# Exact solution of a phase-separation model with conserved-order-parameter dynamics and arbitrary initial concentration

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We obtain an exact time-dependent solution of the zero-temperature Kawasaki-type dynamics of a phase-separation model of a binary mixture of $A$ and $B$ on a linear lattice, starting from a random arbitrary initial concentration $p$ of one of the components. This generalizes a recent result by Privman [Phys. Rev. Lett. **69**, 3686 (1992)] in which only the symmetrical case of equal initial concentrations of $A$ and $B$ was studied. In contrast to the case of two-species diffusion-limited annihilation, the symmetrical case can be obtained from the asymmetrical one by letting $p$ tend to $1/2$ continuously. At any concentration $p$, the number of domain walls between $A$ and $B$ decays exponentially to its $p$-dependent quenched steady value. A Monte Carlo simulation shows excellent agreement between the numerical and the analytical solutions.

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There has been much recent interest in the study of the dynamic behavior of phase-separation models of binary mixtures [1–7]. In a binary mixture of $A$ and $B$ particles, there is assumed to be an energy cost $\epsilon$ whenever a domain wall exists between $A$ and $B$ particles. This system can be mapped into the usual Ising model, but with a conserved order parameter (i.e., fixed magnetization). At low temperature, the $A$ and $B$ particles prefer to be separated, and a transition occurs to a phase-separated state with a decreased number of domain walls. Numerical studies [2,3] have shown this type of phase transition at low temperature for spatial dimensions higher than one. In one dimension, however, the entropy is dominant, and there is no transition. Thus, in one dimension, translation symmetry is preserved, and this makes a few exact solutions possible for some specific dynamics [4,6].

Dynamics that describe the phase-separation model conserve the order parameter. One example is that of Kawasaki [8], which allows the exchange of a pair of nearest-neighbor particles of different type. In contrast to the nonconserved dynamics of the usual Ising system, such as Glauber's [9] (that of flipping an individual spin), for which many exact results are available [9,10], Kawasaki's dynamics is more difficult to study and there is as yet no exact solution at finite temperature. Recently, however, a few exact results [4–6] for a quenched dynamics at zero temperature, which is a limiting case of Kawasaki's dynamics, have become available. Nevertheless, all such exact solutions have been limited to mixtures having symmetrical particle concentrations, i.e., equal particle concentrations of $A$ and $B$. As in a quenched dynamics that is nonergodic, the system evolves eventually to states with energy that is only a local, and not a global, minimum. Hence the evolution of the system will strongly depend on the initial conditions. This then makes the initial concentration an important memory parameter and leads us to ask to what extent the dynamical process depends on the initial concentrations. Are there significant differences between the symmetrical and asymmetrical cases, as has been observed in two-species diffusion-limited annihilation [11]? These are the questions we address in this paper.

Let us now consider the Kawasaki dynamics for a mixture of $A$ and $B$ particles in one dimension. In this procedure, we randomly pick a pair of particles on nearest-neighbor sites. Then, if they are of different types, we exchange the two particles with a probability $\frac{1}{2}[1-\tanh(\frac{1}{2}\beta\Delta)]$, where $\beta$ is the inverse temperature and $\Delta$ is the difference between the energies of the configurations after and before the exchange. At zero temperature there are ergodical and quenched nonergodical dynamics. In the ergodical procedure, exchanges within configurations having equal energies are permitted, while in the nonergodical dynamics, exchanges are allowed only when they reduce the system energy [4,6]. Even at zero temperature, the ergodic dynamics is still too difficult to solve, as the exchanges between degenerate states allow multiple pathways to be followed. Instead, we shall look for exact solutions of the nonergodic dynamics, which reduces the probabilistic exchange to a deterministic exchange. Thus the only time evolution operation in the system is either $\ldots ABAB\ldots \rightarrow \ldots AABB\ldots$ or $\ldots BABA\ldots \rightarrow \ldots BBAA\ldots$. In a description in terms of domain walls, this corresponds to three consecutive domain walls transforming to a single domain wall at the center, thus decreasing the number of domain walls by two. This picture in terms of domain walls simplifies the Monte Carlo simulation significantly and will be implemented in our simulation.

