Phase Separation Model with Conserved Order Parameter on the Bethe Lattice

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We obtain an exact time dependent solution of the zero temperature Kawasaki-type dynamics of a phase separation model on the Bethe lattice with arbitrary coordination number. We also do a direct numerical simulation and show an excellent match between the analytical and numerical results. The nonergodic dynamics leads to a frozen final state whose structure depends crucially on the initial conditions.

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Of late, there has been much interest in studying stochastic dynamical models describing the low temperature phase separation and spinodal decomposition of binary fluid mixtures [1,2]. The dynamics in these models conserves the order parameter. It is this conservation law which makes these models harder to study analytically as opposed to the nonconserved case where several exact results are available, especially in $d=1$ [2–8]. For the conserved models, the dynamics at $T=0$ is essentially irreversible (nonergodic) and often leads to frozen final states whose structure strongly depends on the initial conditions. This frozen domain structure resulting from the $T=0$ dynamics is easy to understand in the context of Kawasaki-type models with spin or particle exchange dynamics, which conserves the total magnetization or the total number of each of the two species of particles. In this case, the dynamics involves both annihilation and diffusion of interfaces between the two phases. Each of the dynamical moves has a certain statistical weight associated with it. At $T=0$, the elementary move which causes the maximum annihilation of interfaces has an infinite Boltzmann factor compared to the other moves. In the absence of diffusion and other moves, if the system at any stage of its time development reaches a configuration where no maximum annihilation move is possible, it just stays in that configuration. Thus, the dynamics is nonergodic in the phase space and the final state depends crucially on the initial configuration. Thus, although the physics is simple, a full time dependent analytical solution would be welcome in understanding the nonergodic nature of the dynamics.

A recent move in this direction is the $d=1$ exact time dependent solution of a zero temperature phase separation model with conserved dynamics of Privman [9] and independently by Krapivsky [10]. Models of this kind were previously studied numerically by Levy, Reich, and Meakin [11,12] for $d=1$ to 5. The $d>1$ models are somewhat different from the $d=1$ case. However, at $T=0$ they are believed to share the common feature of frozen domain structure at large time. In this Letter, we solve this $T=0$ phase separation model exactly on the Bethe lattice, which corresponds in some respects to $d=+\infty$, and compare our exact results to our direct numerical simulations. To our knowledge, it is the first solvable model in $d>1$ in the conserved case. This model on the Bethe lattice was studied numerically at nonzero temperature by Palmer and Frisch [13]. They found complete phase separation, with the density of interfaces tending to zero at large time. Our exact solution at $T=0$ clearly shows that the final state has a frozen domain structure, confirming that $T=0$ dynamics is very different from that of $T>0$. We would like to mention at this point that our solution is not a simple generalization of the $d=1$ solution. Indeed, on the Bethe lattice we will see that topological effects are important, which were absent in the $d=1$ case. This fact makes the $d=1$ model different from those in higher dimensions, and enabled Privman and Krapivsky to obtain their exact solution. In fact, we will recover the $d=1$ exact result as a special case of our more general solution on the Bethe lattice, when the coordination number is 2.

We consider the phase separation model of a binary fluid of A and B with nearest neighbor particle exchange dynamics on the Bethe lattice with coordination number Z. Each site of this Bethe lattice is occupied by either one A or one B particle. Moreover, two neighbors of different species can be exchanged if and only if the number of interfaces in the fluid is decreased by the maximum amount by this move. In the case of a $Z=3$ Bethe lattice, this corresponds to a bond AB with a local environment as shown in Fig. 1(a). In this case, there are five interfaces before the move and only one after [Fig. 1(b)]. Allowing only this kind of move, we do not expect the two phases to completely separate, but to form a frozen structure which can depend on the initial conditions. The natural possible initial conditions are the alternating and the random one, although our result will be applicable to more general initial conditions. In the alternating case, each particle A (B) is surrounded by Z B's (A's). In the random case, each site is randomly occupied by A or B, with equal probabilities. The quantity one is usually interested in is the time dependence of the concentration of interfaces, and especially its asymptotic value ($t=+\infty$). Some other quantities such as the distribution of the sizes of connected clusters of A's are also of interest.

