Decay Process for Three - Species Reaction - Diffusion System

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Abstract

We propose the deterministic rate equation of three-species in the reaction - diffusion system. For this case, our purpose is to carry out the decay process in our three-species reaction-diffusion model of the form $A + B + C \rightarrow D$. The particle density and the global reaction rate are also shown analytically and numerically on a two-dimensional square lattice with the periodic boundary conditions. Especially, the crossover of the global reaction rate is discussed in both early-time and long-time regimes.

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Recently, there has been considerable interest in the front propagation under the initial segregation of two - species reactants in early - time reaction - diffusion process. It is furthermore well - known that the binary reaction has mainly been investigated on the process of ternary reactions\(^1\) and many phenomena in nature.\(^2 - 6\) The early - time behavior for reaction - diffusion system have been argued by Taitelbaum et al,\(^7\) and it has precisely been shown that both the global reaction rate and the reaction front increase as a function of \(t^{1/2}\) at very early times. On the other hand, Cornell et al.\(^8, 9\) have recently treated with the diffusion - limited reaction \(nA + mB\rightarrow C\) for both homogeneous and inhomogeneous conditions under initially separated reactants. They have found that the global reaction rate decreases as \(t^{-1/2}\) at long - time regime, independent of \(n\) and \(m\), and discussed that the upper critical dimension is \(d = 2\) for the reaction - diffusion process. Very recently, Yen et al.\(^10\) also have studied for the asymptotic early - time scaling in the ternary \(A + 2B\rightarrow C\) reaction - diffusion process with initially separated reactants. To our knowledge, it is of fundamental importance to measure extensively more complicated reaction such as multi - components reaction - diffusion process, even though the three - species reaction may occur rarely in the fields of physics, chemistry, and biology.

In the present study, we present the decay process in a reaction - diffusion system with three - species. By a simple perturbation expansion, we derive analytically the particle density and the global reaction rate before the crossover in the reaction - diffusion system of \(A + B + C \rightarrow D\). The scaling exponent for the global reaction rate is also confirmed numerically before and after the crossover via Monte Carlo simulations.

First of all, let us denote that \(\rho_A(x,t), \rho_B(x,t),\) and \(\rho_C(x,t)\) are the particle densities for three - species \(A, B,\) and \(C\) existing at a position \(x\) at time \(t\). As we assume that three - species particles are distributed separately on the axis \(x\), the special initial condition for these particle densities is as follows : \(\rho_A(x,0) = A_0H(x), \rho_B(x,0) = B_0H(x),\) and \(\rho_C(x,0) = C_0[1 - H(x)]\). \(A_0, B_0,\) and \(C_0\) are the initial particle densities, and \(H(x)\) is the Heaviside step function. We assume that both \(A_0\) and \(B_0\) have a uniform mixing state on \(0 < x < \infty\). Since the mean field approximation may be applied to three - species system, \(A + B + C \rightarrow D\), the deterministic rate equation for \(\rho_A(x,t)\) can be expressed in terms of
\[
\frac{\partial}{\partial t} \rho_A(x, t) = D_A \nabla^2 \rho_A(t) - K \rho_A(x, t) \rho_B(x, t) \rho_C(x, t), \quad (1)
\]

where \(D_A\) is the diffusion constant for one-species \(A\). In the above equation \(K\) is the reaction rate which can be considered as small value in reaction-limited reaction.

In particular, when we introduce the dimensionless particle densities \(\alpha(x, t)\), \(\beta(x, t)\), and \(\gamma(x, t)\) from the relations of \(\rho_A(x, t) = A_0 \alpha(x, t)\), \(\rho_B(x, t) = B_0 \beta(x, t)\), and \(\rho_C(x, t) = C_0 \gamma(x, t)\), eq. (1) for \(\alpha(x, t)\) can be rewritten as

\[
\frac{\partial}{\partial t} \alpha(x, t) = d_0 \frac{\partial^2}{\partial \xi^2} \alpha(x, t) - \frac{\omega}{\eta} \alpha(x, t) \beta(x, t) \gamma(x, t), \quad (2)
\]

where the perturbation parameter \(d_0\), \(\eta\), and \(\omega\) are denoted by \(d_0 = (D_A/D_B D_C)^{1/2}\), \(\eta = A_0\), and \(\omega = K/(D_A D_B D_C)^{1/2}\). In the perturbation parameters \(D_B\) and \(D_C\) are the diffusion constants for two-species \(B\) and \(C\). For early-time regime, a perturbation theory can be developed to calculate on the decay process of three-species reactants, provided that the reactive effect is small compared to the diffusion effect. For the sake of concreteness, if it is assumed to be extremely small (i.e. \(\omega \ll 1\)) for the perturbation coefficient, the dimensionless particle densities are expanded in series of powers of \(\omega\) as

\[\alpha = \sum_{n=1}^{\infty} \alpha_n \omega^n, \quad \beta = \sum_{n=1}^{\infty} \beta_n \omega^n, \quad \text{and} \quad \gamma = \sum_{n=1}^{\infty} \gamma_n \omega^n.\]

