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LETTER TO THE EDITOR

Three-species diffusion-limited reaction with continuous density-decay exponentsJae Woo Lee^{†‡} and Vladimir Privman[‡][†] Department of Physics, Inha University, Incheon 402-751, Korea[‡] Department of Physics, Clarkson University, Potsdam, NY 13699-5820, USA

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Abstract. We introduce a model of three-species two-particle diffusion-limited reactions $A + B \rightarrow A$ or B , $B + C \rightarrow B$ or C , and $C + A \rightarrow C$ or A , with three persistence parameters (survival probabilities in reaction) of the hopping particle. We consider isotropic and anisotropic diffusion (hopping with a drift) in one dimension. We find that the particle density decays as a power law for certain choices of the persistence parameter values. In the anisotropic case, on one symmetric line in the parameter space, the decay exponent is *monotonically varying* between the values close to $1/3$ and $1/2$. On another, less symmetric line, the exponent is constant. For most parameter values, the density does not follow a power law. We also calculated various characteristic exponents for the distance of nearest particles and domain structure. Our results support the recently proposed possibility that one-dimensional diffusion-limited reactions with a drift do not fall within a limited number of distinct universality classes.

The kinetics of diffusion-limited reactions has been extensively studied, with recent emphasis on fluctuations in low-dimensional systems [1–7]. In reactions with symmetric annihilation or coagulation of species, including symmetric initial conditions, the density follows a power law $C(t) \sim t^{-\alpha}$, with a non-trivial critical exponent α below the upper critical dimension d_c ; see [3, 5–9]. For instance, for single-species annihilation $A + A \rightarrow 0$ and coagulation $A + A \rightarrow A$, the density decays asymptotically according to the power law $C(t) \sim t^{-1/2}$ for $d = 1 < d_c = 2$, and according to the mean-field power law $C(t) \sim t^{-1}$ for $d > d_c$, etc; see [10–19].

For two-species annihilation $A + B \rightarrow 0$ the density follows the power-law decay $C(t) \sim t^{-d/4}$ for $d < d_c = 4$ and $C(t) \sim t^{-1}$ (mean-field) for $d > 4$ [8, 20–24]. Recently, it was found that in the two-species annihilation model with hard-core particle interactions (same-species exclusion) in $d = 1$ the drift in particle hopping changes the critical exponent α from $1/4$ to $1/3$ [25–27].

There are also several studies of multiparticle reactions such as $kA \rightarrow 0$ or $A + B + C \rightarrow 0$ [28–35]. For instance, for $kA \rightarrow 0$ the upper critical dimension is $d_c = 2/(k - 1)$ [28, 30–32]. For $d > d_c$, the system follows the mean-field rate equation $dC/dt \sim -C^k$ and the density decays as $C(t) \sim t^{-1/(k-1)}$. For $d < d_c$, the fluctuations are important, while at d_c , logarithmic corrections are generally expected in the mean-field power laws. The general reaction $A_1 + A_2 + \dots + A_k \rightarrow 0$ has also been studied by scaling arguments [9, 22, 23].

Recently, a model was introduced for diffusion-limited reactions of two species of particles, $A + B \rightarrow A$ or B , with a drift in diffusion and with hard-core interactions between

same-species particles. The decay exponent of the density was found to vary *continuously* as a function of the probability of which particle, the hopping one or the target, survives in the reaction [36]. This study has suggested that diffusion-limited reactions with drift (anisotropy) in the diffusion of particles do not fall within distinct universality classes in $d = 1$.

In the present work, we extend this observation to a three-species hard-core two-particle reaction model in one dimension. Our model has three adjustable parameters, the survival probabilities, in the reaction, of the hopping particle. All our results were obtained by extensive numerical Monte Carlo simulations utilizing concurrently a cluster of over 50 IBM RISC-6000 workstations at Clarkson University. In the rest of this work, we first define the model generally, and then report numerical results for various parameter values.

