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Cluster approximation solution of a two-species annihilation model

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A two-species reaction-diffusion model, in which particles diffuse on a one-dimensional lattice and annihilate when meeting each other, has been investigated. Mean-field equations for general choice of reaction rates have been solved exactly. The cluster mean-field approximation of the model is also studied. It is shown that the general form of large time behavior of one- and two-point functions of the number operators are determined by the diffusion rates of the two type of species, and is independent of annihilation rates.

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I. INTRODUCTION

Recently properties of systems far from equilibrium have been studied by many people. Although mean-field techniques may give qualitatively correct results for higher dimensions, for low-dimensional systems fluctuations have important roles. Different methods have been used to study reaction-diffusion models, including analytical and approximational methods. Among them, the methods to obtain some quantities can be obtained exactly. For example, in Refs. [1–3], imposing some constraints on the reaction rates leads to a closed set of equations for average number densities in each site. The empty interval method, is another method, which has been also used to analyze the one-dimensional dynamics of diffusion-limited coalescence [4–7]. The most general one-dimensional reaction-diffusion model with nearest-neighbor interactions that can be solved exactly through empty interval method, has been introduced in Ref. [8]. Empty interval method has been also generalized in Ref. [9,10]. Different methods has been introduced to calculate different quantities exactly. However, exactly solvable models are only a special class of reaction-diffusion models, and so people are motivated to use also approximate methods to understand the role played by fluctuations. In Ref. [11] a two-species model has been considered. In this model there are three competing reactions $AA\to\varnothing$, $BB\to\varnothing$, and $AB\to\varnothing$. Asymptotic density decay rates of the two types of species for a special choice of parameters have been studied using the Smoluchowski approximation and also field theoretic renormalization group techniques. A similar model focusing on the same diffusion rates for the two types of species has been studied in Ref. [12]. Field theoretic renormalization group analysis suggest that contrary to the ordinary mean-field technique, the large time density of the minority species decays at the same rate as the majority ones in one-dimensional case. Although an ordinary mean-field technique, generally, does not give correct results for low-dimensional systems, its generalizations such as cluster mean field may give correct results. Anyhow, in the mean-field approximation at most one-point functions may be obtained. To obtain more-point functions one should use other methods. One possible way is, to use a generalization of mean-field known as the cluster mean field approximation.

One of the topics, which have absorbed many interests in recent years, is nonequilibrium phase transitions. There are examples, in which mean-field (MF) solutions are not valid, but its generalization, cluster mean field (CMF) gives qualitatively correct results [13–16]. A coagulation-production model is recently considered in Ref. [13]. Although MF equations do not give correct results, CMF approximation predicts phase transition, supported also by Monte Carlo simulations. Steady state properties in the absorbing phase of one-dimensional pair contact process model are also investigated using Monte Carlo simulations and the cluster approximation. The cluster approximation qualitatively confirms the numerical results [14].

The scheme of the paper is as follows. In Sec. II, the mean-field equations for general parameters have been solved exactly. It is seen that, the large time behavior of the average densities depend both on initial average densities and reaction rates, and are independent of diffusion rates. In Sec. III, the cluster mean-field equations for one- and two-point functions have been solved numerically. It is shown that the general large time behavior is determined by the diffusion rates.

II. THE MEAN-FIELD APPROXIMATION

The model addressed in this article is a two-species exclusion reaction-diffusion model. That is, each site is a vacancy ($\varnothing$) or at most occupied by a particle A or B. The interaction is between nearest sites, and the adjacent sites interact according to the following interactions with the indicated rates:

$$\begin{aligned}
A\varnothing &\leftrightarrow \varnothing A \quad && D_A,\\
B\varnothing &\leftrightarrow \varnothing B \quad && D_B,\\
AA &\to \varnothing\varnothing \quad && \lambda/2,\\
BB &\to \varnothing\varnothing \quad && \lambda'/2,\\
AB &\to \varnothing\varnothing \quad && \delta/2,\\
BA &\to \varnothing\varnothing \quad && \delta/2.
\end{aligned} \tag{1}$$

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We consider translationally invariant initial conditions. In the mean-field approximation, diffusion rates do not have any effect on the evolution equations of average number densities. The mean-field equations for the average densities $a := \langle A \rangle_t$ and $b := \langle B \rangle_t$ are

$$\frac{da}{dt} = -\lambda a^2 - \delta ab, \qquad \frac{db}{dt} = -\lambda' b^2 - \delta ab. \tag{2}$$

The large time behaviors of these equations for special choices of parameters have been studied in Refs. [12,11]. Now, we want to solve these equations exactly and then we will show that there are cases which are not considered in Refs. [12,11], and give qualitatively correct result for large time behaviors, although the exponent of the decay rate is not correct.

