Simulation of phase-ordering dynamics of 2d Ising model under influence of oscillatory shear

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Abstract. In this paper, we study phase-ordering dynamics of 2d Ising model under influence of oscillatory shear by computer simulation. We focus on the time evolution of the equal-time correlation functions to test the dynamical scaling hypothesis and to determine the governing growth laws. We find that at late times the system has two different behaviours which are a non-shear behaviour and a uniformly sheared behaviour. Initial phases and frequencies of oscillatory shear determine the behaviour of the system. On one hand, if the frequency is high, the system behaves as if it is not under shear. On the other hand, if the frequency is approached zero, the behaviour of the system will be determined by the initial phase of oscillatory shear. At the initial phase of 90 degree (or 270 degree), the system also behaves as if it is not under shear. Otherwise, the system behaves as if it is under uniform shear (Oscillatory shear is in the form of cosine function).

1. Introduction
Phase-ordering dynamics is the study dynamics of a system that is suddenly quenched from a homogeneous high-temperature state into a heterogeneous low-temperature region [1]. As the system cannot bring itself in time to be in equilibrium at the new condition, it progressively evolves through a series of intermediate states towards the new equilibrium. It has been found in many systems that the evolution of the system passes the so-called scaling regime, in which there exists a single characteristic length scale $L(t)$ such that the ordering structure is (in a statistical sense) independent of time when lengths are scaled by $L(t)$ . In particular, the equal-time correlation function takes on the scaling form $C(r,t) = f(r/L(t))$ . However, the existence of scaling has not been proved in general but the evidence is compelling in its favour. Thus, it is customarily known as the dynamical scaling hypothesis [1, 2].

In many cases of interest, phase ordering dynamics occurs in the system under the influence of an external field and is significantly affected by its presence. One particular choice of potential applications is the case of applied shear flow, especially in a liquid mixture [3, 4]. In the case of nonconserved coarsening which is of concerned here, the scaling hypothesis and its range of validity have been extensively tested. First, Cavagna, Bray and Travasso employed the Ohta-Jasnow-Kawasaki approximation to investigate the dynamics of a system with a scalar nonconserved order parameter in two and three dimensions [5]. In two dimensions, they expectedly found that $L_x(t) \sim t(ln t)^{1/4}$ and $L_y(t) \sim (ln t)^{-1/2}$ under a uniform shear flow. This is in contrary to the isotropic, non-shear case where $L_x(t) \sim L_y(t) \sim t^{1/2}$ [1]. For the ease of later use, we will refer the former growth laws as the uniform shear growth laws and the latter as the non-shear growth laws. The case of 3d uniformly sheared
nonconserved vector order parameter within the large-N approximation was studied by Piputnchonlathee [6]. On the other hand, Cirillo, Gonnella and Saracco used Metropolis Monte Carlo method to simulate the dynamics of the 2d Ising model also under a uniform shear flow [7]. They found that linear growth law $L_y(t) \cdot t$ in the flow direction and constant transverse size. Note that, in shearing cases of two dimensions, the scaling form of the equal-time correlation function has become $C(x, y, t) = f(x/L_y(t), y/L_x(t))$ where $L_x(t)$ and $L_y(t)$ are the characteristic length in the flow and transverse direction respectively.

As commented by Cavagna, Bray and Travasso [5], not only the effect of oscillatory shear on phase ordering dynamics is interesting in itself but it is also more natural in terms of an experimental setup. Thus, in this study, we aim to investigate the 2d Ising model under the influence of an oscillatory shear using Metropolis Monte Carlo dynamics. The algorithm used in this work was adapted from the work of Cirillo, Gonnella and Saracco [7] to cope with the oscillatory nature of the shear. The purpose of this study is two folds. First, we further explore the extent of the validity of the dynamical scaling hypothesis. Second, it means to provide a platform on the investigation of oscillatory shear for other future works.

