Journal of Statistical Physics, Vol. 81, Nos. 5/6, 1995

Exact Solutions of Anisotropic Diffusion-Limited Reactions with Coagulation and Annihilation

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Received March 2, 1995

We report exact results for one-dimensional reaction–diffusion models $A + A \to$ inert, $A + A \to A$, and $A + B \to$ inert, where in the latter case like particles coagulate on encounters and move as clusters. Our study emphasizes anisotropy of hopping rates; no changes in universal properties are found, due to anisotropy, in all three reactions. The method of solution employs mapping onto a model of coagulating positive integer charges. The dynamical rules are synchronous, cellular-automaton type. All the asymptotic large-time results for particle densities are consistent, in the framework of universality, with other model results with different dynamical rules, when available in the literature.

KEY WORDS: Reactions; anisotropic diffusion; coagulation; synchronous dynamics.

1. INTRODUCTION

Diffusion-limited reactions (DLR) involving aggregation and annihilation processes are important in many physical, chemical, and biological phenomena[1-3] such as star formation, polymerization, recombination of charge carriers in semiconductors, soliton and antisoliton annihilation, biologically competing species, etc. In this paper we generalize and apply a recently introduced method[4,5] in order to study by exact solution effects of anisotropy in some common DLR in one dimension (1D), specifically, $A + A \to A$, $A + A \to$ inert, and a two-species annihilation model $A + B \to$ inert in which like particles coagulate irreversibly. The detailed definitions will be given later.

Scaling approaches and other methods have yielded[1-3,6-12] the upper critical dimension D_c for various reactions. Typical values range from 2 to 4.

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0022-4715/95/1200-0881$07.50/0

For spatial dimensions lower than D_c the kinetics of these reactions is fluctuation-dominated, and we cannot expect the rate equation approach to be valid. Indeed the mean-field rate equation approximation ignores effects of inhomogeneous fluctuations. Fluctuation-dominated DLR have been subject to numerous studies by other methods, notably exact solutions and asymptotic arguments[1,13–22] in 1D. The 1D reactions have also found some experimental applications.[23,24] These studies have assumed isotropic hopping (reactant particle diffusion).

Recently Janowsky[25] concluded, based on numerical results and phenomenological considerations for the two-species annihilation reaction $A+B\to$ inert, that making the hopping fully directed would change the universality class in 1D. Specifically, the large-time particle concentration (assuming equal densities of both species) would scale according to $c(t)\sim t^{-1/3}$ instead of the isotropic-hopping power law $t^{-1/4}$. Few exact and numerical results available in the literature on anisotropic reactions involving only one species[26,27] indicate that the power law is not changed. The model of ref. 25 assumed that like particles interact via hard-core repulsion; this seems to be an essential ingredient for observing the change-over in the universality class.

In this work we report the exact solution for two-particle annihilation with anisotropic hopping. We consider discrete-time simultaneous-updating dynamics, also termed synchronous dynamics, so that our models are cellular-automaton type. The universality classes of behavior at large times and large spatial scales are expected not to depend on most of the details of the model dynamics. Some features, however, are important. For instance, the hard-core constraint plays an important role in determining the universality class of models without reactions (see refs. 1 and 25 and literature cited therein). In our work, however, in order to achieve exact solvability, we took "sticky-particle" rather than hard-core interactions: the like particles coagulate on encounters and diffuse as groups. Our exact calculations yield the $t^{-1/4}$ power law found earlier for similar "sticky-particle" reactions with isotropic hopping.[28,29] This result is probably due to absence of hard-core interations in our model.

For unequal intial concentrations, the large-time behavior changes.[28,29] The crossover between the two regimes is derived analytically. Finally, we also obtain new exact results for single-species two-particle aggregation and annihilation reactions with anisotropy; see also ref. 26. We find that anisotropy does not change the universality class of kinetics of these reactions. A short version of this work was reported.[30]

This paper is organized as follows: in Section 2 we define and review some existing results for the models studied. In Section 3 our method for exact solution is introduced. In Section 4 results for the single-species

models are presented. Finally, Section 5 is devoted to the two-species model. Further scaling analysis of the two-species model and a brief summarizing discussion are given in Section 6.

2. REACTION–DIFFUSION MODELS

In lattice DLR models with like particles it is usually assumed that the particles hop independently, to the extent allowed by their interactions, to their nearest neighbor sites. Whenever two particles meet, they can both annihilate, which corresponds to the reaction $A + A \to$ inert. If, however, only one particle of a pair disappears, we get the reaction $A + A \to A$, usually termed "aggregation." Such single-species reactions have the upper critical dimension $D_c = 2$.[6-9] For $D < 2$ the particle concentration at large times behaves according to $c(t) \sim t^{-D/2}$. Specifically, the 1D kinetics of these reactions is non-mean-field, with the typical diffusional behavior $c(t) \sim t^{-1/2}$. This result is not affected by short-range interactions between the particles and is not sensitive to their initial distribution as long as initial correlations are sufficiently short range.