Consider the following cases.

(I) $\lambda = \lambda'$. The evolution equation for $u := b/a$ is

$$\frac{du}{dt} = (\lambda - \delta) u (1-u) a. \tag{3}$$

Using Eqs. (2) and (3), it is seen that

$$\frac{du}{da} = -\frac{(\lambda - \delta) u (1-u)}{(\lambda + \delta u) a}, \tag{4}$$

which can be integrated to

$$\left| \frac{u-1}{u_0 - 1} \right|^{1+\delta/\lambda} \left(\frac{u_0}{u} \right) = \left(\frac{a}{a_0} \right)^{1-\delta/\lambda}, \tag{5}$$

where u_0 and a_0 are the initial values of u and a, respectively. Now, we can obtain the large time behavior of the average densities. It is seen that the large time behavior of u depends on the ratio δ/λ.

(1) $\delta > \lambda$. At large times, obviously $a \to 0$, so it is seen from Eq. (5) that depending on the initial value u_0, two cases may occur

$$\text{at large times } u \to \infty \Rightarrow u \sim a^{\lambda/\delta - 1}, \quad b \sim a^{\lambda/\delta},$$

$$\text{at large times } u \to 0 \Rightarrow u \sim a^{\delta/\lambda - 1}, \quad b \sim a^{\delta/\lambda}.$$

Assuming an imbalance in the initial average densities, for example, $a_0 > b_0$ ($u_0 < 1$), Eq. (2) gives the large time behavior of $a(t)$, and $u(t)$ as

$$a(t) \sim t^{-1}, \qquad u(t) \sim t^{1-\delta/\lambda}, \tag{6}$$

which means that for $\delta > \lambda$, in the mean-field approximation the minority species dies out earlier than the majority one, and the decay exponent of $u(t)$ is independent of diffusion rates.

(2) $\delta < \lambda$. As a consequence of the large time behavior of a, $a \to 0$, it is seen from Eq. (5) that at large times $u \to 1$. Defining $\epsilon := |1-u|$,

$$\epsilon \sim a^{(1-\delta/\lambda)/(1+\delta/\lambda)}. \tag{7}$$

To obtain the large time behavior of a and u, we should use again Eqs. (2) and (3), which give

$$a(t) \sim t^{-1}, \qquad |1-u(t)| \sim t^{-(1-\delta/\lambda)/(1+\delta/\lambda)}, \tag{8}$$

which means that at large times both the minority and the majority species decay with the same rate. The exponent of decay rate does not depend on the diffusion rates.

(II) $\lambda \neq \lambda'$. For this case one arrives at

$$\frac{du}{da} = -\frac{[(\lambda - \delta) - (\lambda' - \delta) u] u}{(\lambda + \delta u) a}, \tag{9}$$

which after integration gives

$$\left| \frac{1 - \frac{(\lambda' - \delta) u}{\lambda - \delta}}{1 - \frac{(\lambda' - \delta) u_0}{\lambda - \delta}} \right|^{(\delta^2 - \lambda' \lambda)/(\delta - \lambda')} \left(\frac{u}{u_0} \right)^{-\lambda} = \left(\frac{a}{a_0} \right)^{-\delta + \lambda}. \tag{10}$$

Now, it is easy to obtain large time behavior of the average densities. Generally, there are three cases

(1) $\delta > \lambda, \lambda'$. Depending on the initial average densities, the large time behavior of the average densities ratio is $u(t) \to 0$ ($b \sim a^{\delta/\lambda}$) or $u \to \infty$ ($b \sim a^{\lambda'/\delta}$), which means that one kind of species decay faster.

(2) $\delta < \lambda, \lambda'$. Defining $\epsilon := u - (\lambda - \delta)/(\lambda' - \delta)$, at large times $\epsilon(t) \sim a^{[(\delta - \lambda)(\lambda' - \delta)]/[\lambda \lambda' - \delta^2]}$. In this case two kinds of species decay with the same rate.

