Reaction-diffusion processes of three species on small-world networks

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We study the decay process for the reaction-diffusion process of three species on the small-world network. The decay process is manipulated from the deterministic rate equation of three species in the reaction-diffusion system. The particle density and the global reaction rate on a two-dimensional small-world network adding new random links is discussed numerically, and the global reaction rate before and after the crossover is also found by means of the Monte Carlo simulation. The time-dependent global reaction rate scales as a power law with the scaling exponent 0.66 at early time regime while it scales with \(-0.50\) at long time regime, in all four cases of the added probability \(p = 0.2 - 0.8\). Especially, our result presented is compared with the numerical calculation of regular networks.

I. INTRODUCTION

In the past decades, several papers have been devoted to the theoretical and numerical investigation on the reactant segregation phenomena in anomalous kinetics. An important contribution to this field of research has been given by Ovchinnikov and Zeldovich, who developed the segregation phenomenon. It is well known that the binary reaction has primarily been investigated on the process of binary reactions and many phenomena in nature. Until now, the segregation of reactants has been investigated in a reaction-diffusion process based on the experimental observation. Cornell et al. have precisely shown both the global reaction rate and the reaction front increased as a function of \(t^{1/2}\) at very early times. At that time, Cornell et al. have argued the diffusion-limited reaction \(nA + mB \rightarrow C\) for both homogeneous and inhomogeneous conditions under initially separated reactants. They have discussed that the global reaction rate decreases as \(t^{-1/2}\) in long time limit, independent of \(n\) and \(m\), and that the upper critical dimension is \(d_c = 2\) for the reaction-diffusion process.

Recently, Zumofen et al. have studied mainly the particle density and the pair correlation function on the two-particles reaction process. Particularly, they found that the particle density is distributed as \(P(n) \sim n^{-1-\gamma}\), \(n > 0, 1 < \gamma < 2\), for Lévy walks and that the segregation disappears in \(d = 3\) dimension for \(\gamma < 3/2\). Yen et al. have studied for the asymptotic early-time scaling in the ternary reaction-diffusion process with initially separated reactants. Moreover, Kim et al. have argued the decay process in a reaction-diffusion system with three species on the regular square lattice. By a simple perturbation expansion, we have analytically derived the particle density and the global reaction rate before and after the crossover in the reaction-diffusion system of \(A + B + C \rightarrow 0\).

For last few years, a growing interest has been concentrated on small-world and scale-free network models, and these models have recently been widely studied in various applications of methods from physics to other natural, social and applied sciences. In fact, the phenomenon of small-world and scale-free networks is different in their nature compared to regular lattice models, due to the small diameter of networks and the existence of hubs. Furthermore, Catanzaro et al. have analyzed that the inverse particle density scales linearly as \(1/\rho(t) \sim t\). From this result, they have found that the inverse particle density in uncorrelated scale-free network crosses over to a linear behavior. Very recently, Gallos and Argyrakis have dis-
cussed the reaction-diffusion process of the two species on the scale-free network between the the correlated and the uncorrelated configuration models. They have especially revealed that two models are identical when $\gamma = 3.0$.

In this paper, the decay process for the reaction-diffusion process of three species on the small-world network is studied. We also consider the particle density and the global reaction rate on the two-dimensional small-world lattices added by new random links. In Section 2, we discuss the reaction-diffusion process of three species on small-world networks. We present some results obtained by the numerical simulations and the concluding remark in the final section.

II. REACTION-DIFFUSION SYSTEM OF THREE SPECIES

In the reactions of $A + A \rightarrow 0$ and $A + B \rightarrow 0$ types on a $d$ dimensional regular lattice, the surviving particle density scales in long time limit as

$$\frac{1}{\rho(t)} - \frac{1}{\rho_0} \sim t^\alpha,$$

where $\rho_0$ is the initial particle density. It is well known that the scaling exponent $\alpha = d/d_c$ for $d \leq d_c$ and 1 for $d > d_c$, and that the critical dimension $d_c = 2$ for $A + A$ and 4 for $A + B$.

Next the $A + B \rightarrow 0$ process on a regular network f19) is introduced for Lévy walks using the following reaction-diffusion equation,

$$\frac{\partial}{\partial t} A(\vec{r}, t) = D \hat{L} A(\vec{r}, t) - \kappa A(\vec{r}, t) B(\vec{r}, t),$$

$$\frac{\partial}{\partial t} B(\vec{r}, t) = D \hat{L} B(\vec{r}, t) - \kappa A(\vec{r}, t) B(\vec{r}, t),$$

where $A(\vec{r}, t)$ and $B(\vec{r}, t)$ are the particle densities, $D$ a generalized diffusion coefficient, $\kappa$ a reaction rate, and $\hat{L}$ the operator for the Lévy-enhanced diffusion. The time-dependent particle densities can be calculated as

$$A(t) = B(t) \sim t^{d/2\gamma}, \quad \text{for } \gamma > d/2,$$

where three marginal values are $\gamma = 1$ for $d = 2$, $\gamma = 3/2$ for $d = 3$, and $\gamma = 2$ for $d = 4$.

