Temperature dependence of the amplitude of power-law growth in the spin-flip kinetic Ising model

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A definition of the average size R of the domains observed during a first-order phase transition, which is based on the time-dependent excess internal energy, is introduced. The temperature dependence of the growth law for $R(t,T)$, where t is time and T is the quench temperature, has been investigated over a wide range of temperature below and near T_c, in the two-dimensional spin-flip Ising model. The results obtained support the Allen-Cahn growth law, $R(t,T)^2 \sim \alpha(T)t$, and allow an estimate of the temperature dependence of the nonuniversal coefficient $\alpha(T)$. Nonmonotonic behavior of α is observed at low temperature, which is attributed to lattice anisotropy.

I. INTRODUCTION

When the kinetic Ising model is quenched from an initial state at a temperature T_∞ above the critical temperature T_c to a temperature $T < T_c$, the average size of ordered domains $R(t,T)$ grows in time according to a power law $R(t,T) = [\alpha(T)t]^n$. There is now strong theoretical and experimental evidence that in the asymptotic long-time regime any linear scale of the pattern becomes proportional to R. Furthermore, in systems with a nonconserved order parameter that belong to the universality class of model A,[1] $n = 1/2$, and is independent of T. These results have been derived in different ways by many authors,[2–5] but the main theoretical insight is due to Allen and Cahn.[3] It should be mentioned that the universality class of model A encompasses a large number of systems including, for example, order-disorder transitions in binary alloys, time-dependent Ginzburg-Landau equations, and the spin-flip kinetic Ising model. Common (and presumably universal) features shared by all these systems have been observed in a number of experiments[3,6–13] as well as computer simulations.[14–26]

The independence of the growth exponent n on temperature can be heuristically understood as follows. In systems described by a scalar-nonconserved order parameter, relevant length scales other than R are the thermal-correlation length of the initial state (at T_∞), and more importantly, since we shall always consider $T_\infty = \infty$ hereafter, the finite correlation length at T, $\xi(T)$. Since $\xi/R \to 0$ as $t \to \infty$ for $T < T_c$, it is natural to expect that only one length scale determines the universal scaling properties. Since temperature-dependent effects (or fluctuations of thermal origin) are asymptotically irrelevant in the scaling regime, it is frequently said that domain growth is controlled by a zero-temperature fixed point, and that the growth exponent follows from dimensional analysis. Nevertheless, there is a nonuniversal dependence of the amplitude of the growth law on temperature which can be important in some cases, and that we investigate in this paper. The explicit form for the asymptotic growth law is

$$R^2 = \alpha(T)\, t \tag{1}$$

for sufficiently late times. It is the purpose of this paper to numerically obtain the temperature dependence of the nonuniversal parameter $\alpha(T)$ for an important specific system, the two-dimensional spin-flip kinetic Ising model, and to investigate its dependence on anisotropy.

We first briefly review the relevant theory. Allen and Cahn obtained an equation for the normal speed of an element of antiphase boundary v_n, in terms of its local mean curvature K and a mobility coefficient α_0. Their analysis begins with a time-dependent Ginzburg-Landau equation for a system described by a nonconserved scalar order parameter. They found that v_n is proportional to K:

$$v_n = \alpha_0 K, \tag{2}$$

where K is defined to be negative for a sphere. In their theory, α_0 is independent of surface tension $\gamma(T)$, and of the thickness of domain walls [which one would expect to be $\mathcal{O}(\xi)$ at sufficiently high temperatures when lattice effects are unimportant]. This is what is experimentally observed in systems with negligible anisotropies.[8] In this sense, their theory provided an important improvement to earlier studies, which indeed predicted dependences such as $\alpha_0 \propto \gamma$.

The only temperature dependence in the theory of Allen and Cahn comes from the mobility,

$$\alpha_0(T) \propto e^{-A/k_B T}, \tag{3}$$

for low T, where k_B is Boltzmann's constant and A is a (possibly zero) activation energy for the microscopic processes responsible for interface motion. Such a temperature dependence of the mobility has been seen to be important, for example, in a recent experiment on the late-stage kinetics of the $B2/DO_3$ transition in Fe_3Al.[13] There, the rate of growth was found to decrease exponentially with temperature over a wide range of temperatures.