The key to exact solutions of the quenched dynamics is to introduce a set of probabilities $\wp(n,t)$ that the occupancy of a randomly selected consecutive $n$ ($\geq 3$) lattice sites is fully alternating, i.e., is occupied, at time $t$, by $n$ particles $ABAB\ldots$ or $BABA\ldots$ [6]. In the domain-wall representation, this probability function is essentially the same as the probability function $E(n-1,t)$, introduced in solving one-species diffusion-limited coagulation [12], that $n-1$ randomly selected consecutive lattice sites are empty.

In the asymmetric case of unequal particle concentra-

 

tion, we must distinguish whether the cluster of $n$ consecutive sites, occupied by $A$ and $B$ particles in a fully alternating sequence, is ended by an $A$ particle or a $B$ particle. To overcome this lack of symmetry, we need more probability functions.

Let us define $P_{\alpha\beta}(n,t)$ as the probability of finding $n+2$ ($n \geq 1$) randomly selected consecutive sites being occupied, at time $t$, by $A$ and $B$ in a fully alternating order, and which starts from an $\alpha$ particle and ends at a $\beta$ particle, where each $\alpha$ and $\beta$ represent either $A$ or $B$. Clearly, when $n$ is even (odd) only $P_{AB}(n,t)$ and $P_{BA}(n,t)$ [$P_{AA}(n,t)$ and $P_{BB}(n,t)$] are meaningful. In quenched dynamics, the time evolution of $P_{\alpha\beta}(n,t)$ is determined by the hierarchy

$$-\frac{dP_{\alpha\beta}(n,t)}{dt} = (n-1)P_{\alpha\beta}(n,t) + P_{\bar{\alpha}\beta}(n+1,t) + P_{\alpha\bar{\beta}}(n+1,t) + 2P_{\alpha\beta}(n+2,t) \ , \tag{1}$$

where $\bar{\alpha}$ is $A$ ($B$) if $\alpha$ is $B$ ($A$), and similarly for $\bar{\beta}$. Three parts contribute to the decreasing rate of probability $P_{\alpha\beta}(n,t)$. The first comes from operations in which all three domain walls involved are within the cluster chosen, the second comes from operations in which two of the three domain walls are within the cluster, and the final parts come from operations in which only one of the three domain walls is within the cluster. These are represented by the first term, the second and the third terms, and the fourth term on the right hand side of Eq. (1), respectively. Since a cluster chosen with an even number of sites $n = 2m$ is quite different from that with an odd number of sites, we define further

$$\begin{aligned} P(m,t) &\equiv P_{AB}(n,t) + P_{BA}(n,t) \\ &= 2P_{AB}(n,t) \ , \\ Q(m,t) &\equiv P_{AA}(n+1,t) \ , \\ R(m,t) &\equiv P_{BB}(n+1,t) \ , \end{aligned} \tag{2}$$

where the equality follows from the fact that there is still reflection symmetry in the system. These probability functions satisfy the equations

$$\begin{aligned} -\frac{dP(m,t)}{dt} &= (2m-1)P(m,t) + 2[Q(m,t)+R(m,t)] \\ &\quad +2P(m+1,t) \ , \\ -\frac{dQ(m,t)}{dt} &= 2mQ(m,t) + P(m+1,t) + 2Q(m+1,t) \ , \\ -\frac{dR(m,t)}{dt} &= 2mR(m,t) + P(m+1,t) + 2R(m+1,t) \ . \end{aligned} \tag{3}$$

Let the system start from a randomly distributed mixture of particles $A$ and $B$ such that the concentration of $A$ and $B$ particles are $p$ and $q$ ($= 1-p$), respectively. The initial conditions are given by

$$\begin{aligned} P(m,0) &= 2pq(pq)^m \ , \\ Q(m,0) &= p^2q(pq)^m \ , \\ R(m,0) &= pq^2(pq)^m \ . \end{aligned} \tag{4}$$