Our model is an extension of the two-species model on the one-dimensional lattice. Each lattice site can be occupied by a single particle (A or B or C), or be empty. Monte Carlo simulations were performed for the cases of isotropic and maximally anisotropic hopping. In the isotropic case, a randomly-selected particle attempts to hop to the left or right nearest-neighbour site with equal probabilities $1/2$. In the general anisotropic case, the particle attempts to hop to the right with probability $(1 + a)/2$ or to the left with probability $(1 - a)/2$. In this work we took the maximal bias $a = 1$, i.e. the chosen particle only attempts to hop to the right.

If the target site is empty then the hopping attempt succeeds and the chosen particle is moved one lattice spacing. If the target site is occupied by a particle of the same species as the chosen particle then the hopping attempt fails; this rule models the hard-core interaction between same-species particles. If the target site is occupied by a particle of a different species then the hopping is accompanied by reaction defined by the following probabilistic rules (shown here for hopping to the right):

$$AB \rightarrow \begin{cases} 0A & \text{Prob } p \\ 0B & \text{Prob } 1 - p \end{cases} \quad \text{and} \quad BA \rightarrow \begin{cases} 0B & \text{Prob } p \\ 0A & \text{Prob } 1 - p \end{cases} \quad (1)$$

$$BC \rightarrow \begin{cases} 0B & \text{Prob } q \\ 0C & \text{Prob } 1 - q \end{cases} \quad \text{and} \quad CB \rightarrow \begin{cases} 0C & \text{Prob } q \\ 0B & \text{Prob } 1 - q \end{cases} \quad (2)$$

$$CA \rightarrow \begin{cases} 0C & \text{Prob } r \\ 0A & \text{Prob } 1 - r \end{cases} \quad \text{and} \quad AC \rightarrow \begin{cases} 0A & \text{Prob } r \\ 0C & \text{Prob } 1 - r \end{cases} \quad (3)$$

where $0 \leq p, q, r \leq 1$. The probabilities p , q , and r represent the persistence (probability of survival) of the hopping particle. Thus the reactions involved are $A + B \rightarrow A$ or B , $B + C \rightarrow B$ or C , and $C + A \rightarrow C$ or A .

In the Monte Carlo simulations, we used lattices of 10^5 sites with periodic boundary conditions. One Monte Carlo time step corresponded, statistically, to the number of hopping attempts equal to the number of remaining particles, so that, on average, each particle's hopping attempt rate (per unit time) was 1. Initial densities were 90% of the full occupancy, with randomly distributed equal densities of the three species. Data were collected for up to 10^5 Monte Carlo time steps and averaged over at least 100 runs for each choice of the persistence parameter values.

Let us point out that if the initial density of the C particles, for instance, is zero, then our model becomes two species, identical to that studied in [36]. In this two-species (A and B) case, the initial symmetry $A \leftrightarrow B$, assuming equal densities, is maintained dynamically for all values of p . Indeed, the number of $A \cdots B$ configurations (here \cdots represent empty or no sites) which lead to a reaction when A 'catches up' with B (we consider the fully

anisotropic hopping case here [36]) is equal, on the one-dimensional lattice, to the number of $B \cdots A$ configurations: they simply alternate.

In the new, three-species model, the symmetries are less robust. Indeed, starting from a symmetric initial distribution, the system can evolve dynamically into a state which is not symmetric with respect to the three species involved. In this regard, our results shed an interesting light on the nature of the non-universal-exponent behaviour. Similar to the two-species case, we find non-universal exponents only when all the following conditions are satisfied, and presumably it is the interplay of all three of them that leads to non-universality: the hopping must be anisotropic, the same-species interaction must be hard core, and the *full symmetry* must be maintained. Thus, we find non-universal exponents only on the symmetric line $p = q = r$ in the parameter space. On some other lines, we find constant-exponent (universal) behaviour, while in most of the parameter space, lack of symmetry results in a non-power-law density variation (so that critical exponents are not defined). We note, however, that for a certain three-species system in two dimensions, with *three-particle reactions*, continuous exponents were found [37] for a specific line in the parameter space, without introduction of spatial anisotropy in the dynamics.