Consider a cluster of n connected sites. This will be a fully alternating cluster if and only if all its sites have opposite particles on all Z of their nearest neighbors. The

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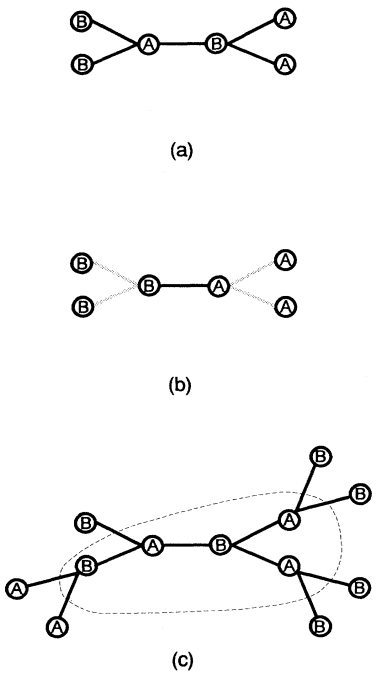

FIG. 1. (a) The two letters of the central AB bond can be exchanged since this move decreases the number of interfaces by the maximum number, which is 4 in the $Z=3$ Bethe lattice. (b) The configuration of (a), after the move. (c) The dotted line encircles a fully alternating cluster with $n=5$.

cluster is also characterized by its shape or topology T. An example of such a cluster with $n=5$ is shown in Fig. 1(c), for the Bethe lattice with $Z=3$. Now, we define $P(n,T,t)$, the probability that at time t a randomly chosen cluster of size n and topology T is a fully alternating cluster. In the $d=1$ case, there is only one possible topology for a given cluster size, so that $P(n,T,t)$ only depends on n and t. The crucial observation in solving the $d=1$ model [9,10] was that the time evolution of the $P(n,t)$'s is much easier to write than that of the $P_{ex}(n,t)$'s [14], the probability of occurrence of a fully alternating cluster of size n that is not part of a larger fully alternating cluster. In the present case, the extra dependence on topology makes the problem apparently much harder. The evolution equation for $P(n,T,t)$, in the bulk, reads

$$-\frac{\partial P}{\partial t}(n,T,t)=b(n,T)P(n,T,t)+\sum_{T'\in\mathcal{C}'(T)}P(n+1,T',t)+\sum_{T''\in\mathcal{C}''(T)}P(n+2,T'',t)\,, \tag{1}$$

where $b(n,T)$ is the number of internal bonds of the considered cluster. In general, it depends on both n and T. However, for the Bethe lattice, $b(n,T)=n-1$. The first term on the right-hand side of (1) refers to the decay of probability due to the exchange of particles within the cluster. The two last terms are due to exchanges which involve the neighbors of the cluster. The neighbors of the cluster are the sites outside the cluster with at least one neighbor inside the cluster. For instance, the second term describes the exchange of a neighbor of the cluster with one particle inside the cluster. So, the summation in the second term runs over the set $\mathcal{C}'$ of all fully alternating clusters of size $n+1$ which contain the alternating cluster of size n and topology T. The number of terms in the sum is equal to the number of outgoing bonds from the cluster. Thus, a given T' may appear more than once in the sum depending on whether the neighbor site has more than one neighbor in the cluster. For the Bethe lattice, we note that there are $n'=n(Z-2)+2$ such clusters in $\mathcal{C}'(T)$, for a given T, and each T' appears only once in the summation. Similarly, the third term refers to the exchange of a neighbor of the cluster with a site outside the cluster, and the summation runs over the fully alternating clusters of size $n+2$, which contain the elements of $\mathcal{C}'(T)$. For the Bethe lattice, there are $n''=(Z-1)n'$ such clusters in $\mathcal{C}''(T)$. Thus, we notice that on the Bethe lattice, these numbers n' and n'' do not depend on the topology T explicitly. For lattices containing loops, such as hypercubic lattices, n' and n'' do depend on the topology. This fact is crucial in obtaining our exact solution for the Bethe lattice.

