Exact Results for 1D Conserved Order Parameter Model

Vladimir Privman

Department of Physics, Clarkson University, Potsdam, New York 13699–5820, USA

ABSTRACT

Recent exact results for a particle-exchange model on a linear lattice, with only irreversible moves reducing the local energy allowed, are reviewed. This model describes a zero-temperature Kawasaki-type phase separation process which reaches a frozen, initial-condition-dependent state at large times.

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This short review covers selected recent results of interest in phase coarsening, spinodal decomposition, nucleation.[1–3] These processes can be modeled quite successfully by irreversible, zero-temperature, low dimensional lattice systems.[4–6] Variants of nonconserved order parameter dynamical models in 1D, with effectively $T=0$ Glauber-type spin dynamics, have been solved exactly for the structure factor and average domain size, as functions of time.[6–7] The mechanism leading to cluster growth in 1D is pairwise annihilation of interfaces separating ordered domains; the interfacial motion is simple diffusion.

Spin-exchange, Kawasaki-type models, no longer allow for a simple, diffusional interpretation of the dynamics. Derivation of exact result even in 1D is more difficult than for the nonconserved models; few very recent results were obtained, in 1D and on the Bethe lattice, for a model with maximal limitation of the dynamical moves allowed.[8–11] These new results will be surveyed here and illustrated by working though the steps of a 1D solution.[8,11] Somewhat different nomenclature and several generalizations can be found in Ref. 10. The 1D solutions can also be obtained by a different, cluster-size-distribution approach[12] based on the low-T Ising-model studies of Ref. 13.

Detailed Bethe-lattice results were obtained in Ref. 9; these will not be described here. The method of solution both in 1D and on Bethe lattices bears similarity to the techniques employed in kinetics of reactions with immobile reactants[14–15] and in random sequential adsorption reviewed, e.g, in Refs. 16–17.

Let us emphasize that for <u>nonconserved</u> models, ordering in 1D in the Glauber-type dynamics involves interface annihilation which is a process lowering the local energy and therefore has Boltzmann factor $+\infty$ associated with its transition probability at $T=0$. Interface diffusion does not change the local energy and therefore has Boltzmann factor 1. Finally, interface generation (birth) has Boltzmann factor 0 (due to energy cost) at $T=0$. The $T=0$ models[6–7] with unlimited domain growth, $\sim\sqrt{t}$, for large times

t, correspond to allowing for both annihilation and diffusion. Models with annihilation only lead to frozen states.[14–15]

For conserved, spin-exchange, Kawasaki-type models, ordering processes even at $T = 0$ are more complicated than for the nonconserved case. Specifically, let us consider the binary AB-mixture model: each site of the lattice is occupied by particle A or particle B. The dynamics generally involves nearby particle exchanges; the locally conserved order parameter is the difference of the A- and B-particle densities. If one only eliminates energy-increasing moves, one is still left with a model which was not solved exactly. Several numerical studies and analytical expansion results were reported[18–22] for such particle-exchange models in D up to 5. As in the nonconserved case, some of the properties of the 1D models are different from D > 1. However, the general expectation of the "freezing" of the domain structure at large times applies, for conserved $T = 0$ dynamics, in all space dimensions studied.

We now turn to the strictly 1D case. Let us assume that initially the linear lattice sites are occupied by particles A and B in exact alternating arrangement. We will solve the dynamics of this model[8] under the assumption that unlike particle contacts cost energy. The only dynamical moves allowed will be those nearest-neighbor exchanges which reduce the energy, i.e., $A \rightleftharpoons B$ exchanges in the configurations

$$\ldots ABAB \ldots \to \ldots AABB \ldots \quad , \tag{1}$$

$$\ldots BABA \ldots \to \ldots BBAA \ldots \quad . \tag{2}$$

Indeed, these exchanges, of AB or BA pairs which are part of a fully alternating sequence of 4 particles, reduce the local number of unlike contacts from 3 to 1. The exchanges are irreversible.

A model with this dynamics can be also solved for random initial placement of particles,[8] with arbitrary initial density of A and B species,[11] which must fully cover the lattice. In all cases, as the time goes by the number of "reactive" regions decreases. For large times, a frozen state is approached at an exponential rate.[8,11] Particle exchanges do not affect the species concentrations. Therefore the dynamical quantity of interest if the density of "interfaces," i.e., of unlike particle contacts, in the system, $I(t)$. We will present the solution for the initially fully alternating state with $I(0) = 1$.

