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Nucleation of Kinetic Ising Model under Oscillating Field

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We have studied the nucleation process of a two-dimensional kinetic Ising model subject to a bias oscillating external field, focusing on how the nucleation time depends on the oscillation frequency. It is found that the nucleation time shows a clear-cut minimum with the variation of oscillation frequency, wherein the average size of the critical nuclei is the smallest, indicating that an oscillating external field with an optimal frequency can be much more favorable to the nucleation process than a constant field. We have also investigated the effect of the initial phase of the external field, which helps to illustrate the occurrence of such an interesting finding.

Key words: Kinetic Ising model, Nucleation, Oscillating field

I. INTRODUCTION

Nucleation is a fluctuation-driven process that initiates the decay of a metastable state into a more stable one [1]. Many phenomena in nature are associated with nucleation, such as crystallization [2], glass formation [3, 4], and protein folding [5]. The Ising model is a simple but powerful model which has been widely used to study the nucleation process. For instance, the nucleation pathway of the Ising model in a three-dimensional lattice has been studied by the transition path sampling approach in which analysis of the transition state ensemble (TSE) indicate that the critical nuclei are rough and anisotropic [6]. Ising model in the geometry of a long stripe exhibits a rather different "phase behavior" from bulk phase transition, and it was demonstrated that this system exhibits properties of the 2D Ising bulk system as well as properties of the 1D-Ising system [7]. The existence of a pore may change the nucleation mechanics, leading to two-stage nucleation and the overall nucleation rate can arrive at a maximum level in intermediate pore size [8]. Ising model has also been used to test the applicability of the classical nucleation theory by Shneidman *et al.* [9], and so on.

Despite great progress, the physics of nucleation has been made in "quasi equilibrium" systems. Nucleation also takes place in systems out of equilibrium. In recent decades, nucleation in driven systems where external forces break the detailed balance has gained more and more attention, including nucleation of glasses [4], semicrystalline polymers [10], and microcellular foaming process under shear. Simulations and experiments reveal that shear has a significant impact on nucleation and nonequilibrium phase transitions [10, 11]. Blaak *et al.* found shear can suppress nucleation and lead to a larger critical nucleus [12]. Mazzanti *et al.* reported that crystalline orientation and phase transition acceleration induced by shear are demonstrated to occur in different edible fats using synchrotron X-ray diffraction [13]. In the 2D (two-dimension) Ising system, shear can enhance nucleation rate and at intermediate shear rate the nucleate-rate peaks [14].

Oscillating field usually acts as an important type of driven force in nonequilibrium systems. Ising models subject to an oscillating field have been used to study the so-called dynamic phase transition (DPT). After first observed by Tomé [15], DPT had been extensively studied by mean field analysis [15, 16], Monte Carlo (MC) simulations [17−19], and other analytical methods [20, 21]. It is found that the critical exponent of the DPT is consistent with the equilibrium Ising value, which is universal with respect to the choice of the stochastic dynamics [22]. Nevertheless, nucleation process of the Ising system under oscillating field has not been studied yet.

In the present work, we have investigated the nucleation of a 2D kinetic Ising model subject to an oscillating external field using MC simulations. We have mainly focused on how the nucleation time τ_n, defined as the ensemble averaged escape time from the metastable state, depends on the oscillating frequency ω for fixed oscillation amplitude. Interestingly, τ_n shows a clear-cut minimum at $\omega=\omega_c$, demonstrating that an oscillating field with an intermediate frequency can be the most favorable to the nucleation process. In ac-