In fact, Eq. (1) is very general and applies to hypercubic lattices as well. However, the explicit topology dependence makes it harder to tackle analytically. But, for the Bethe lattice, we notice that if the initial condition is topology independent, i.e., $P(n,T,0)$ is independent of T, then $P(n,T,t)$ remains independent of T for all subsequent times. This is because the dynamics given by (1) does not generate any topology dependence. This is of course the case for the two most "natural" initial conditions considered here, for which we have $P_{alt}(n,T,0)=1$ and $P_{ran}(n,T,0)=2^{-[n(Z-1)+1]}$. Note that the fact that the ratio of n' and n'' does not explicitly depend on n is special to the Bethe lattice case and is another reason for obtaining the exact solution. Finally, if the initial condition is topology independent, (1) reduces to an effective (but exact) evolution equation, which now only involves the size of the considered cluster:

$$-\frac{\partial P}{\partial t}(n,t)=(n-1)P(n,t)+[n(Z-2)+2]P(n+1,t)+(Z-1)[n(Z-2)+2]P(n+2,t)\,. \tag{2}$$

For $Z>2$, the solution of this equation consistent with the initial conditions is of the form

$$P(n,t)=a\exp\left[\frac{Z}{Z-2}t\right]s(t)^{n+2/(Z-2)}\,, \tag{3}$$

where $a_{ran}=2^{Z/(Z-2)}$ and $a_{alt}=1$ and $s(t)$ satisfies a simple differential equation:

$$\frac{ds}{dt}=-s-(Z-2)s^2-(Z-1)(Z-2)s^3\,,\qquad s_{alt}(0)=1,\quad s_{ran}(0)=2^{-(Z-1)}\,. \tag{4}$$

The function $t(s)$ can be easily computed from (4), but there is no simple way of expressing s as a function of t. An important feature of $s(t)$ is that it behaves like $s_{\text{init}}\exp(-t)$ when $t\to+\infty$, where the constant depends on the initial conditions and can be exactly computed in the alternating and random case. It shows that all the $P(n,t)$'s go to 0, except $P(1,t)$ which goes to a constant which measures the density of A's surrounded by Z B's at infinite time. A more interesting quantity is certainly the density of interfaces, $I(t)$. Since all alternating configurations with $n=2$ will flip as shown in Fig. 1, decreasing the number of bonds by $2(Z-1)$, the evolution equation of $I(t)$ is

$$\frac{dI}{dt}(t)=-2(Z-1)P(2,t),\quad I_{\text{alt}}(0)=1,\quad I_{\text{ran}}(0)=\tfrac{1}{2}\,. \tag{5}$$

Combining the form of $P(2,t)$ given in (3) with the last equation, and taking into account the different initial conditions, we obtain

$$\begin{aligned}
&I(t)=I(0)-\frac{C}{f(s(0))}\int_{s(t)}^{s(0)}[1+(Z-2)u+(Z-1)(Z-2)u^2]^{(4-Z)/2(Z-2)}f(u)\,du\,,\\
&f(u)=\exp\left\{\frac{Z}{\sqrt{(Z-2)(3Z-2)}}\tan^{-1}\left[\left(\frac{Z-2}{3Z-2}\right)^{1/2}[2(Z-1)u+1]\right]\right\},\\
&C_{\text{alt}}=2(Z-1)^{-2/(Z-2)}\,,\\
&C_{\text{ran}}=\frac{(Z-1)2^{2(Z-1)/(Z-2)}}{[2^{2(Z-1)}+(Z-2)2^{Z-1}+(Z-1)(Z-2)]^{Z/2(Z-2)}}\,.
\end{aligned} \tag{6}$$

