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The study of a three-body interaction Hamiltonian on a lattice.

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The study of a three-body interaction Hamiltonian on a lattice

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We investigate the phase diagram and the segregation kinetics of a system of particles with three-body interactions on a two dimensional square lattice. We compare this to the usual case of pair interactions which have particle-hole symmetry. Our simulations suggest that the kinetics belong to the same universality class as the symmetric model with pair interactions.

I. INTRODUCTION

Many properties of the time evolution of a phase-segregating binary alloy, such as Zn-Al, following a quench from a high temperature into the miscibility gap are well described by the corresponding behavior of simple Ising models with ferromagnetic pair interactions. The kinetics of such models have been studied extensively on both the square and cubic lattice [1–8]. The phase diagram of these models are inherently even functions of the magnetization, corresponding in the binary alloy language, to a symmetry in the two components. In the present work, we study the phase segregation kinetics of a lattice gas with pure three-particle interactions in which there is no such symmetry.

Our model is defined on a square lattice. At each site i there is a spin variable $\sigma_i = (-1, 1)$ or alternatively in the lattice gas language an occupation variable $\eta_i = \frac{1}{2}(1 + \sigma_i) = (0, 1)$. The Hamiltonian of our system is

$$H = -J\Sigma_{ijk}\eta_i\eta_j\eta_k - \mu\Sigma_i\eta_i, \;\; J > 0 \tag{1}$$

where $< i, j, k >$ denotes all triplet of sites forming a right triangle in each unit square and μ is the chemical potential. For the simulations, we used an $L \times L$ square lattice with periodic boundary conditions. This corresponds to having $4L^2$ terms in the first sum in (1).

In terms of spin variable σ_i, H will contain both two and three spin interactions as well as a magnetic field one spin term.

Before we study the kinetics of phase segregation in this system, we need information about it's equilibrium phase diagram which we describe in the next section.

II. EQUILIBRIUM PROPERTIES

The Pirogov-Sinai theory [10] provides a general framework for constructing the low temperature phase diagram of a system from information about the ground states of its Hamiltonian. We can decompose the Hamiltonian on the 2D square lattice into a sum over terms contributed by each unit square (cell) and then sum over all the cells in the lattice. Now the problem reduces to finding the ground state configuration of each unit cell; at the end one has to make sure the ground state can be consistently constructed using these unit cell configurations. An analysis of the 2^4 possible configurations shows that for $\mu < -4J$, the ground state corresponds to all the sites empty ($\eta_i = 0$) and for $\mu > -4J$, all the sites are occupied($\eta_i = 1$). At $\mu = -4J$ there is a degeneracy with both these states having the same value of energy, which is zero.

At low temperatures one of two things can happen, one can have equilibrium states which are close to the ground states or the ground state order is completely destroyed. The PS theory proves that if there are a finite number of periodic ground states and the Peierls condition [10] is satisfied, (i.e. the energy of configurations consisting of one ground state in a region V surrounded by another ground state outside V, is proportional to the boundary area of V), then the ground state order is not destroyed. The low temperature phase diagram will then be a perturbation about zero temperature and the PS theory provides a method to construct the exact low-temperature phase diagram of such a system. The two ground states in our model are G_1 with all sites empty and G_2 with all sites occupied. Following PS theory, we look at the free energy contribution of the low energy excitations to a certain order. Then the coexistence line corresponds to the free energy per site for the two phases being equal. This gives in our case, to lowest order in the possible excitations of each ground state, the equation,

$$\exp(-\frac{1}{T}(12J+\mu))+\frac{\mu}{J}+4=\exp(-\frac{1}{T}(\mu))+\ \textit{higher order terms} \tag{2}$$

Hence to the first non-trivial order in $\exp(-\frac{J}{T})$, the critical value of the chemical potential is given by $\mu = -4J + J\exp(-\frac{4J}{T})$. Higher orders can be computed in a straightforward but tedious way to obtain the low temperature (say up to a half or a third of the critical temperature) phase diagram. The existence of a maximum temperature for coexistence of phases follows from the fact that at very high temperature there is a unique equilibrium state. To say something about the critical temperature in the absence of an exact solution for the model, we use the mean-field approximation. This ignores all correlations and gives us the free energy as a function of an order parameter (the average magnetization m in the spin language) for each site. $m = \frac{1}{N}\sum_i \sigma_i$, where N is the total number of sites. In the lattice gas language the order parameter is the average density of particles on the lattice given by $\phi = \frac{1}{N}\sum_i \eta_i = \frac{1+m}{2}$.