Consider now the two-particle annihilation model, to be termed the AB model. Particles hop randomly to one of their nearest neighbor sites. Whenever two particles meet, unlike species annihilate, $A + B \to$ inert. When like species meet, some interaction must be assumed. The simplest interaction is hard core: diffusion attempts leading to multiple occupancy of lattice sites are discarded. For such reactions, assuming equal average A and B concentrations and uniform initial conditions, the upper critical dimension is $D_c = 4$.[6-9] The (equal) particle concentrations scale according to $c(t) \sim t^{-D/4}$. A surprising, largely numerically based recent result of Janowsky[25] is the new exponent $\approx 1/3$, replacing 1/4, for anisotropic particle hopping in 1D. For unequal initial concentrations, the density of the minority species is expected to decay faster than the symmetric-case power law; some specific results will be referred to later.

In order to obtain a solvable model in 1D, let us now consider the AB annihilation model with the "sticky particle" interaction. Thus, like particles coagulate irreversibly on encounters, for instance,

$$nA + mA \to (n+m)A \tag{2.1}$$

and the clusters thus formed then diffuse as single entities with the single-particle hopping rates. When unlike clusters meet at a lattice site, the outcome of the reaction is

$$nA + mB \to \begin{cases} (n-m)A & \text{if } n > m \\ \text{inert} & \text{if } n = m \\ (m-n)B & \text{if } n < m \end{cases} \tag{2.2}$$

Recent numerical results and scaling considerations for these reactions[31] in $D = 1, 2, 3$ seem to suggest that they are mean field in $D = 2, 3$. However, in $D = 1$ the power-law exponent for the density is 1/4, obtained by exact solution[28,29] which also yielded a faster power-law decay $\sim t^{-3/2}$ for the minority species in case of unequal densities of A and B.

As mentioned earlier, in order to obtain exact solutions for our single-species and AB models, we first solve another model,[4] of coagulating nonnegative integer charges in 1D,[4,5] with anisotropic hopping. All our models are defined with synchronous dynamics to be described in detail in the next section, along with detailed dynamical rules and their exact solution. From the coagulating-charge model one can derive results for the reactions $A + A \to A$ and $A + A \to$ inert with anisotropic hopping; see Section 4. Some of our expressions are new, while other are consistent with results available in the literature. We next use the approach of refs. 28 and 29 to extend the coagulating-charge solution to the "sticky" AB model. We find that hopping anisotropy does not change the density exponent in 1D: it remains 1/4; see Section 5.

3. SYNCHRONOUS DYNAMICS OF COAGULATING CHARGES

Let us consider a one-dimensional lattice with unit spacing. Following ref. 4, we consider diffusion of nonnegative charges on this lattice. Initially, at $t = 0$, we place positive unit charge at each site with probability p or zero charge with probability $1 - p$. Furthermore, we consider synchronous dynamics, i.e., charges at all lattice sites hop simultaneously in each time step $t \to t + 1$, where $t = 0, 1, 2, \ldots$. However, the probabilities of hopping to the right, r, and to the left, $l = 1 - r$, are not necessarily equal. Since this dynamics decouples the even–odd and odd–even space-time sublattices, it suffices to consider only those charges which are at the even sublattice at $t = 0$. Thus we only consider the lattice sites $j = 0, \pm 2, \pm 4, \ldots$, at times $t = 0, 2, 4, \ldots$, and lattice sites $j = \pm 1, \pm 3, \pm 5, \ldots$ at times $t = 1, 3, 5, \ldots$.

One can view the diffusional hopping as taking place on a directed square lattice with the time direction along the "directed" diagonal. This lattice is illustrated in Fig. 1; note that the charges arriving at site j at time t can only come from the sites $j - 1$ and $j + 1$ at time $t - 1$. Finally, the "interaction" between the charges is defined by the rule that all charge accumulated at site j at time t coagulates. There can be 0, 1, or 2 such charges arriving from the two nearest neighbors of j in the time step

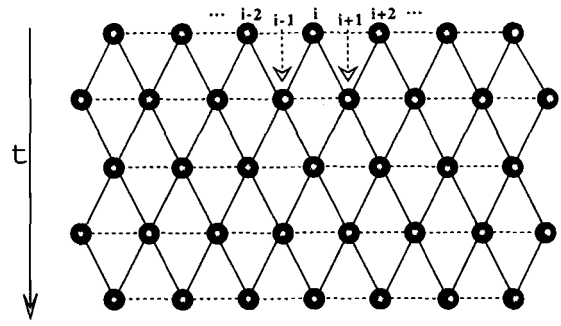

Fig. 1. The 1D even–odd sublattices represented as the two-dimensional space-time lattice directed along the time axis. The solid-line bonds show possible hopping event directions.

$t-1 \to t$, depending on the random decisions regarding the directions of hopping from sites $j \pm 1$ in this time step.

This model can also be viewed as diffusion–coagulation of unit-charge "particles" C, where the coagulation is presented by the reaction

$$nC + mC \to (n+m)C \tag{3.1}$$

Such reactions, without the limitation of positive or integer charges, and with an added process of feeding-in charge at each time step, with values drawn randomly at each site from some fixed distribution, have been considered as models of self-organized criticality and coagulation.[5,32,33] These studies were limited to isotropic hopping, i.e., $r = l = 1/2$. Our interest in these reactions is in that their dynamics can be mapped[4,28,29] onto that of both the single-species (Section 4) and "sticky" AB (Section 5) reaction–diffusion models introduced in Section 2. However, before discussing and utilizing this mapping, let us present the exact solution of the model of coagulating charges with anisotropic hopping, following the ideas of refs. 4 and 5.