(3) $\lambda < \delta < \lambda'$. At large times the average densities ratio $u(t) \to 0$, and $b \sim a^{\delta/\lambda}$.

As it is seen, in the MF approximation only for a special choice of parameters, which is independent of diffusion rates, the two types of species decay with the same rate. The case with $\lambda = \lambda' < \delta$, and $D_A = D_B$ has been considered in Ref. [12]. Using field theoretic renormalization group analysis, it is shown that in one dimension both type of species decay with the same rate. Monte Carlo data also supports the field theory predictions in the one-dimensional model.

III. THE CLUSTER MEAN-FIELD APPROXIMATION

Now, we want to use cluster mean-field approximation. If the diffusion rate for both type of species is the same, $N = 2$ cluster mean-field approximation gives the same value for the decay rates for both type of species, even if there is an imbalance in the initial average densities. If two type of species diffuse with different rates, irrespective of the initial values, at large times particles with greater diffusion rates decay more rapidly. For the nearest-neighbor interactions,

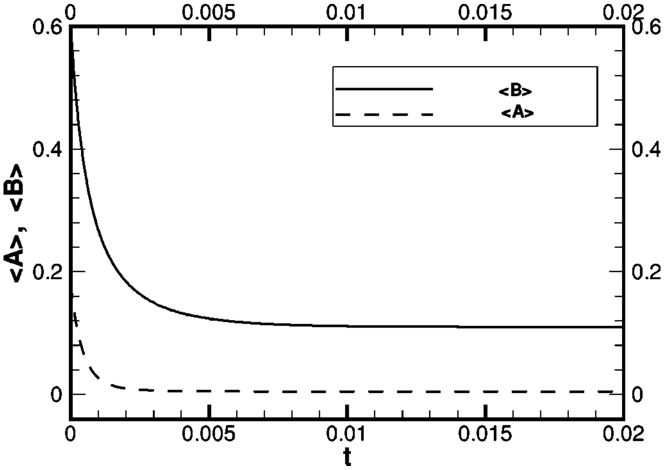

FIG. 1. Average densities $\langle A\rangle$ and $\langle B\rangle$ as a function of time. The rates are $D_A=D_B=1$, $\lambda=\lambda'=1000$, and $\delta=3000$.

the evolution equation of k-point functions $\langle n_1 n_2 \cdots n_k\rangle$ contains at most $(k+1)$-point functions. So, generally, this set of equations will be a hierarchy, which cannot be solved exactly. One way to overcome this difficulty is to impose constraints on the reaction rates that leads to disappearance of $(k+1)$-point functions from the evolution equation of k-point functions. This method has been used to calculate some correlators exactly in Ref. [1]. Another possible way is to use the cluster approximation. In the k-site cluster approximation, the set of evolution equations truncates and one encounters with a closed set of equations which may be solvable, at least numerically. Any how, for a two-site cluster approximation, a three-site joint probability for a sequence of nearest-neighbor sites is approximated by

$$P(A,B,C)=P(A|B,C)P(B,C)\simeq\frac{P(A,B)P(B,C)}{P(B)}, \tag{11}$$

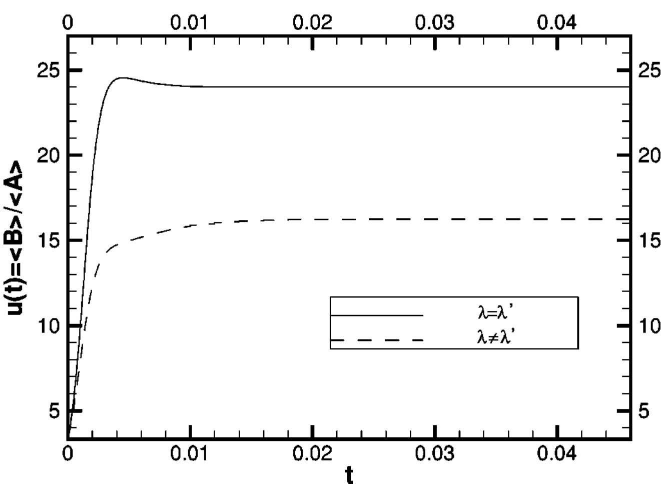

FIG. 2. Ratio of average densities, $u(t)=\langle B\rangle/\langle A\rangle$, as a function of time. For the dashed line, the rates are $D_A=D_B=1$, $\lambda=1000$, $\lambda'=500$, and $\delta=3000$.