The free energy(per site) in this approximation, is given by

$$f(m,T)=\frac{T}{2}\left((1+m)log(1+m)+(1-m)log(1-m)\right)-\frac{J}{2}(1+m)^3 \tag{3}$$

We obtain the critical temperature T_c as the temperature above which there is a unique minimum of the free energy(3) as a function of m. This corresponds to the free energy being a convex function of m (i.e. $\frac{\partial^2 f}{\partial m^2} > 0$ for $T \geq T_c$). The mean field critical temperature is $\frac{32J}{9}$. But as in the Ising case we expect the true T_c to be bigger than the mean field value by about a factor of two. Below this critical temperature on the coexistence line, there are two equilibrium states each corresponding to a definite magnetization Using the mean field expressions, we can set up equations corresponding to the coexistence line.

$$2\frac{f(m_+,T)-f(m_-,T)}{m_+-m_-}=\mu \tag{4}$$

$$2\frac{\partial f(m_+,T)}{\partial m}=\mu \tag{5}$$

$$2\frac{\partial f(m_-,T)}{\partial m}=\mu \tag{6}$$

where μ corresponds to the coexistence chemical potential and m_+ and m_- the two spontaneous magnetizations. It not does not seem possible to solve analytically for the coexistence line. It is however possible to extract the low temperature behavior. This turns out to be surprisingly close to the exact results obtained using PS theory. We obtain the equation as $\mu = -4J + 4J\exp(-\frac{4J}{T})$ up to the leading order in $\exp(-\frac{J}{T})$. For finite temperatures below T_c, we solve the equations numerically. This yields Fig. 1 for the coexistence line and Fig. 2 for the order parameter values(spontaneous magnetizations) corresponding to the coexistence. The phase diagram clearly has no particle-hole symmetry.

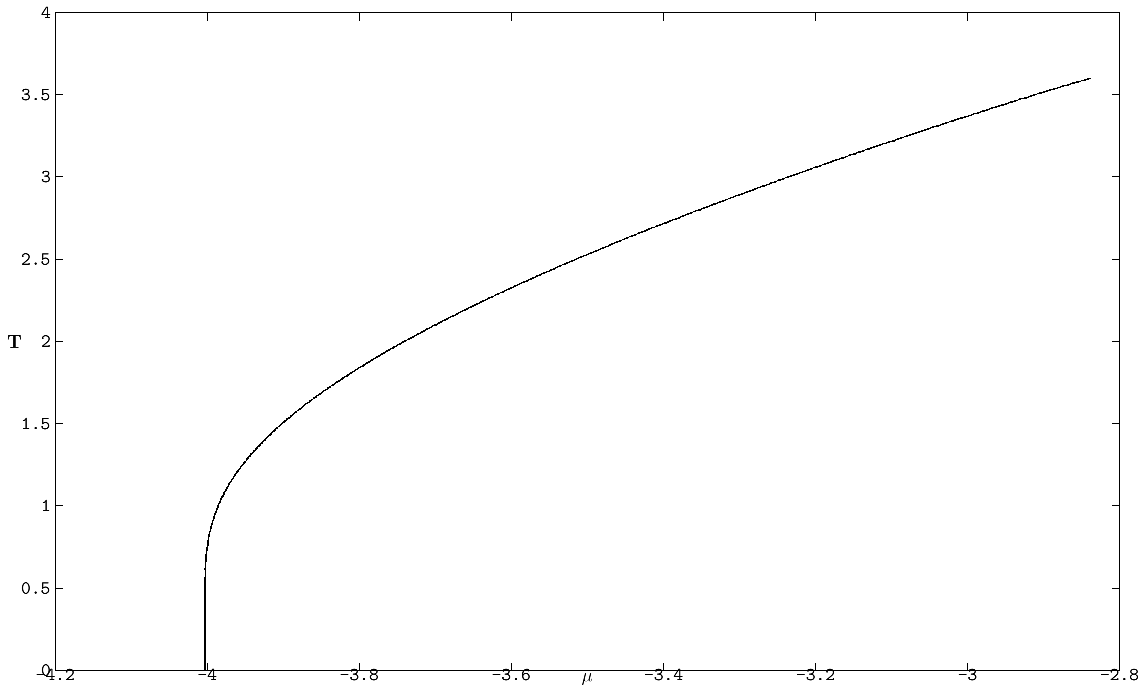


FIG. 1. The Mean-field Coexistence line on a Chemical potential-Temperature plot. Both axes μ and T are plotted in units of J.

