-flower network. The slope increases as the fraction f of rewired links increases from $f = 0$ to $f = 0.5$. For the $f = 0$ and $f = 0.5$ cases, the slopes are close to $\alpha \approx 0.43$ and 1.04, respectively. Since $\gamma \approx 3.58 > 3$, $\alpha = 1$ is the MF result.

distribution. Figure 4 shows that the exponent α changes from $\alpha \approx 0.43$ to the MF value $\alpha = 1$ as the number of rewired links increases. Moreover, Q_{AB} does not decrease monotonically for the rewired networks as shown in figure 5.

The World Wide Web [26] is a prototypical example of a fractal network in the real world. We obtain that the particle density decreases slowly as $\rho(t) \sim t^{-0.54}$ on this network (figure 6). The Internet at the autonomous system (AS) level[2] is, however, not one. This may be caused by the geographical effect. Due to this non-fractality, the segregation does not occur in the Internet, and thus the particle density decreases quickly with exponent $\alpha \approx 1.8$ for the Internet topology in the year 2004 as shown in figure 6. This property can be used beneficially when one designs a protocol for a P2P network, a virus–antivirus annihilation robot, etc [27].

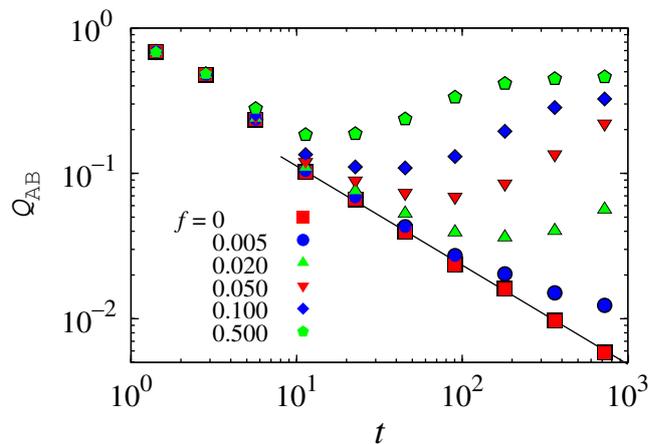[2] The NLANR provides Internet routing related information based on BGP data (see http://moat.nlanr.net/).

Figure 5. Plot of Q_{AB} as a function of t for the rewired networks used in figure 4. The slope of the solid line is -0.65.
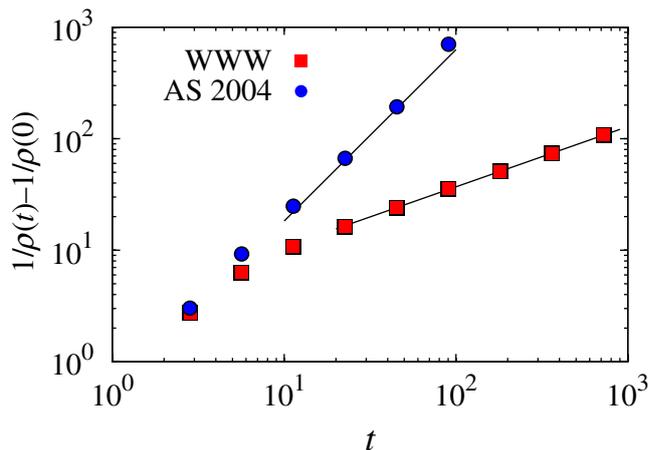

Figure 6. The particle densities as a function of time on the World Wide Web (■) and the Internet at the AS level collected in the year 2004 (●). The slopes of guidelines are 0.54 for the World Wide Web and 1.8 for the Internet.

It is worth noting that whereas the decaying behavior obeying formula (1) applies to the BA model when m, the number of incoming links at each time step, is larger than 1, it is not so for the BA tree network with $m = 1$. This is because the tree structure has no alternative paths, which enhances segregation. Thus, the particle density decays slowly with exponent $\alpha \approx 0.5$, even though the BA tree is not fractal.

In summary, the segregation effect in the two-species annihilation reaction dynamics has to be taken into account when the dynamics takes place on fractal, modular, or tree networks. In this case, the role of hubs is different from that of random SF networks and the particle density decays slowly in a power-law manner with exponent less than 1, even though these networks are SF.

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Acknowledgment

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