In figure 1, we plot the density as a function of time for varying persistence parameter values, for the fully symmetric case $p = q = r$ and anisotropic hopping. The log–log plot clearly shows the asymptotic power-law (straight-line) behaviour. However, the slope depends on the persistence parameter. The decay exponents were estimated by extrapolation of the local slopes, similar to [36]. In table 1, we list the exponents for various values of the persistence parameter. We actually calculated several physical quantities which characterize fluctuations in the system, similar to [36]. These include the density $C(t) \sim t^{-\alpha}$, the average distance between nearest particles of the same species $\langle l_{AA}(t) \rangle \sim t^\beta$, the average distance between nearest particles of different species $\langle l_{AB}(t) \rangle \sim t^\gamma$, the average domain size of same-species particles $\langle L_A(t) \rangle \sim t^\delta$, the average number of particles per such domain $\langle N_A(t) \rangle \sim t^\eta$, the average number of pairs of same-species particles $\langle N_{AA}(t) \rangle \sim t^{-\mu}$, and the average number of pairs of different-species particles $\langle N_{AB}(t) \rangle \sim t^{-\nu}$. In the latter two quantities the pairs need not be nearest neighbour, they can be separated by empty lattice sites. All these exponents vary non-universally along the line $p = q = r$; their values will be further discussed in the following paragraphs.

Table 1. Exponent estimates for several values of the persistence parameters, with $p = q = r$. The exponents are defined according to $C \sim t^{-\alpha}$, $\langle l_{AA} \rangle \sim t^\beta$, $\langle l_{AB} \rangle \sim t^\gamma$, $\langle L_A \rangle \sim t^\delta$, $\langle N_A \rangle \sim t^\eta$, $\langle N_{AA} \rangle \sim t^{-\mu}$, $\langle N_{AB} \rangle \sim t^{-\nu}$; see text for further details.

p	α	β	γ	δ	η	μ	ν
1	0.499(2)	0.49(1)	0.50(1)	0.503(6)	0.005(4)	0.497(4)	0.499(5)
0.75	0.456(3)	0.46(1)	0.47(1)	0.51(1)	0.064(3)	0.440(8)	0.525(5)
0.5	0.402(3)	0.42(1)	0.44(1)	0.54(1)	0.16(1)	0.381(7)	0.558(5)
0.25	0.360(4)	0.387(3)	0.42(1)	0.56(1)	0.23(1)	0.341(2)	0.578(4)
0	0.340(4)	0.360(2)	0.405(6)	0.57(1)	0.26(1)	0.316(4)	0.60(3)

The isotropic-hopping case was studied numerically only for $p = q = r$ in this work. We found that the exponents do not depend on the persistence parameter. The characteristic exponents for the isotropic hopping were estimated as $\alpha = 0.350(5)$, $\beta = 0.366(5)$, $\gamma = 0.438(8)$, $\delta = 0.496(4)$, $\eta = 0.164(8)$, $\mu = 0.328(3)$, and $\nu = 0.512(6)$, where the uncertainties always refer to the last digit. The density-decay exponent, α , value is somewhat larger than $1/3$. Furthermore, it is somewhat smaller than the prediction $\alpha = 3/8 = 0.375$