The structures of the dynamic evolution equations, Eq. (3), and the initial conditions, Eq. (4), suggest that we look for solutions of the form

$$\begin{aligned} P(m,t) &= u(t)\gamma^m(t) \ , \\ Q(m,t) &= v(t)\gamma^m(t) \ , \\ R(m,t) &= w(t)\gamma^m(t) \ . \end{aligned} \tag{5}$$

Upon substitution of Eq. (5) in Eqs. (3) and (4), one finds

$$\begin{aligned} -\dot{\gamma}(t) &= 2\gamma(t) \ , \\ -\dot{u}(t) &= -u(t) + 2\,[v(t)+w(t)] + 2\gamma(t)u(t) \ , \\ -\dot{v}(t) &= u(t)\gamma(t) + 2v(t)\gamma(t) \ , \\ -\dot{w}(t) &= u(t)\gamma(t) + 2w(t)\gamma(t) \ , \end{aligned} \tag{6}$$

where an overdot represents the time derivative, with initial conditions

$$\begin{aligned} \gamma(0) &= pq \ , \\ u(0) &= 2pq \ , \\ v(0) &= p^2q \ , \\ w(0) &= pq^2 \ . \end{aligned} \tag{7}$$

These equations are simplified if rewritten in terms of functions $v(t)+w(t)$ and $v(t)-w(t)$. The solutions are

$$\begin{aligned} P(m,t) &= \frac{1}{2}\left[(2pq+\sqrt{pq})\,e^{-2\sqrt{pq}\tau} + (2pq-\sqrt{pq})\,e^{2\sqrt{pq}\tau}\right] e^{-2pq\left(\tau-\frac{1}{2}\tau^2\right)}(pq)^m(1-\tau)^{2m-1} \ , \\ Q(m,t) &= \frac{1}{2}\left[\frac{1}{2}\left[(2\sqrt{pq}+1)\,e^{-2\sqrt{pq}\tau} - (2\sqrt{pq}-1)\,e^{2\sqrt{pq}\tau}\right] + (p-q)\right] e^{-2pq\left(\tau-\frac{1}{2}\tau^2\right)}(pq)^{m+1}(1-\tau)^{2m} \ , \\ R(m,t) &= Q(m,t)\,|_{p\leftrightarrow q} \ , \end{aligned} \tag{8}$$

where $\tau$ is a reduced time defined as

$$\tau \equiv 1 - e^{-t} \tag{9}$$

and $Q(m,t)\,|_{p\leftrightarrow q}$ represents interchanging $p$ and $q$ in the expression $Q(m,t)$. The asymmetrical effects are contained in the terms having factors $2pq-\sqrt{pq}$ or $p-q$. In the symmetrical case, $p=q=1/2$, all these terms disappear and all the probability functions $P_{\alpha\beta}(n,t)$ reduce to one common expression $\wp(n-2,t)/2$, reproducing Privman's results [6]. Noting that $\tau = 1-e^{-t} \to 1$ when

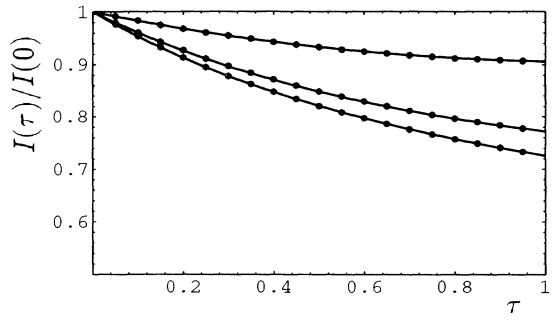


FIG. 1. These curves show the normalized density of domain walls $I(\tau)/I(0)$ for random initial conditions with various concentrations $p$ (from top to bottom, $p = 0.1$, 0.3, and 0.5, respectively), as a function of the reduced time $\tau$ $(= 1 - e^{-t})$. The solid curves are the theoretical results from Eq. (12) and the dots indicate the results of Monte Carlo simulations.