For each time t and at each lattice site j (of the relevant sublattice) we define stochastic variables

$$\tau_j(t) = \begin{cases} 1 & \text{probability } r \\ 0 & \text{probability } l \end{cases} \tag{3.2}$$

which represent the hopping direction decisions. Then the stochastic equation of motion for the charges $q_j(t)$, equal to the number of C particles at site j at time t, is

$$q_n(t+1) = \tau_{n-1}(t)\, q_{n-1}(t) + [1 - \tau_{n+1}(t)]\, q_{n+1}(t) \tag{3.3}$$

The total number of C particles, or the total charge, in an interval of k consecutive proper-parity-sublattice sites, starting at site j at time t, is given by

$$S_{k,j}(t) = \sum_{i=0}^{k-1} q_{j+2i}(t) = q_j(t) + q_{j+2}(t) + \cdots + q_{i+2k-2}(t) \tag{3.4}$$

Due to conservation of charge in this process, the equations of motion (3.3) yield the relation

$$\begin{aligned} S_{k,n}(t+1) = {} & \tau_{n-1}(t)\, q_{n-1}(t) \\ & + q_{n+1}(t) + \cdots + q_{n+2k-3}(t) \\ & + [1 - \tau_{n+2k-1}(t)]\, q_{n+2k-1}(t) \end{aligned} \tag{3.5}$$

This result indicates that only the two random decisions at the endpoints are involved in the dynamics of charges in consecutive-site intervals. The exact solvability of coagulating-charge models is based on this property, as first observed in ref. 5. Other solution methods were used in related interface-growth models,[34] which will not be discussed here.

Let us introduce the function

$$I(s, m) = \delta_{s,m} \tag{3.6}$$

and averages

$$f_{k,m}(t) = \langle I(S_{k,j}(t), m) \rangle \tag{3.7}$$

The average $\langle \cdots \rangle$ is over the stochastic dynamics, i.e., over random choices of the decision variables $\tau_i(t)$, as well as over the random initial conditions. Such the latter are uniform, the averages $f_{k,m}(t)$ in (3.7) do not depend on the lattice site j. Functions other than the Kronecker delta have been used for $I(s, m)$ in the literature.[4,5,32,33] With our choice (3.6), the resulting averages $f_{k,m}(t)$ correspond to the probability to find exactly m charge units in an interval of k consecutive sites. For instance, $f_{1,m}(t)$ is the density (fraction) of sites with charge m.

Note that (3.5) essentially represents the following simple rule: charge "fed" into an interval of k sites comes from $k+1$ sites, at the preceding time-variable value, with probability rl, from $k-1$ sites with probability rl, and from two possible groups of k sites, with probabilities r^2 and l^2; this is illustrated in Fig. 2. Furthermore, the variables $\tau_i(t)$ and $S_{k,n}(t)$ are

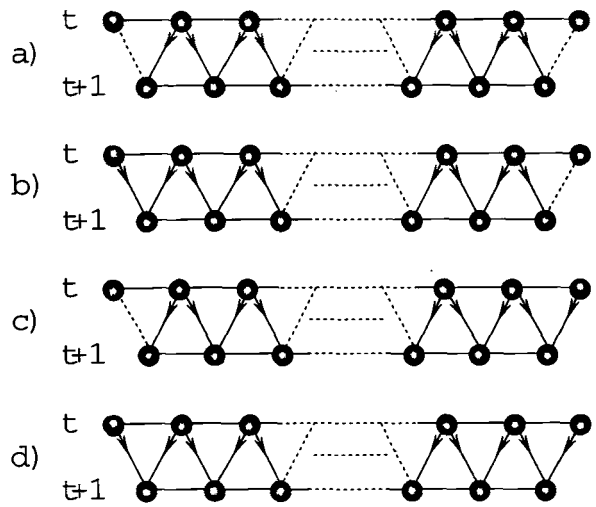

Fig. 2. The charge in a continuous span of k lattice sites at time $t+1$ can come from (a) $k-1$ sites at time t, with probability rl. Note that the directions of hopping from these $k-1$ sites, shown by double arrows, are immaterial. Only the two exterior sites of the larger, $(k+1)$-interval shown determine the probability rl. Another possibility is (b) for the charge to come from k sites at time t. In this case both end sites of the $(k+1)$-interval hopped to the right. The probability of (b) is therefore r^2. Similarly, the probability of the charge coming from the other k-interval, event shown as (c), is l^2. Finally, (d) the charge can also come from all $k+1$ sites shown at time t, with probability rl.

statistically independent because the latter only depends on "decision-making" variables τ_i at earlier times. Therefore, the averages introduced in (3.7) satisfy, for any function $I(s, m)$, the following equations of motion:

$$f_{k,m}(t+1) = rl[f_{k+1,m}(t) + f_{k-1,m}(t)] + (r^2 + l^2) f_{k,m}(t) \tag{3.8}$$