We assume asynchronous, continuous-time dynamics. Each allowed exchange event proceeds with the rate R per unit time (which will be absorbed in the dimensionless time variable, $Rt \to t$), and independently of other exchange events. The method of solution for various initial conditions, and for several related models,[8−11,15] involves consideration of probabilities $P_k(t)$ that a randomly selected continuous group of k lattice sites is fully "reactive." In the case chosen for illustration here, there is the $A \rightleftharpoons B$ symmetry, while fully reactive here means, for $k \geq 4$, fully alternating. (We will also have to use the fully-alternating probability for 3 consecutive sites, $P_3(t)$, although "reactivity" cannot be decided from 3 sites only.) In other applications, one considers different objects, and no $A \rightleftharpoons B$ symmetry in some instances.

Thus, $P_k(t)$ here is defined as the probability that a randomly chosen, consecutive k-site sequence of sites is, at time t, occupied by particles in the configurations $ABAB\ldots$ or $BABA\ldots$. Note that the density of interfaces is then obtained from the relation

$$\frac{dI(t)}{dt} = -2P_4(t) \quad , \tag{3}$$

which is self-explanatory in view of (1)-(2). The factor 2 is due to the reduction from 3 to 1 of the number of interfaces in each allowed particle exchange event.

The key to solubility is in that for some dynamical rules (where details of course depend on the model), the probabilities $P_k(t)$ are determined locally, from the configuration of the clusters which include the k-cluster. Furthermore, in one dimension the "topology" of the surrounding clusters is trivial. This allows to write a closed hierarchy of rate equations; in our case it is

$$-\frac{dP_k(t)}{dt} = (k-3)P_k(t) + 2P_{k+1}(t) + 2P_{k+2}(t) \quad . \tag{4}$$

This recursion must be considered for $k \geq 3$ and with the initial condition

$$P_k(0) = 1 \quad , \tag{5}$$

because in the selected example of the fully alternating initial configuration, all the k-site clusters are fully reactive initially.

The rate equations (4) incorporate exchange processes with all the "deciding" four sites, see (1)-(2), within the original k-cluster. There are $k-3$ such 4-site groups in the k-site cluster. In addition, up to two exchange events may be possible with the "deciding" 4-site group extending outside the original cluster even though the actually exchanging A and B particles are within it, at the end. The "decision making" is then within the larger, $(k+1)$-clusters which include the original k-cluster. The second term on the right-hand side of (4) accounts for these events. Finally, up to two end-particles in the k-cluster can exchange with nearby particles outside it. It is obvious that the "decision" is then based on the configuration of the two appropriate $(k+2)$-site clusters. The third term in (4) accounts for such external exchanges.

Typically, 1D hierarchies such as (4) can be solved by assuming a form exponential in k,

$$P_k(t) = P_k(0) C(t) E^k(t) \ . \tag{6}$$

In our example, we find[8]

$$C(t) = \exp\left(2e^{-t} + e^{-2t} - 3 + 3t\right) \ , \tag{7}$$

$$E(t) = e^{-t} \ , \tag{8}$$

which can be checked by substitution in (4).

For the density of interfaces, we get, via (3), the result

$$I(t) = 1 - 2e^{-4} \int\limits_{1+e^{-t}}^{2} e^{z^2} dz \ . \tag{9}$$

Specifically, for large times the ordering process stops at the residual density of unlike-particle contacts $I(\infty) \simeq 0.450898$. More generally, both the saturation value and time-variation are initial-condition dependent;[8,11] explicit results can be found in Refs. 8–11, 15.

In summary, we surveyed an approach to deriving exact time-dependent solutions for 1D models with $T = 0$ Kawasaki dynamical moves restricted to the extreme irreversibility and lack of ergodicity. The 1D results are useful as test models for approximation schemes and numerical studies in D$>$ 1. Indeed, standard approximation schemes developed for random sequential adsorption, for instance (reviewed in Refs. 15–16), have been based on hierarchies of equations similar to those that appear in irreversible Kawasaki dynamics considered here. In D$>$ 1, they involve complicated cluster shapes and must be truncated within closure schemes. However, 1D exactly solvable hierarchies have provided a useful guide to these approximation schemes.

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