Just before passing by, we would like to mention that the authors has also done a theoretical work on phase ordering dynamics of the system with vector order parameter under oscillatory shear in the large-N limit [8].

The rest of the article is organised as follows. Section 2 shows details of the simulation used in this work and then the results and discussion are presented in Section 3. Finally, we conclude and remark on our study in Section 4.

2. The simulation

The model is set in a square lattice $A$ of side length $\ell$ with periodic boundary condition in $x$-axis and free in $y$-axis. “Spin” of each site can be either +1 or -1. We define $\Omega$ to be the set of all possible configurations of the model and $\sigma_{x,y}$ is the value of “spin” at site $(x,y)$ of the configuration $\sigma$. With this, the Hamiltonian of the model may be written as

$$H(\sigma) = -J \sum_{x=1}^{\ell} \sum_{y=1}^{\ell} \sigma_{x,y} \sigma_{x+1,y} - J \sum_{x=1}^{\ell} \sum_{y=1}^{\ell} \sigma_{x,y} \sigma_{x,y+1}$$

where there is no external interaction, the internal interaction $J$ is the same for every pair of “spins” and $\sigma_{x+1,y} = \sigma_{x,y}$ which is the periodic boundary condition.

We define the time unit to be one Monte Carlo Step (MCS), i.e., a full sweep of the Metropolis algorithm and set the period of the shear procedure to be $\tau$ (a factor of $\ell^2$).

(I) Set $t = 0$, $i = 0$ and randomize the initial state $\sigma_0$.

(II) Set $i = i+1$ and choose a site of the lattice randomly with uniform probability $\ell^{-2}$ and perform the elementary single-site step of the thermalization dynamics (for more details, see [9])

(III) If $i$ is multiple of $\tau$, $\lambda$ is set to be the integer value of $A \cos(\omega(t+i\ell^{-2})+\theta)$ where $A$ is a real number, $\omega$ and $\theta$ are angular frequency and initial phase of the shear respectively. Then, a layer is randomly chosen with uniform probability $\ell^{-1}$. Finally, if $Y$ is the chosen layer, all the layers with $y \geq Y$ are shifted $\lambda$ sites to the right or the left depending on its sign.

(IV) If $i < \ell^2$, go to (II). Otherwise, we denote the configuration of the system by $\sigma_{i+1}$.

(V) Set $t = t+1$, set $i = 0$, and go to (II).
We calculate equal-time correlation functions in the flow and transverse directions by ensemble and spatial average as defined below.

\[ C_r(t) = \frac{1}{3\ell^2} \sum_{k=1}^{3/\ell^2} \sum_{s=1}^{3/\ell^2} \sum_{y=1}^{3/\ell^2} \left\{ \sigma_{x,s}^{(k)}(t) \sigma_{y,r}^{(k)}(t) + \sigma_{x,s}^{(k)}(t) \sigma_{y,r}^{(k)}(t) \right\} \]

where \( 0 \leq r \leq \ell/4 \) and \( k \) is the number of initial configuration.

3. Results and Discussion

In this simulation, we set the system size \( \ell = 2048 \) and observing time interval from 0 to 1,000 MCS to go with the shear rate parameter \( \gamma = 1/\ell \). The frequency of the oscillatory shear employed in this work is 48, 24, \( 2 \times 10^{-5} \) and \( 10^{-5} \) 1/MSC. For each frequency, seven different values of initial phase are used, i.e., 0, 5, 10, 45, 80, 85 and 90 degrees. Finally, the final temperature of the system \( \beta J = 2, 10 \) and \( \infty \), corresponding to \( T = 0 \), are chosen, where \( \beta = 1/(k_B T) \), \( T \) is temperature and \( k_B \) is Boltzmann’s constant. (The critical temperature of 2d Ising model corresponds to \( \beta J \approx 0.44 \))