Interestingly, the m dependence is parametric in (3.8). However, it does enter the initial conditions. It is also convenient[4] to define $f_{0,m}(t) = I(0, m)$ in order to extend the applicability of (3.8) to all $t \geqslant 0$. For our specific choices, we have the following expressions. First, the initial conditions of placing charge 1 or 0 at each site, with respective probabilities p and $1-p$, correspond to

$$f_{k,m}(0) = \begin{cases} p^m(1-p)^{k-m}\binom{k}{m}, & 0 \leqslant m \leqslant k \\ 0, & m > k \end{cases} \tag{3.9}$$

where $\binom{k}{m} = k!/[m!(k-m)!]$. Second, the boundary condition is that a null interval cannot have charges, i.e.,

$$f_{0,m}(t \geqslant 0) = \delta_{0,m} \tag{3.10}$$

In order to solve the equations of motion (3.8) we introduce the double generating function of $f_{k,m}(t)$, over the time variable t and over the number of charges m, with fixed number of sites k,

$$g_k(u, w) = \sum_{t=0}^{\infty} \sum_{m=0}^{\infty} f_{k,m}(t)\, u^t w^m \tag{3.11}$$

It is also convenient to introduce the variable $a = r - l$ directly measuring the hopping anisotropy,

$$r = (1+a)/2 \qquad \text{and} \qquad l = (1-a)/2 \tag{3.12}$$

A straightforward but tedious calculation then yields the following difference equation, which derives from the equations of motion (3.8), with (3.9):

$$g_{k+1}(u, w) + 2\frac{(1+a^2)\,u - 2}{(1-a^2)u} g_k(u, w) + g_{k-1}(u, w)$$
$$= -\frac{4}{(1-a^2)u}(wp + 1 - p)^k \tag{3.13}$$

The initial and boundary conditions "translate" as follows:

$$g_k(0, w) = (wp + 1 - p)^k \tag{3.14}$$

$$g_0(u, w) = \frac{1}{1-u} \tag{3.15}$$

The solution of (3.13) is obtained as a linear combination of the special solution $\Omega(wp + 1 - p)^k$ proportional to the right-hand side, and that solution of the homogeneous equation which is regular at $u = 0$. The coefficient Ω is obtained by substitution,

$$\Omega = -\frac{4(wp + 1 - p)}{(1-a^2)\,u(wp + 1 - p - \Lambda_+)(wp + 1 - p - \Lambda_-)} \tag{3.16}$$

where it is convenient to express the denominator in terms of the roots $\Lambda_\pm$ of the characteristic equation of (3.13),

$$\Lambda^2 + 2\frac{(1+a^2)\,u - 2}{(1-a^2)u}\Lambda + 1 = 0 \tag{3.17}$$

These roots are given by

$$\Lambda_{\pm} = \frac{2-(1+a^2)\,u \pm 2[(1-u)(1-a^2u)]^{1/2}}{(1-a^2)u} \tag{3.18}$$

and the root Λ_-, which is nonsingular as $u \to 0$, also gives the homogeneous solution proportional to Λ_-^k. The proportionality constant is determined by (3.15). In summary, the solution takes the form

$$g_k(u, w) = \left(\frac{1}{1-u} - \Omega\right)\Lambda_-^k + \Omega(wp + 1 - p)^k \tag{3.19}$$

The w dependence of this result is via Ω [see (3.16)] and it is of a simple rational form. Therefore, derivation of the dependence on the number of charges, "generated" by w, is relatively simple. In our applications we will concentrate on densities of reactants at single lattice sites, derived from $f_{k=1,m}(t)$. The m dependence then follows by expanding (3.19) in powers of w. However, the u dependence of (3.19) with (3.16), (3.18), is more complicated. Therefore we will use the generating functions for the time dependence and most of our explicit time-dependent expressions will be derived as asymptotic results valid for large times. Indeed, the power series in u are then controlled by the singularity at $u = 1$, and analytical results can be derived by appropriate expansions. Specifically, let us introduce the time-generating function for the quantities $f_{1,m}(t)$, which represent the probability to find charge m at a lattice site at time t. We define

$$G_m(u) = \sum_{t=0}^{\infty} f_{1,m}(t)\, u^t \tag{3.20}$$

The central result of this section is thus

$$G_m(u) = \delta_{m,0}\left[\frac{\Lambda_-}{1-u} - \frac{4}{(1-a^2)u}\right] - (-1)^m \frac{4\Lambda_+ p^m}{(1-a^2)\,u(1-p-\Lambda_+)^{m+1}} \tag{3.21}$$

where $\Lambda_{\pm}$ were given in (3.18). Note that $G_m(u)$ is just the mth Taylor series coefficient in w of the function $g_1(u, w)$.