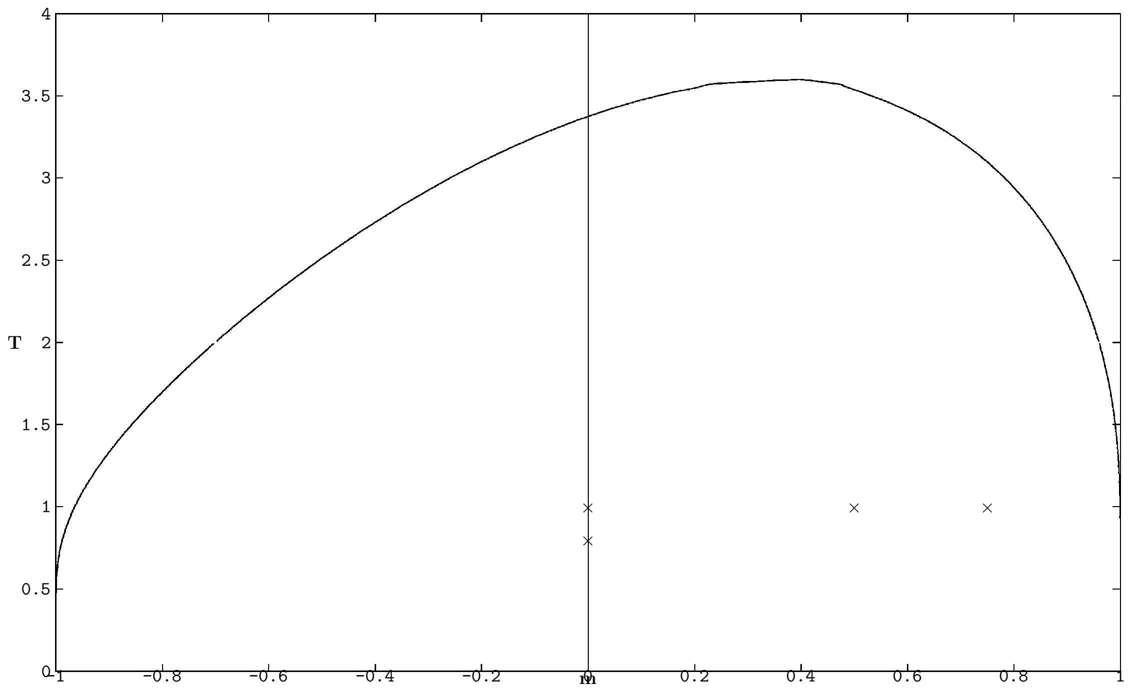
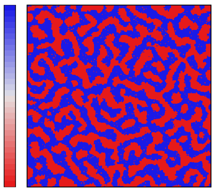


FIG. 2. Mean-field phase diagram on a magnetisation-Temperature plot. The axis T is in units of J. The crosses indicate the points inside the coexistence region to where the system was quenched in our simulations.

III. PHASE SEGREGATION KINETICS

When a homogeneous system is quenched, i.e. suddenly cooled from a high temperature into the coexistence region, it becomes thermodynamically unstable and evolves towards a new equilibrium state, consisting of regions rich in one or the other constituents of the mixture. In this section we discuss the time evolution of our system following such a quench; identifying empty (spin down) sites with one component and occupied (spin up) sites with the other component.



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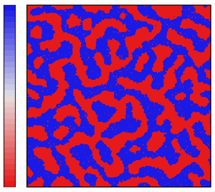

B

FIG. 3. Snapshots of the phase segregating system after A)4096 MCS and B)16384 MCS on a L=256 square lattice. Fraction of sites occupied ϕ = 0.5, temperature T=1.0J. The dark color indicates occupied sites and the light regions are empty sites.

We have carried out extensive simulations of the quenching process for our model, using the Kawasaki spin-exchange dynamics [11], where the total magnetization is conserved. Our results consist of 50 independent samples at $\phi = 0.5, T = 1.0J$, 30 independent samples each at $\phi = 0.75, T = 0.1J$, $\phi = 0.875, T = 0.1J$ and $\phi = 0.5, T = 0.8J$ independent There is now a good understanding of many aspects of phase ordering in spin systems with two-body interaction Hamiltonians [6–9]. The coarsening domains are characterized at late times, by a time dependent characteristic length scale. We can observe this qualitatively in simulations of our model, if we look at the domains at different times, which appear to be self-similar in Fig. 3. A statistical quantity used to quantify this behavior is the time dependent structure function. This is defined for N lattice sites, as