Figure 1. (a) Equal-time correlation function in the flow direction where the frequency is \( 10^{-5} \) 1/MCS and initial phase is equal to 0 degree - each line plotted 200 MCS differently, (b) the graphs scaled by the uniform shear growth law and (c) the graphs scaled by the non-shear growth law

Figure 2. (a) Equal-time correlation function in the flow direction where the frequency is \( 10^{-5} \) 1/MCS and initial phase is equal to 90 degree - each line plotted 200 MCS differently, (b) the graphs scaled by the uniform shear growth law and (c) the graphs scaled by the non-shear growth law
Figure 1 (a) and figure 2 (a) show the plots of the equal-time correlation function in the flow direction of the system at different times, i.e., 200, 400, 600, 800 and 1000 MCS. The frequency used in both cases is $10^{-5}$ 1/MSC but the initial phase is 0 degree in the former and 90 degree in the latter. As suggested by theoretical results of [8], we tried to collapse the graphs with two different growth laws and the results are shown in figure 1 (b) and figure 2 (b) for the uniform shear growth law and in figure 1 (c) and figure 2 (c) for the non-shear growth law. We can see by our naked eyes that the collapse in the former case is well suited by the uniform shear growth law while the latter case by the non-shear growth law. This scenario seems to be common in all cases we consider in this work, except a few. Therefore, we may safely say that there exist two characteristic length scales $L_x(t)$ and $L_y(t)$ which dictate the evolution of the system at late times. In other words, the dynamical scaling hypothesis prevails when the system is under the influence of oscillatory shear, irrespective of temperature, frequency and initial phase.

From all our results, we may draw another important finding about this simulation of phase ordering dynamics. The growth laws, $L_x(t)$ and $L_y(t)$, for high frequency cases (48 and 24 1/MCS) are given by the non-shear growth laws while for low-frequency cases ($2 \times 10^{-5}$ and $10^{-5}$ 1/MCS) are governed by the uniform shear growth laws except for the cases of initial phase of 85 and 90 degrees. For the 90-degree-initial-phase low-frequency case, the uniform shear growth laws are justified. On the other hand, it is rather hard to decide which growth laws are the more suitable growth laws for the 85-degree case. This finding is essentially in agreement with the results of [8], which indeed gave the motivation and idea for doing this work.

Last but not least, to make sure that finite size effects did not hamper our results, we had also performed some simulations on the system with $\ell = 4096$ and found that it confirmed our results on smaller systems. Another point worth mentioning is the growth laws for the uniform shear flow cases. We found that the growth laws $L_x(t) - t$ and $L_y(t) - \text{constant}$ without logarithmic corrections are also very acceptable. This is in consistent with the results of Cirillo, Gonnella and Saracco [7], and, actually, it was also noted by Cavagna, Bray and Travasso [5].

4. Conclusion

In this work, we have performed Monte Carlo simulations on 2d Ising model to investigate its phase ordering dynamics. We found that under the influence of applied oscillatory shear, the dynamical scaling hypothesis is generally satisfied at late times. Most of cases are governed by either the uniform shear growth laws $L_x(t) - t (\ln t)^{1/4}$ and $L_y(t) - (\ln t)^{-1/4}$ or the non-shear growth laws $L_x(t) - L_y(t) - t^{1/2}$. Initial phases and frequencies of oscillatory shear essentially determine the behaviour of the system. On one hand, when the applied frequency of shearing is high, the system behaves as if it is under no shear. There is no difference of growing in the flow direction and perpendicular directions. On the other hand, when the applied frequency is low, the behaviour of the system seem to be controlled by the initial phase of oscillatory shear. At the initial phase of 90 degree (or 270 degree), the system behaves as if it is not under shear. At other initial phase values, the system behaves as if it is under uniform shear, which means that there is difference of dynamical scaling in flow direction and perpendicular direction. Hence, this suggests that some kind of "nonequilibrium phase transition" may occur when the frequency of shearing is low. The existence and nature of the transition in a more general setting requires more work to be done.

Acknowledgements

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