4. SINGLE-SPECIES REACTIONS

In this section we map the coagulating-charge model onto the two single-species reactions introduced in Section 2. This approach follows recent work,[4] although related ideas have been used in earlier literature,

for instance, in ref. 35. Let us consider first the two-particle aggregation reaction $A + A \to A$. In the coagulating-charge model we now regard each "charged" site as occupied by an A particle and each "uncharged" site as empty of A particles. Specifically, any charge $m > 0$ represents an A particle. No charge at a site, $m = 0$, corresponds to absence of an A particle. The dynamics of the coagulating charges then maps onto the dynamics of the reaction $A + A \to A$ on the same lattice, with the initial conditions of placing particles A randomly with probability p, or leaving the lattice sites vacant with probability $1 - p$, so that the initial density of the A particles is

$$c(0) = p \tag{4.1}$$

We now observe that the quantity $f_{1,0}(t)$ gives the density of empty sites in both models. Therefore, the particle density (per lattice site) $c(t)$ in the aggregation model is given by

$$c(t) = 1 - f_{1,0}(t) \tag{4.2}$$

The generating function is therefore easily derivable from (3.21),

$$\begin{aligned} E(u) &= \sum_{t=0}^{\infty} c(t)\, u^t = \frac{1}{1-u} - G_0(u) \\ &= \frac{1 - A_-}{1-u} + \frac{4(1-p)}{(1-a^2)\, u(1-p-A_+)} \end{aligned} \tag{4.3}$$

The function $E(u)$ is actually regular at $u = 0$. Thus the Taylor series is controlled by the singularity at $u = 1$, near which we have the leading-order term

$$E(u) = \frac{2}{(1-a^2)^{1/2}} \left[\frac{1}{(1-u)^{1/2}} + \mathcal{O}(1) \right] \tag{4.4}$$

This yields the leading-order large-time behavior,

$$c(t) \approx \frac{2}{[(1-a^2)\, \pi t]^{1/2}} \tag{4.5}$$

While we are not aware of other exact solutions for this model with anisotropic hopping, the result (4.5) is not surprising. Indeed, the leading-order large-time behavior is expected to be universal in that it does not depend on the initial density p. Furthermore, the diffusion constant $\mathcal{D}(a) = (1-a^2)\, \mathcal{D}(0)$ decreases proportionally to $1 - a^2$ when the anisotropy is

introduced (single-particle diffusion is then of course also accompanied by drift). Therefore, as a function of $\mathscr{D}(a)t$, the result (4.5) also does not depend on the anisotropy and in fact it is the same as expressions found for other $A + A \to A$ reaction models with different detailed dynamical rules (with isotropic hopping), e.g., ref. 20.

Let us now turn to the two-particle annihilation model $A + A \to$ inert. The appropriate mapping here is to identify odd charges with particles A and even charges with empty sites. Indeed, the dynamics of the coagulating-charge model is then mapped onto the reaction $A + A \to$ inert. Thus, each lattice site with an odd charge $q = 1, 3, 5,...$ will be replaced by a site with one A particle. Each lattice site with an even charge $q = 0, 2, 4,...$ is empty of A particles. The rules of charge coagulation then reduce to the desired reaction. Furthermore, relation (4.1) applies. However, the generating function $E(u)$ for particle density is given by a different expression,

$$E(u) = \sum_{j=0}^{\infty} G_{2j+1}(u) = \frac{4\Lambda_+ p}{(1-a^2)\, u[(1-p-\Lambda_+)^2 - p^2]} \tag{4.6}$$

The large-time behavior is similar to the aggregation reaction, with the universal expression which only differs from (4.5) by a factor of 2,

$$c(t) \approx \frac{1}{[(1-a^2)\,\pi t]^{1/2}} \tag{4.7}$$

While the large-time behavior of both models is model independent and otherwise universal as described earlier, the finite-time results do depend on details of the dynamical rules. For our particular choice of synchronous dynamics on alternating sublattices (Fig. 1), there exists an exact mapping relating the isotropic-hopping aggregation and annihilation reactions.[4] This mapping was also found for the anisotropic-hopping results obtained here. Specifically, we find (by comparing their generating functions)

$$2c_{\text{inert}}(t; p) = c_A(t; 2p) \tag{4.8}$$

where the subscripts denote the outcome of the reaction, while the added argument stands for the initial density. Thus if we consider an annihilation reaction with, initially, at $t = 0$, half the particle density as compared to an aggregation reaction with the same synchronous dynamical rules, then the density ratio will remain exactly 1/2 for all later times, $t = 1, 2,...$, as well.

We note that due to complexity of expressions involved, results like (4.4) and especially (4.8) in this section as well as many other expressions in the next two sections could only be derived by using symbolic computer programs Maple and Mathematica.

5. TWO-SPECIES ANNIHILATION MODEL

In this section we present results for the AB model defined in Section 2. We assume that initially particles are placed with density p, but now a fraction α of them are type A and a fraction β are type B. Clearly,

$$\alpha + \beta = 1 \tag{5.1}$$

Furthermore, the initial A- and B-particle concentrations are, respectively, αp and βp. The concentration difference is constant during the reaction; it remains $(\alpha - \beta)p$. At large times, this is also the limiting value of the density of the majority species, while the density of the minority species vanishes. In what follows we assume

$$\alpha \geqslant \beta \tag{5.2}$$

which can be done without loss of generality. Indeed, the results for $\alpha < \beta$ can be obtained by relabeling the particle species. Thus, either the concentrations are equal or the majority species is always A. Our goal will be to calculate the density $c(t)$ of the majority species A.