$$S(\mathbf{k},t) = 1/N \left\langle |\Sigma e^{i\mathbf{k}\cdot\mathbf{r_j}}(\sigma_j - \bar{\sigma})|^2 \right\rangle \tag{7}$$

$$\bar{\sigma} = (1/N)\Sigma\sigma_j \tag{8}$$

The spherically averaged form of this function has been found for systems with pair interactions to satisfy a scaling relation of the form

$$S(k,t) \sim k_m(t)^{-d} F(k/k_m(t)) \tag{9}$$

where d is the spatial dimension of the system. Our observations are in agreement with this type of behavior. The $S(k,t)$ generated in our simulations, at different times collapse on top of each other (see Fig. 4), after an appropriate rescaling indicated in equation (9). We obtain the characteristic wave vector k_m as the first moment of the structure function.

$$k_m =< k >= \frac{\int kS(k,t)}{\int S(k,t)} \tag{10}$$

When we compare the scaled structure factor for our model with the usual Ising model, we obtain curves that are identical within the statistical errors.

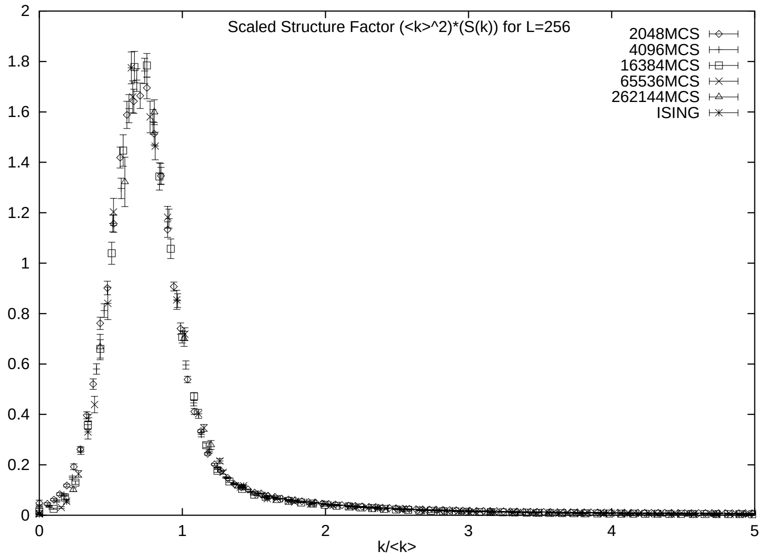

FIG. 4. Collapse of the scaled structure functions at different times during the quenching. $\phi = 0.5$, T=1.0

For sharp interfaces (i.e. when the width of the interface $\epsilon << (k_m)^-1)$, Porod's law predicts a power tail $k^{-(d+1)}$ in d dimensionsi for the tail of S(k,t) in the regime where $\frac{1}{R(t)} \leq k \leq \frac{1}{\epsilon}$ In Fig. 5 we obtain the predicted Porod's tail [12] for our model in 2 dimensions.

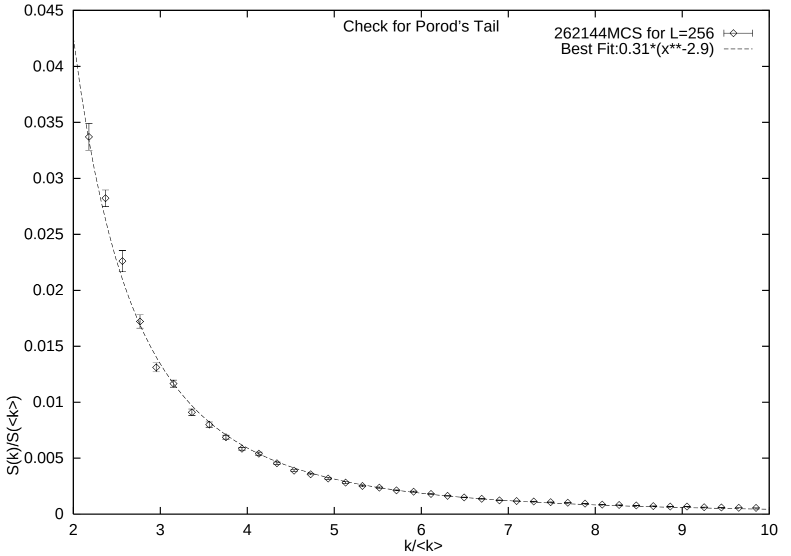

FIG. 5. Porod's tail behavior of k^{-3} after 262144 Monte Carlo Steps for L=256, $\phi = 0.5$, T=1.0.