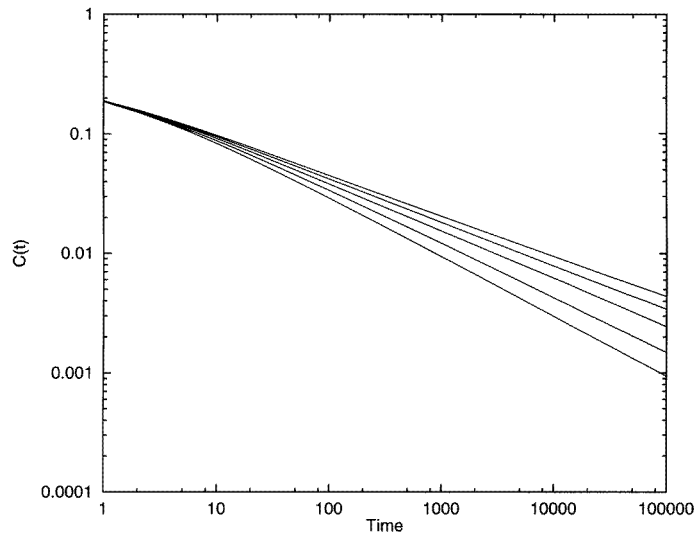


Figure 1. Log-log plot of the decay of the A-particle density against time, for $p = q = r = 1$ (bottom curve), 0.75, 0.5, 0.25, 0 (topmost curve).

for three-species two-particle annihilation $A_i + A_j \rightarrow 0$ ($i \neq j$) [32]. As already mentioned, exponent values exactly (or very close to) $1/3$ appear in the fully anisotropic $A + B \rightarrow 0$ reaction. The value α near $1/3$ was also found for the two-species variant of our model with anisotropy and with $p = 1/2$, and in the anisotropic three-species case with $p = q = r = 0$ (see table 1).

Thus, it seems likely that both the isotropic-hopping results and the anisotropic results, with the latter limited to certain special points in the parameter space, will be eventually identified within some established universality classes of various diffusion-limited reactions.

However, for anisotropic hopping, the exponents are non-universal when the persistence parameter values are varied in the full range from 0 to 1, both in the symmetric three-species case and in the two-species case (where the symmetry is built-in). Of course, there is always the danger that the observed behaviour, interpreted as non-universality, is actually a slow crossover phenomenon. However, we note that our simulation is sufficiently ‘large scale’ as compared to other simulations (including our own in this work) which have found both universal and non-universal behaviour. So, we feel confident that the observed non-universality is well established within the limits of modern computational capabilities.

Some general exponent properties can still be discussed even if the universality class association is ambiguous. Owing to the effective repulsion, one expects that $\langle l_{AA}(t) \rangle \leq \langle l_{AB}(t) \rangle$, i.e. $\beta \leq \gamma$. This inequality is always satisfied by our results (including the case of less symmetry discussed later). There is another inequality, $\beta \geq \alpha$, which holds because the average interparticle distance is related to the (fluctuating) particle density $c_A(t)$ according to $\langle l_{AA} \rangle = \langle 1/c_A(t) \rangle \geq 1/\langle c_A(t) \rangle$ [38, 39]. Our simulation results also satisfy this relation within error bars.

Since the density is approximately equal to the number of particles per domain divided by the average domain size, i.e. $C_A \sim \langle N_A \rangle / \langle L_A \rangle$ [36, 39], the exponents δ and η should satisfy the relation $\alpha = \delta - \eta$. Our data are consistent with this relation. The rate of change of the A-particle density is proportional to the number of the pairs $A \cdots B$, $\langle N_{AB} \rangle$, divided by the diffusion time which is of order $\langle l_{AB} \rangle^2 / \mathcal{D}$, where \mathcal{D} is the diffusion constant. This

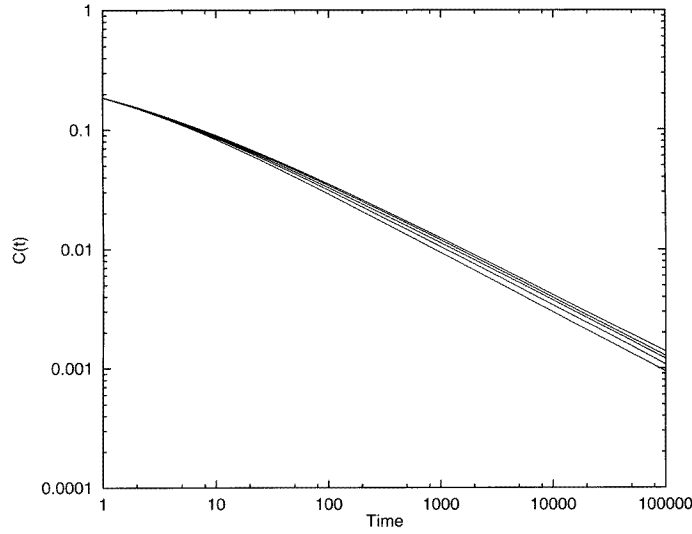


Figure 2. Log-log plot of the decay of the A-particle density against time, for $p = q = 1$ and $r = 1$ (bottom curve), 0.75, 0.5, 0.25, 0 (topmost curve).