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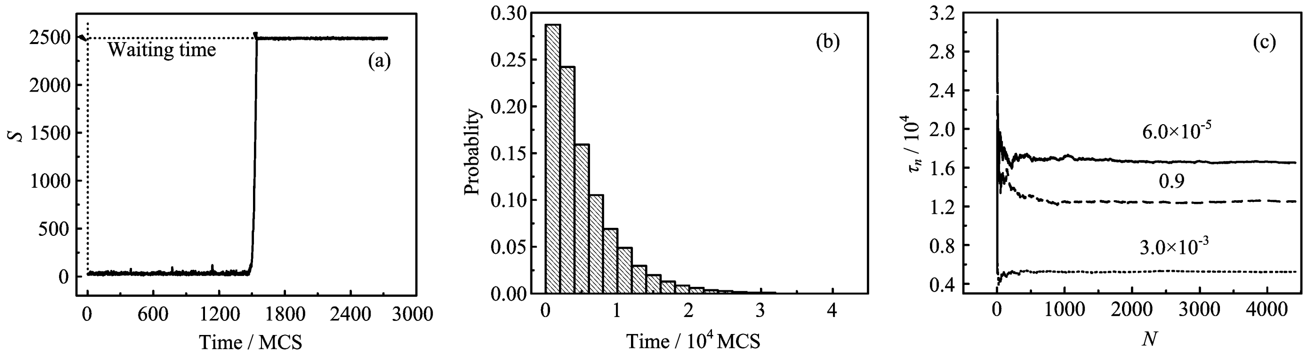

FIG. 1 (a) Time series S of up spins in a nucleation process. (b) Distribution of N_t at ω=3.0×10^{-3} for N=10×10^4 simulation runs. (c) Dependency of the average nucleation time τ_n on N for ω=6.0×10^{-5}, 3.0×10^{-3}, and 0.9.

cordance with this, we have investigated the mean size of the critical nuclei by analysis of the transition state ensemble. As expected, the average size of the critical nuclei is the smallest at ω_c. In addition, the effect of the initial phase ϕ of the external field on τ_n is also explored.

II. MODEL AND SIMULATION DETAILS

A ferromagnetically interacting nearest neighbor 2D Ising model in the presence of a time varying magnetic field can be represented by the Hamiltonian,

$$H = -J\sum_{\langle i,j\rangle} s_i s_j - h(t)\sum_i s_i \tag{1}$$

here, J=1 is the coupling constant, s_i is the spin variable at site i which can be either +1 (up) or −1 (down), $\langle i,j\rangle$ represents nearest-neighbor pairs, and $\sum_i$ runs over all lattice sites. The external magnetic field $h(t)$ includes two components:

$$h(t) = h_0 + h_1\sin(\omega t + \phi) \tag{2}$$

h_0>0 is a static field which is more favorable for up spins than down spins, and the second term is an oscillating field with amplitude h_1, frequency ω, and initial phase ϕ.

Initially, we set all the lattice spins down in h_0 always larger than h_1. By this setting, the initial state is metastable and the stable state is the one with most spins up. At a finite temperature, a phase transition will take place via a nucleation process from the initial state to the stable one. The configuration of the system is updated by Glauber standard dynamics: each attempt spin flip from s_i to $-s_i$ is accepted with probability

$$W(s_i \to -s_i) = \frac{\exp(-\beta\Delta E_i)}{1+\exp(-\beta\Delta E_i)} \tag{3}$$

where ΔE_i is the energy change of the system if the spin flip is accepted and β=1/$k_\mathrm{B}T$ with k_B the Boltzmann's constant and T the temperature. During the simulation, each lattice site is updated sequentially, and one such full scan over the lattice is defined as a Monte Carlo step (MCS). If not stated otherwise, all simulations are performed on a 50×50 lattice with h_0=0.17, h_1=0.04, and ϕ is randomly chosen from a uniform distribution from 0 to 2π. T=2/3T_c=1.54 where T_c is the critical temperature of the 2D Ising system out of the external field. Periodic boundary condition is imposed. Nucleation time for each frequency is obtained via averaging over 3000 independent simulation runs.

III. RESULTS

To describe the nucleation process, we chose the number of up spins S as the order parameter. The time series S for a typical nucleation process is shown in Fig.1(a), from which we can see that S fluctuates at low level in the early stage, which indicates the system is in the metastable state, followed by a sudden jump after a period of waiting time to the stable state with high value of S. Usually, the waiting time is randomly distributed as shown in Fig.1(b) for ω=3.0×10^{-3} for N=10×10^4 simulation runs. In Fig.1(c), the dependencies of τ_n on N are shown respectively for ω=6.0×10^{-5}, 3.0×10^{-3}, and 0.9. Obviously, τ_n converges after about 2000 runs. We thus define the average waiting time over N=3000 runs as the nucleation time τ_n (the nucleation rate R is simply 1/τ_n).