The characteristic length scale, which is just $(2\pi k_m)^{-1}$, is found to grow asymptotically with time like a power of t.

$$R(t) \sim t^{\alpha} \tag{11}$$

In Fig. 6 we determine the growth exponent α by employing a three free parameter unbiased best fit of the form $R(t) \sim A + B \cdot t^C$ to the length scales obtained from our simulations. The unbiased value of the exponent obtained as a result is strikingly close to the value of $\frac{1}{3}$ predicted by the Lifshitz-Slyozov (LS) theory [9].

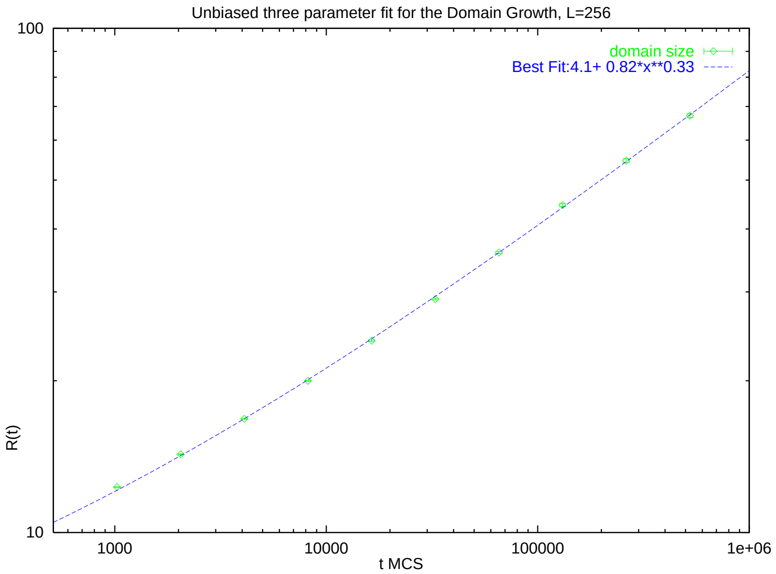

FIG. 6. Domain growth on a L=256 lattice. $\phi = 0.5$, T=1.0

To check the true universal character of the results, we compare the growth of the characteristic length scales in our model for quenching to different temperatures and with different densities. In Fig. 7, we obtain a collapse plot of $R(t)$ vs $t^{1/3}$ by normalizing the slope of the data sets to 1 and the y-intercept to 0.

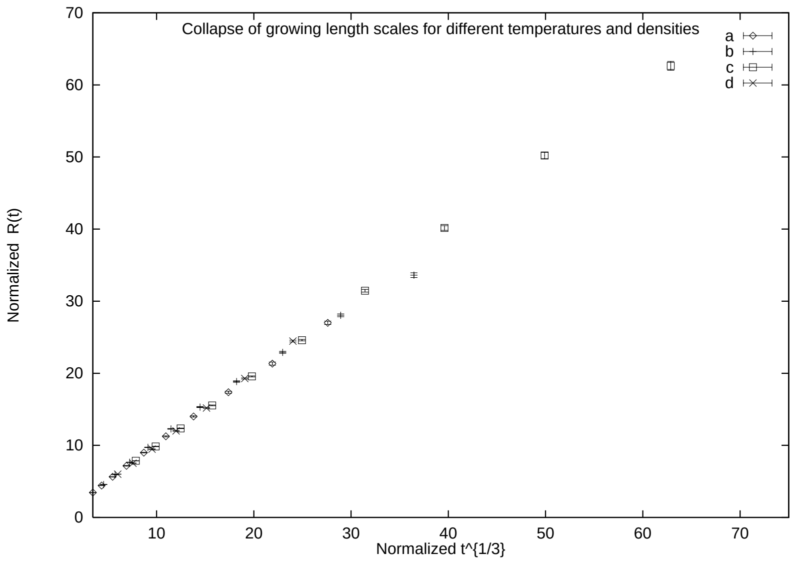

FIG. 7. Growth of characteristic length scales for different densities and temperatures L =256 square lattice a) $\phi = 0.875, T = 1.0$, b) $\phi = 0.75, T = 1.0$, c) $\phi = 0.5, T = 1.0$, d) $\phi = 0.5, T = 0.8$. The Y-axis has been normalized so that the y-intercept is 0 and the x-axis has been normalized so that the slope is 1.

In conclusion , for the simple model with pure three-body lattice gas Hamiltonian, we obtain kinetic behavior which is very similar to that found for models with pair interactions. This confirms the expected universal character of phase segregation with particle conservation diffusive dynamics such as those given by spin-exchanges in our model.

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