The dynamics of the AB model can be related to that of the coagulating-charge model of Section 3 by adapting the ideas of refs. 28 and 29. First, we note that the dynamics of the "sticky" $A + B \to$ inert model can be viewed as coagulation. Thus, if a group of n particles A and m particles B meet, they can be viewed as coagulating and continuing to move together. Of course, at later times this combined group may become part of a larger coagulated cluster of particles. However, if their contribution to the particle count is according to (2.2), the annihilation is properly accounted for by this counting both upon original and later coagulation events with other clusters. Alternatively, one can view these particles as new charges, $+1$ for A and -1 for B. If the total charge of a coagulated cluster is positive, then we view it as a group of A particles (equal in their number to the charge value). If the charge is negative, we consider the cluster a B particle, while if the charge is 0, we regard this cluster as nonexistent (inert) in the AB model.

The probability of having an m-particle (charge m) cluster in the original positive-charge-only model was given by $f_{1,m}(t)$. Each such m-particle cluster can have charge $n = -m, -m+2, \ldots, m-2, m$, where we now refer to the new, $\pm$ charge definition rather than to the positive charges of the original coagulation model. The key observation is that having a "species" label assigned to a particle at time $t = 0$ is statistically independent of its motion and affiliation as part of clusters at later times. Statistical averaging over the particle placement initially and their motion

at later times while coagulating to form particle clusters is uncorrelated with the choice, with probabilities α and β, of which species label to allocate to each particle at time $t=0$.

Thus the density (per site) of m-size clusters with exactly n units of charge, where m size is that of the original coagulation models, while the charge $-m \leqslant n \leqslant m$ is the new $\pm$ type, is given by

$$\Psi_{m,n}(t) = \alpha^{(m+n)/2}\beta^{(m-n)/2}\frac{m!}{((m+n)/2)!\,((m-n)/2)!}f_{1,m}(t) \tag{5.3}$$

Therefore the density per site of A particles, i.e., the density per site of the $+$ charge, can be written as

$$c(t) = \sum_{n=1}^{\infty} n\left[\sum_{m=n,n+2,\ldots} \Psi_{m,n}(t)\right] \tag{5.4}$$

Similar to Section 4, let us denote the time-generation function of $c(t)$ by $E(u)$; see (4.3). By using results from Section 3, and after some algebra, we get the following expression for the generating function:

$$E(u) = \frac{4\Lambda_+}{(1-a^2)\,u(p+\Lambda_+-1)}\left(x\frac{\partial}{\partial x} - y\frac{\partial}{\partial y}\right)S(x,y) \tag{5.5}$$

Here we introduced the function

$$S(x,y) = \sum_{n=1}^{\infty}\sum_{j=0}^{\infty} x^{n+j}y^j\binom{n+2j}{j} \tag{5.6}$$

and the variables

$$x = \frac{p\alpha}{p+\Lambda_+-1} \tag{5.7}$$

$$y = \frac{p\beta}{p+\Lambda_+-1} \tag{5.8}$$

To make progress, we have to evaluate the double sum in (5.6). This is accomplished as follows. First, we write the sum

$$S(x,y) = \sum_{n=1}^{\infty} s_n x^n \tag{5.9}$$

where

$$s_n = \sum_{j=0}^{\infty}\frac{(xy)^j\,\Gamma(2j+n+1)}{j!\,\Gamma(j+n+1)} \tag{5.10}$$

Now, by using the duplication formula for the gamma function, we have

$$s_n = \sum_{j=0}^{\infty} \frac{((n+1)/2)_j ((n+2)/2)_j (4xy)^j}{j!\,(n+1)_j} \tag{5.11}$$

where $(z)_j = \Gamma(z+j)/\Gamma(z)$. The sum in s_n is a special case of the hypergeometric function,

$$s_n = {}_2F_1(\nu, \nu+1/2; 2\nu; \zeta) \tag{5.12}$$

where $\nu = (n+1)/2$ and $\zeta = 4xy$.

Fortunately, this can be expressed in elementary terms; all subsequent references in this paragraph are to formulas in Chapter 15 of ref. 36. First, using Gauss' linear transformation (15.3.6), we obtain

$$\begin{aligned} s_n = {} & \frac{\Gamma(2\nu)\,\Gamma(-1/2)}{\Gamma(\nu)\,\Gamma(\nu-1/2)}\, {}_2F_1\left(\nu, \nu+\frac{1}{2}; \frac{3}{2}; 1-\zeta\right) \\ & + \frac{\Gamma(2\nu)\,\Gamma(1/2)}{\Gamma(\nu)\,\Gamma(\nu+1/2)} (1-\zeta)^{-1/2}\, {}_2F_1\left(\nu, \nu-\frac{1}{2}; \frac{1}{2}; 1-\zeta\right) \end{aligned} \tag{5.13}$$

Next, from the recursion relation (15.2.20),

$$\begin{aligned} & {}_2F_1\left(\nu, \nu-\tfrac{1}{2}; \tfrac{1}{2}; 1-\zeta\right) \\ & \quad = \zeta\, {}_2F_1\left(\nu, \nu+\tfrac{1}{2}; \tfrac{1}{2}; 1-\zeta\right) \\ & \qquad + (1-2\nu)(1-\zeta)\, {}_2F_1\left(\nu, \nu+\tfrac{1}{2}; \tfrac{3}{2}; 1-\zeta\right) \end{aligned} \tag{5.14}$$