As already shown in Fig.1(c), τ_n for an intermediate ω, 3.0×10^{-3}, is smaller than that for a larger frequency ω and a smaller one. It seems that there exists an optimal frequency for the external field which is the most favorable for the nucleation process. To show this, we plot τ_n as a function of ω in Fig.2, where the dash-dot line denotes the nucleation time under the static field h_0. Indeed, τ_n exhibits a clear-cut minimum at some optimal frequency ω=ω_c. It is also shown that an external field with large frequency has no effect on the nucleation

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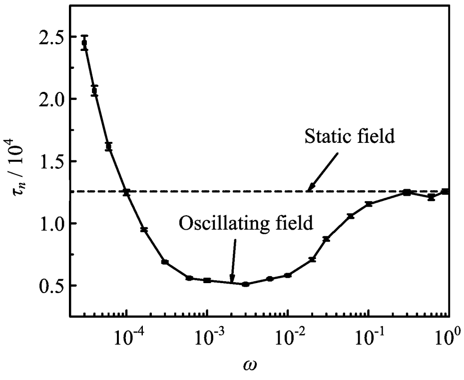

FIG. 2 Nucleation time τ_n as a function of the frequency ω. The dash-dot line represents the average waiting time in the static field h_0.

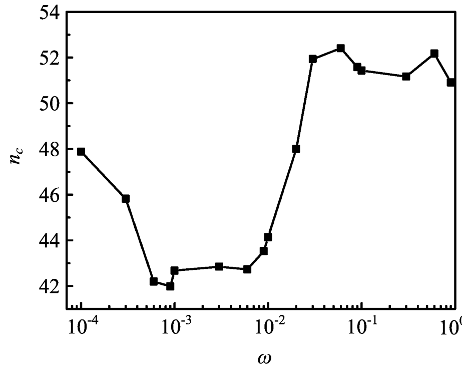

FIG. 3 The mean size of critical cluster n_c is plotted as function of frequency ω.

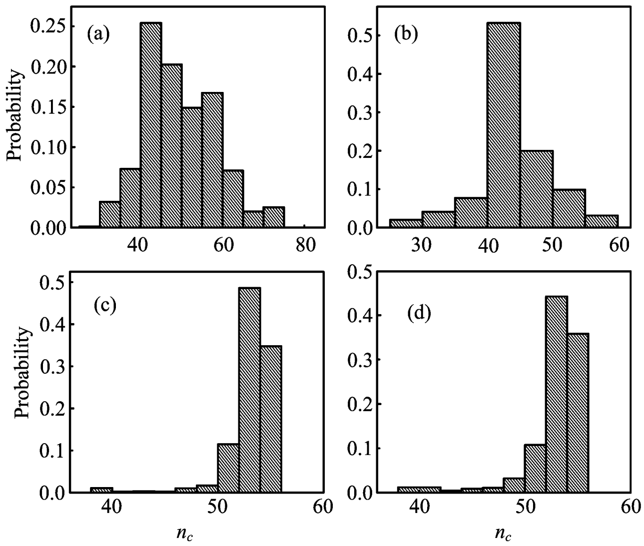

FIG. 4 Distribution of the size of critical nucleus at different frequency. (a) ω=1.0×10^{-4}. (b) ω=3.0×10^{-3}. (c) ω=0.9. (d) Static field h_0.

process. This is reasonable because in this case the period of the field is much smaller than τ_n and the system already oscillates many times in the metastable region before jumping to the stable state. In this case, the system can only experience an average field h_0. On the other hand, a slow-varying external field is not helpful for the nucleation process, the reason of which will be given below along with the discussion about the initial phase.