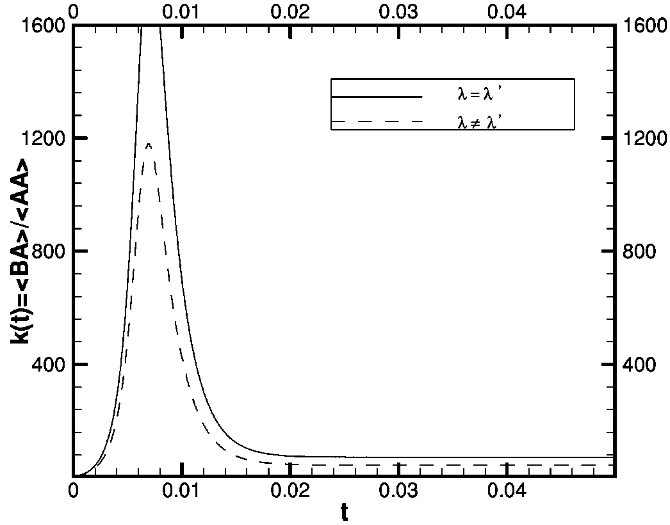

FIG. 3. $K(t)=\langle BA\rangle/\langle AA\rangle$ as a function of time.

where $P(A|B)$ is the conditional probability. In the mean-field approximation there are three variables $\langle A\rangle$, $\langle B\rangle$, and $\langle\emptyset\rangle$, only two of them are generally independent. In the two-site cluster approximation, or pair approximation, the variables are $\langle A\rangle$, $\langle B\rangle$, $\langle\emptyset\rangle$, $\langle A\emptyset\rangle$, $\langle B\emptyset\rangle$, $\langle\emptyset\emptyset\rangle, \dots$, among them there are six independent variables which we choose to be $\langle A\rangle$, $\langle B\rangle$, $\langle AA\rangle$, $\langle BB\rangle$, $\langle AB\rangle$, and $\langle BA\rangle$. In fact in the pair approximation, besides the average densities the two-point functions can also be obtained. The equations of motion for the average densities when $D_A=D_B=:D$ are

$$\begin{aligned}\frac{d\langle A\rangle}{dt}&=-\lambda\langle AA\rangle-\frac{\delta}{2}\langle AB\rangle-\frac{\delta}{2}\langle BA\rangle,\\ \frac{d\langle B\rangle}{dt}&=-\lambda\langle BB\rangle-\frac{\delta}{2}\langle AB\rangle-\frac{\delta}{2}\langle BA\rangle.\end{aligned} \tag{12}$$

Similarly to the mean-field approximation, the diffusion rates do not appear in the evolution equations of the average den-

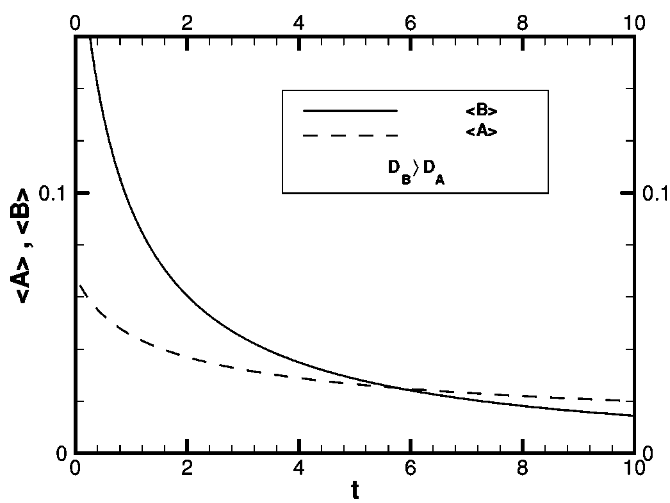

FIG. 4. Average densities as a function of time. The rates are $D_A=0.1$ and $D_B=1$.