The asymptotic value of $I(t)$ is obtained by substituting $s(+\infty)=0$ at the lower limit of the integral. We note that in the $Z=2$ case, which corresponds to $d=1$, (1) is trivially equivalent to (2) and reproduces the recent result by Privman [9,10]. However, as shown by (3)–(6) the nature of the solution is very different in the $Z>2$ case. Note that the solution (6) goes smoothly to Privman's solution despite the apparent singularity at $Z=2$. Some values of $I(+\infty)$ are given in Table I. The main feature is that the density of interfaces is an increasing function of Z in the random case. In the alternating case, it has a minimum for $Z=3$. In addition, except for $Z=4$, one has $I_{\text{alt}}>I_{\text{ran}}$, which means that the alternating initial configuration is more frustrated than a typical random configuration. For very large Z, the final density of interfaces is the same as the initial one. This is due to the fact that one exchange forbids many further exchanges in the neighborhood. Therefore, the final frozen state the system reaches is close to the initial one.

In the following, we restrain ourselves to the $Z=3$ case for which we have performed numerical simulations on lattices of size up to $M=2^{21}$ sites. We would like to stress the fact that our study concerns the bulk properties of the Bethe lattice which are defined in the following way. First let us make the size of the Bethe lattice go to infinity. Take a finite subset of this lattice of size N and average a given quantity, say $I(t)$, on this subset. The bulk value of the observable is the limit of this average when $N\to+\infty$. If one starts from a finite sample the average will depend on how many surface shells are retained to perform the average. In Table II, we present $I(+\infty)$ as a function of the number of discarded shells for the two initial conditions considered here. The boundary effects are stronger in the alternating case as one might expect, but the numerical results are very close to our exact result after 7–8 shells are discarded. In the random case, the limiting value seems to be reached much faster.

Note that our simulation was performed by picking successive random bonds on the lattice, which are flipped when possible. Indeed, our solution (1)–(6) describes the

TABLE I. Asymptotic density of interfaces given by (6), for the alternating and random initial conditions as a function of Z.

Z	I_{alt}	I_{ran}
2	0.450898	0.362957
3	0.436061	0.427627
4	0.465548	0.468485
5	0.499634	0.487955
6	0.531444	0.495841
∞	1	0.5

TABLE II. Asymptotic density of interfaces for the alternating and random initial conditions as a function of the number of discarded surface shells to perform the average (2000 samples of $N=2^{21}=2097152$ sites for $Z=3$). The standard error is less than 3.0×10^{-4} in all cases, and decreases when shells are added.

	I_{alt}	I_{ran}
0	0.5493	0.4581
1	0.4235	0.4399
2	0.3017	0.4219
3	0.4337	0.4276
4	0.4596	0.4278
5	0.4124	0.4277
6	0.4337	0.4275
7	0.4420	0.4276
8	0.4359	0.4276

continuous time asynchronous dynamics of interfaces, where the exchange moves are independent of each other, with an exponential waiting time distribution. In our simulations, after $4M$ bonds are visited randomly, one last ordered sequential inspection starting from a root site is made in order to flip the few bonds which were not visited by the random inspection (in general less than 10). If one performs such a sweep directly on the initial configuration, the value of I after the sweep is very different from our result. For instance, for $Z=3$ and in the alternating case, the value of I after the sweep is exactly $\frac{1}{5}$ instead of the larger value $I(+\infty)=0.436061\ldots$ given by (6). In the random case, this value can be expressed as a simple series and goes to $0.447\ldots$, which is bigger than our result $0.427627\ldots$.

In summary, an exact time dependent solution has been obtained for the concentration of interfaces in a $T=0$ phase separation model with conserved order parameter on the Bethe lattice. It would be interesting to compute also the full time dependent correlation functions, e.g., the probability of occurrence of a cluster of a given size, containing only A's (or B's). These correlation functions can be computed exactly for the $d=1$ case [14]. The finite temperature dynamics where diffusional moves are allowed seems hard to solve exactly. But, at least an approximate solution with only certain moves allowed would be interesting and welcome.

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