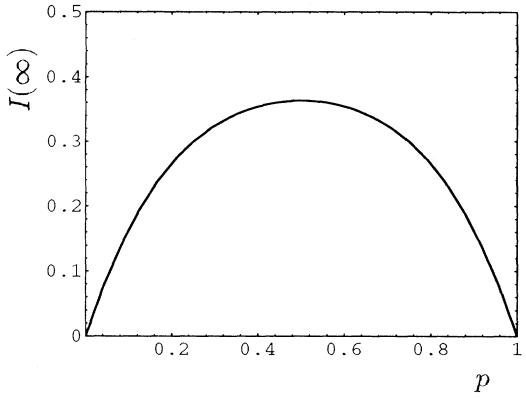


FIG. 2. This figure shows the asymptotical values of the density $I(t = \infty)$ of the domain wall, for random initial conditions, as a function of the initial concentration $p$.

$t \to \infty$, we find that all the probability functions decay exponentially to zero [or to their quenched steady values, as happens for $Q(1,t)$ and $R(1,t)$ only] and the asymmetry has no effect in the exponents describing the decay; it affects only the coefficients.

For the phase-separation model, the main interest lies in the time-dependent density of domain walls denoted by $I(t)$. This density of domain walls determines the energy of the system. In quenched dynamics, the rate equation for $I(t)$ is

$$-\frac{dI(t)}{dt} = 2P(1,t) \ . \tag{10}$$

From Eqs. (3) and (10), one finds that $I(t)$ is actually determined by $P(m,t)$ and $Q(m,t) + R(m,t)$ only. For a random initial distribution the initial condition is

$$I(0) = 2pq \ . \tag{11}$$

The solution is

$$\frac{I(\tau)}{I(0)} = 1 - \frac{1}{2}\int_0^\tau d\tau' e^{-2pq(\tau' - \frac{1}{2}\tau'^2)}[(2pq + \sqrt{pq})e^{-2\sqrt{pq}\tau'} + (2pq - \sqrt{pq})e^{2\sqrt{pq}\tau'}] \ , \tag{12}$$

which can be expressed in terms of error functions. We have plotted this normalized domain-wall density as a function of the reduced time $\tau$ in Fig. 1. In this figure we also show the results of a Monte Carlo simulation. One can see the excellent agreement between the numerical simulation results and the analytical results. In all our Monte Carlo simulations, a one-dimensional lattice with periodic boundary conditions and $N = 10^6$ sites was used. Thus, the standard error is about $10^{-3}$. The simulations were carried out in the domain-wall picture rather than in terms of $A$ and $B$ occupancies. However, the initial domain-wall configurations were generated from random initial configurations of $A$ and $B$. The time is normalized according to the lattice size $N$.

The quenched steady value is given by

$$I(t = \infty) = I(\tau = 1) \ , \tag{13}$$

which depends on the initial concentration $p$. This dependence is shown in Fig. 2. The asymptotic value $I(t = \infty)$ takes its maximum at the symmetrical point $p = 1/2$, indicating that this case is in the most frustrated situation. Again, the effect of asymmetry arises from the presence of the factor $2pq - \sqrt{pq}$ in Eq. (12) and vanishes when $p = 1/2$. When the time is large, the domain-wall density asymptotically approaches to its $p$-dependent steady value in the manner

$$I(t) - I(\infty) \sim \frac{1}{2}e^{-pq}[(2pq + \sqrt{pq})e^{-2\sqrt{pq}} + (2pq - \sqrt{pq})e^{2\sqrt{pq}}]e^{-t} \ , \tag{14}$$

i.e., as an exponential decay with an amplitude depending on the particle concentration.

In summary, we have obtained an exact expression for the time dependence and initial concentration dependence of the domain-wall density for a one-dimensional phase-separation model of a binary mixture with zero-temperature quenched Kawasaki dynamics. This generalizes the previously determined result [4,6] for the symmetrical case of equal concentrations of $A$ and $B$. The asymmetry in the concentrations has been shown to cause no major qualitative changes in the asymptotic behavior of this system.

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