Now, by (15.1.10),

$$\begin{aligned} & {}_2F_1\left(\nu, \nu+\frac{1}{2}; \frac{3}{2}; 1-\zeta\right) \\ & \quad = \frac{(1-\zeta)^{-1/2}}{2(1-2\nu)} \left\{ \left[1+(1-\zeta)^{1/2}\right]^{1-2\nu} - \left[1-(1-\zeta)^{1/2}\right]^{1-2\nu} \right\} \end{aligned} \tag{5.15}$$

while (15.1.9) yields the analytical expression

$${}_2F_1\left(\nu, \nu+\tfrac{1}{2}; \tfrac{1}{2}; 1-\zeta\right) = \tfrac{1}{2}\left\{ \left[1+(1-\zeta)^{1/2}\right]^{-2\nu} + \left[1-(1-\zeta)^{1/2}\right]^{-2\nu} \right\} \tag{5.16}$$

and so we have

$$\begin{aligned} & {}_2F_1\left(\nu, \nu+\tfrac{1}{2}; \tfrac{1}{2}; 1-\zeta\right) \\ & \quad = \tfrac{1}{2}\zeta \left\{ \left[1+(1-\zeta)^{1/2}\right]^{-2\nu} + \left[1-(1-\zeta)^{1/2}\right]^{-2\nu} i \right\} \\ & \qquad + \tfrac{1}{2}(1-\zeta)^{1/2} \left\{ \left[1+(1-\zeta)^{1/2}\right]^{1-2\nu} - \left[1-(1-\zeta)^{1/2}\right]^{1-2\nu} \right\} \end{aligned} \tag{5.17}$$

Putting all this together, we find

$$s_n = 2^{2\nu-1}(1-\zeta)^{-1/2}\left[1+(1-\zeta)^{1/2}\right]^{1-2\nu}$$
$$= (1-4xy)^{-1/2}\left(\frac{2}{1+(1-4xy)^{1/2}}\right)^n \tag{5.18}$$

and finally,

$$S(x,y) = (1-4xy)^{-1/2}\sum_{n=1}^{\infty}\left(\frac{2x}{1+(1-4xy)^{1/2}}\right)^n$$
$$= \frac{2x}{(1-4xy)^{1/2}\left[1-2x+(1-4xy)^{1/2}\right]} \tag{5.19}$$

It is useful to introduce the parameter $b=\alpha-\beta\geqslant 0$, which measures the excess of A over B at time $t=0$,

$$\alpha=(1+b)/2 \qquad \text{and} \qquad \beta=(1-b)/2 \tag{5.20}$$

Consider first the equal-concentration case $b=0$. The large-time behavior of the concentration $c(t)$ is governed by the singularity at $u=1$ of the generating function $E(u)$. The form of the latter was evaluated near $u=1$ from the expressions derived in this section, with the result

$$E(u) = \frac{1}{(1-u)^{3/4}}\left[\frac{\sqrt{p}}{2(1-a^2)^{1/4}} - \frac{1-p}{4\sqrt{p}(1-a^2)^{3/4}}(1-u)^{1/2} + \mathcal{O}(1-u)\right] \tag{5.21}$$

The leading-order behavior of the A-particle concentration follows from the first term in (5.21), while the second term will be further discussed in Section 6. We get

$$c(t) \approx \frac{\sqrt{p}}{2\Gamma(3/4)(1-a^2)^{1/4}\,t^{1/4}} \tag{5.22}$$

The most significant feature of this result is that, similar to the single-species reactions considered in Section 4, the anisotropy, a, dependence can be fully absorbed in the diffusion constant, in terms of $\mathscr{D}(a)t = (1-a^2)\,\mathscr{D}(0)t$. The exponent 1/4 was derived in refs. 28 and 29 for different (isotropic) dynamical rules.

A similar expansion for fixed $b > 0$ yields

$$E(u) = \frac{bp}{1-u} + \frac{1-b^2}{(1-a^2)\,b^3 p} - \frac{2(1-b^2)(2-b^2p)}{(1-a^2)^{3/2}\,b^5 p^2}(1-u)^{1/2} + \mathcal{O}(1-u) \tag{5.23}$$

The leading term in (5.23) corresponds to the constant contribution $c(t) = bp + \cdots$, which is expected since A is the majority species. In fact, expansions near $u = 1$ are nonuniform in the limits $b \to 0^+$ and $b \to 0^-$. In deriving (5.23) we used for the first time the fact that the majority species is A. The approach to the constant-asymptotic-density value is given by the third term in (5.23),

$$c(t) - bp \approx \frac{(1-b^2)(2-b^2p)}{\sqrt{\pi}\,b^5 p^2 (1-a^2)^{3/2}\,t^{3/2}} \tag{5.24}$$

Note that this difference is just the density of the minority species B. As before, the anisotropy dependence of this leading-order power-law correction is fully absorbed in the diffusion rate, while the exponent is consistent with the results of refs. 28 and 29. Details of the crossover in the limit $b \to 0$ are discussed in the next section.