The solutions for \(\alpha(\xi, \tau), \beta(\xi, \tau)\), and \(\gamma(\xi, \tau)\) are obtained that

\[
\alpha(\xi, \tau) = \phi\left(\frac{\xi}{2(d_0 \tau)^{1/2}}\right), \quad \beta(\xi, \tau) = \phi\left(\frac{\xi}{2(d_0 \tau)^{1/2}}\right), \quad (3)
\]

and

\[
\gamma(\xi, \tau) = 1 - \phi\left[\frac{\xi}{2\left(d_0 \frac{1}{\tau}\right)^{1/2}}\right], \quad (4)
\]

where the dimensionless time \(\tau\) and space variables \(\xi\) are, respectively, given by \(\tau = t A_0 B_0 C_0 (D_A D_B D_C)^{1/2}, \quad \xi = x(A_0 B_0 C_0)^{1/2}\), and \(\phi(x) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{x} dx e^{-x^2} \).

In general, the global reaction rate \(R(t)\) also can be defined by \(R(t) = \int_{-\infty}^{\infty} dx R(x, t)\), where the local reaction rate is the statistical quantity given by \(R(x, t) = K \alpha(x, t) \beta(x, t) \gamma(x, t)\). For simplicity,
we can get the global reaction rate from lowest order of perturbation terms. Hence, this is calculated as

\[
R(\tau) = A_0 B_0 C_0 (D_A D_B D_C)^{1/2} \omega (R_0 + \omega R_1 + ...) \sim \tau^{1/2}
\]

in early - time regime.

In order to confirm numerically the analytical result of the global reaction rate, we concentrate mainly on the Monte Carlo simulation in reaction - diffusion process of \( A + B + C \to D \). It is supposed that three - species reactants are distributed randomly on two - dimensional square lattice with the periodic boundary conditions. We also assume that the intermediate process existing concurrently the combined two - species reactants can be formed, when two - species reactants meet each other on the same lattice points. If two - species reactants meet the third reactant, these reactants react and leave immediately on lattice point. In this reaction - diffusion process, we only restrict ourselves to the case that the diffusion constant takes the same value for each reactant.

In our reaction - diffusion system, the respective particle density of 30\% for \( A, B, \) and \( C \) is distributed randomly on a square lattice having 200 \( \times \) 200 lattice points. When our simulations are performed on \( 2 \times 10^2 \) realizations, our reaction constant is \( 1/1500 \). As shown in Fig.1, we can directly observe the crossover for the global reaction rate from our simulation result. Therefore, it is found numerically from Fig.2 that the scaling exponent for the slope before the crossover is 0.49 that is close nearly to 0.5 , the result of eq. (5) derived from our three - species process. The scaling exponent for the slope after the crossover also is \(-0.54\), as shown in Fig.3.

In conclusion, we have analytically derived the global reaction rate before the crossover in reaction - diffusion system of the form \( A + B + C \to D \). It is really found from our simulation result that the global reaction rate is approximately proportional to \( t^{1/2} \) at early - time regime, and to \( t^{-1/2} \) at long - time regime by scaling arguments. However, future work is in progress to extend to the systematic method of renormalization field theory for multi - components reaction - diffusion process, and we also will attempt to investigate extensively on fractal lattice models.11)

This work is supported in part by the academic research fund of
Ministry of Education of Korea.

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Figure Captions

Fig.1.

The global reaction rate $R(t)$ verse time $t$ for the reaction - diffusion process of the form $A + B + C \rightarrow D$. Our numerical simulation is done for $2 \times 10^2$ configurations on $200 \times 200$ square lattice with the periodic boundary conditions.

Fig.2

Plot of $\ln R(t)$ verse $\ln t$ before the crossover. The slope of solid line is 0.49.

Fig.3

Plot of $\ln R(t)$ verse $\ln t$ after the crossover. The scaling exponent we obtained is approximately $-0.54$. 