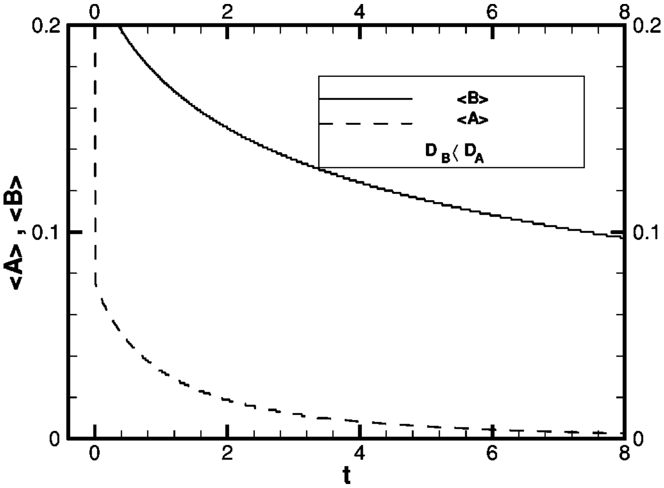

FIG. 5. Average densities as a function of time. The rates are $D_A = 1$ and $D_B = 0.1$.

sities. But in fact, they affect the average densities through the evolution equations of two-point functions, which are

$$\frac{\mathrm{d}\langle AA\rangle}{\mathrm{d}t} = -\frac{\lambda}{2}\langle AA\rangle - \lambda\langle AAA\rangle - \frac{\delta}{2}\langle AAB\rangle - \frac{\delta}{2}\langle BAA\rangle - D\langle AA\varnothing\rangle - D\langle \varnothing AA\rangle + 2D\langle A\varnothing A\rangle, \tag{13}$$

$$\frac{\mathrm{d}\langle BB\rangle}{\mathrm{d}t} = -\frac{\lambda}{2}\langle BB\rangle - \lambda\langle BBB\rangle - \frac{\delta}{2}\langle BBA\rangle - \frac{\delta}{2}\langle ABB\rangle - D\langle BB\varnothing\rangle - D\langle \varnothing BB\rangle + 2D\langle B\varnothing B\rangle, \tag{14}$$

$$\frac{\mathrm{d}\langle AB\rangle}{\mathrm{d}t} = -\frac{\delta}{2}\langle AB\rangle - \frac{\delta}{2}\langle BAB\rangle - \frac{\delta}{2}\langle ABA\rangle - D\langle AB\varnothing\rangle - D\langle \varnothing AB\rangle + 2D\langle A\varnothing B\rangle, \tag{15}$$

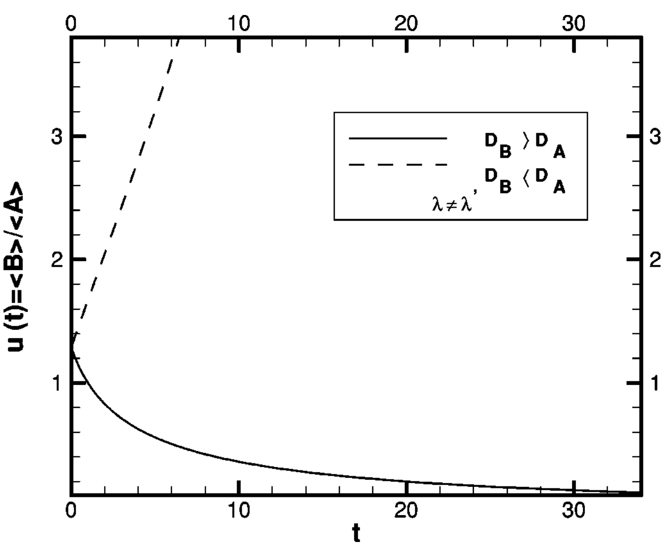

FIG. 6. $u(t) = \langle B\rangle/\langle A\rangle$ as a function of time. The rates are $\lambda = 2400$, $\lambda' = 1000$, $\delta = 2500$, and the greater diffusion rate is 1, and the smaller one is 0.1.