To further illustrate the existence of the optimal frequency, we tried to figure out the critical nucleus at different frequency by TSE sampling. TSE consists of a set of configurations located at the top of the free energy barrier along the nucleation pathway, wherein each configuration has the same probability to reach the final and the initial state. In simulations, we determine the transition state by computing the committor probability P_B which is the probability of reaching the final state before returning to the initial one for 4000 independent trials starting from this configuration. If a configuration with P_B=0.5±0.02, we take it as one belonging to the TSE. Analysis of the TSE containing 2000 configurations gives the information of the critical nucleus, the mean size n_c and distribution of which are obtained by the Hoshen-Kopelaman method [23].

Figure 3 shows the frequency ω dependence of n_c, which also exhibits an minimum for near ω_c. According to classic nucleation theory, a smaller critical nucleus size generally corresponds to a larger nucleation rate. Thus the tendency shown in Fig.3 is in agreement with Fig.2, which supports the existence of an optimal frequency. Accordingly, typical distributions of the nucleus size are shown in Fig.4 for ω=1.0×10^{-4}, 3.0×10^{-3}, 0.9 and h_0, respectively. For a low ω as shown in Fig.4(a), the distribution is relatively broad, indicating that a critical nucleus to some extent is not well-defined in this case. Near the optimal frequency, the distribution is more sharp around a relatively smaller value, see Fig.4(b). When ω is large, the distribution is biased to larger size, as depicted in Fig.4(c), which is very similar to the case for a static external field, see Fig.4(d).

To understand why τ_n in an oscillating field with very low frequency is much larger than that in a static field h_0, we have evaluated the effect of the initial phase ϕ on τ_n. Note that if ω tends to zero, the system is simply subjected to a field $h'=h_0+h_1\sin\phi$. For the simulation results above, ϕ is randomly chosen from a uniform distribution from 0 to 2π. We now fix ϕ to see how it would influence τ_n, which is demonstrated in Fig.5. For very low frequencies, for instance ω=6.0×10^{-5}, 1.0×10^{-4}, and 3.0×10^{-4}, the curve of τ_n versus ϕ shows a sinusoidal-like shape, but being unsymmetric with respect to $\phi=\pi$. With decreasing frequency, the peak (right side) height of τ_n increases more rapidly than the valley (left side) depth decreases. Note that the ensemble average of the nucleation time for random initial phase equals the area below the curve. Therefore, the asymmetric distribution of τ_n with respect to ϕ is the

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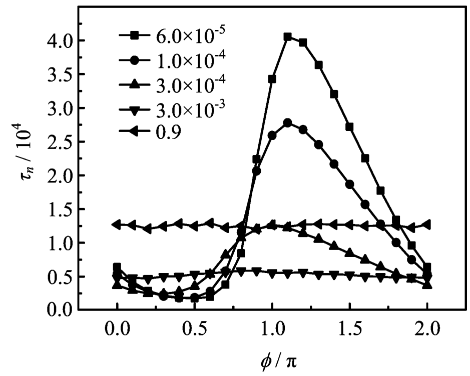

FIG. 5 The effect of initial phase ϕ in a definite frequency on the average nucleation time τ_n of varying initial phase. ω=6.0×10^{-5}, 1.0×10^{-4}, 3.0×10^{-4}, 3.0×10^{-3}, and 0.9. Each dot is also averaged by 3000 simulations.

very reason that leads to the increment of τ_n with decreasing ω shown in Fig.2. We also notice that for a relatively large ω, as also shown in Fig.5 for ω=3.0×10^{-3} and 0.9, τ_n is not sensitive to the fixed initial phase ϕ, but τ_n keeps an apparently smaller value for the former frequency which is closer to ω_c than the latter one.

IV. CONCLUSION

Nucleation of a 2D kinetic Ising model subject to a bias oscillating field has been studied. We find that there exists an optimal frequency of the external field which is the most favorable to the nucleation process. This is demonstrated by a clear-cut minimum of the nucleation time, as well as a smallest average size of the critical nucleus. We have also investigated the effect of initial phase of the external field on the nucleation time, which helps to illustrate why a slow varying field also slows down the nucleation process. Since the Ising model is widely used in many physical, chemical and biological systems, and periodic loading is often used to perform system control, our study may open new perspectives in the study of nonequilibrium nucleation process.

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