6. CROSSOVER SCALING IN THE TWO-SPECIES REACTION

As emphasized in the preceding section, the limit $u \to 1$ is nonuniform at $b = 0$, i.e., the pattern of the asymptotic large-time behavior changes at equal A- and B-particle concentrations. It is of interest to explore this behavior in greater detail within the standard crossover scaling formulation. In this approach, one seeks a combination of powers of variables each of which vanishes in the limit of interest, such that this so-called scaling combination can be kept fixed in the double limit. The appropriate choice is expected to yield a nontrivial variation of quantities of interest in the limit, as functions of the scaling combination.

In our case, the appropriate scaling combination turns out to be proportional to $b/(1-u)^{1/4}$, as determined by inspection of various limiting expressions. It proves convenient to absorb certain constants into the precise definition of the scaling combination σ,

$$\sigma = \sqrt{p}(1-a^2)^{1/4}\,b/(1-u)^{1/4} \tag{6.1}$$

The time-generating function $E(u)$ studied in Section 5 will be now analyzed in the double limit $b \to 0$ and $u \to 1^-$, taken with fixed values of σ. From expressions derived in Section 5 one obtains

$$E(u) \approx p^{-1}(1-a^2)^{-1}\,b^{-3} R(\sigma) \tag{6.2}$$

where R is termed the scaling function. Note that the first two prefactors are constants in the limit of interest. However, the power b^{-3} is necessary to ensure scaling function values of order 1 for σ of order 1.

The scaling function R can be derived exactly,

$$R(\sigma)=\frac{\sigma^3[\sigma+(4+\sigma^2)^{1/2}]^2}{4(4+\sigma^2)^{1/2}} \tag{6.3}$$

Note that it is analytic at $\sigma=0$, where $\sigma \propto b$. Thus, at the expense of introducing the nonanalytic factor in σ which is power law in $1-u$ [see (6.1)], we managed to "blow up" the regime of small b. The scaling limit provides, as usual, a better understanding of the crossover in the limit $b \to 0$. Note that for $\sigma \ll 1$ the following small-argument expansion of $R(\sigma)$ applies:

$$R(\sigma)=\tfrac{1}{2}\sigma^3+\tfrac{1}{2}\sigma^4+\mathcal{O}(\sigma^5) \tag{6.4}$$

It is interesting to note that the leading term here actually reproduces the first term in (5.21). The latter was the limiting form for $u \to 1$ at $b=0$. Indeed, the b dependence cancels out, while the $(1-u)$ dependence is the identical, simple power law in both limits. However, the second term in (5.21) does not seem to correspond to the next scaling-expansion contribution; see (6.4). Corrections to the leading scaling behavior contribute to this term in the $b=0$ expansion.

In the opposite limit, $\sigma \to +\infty$, we get the expansion

$$R(\sigma)=\sigma^4+1-4\sigma^{-2}+\mathcal{O}(\sigma^{-4}) \tag{6.5}$$

The first term here reproduces the leading term in (5.23). Indeed, the limit $\sigma \to +\infty$ corresponds to $u \to 1$ at fixed small positive b. Interestingly enough, the next two terms in (5.23) are also reproduced in their small-b form by the next two terms in (6.5). For instance, the second term in (6.5) yields $1/[(1-a^2)\,b^3 p]$ in $E(u)$. Similarly, the third term in (5.23) is reproduced with numerator 4, which is the correct small-b limiting value. Thus the minority-species concentration (5.24) with, for small b, the numerator replaced again by 4 is also contained in the scaling form. Of course, corrections to scaling, not discussed here, yield improved results.

The main point of the scaling description is that it provides a uniform limiting approximation in the double limit $b \to 0$ and $u \to 1$. Specifically, the region of nonuniform behavior near $b=0$ is exploded by the large factor $\sim(1-u)^{-1/4}$. In terms of σ, the behavior is smooth and well defined. For instance, the result (6.3) applies equally well for $\sigma<0$, which corresponds to A becoming the minority species. The limit of $u \to 1^-$ at small fixed

$b<0$ is described by the limit $\sigma \to -\infty$. The appropriate expansion takes the form

$$R(\sigma) = -1 + 4\sigma^{-2} + \mathcal{O}(\sigma^{-4}) \tag{6.6}$$

similar in structure to (6.5), but without the constant-density first term.

The scaling formulation developed in this section for the particular one-dimensional "sticky-particle" model studied should apply to other models with hard-core interactions and in higher dimensions. However, the results must be viewed with caution. The exponent values are likely to be different. Furthermore, the leading behavior of the asymmetric-model minority-species density [see (5.24)] will not be power law. Rigorous considerations[17,21] and mean-field models suggest exponential behavior for $b \neq 0$. This will result in different asymptotic forms for large $|\sigma|$. Of course, these expectations only emphasize that the sticky-particle and hard-core models belong to different universality classes.

In summary, we derived exact results for several reaction–diffusion models in one dimension. The leading-order large-time particle densities show expected power-law and universal behaviors. Anisotropy of hopping has no effect on the universality class of the models studied, and it can be largely absorbed into the definition of the diffusion constant. While finite-time results are expected[26] to be more sensitive to the value of the anisotropy parameter a, they are cumbersome to derive and of less interest than the leading-order expressions. One interesting exception is the duality relation (4.8), which applies for all finite time values in our synchronous-dynamics models.

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