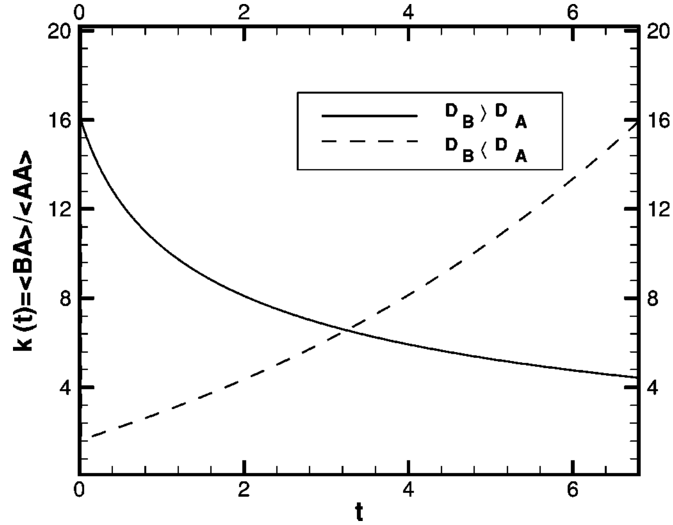

FIG. 7. $K(t) = \langle BA\rangle/\langle AA\rangle$ as a function of time. The rates are $\lambda = 250$, $\lambda' = 100$, $\delta = 300$, and the greater diffusion rate is 1, and the smaller one is 0.1.

$$\frac{\mathrm{d}\langle BA\rangle}{\mathrm{d}t} = -\frac{\delta}{2}\langle BA\rangle - \frac{\delta}{2}\langle BAB\rangle - \frac{\delta}{2}\langle ABA\rangle - D\langle BA\varnothing\rangle - D\langle \varnothing BA\rangle + 2D\langle B\varnothing A\rangle. \tag{16}$$

To solve these equations in the cluster approximation, one should first approximate three-point functions and then all the equations should be expressed in terms of independent variables. For example, $\langle AB\varnothing\rangle$ can be written as

$$\langle AB\varnothing\rangle \approx \frac{\langle AB\rangle\langle B\varnothing\rangle}{\langle B\rangle} \tag{17}$$

and then using probability conservation, $\langle B\varnothing\rangle$ should be expanded,

$$\langle B\varnothing\rangle = \langle B\rangle - \langle BA\rangle - \langle BB\rangle. \tag{18}$$

A. $D_A = D_B$

Figure 1 and 2 show results for $\langle A\rangle$, $\langle B\rangle$, and the density ratios $u(t) := \langle B\rangle/\langle A\rangle$ obtained using numerical solutions of Eqs. (12)–(16). As it is seen both types of species decay with the same rate irrespective of equality or inequality of reaction rates λ and λ'. In the MF approach, $K(t) := \langle BA\rangle/\langle AA\rangle$ is not an independent quantity and is $\langle B\rangle/\langle A\rangle$. But in the CMF approach it is an independent one and the numerical result obtained for it is plotted in Fig. 3. As it is seen, in the CMF approximation it approaches a constant value at large times, means that both $\langle AA\rangle$ and $\langle BA\rangle$ decay with the same rate. Equality of their decay rates is independent of equality or inequality of reaction rates λ and λ'.

B. $D_A \neq D_B$

As MF equations are independent of diffusion rates, their solutions remain unaltered. But in the pair approximation, only Eqs. (12) remains unaltered. The diffusion rate D in Eqs. (13) and (14) should be changed properly to D_A or D_B, and the Eqs. (15) and (16) become

$$\frac{d\langle AB\rangle}{dt} = -\frac{\delta}{2}\langle AB\rangle - \frac{\delta}{2}\langle BAB\rangle - \frac{\delta}{2}\langle ABA\rangle - D_B\langle AB\varnothing\rangle - D_A\langle \varnothing AB\rangle + (D_A + D_B)\langle A\varnothing B\rangle, \tag{19}$$

$$\frac{d\langle BA\rangle}{dt} = -\frac{\delta}{2}\langle BA\rangle - \frac{\delta}{2}\langle BAB\rangle - \frac{\delta}{2}\langle ABA\rangle - D_A\langle BA\varnothing\rangle - D_B\langle \varnothing BA\rangle + (D_A + D_B)\langle B\varnothing A\rangle. \tag{20}$$

These set of equations has been solved numerically, and the numerical results for the average densities has been plotted in Figs 4 and 5. As it is seen, at large times, species with greater diffusion rate dies out faster. If species with greater diffusion rate are in majority initially, there is a crossover, as it is seen from Fig. 4. The general behavior of the average densities ratio is independent of λ, λ', and δ, and the general form of large time behavior is determined by the diffusion rates. See Fig. 6. The numerical results for $K(t)$ have been summarized in Fig. 7.

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