yields the exponent relation $\alpha = 2\gamma + \nu - 1$ [39]. Another exponent relation follows by observing that the same rate can be estimated as the inverse of $\langle L_A \rangle \langle l_{AB} \rangle^2 / \mathcal{D}$, which yields $\alpha = 2\gamma + \delta - 1$ [26]. Combining the above relations, we get $\nu = \delta$ and $2\gamma + \eta = 1$. The latter equalities are satisfied by our results to within 10%. Note that these exponent relations are based on a combination of mean-field and diffusive arguments and they are therefore phenomenological.

For the symmetric dynamics with $p = q = r = 0$ and anisotropic hopping, the exponents are equal to those for the isotropic hopping case within error bars. The estimated exponent of the density is close to $\alpha = 1/3$. When values of the persistence parameters increase along the diagonal (symmetric) line in the parameter space the exponent of the density α increases continuously in the anisotropic case. At $p = q = r = 1$ the density exponent estimate is close to $\alpha = 1/2$ (the latter value is likely exact). The decay of the density $\sim t^{-1/2}$ is then similar to that of the single-species coalescence or annihilation, $A + A \rightarrow A$ or 0 , and the two-species annihilation version of our model [36], discussed earlier, at $p = 1$. In this case no large domains of the same species of particle are formed. Indeed, the exponent η estimates are close to zero. Even in this well mixed situation, non-mean-field fluctuations can arise in the form of non-mean-field interparticle distribution [12, 34]. For $p = q = r = 1$, the ‘catching up’ argument for the impossibility of large same-species domains applies, similarly to the two-species case. This argument is not reviewed here; see [36].

For anisotropic hopping, we explored points in the parameter space of p , q , and r outside the symmetric line $p = q = r$. The only other regions in the parameter space where power-law behaviour is found are the line $p = q = 1$, r -varying, and two lines obtained by relabelling. In figure 2, we plot the density against time for $p = q = 1$ and several r values. For large time, a power-law behaviour is obtained with the same exponents for $r < 1$ as in the case $p = q = r = 1$, within error limits. It is important to recall that for $p = q = r = 1$ the system is fully mixed: there are no large same-species domains formed. For $r < 1$, the B species is no longer symmetric (while the $A \leftrightarrow C$ symmetry is still

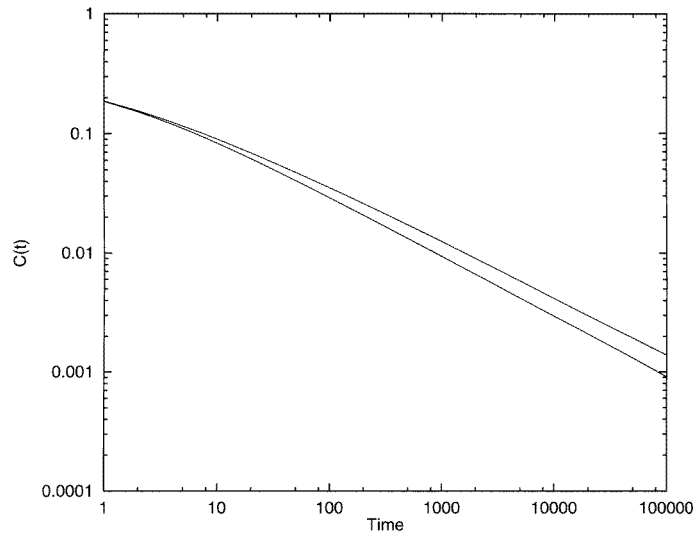


Figure 3. Log-log plot of the decay of the A (upper curve) and B (lower curve) particle densities for $p = q = 1$, $r = 0$.