From the decay process20 of $A + 2B \rightarrow C$, the diffusion equations under the initial reactant segregation are as follows:

$$\frac{\partial}{\partial t} A(x, t) = D_a \nabla^2 A(x, t) - k A(x, t) B^2(x, t),$$

$$\frac{\partial}{\partial t} B(x, t) = D_b \nabla^2 B(x, t) - k A(x, t) B^2(x, t),$$

where $A(x, t)$ and $B(x, t)$ are the particle densities, $k$ is the microscopic reaction constant, and $D_a$ and $D_b$ are the diffusion coefficients of reactants $A(x, t)$ and $B(x, t)$, respectively. Then, from the lowest order of the perturbation theory, the global reaction rates $R(t)$ on both the early time and long time behaviors scaled as a power law $t^{1/2}$ and $t^{-1/2}$, respectively. Using the Monte carlo method, it was found that the slopes are, respectively, 0.5 and $-0.48$ before and after the crossover.

Let us denote that $A(x, t)$, $B(x, t)$, and $C(x, t)$ are the particle densities for three-species $A$, $B$, and $C$ existing at a position $x$ at time $t$. We assume that three species are initially distributed separately on the axis $x$. Then, the deterministic rate equation for $A(x, t)$ can be expressed in terms of

$$\frac{\partial}{\partial t} A(x, t) = D_A \nabla^2 A(x, t) - K A(x, t) B(x, t) C(x, t),$$

where $D_A$ is the diffusion constant for one species $A$, and $K$ is the reaction rate. The solution for $A(x, t)$, $B(x, t)$, and $C(x, t)$ is obtained that

$$A(x, t) = B(x, t) = C(x, t) \sim \phi(\frac{x}{t^{1/2}})$$

in large time limit, where $\phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-x^2}$. Similar to the result of the previous work,20 the time dependence of the global reaction rates $R(t)$ was shown to behave as

$$R(t) \sim t^{1/2} \text{ and } t^{-1/2}$$

in early time and long time limits.21

III. NUMERICAL RESULTS AND CONCLUDING REMARKS

In order to confirm numerically the global reaction rate, we mainly use the Monte Carlo simulation method in reaction-diffusion process of $A + B + C \rightarrow 0$ on the small-world network adding new random links. First of all, we assume that three species reactants are distributed randomly on two dimensional square lattice with the periodic boundary condition. After one species reactant is chosen at random, the direction of its move is chosen at random with equal probability to one of its linked neighbor lattice points. When two species reactants meet each other on the same lattice point, the intermediate process existing concurrently the combined two species reactants can be formed. If two species reactants meet the third reactant, these reactants react and leave immediately on lattice point. If one species or two species reactants cannot meet the other reactant, the reactants diffuse randomly to one of its linked neighbor lattice points. The diffusion constant in our case takes the same value for each reactant, and the respective particle density of $13.33(40/3)^{1/2}$ for $A$, $B$, and $C$ is distributed randomly on a square lattice having $200 \times 200$ lattice points with the boundary condition. After our simulation is performed
FIG. 1: Plot of the global reaction rate $R(t)$ for the reaction-diffusion process of $A + B + C \rightarrow 0$. Our numerical simulation is performed on $2 \times 10^5$ configurations in $200 \times 200$ square lattice that is added by new random links for the added probability $p = 0$ (black circles), 0.2 (squares), 0.4 (circles), 0.6 (down triangles), and 0.8 (up triangles).

on $2 \times 10^5$ realizations and $K = 1/1500$, we directly observed the crossover for the global reaction rate from our simulation result. It is numerically found that the scaling exponent for the slope before and after the crossover is, respectively, 0.66 and −0.54 on the regular network ($p = 0$). As shown in Fig. 1, the time-dependent global reaction rate scales as a power law with the scaling exponent 0.66 at early time regime while it scales with −0.50 at long time regime, in all four cases of the added probability $p = 0.2$, 0.4, 0.6, and 0.8.

In conclusion, we have numerically estimated the global reaction rate before and after the crossover in reaction-diffusion system of $A + B + C \rightarrow 0$ on square lattice added by new random links. It is really found from our simulation result that the scaling exponent of the global reaction rate on small-world network added by new random links is the similar to that of the regular network at early time regime. At long time regime, the decay process on small-world network proceeds slightly faster than in the case of the regular network.

In future, our work is in progress to extend the correlated and the uncorrelated configuration models. We also will attempt to investigate small-world and scale-free networks in several scientific fields for three species reaction-diffusion process.

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