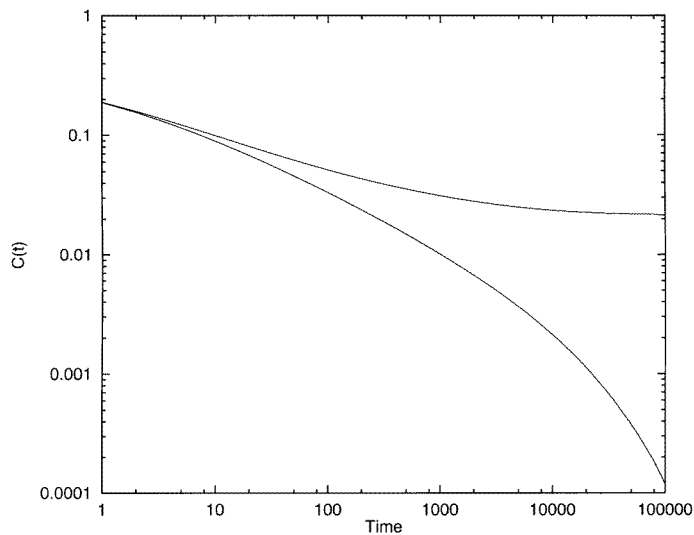


Figure 4. Log-log plot of the variation of the C-particle density (upper curve) and A (and B) density (lower curve) against time, for $p = 1$, $q = r = 0$.

preserved). Numerical indications are that the density of B still follows approximately the same power law as A and C, see figure 3 for the case $r = 0$, but with a smaller amplitude. The well mixed state seems to persist for $r < 1$.

As already mentioned, probes at several other p , q , and r values with varying degrees of symmetry (though we did not do a ‘dense’ scan of the full cube $0 \leq p, q, r \leq 1$) seem to suggest that outside the lines $p = q = r$, $p = q = 1$ (and also $p = r = 1$ and $q = r = 1$ by symmetric relabelling), the behaviour of the density is no longer power law. Let us

consider, for illustration, the point $p = 1$, $q = r = 0$. The symmetry here seems not lower than, for instance, the line $q = r = 1$. In both cases, C is special while A and B remain symmetric. However, for $p = 1$, $q = r = 0$, our numerical data suggest that C particles survive with non-zero final density, see figure 4, while A and B are eliminated faster than a power law for large times, as shown in figure 4. Attempts to fit the A density to a stretched exponential were inconclusive (the fitted exponent of the stretched-exponential power was very small). Generally, for p , q , and r values which are not symmetrically positioned in the parameter space there is no reason to expect equal large-time densities of the species even for equal-density initial conditions.

Finally, let us list some preliminary findings [40] which hopefully illuminate the robustness of the results of this work to changes in the reaction rules. Numerical Monte Carlo simulations [40] suggest that the following symmetric three-species reaction, $A + B \rightarrow C$, $B + C \rightarrow A$, $C + A \rightarrow B$, has the critical exponent $\alpha = \frac{1}{2}$ regardless of the drift. However, for the three-species two-particle annihilation reaction, $A + B \rightarrow 0$, $B + C \rightarrow 0$, $C + A \rightarrow 0$, the exponents seems to depend on the drift [40].

In summary, we studied three-species diffusion-limited reactions with emphasis on the effects of hopping anisotropy and variation of the survival probabilities of the hopping particles. The ‘critical’ power-law behaviour was observed only along special, symmetric lines in the parameter space. In the full three-species symmetry case the critical exponents vary continuously, with that for the particle density increasing from about $1/3$ to $1/2$ when $p = q = r$ increase from zero to one. On the less symmetric line $p = q = 1$, the exponents for varying $r < 1$ are the same as for $p = q = r = 1$.

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