At higher temperatures, however, the Allen-Cahn theory fails to describe the effect of thermal fluctuations. In order to incorporate their effect, a noise contribution was added to Eq. (2). As argued previously, such a contribution is not expected to change the growth exponent n, but can change the temperature dependence of α_0, leading to a new coefficient $\alpha(T)$, where the effects of fluctuations are properly incorporated. Two important manifestations of thermal fluctuations are capillary wave roughening, which can be important $0 < T < T_c$, and critical fluctuations, which will be important for $T \lesssim T_c$.

The contribution from roughening fluctuations has already been studied within the framework of Ginzburg-Landau models.[27,28] In our model, thermal fluctuations cause the interface to wander randomly, a fact that is expected to cause a decrease in $\alpha(T)$ as temperature is increased. For example, Grant and Gunton[27] incorporated additive noise into Eq. (2) and obtained $\alpha(T)$ for both a random distribution of interfaces and an initially circular distribution of domains. For low temperatures, both results yielded behavior of the form

$$\alpha(T) \propto (1 - bT), \tag{4}$$

where b is a constant.

Near T_c, critical fluctuations should also be important. Their effect can be estimated as follows:[29] Power law growth is expected to hold near T_c provided that all lengths are rescaled with the diverging correlation length $\xi \sim (T_c - T)^{\nu}$, and times with the correlation time $\tau \sim \xi^z$, where ν and z are critical exponents. Therefore, close to T_c,

$$(R/\xi)^2 \sim (t/\tau) \tag{5}$$

or

$$\alpha \propto \xi^{2-z} \sim (T_c - T)^{\phi} , \tag{6}$$

where $\phi = \nu(z-2) > 0$. For a nonconserved order parameter, it is expected that $z \gtrsim 2$ for dimensions $d = 2$ and 3. For example, in $d = 2$ where $\nu = 1$, we[30] have recently obtained $z \approx 2.13$, and so $\phi \approx 0.13$, which is rather small. This implies that the critical region in the temperature for observing such behavior is also small. Indeed, we do not think that critical fluctuations play an important role in the numerical study presented below.

These three effects, Arrhenius dependence at low temperature, capillary wave roughening at intermediate temperatures, and critical fluctuations at high temperatures, summarize our theoretical understanding of the temperature dependence $\alpha(T)$. Below, we numerically investigate $\alpha(T)$ for the two-dimensional spin-flip Ising model, and find an important contribution due to anisotropy, particularly as it is related to the underlying lattice structure, which has not been previously studied.

Finally, we also have to note some earlier numerical studies of the temperature dependence of $\alpha(T)$. For example, Kaski *et al.*[18] analyzed the variation of the dynamic structure factor and of the magnetization squared[19] of an Ising model quenched at different temperatures. Although they used a system of reasonable size ($N = 60^2$ spins), their results for the temperature dependence of α were not conclusive. More recently, an analysis of a related model[26] concentrated on the time dependence of the average size of the domains. The results obtained indicate a decrease of the growth coefficient α with temperature.

II. METHOD

In order to study the influence of the quenching temperature on growth rate, we study a ferromagnetic spin-flip Ising model in two spatial dimensions, with periodic boundary conditions. The Hamiltonian is $\mathcal{H} = -J\sum_{i,j}\sigma_i\sigma_j$, where the sum extends over all pairs (i,j) of nearest neighbors in the system, $J > 0$ is the coupling constant, and the $\sigma_i = \pm 1$ represent the two possible orientations of the N spins on sites $i = 1, 2, \ldots, N$ of a square lattice. At time $t = 0$, the initial configuration is comprised of randomly oriented spins (i.e., at $T_\infty = \infty$) and this system is then quenched at various temperatures $T < T_c$. The evolution of the system of spins is defined according to a Metroplis-type algorithm: A spin is chosen at random and flipped with probability $\min(1, \exp \Delta\mathcal{H}/T)$, where $\Delta\mathcal{H}$ is the energy difference between the spin configuration before and after flipping the spin. The unit of time is one Monte Carlo time step (MCS), defined to be equal to N attempts at flipping one spin. We calculate the internal energy density (i.e., per spin) $u(t) = \langle\mathcal{H}\rangle/N$, with $N = 256^2$, and where the brackets denote an average over 320 independent runs.

A. Measure of the domain size

Previous numerical studies used a variety of methods to measure the size of the domains, including the inverse perimeter density (defined from the number of broken bonds in the system, a "broken bond" being a pair of nearest-neighbor spins with different orientations), the ensemble average of the magnetization squared, and the intensity of the peak of the structure factor. It is commonly accepted that the value of the average domain size obtained from the perimeter density is less susceptible to statistical fluctuations than, for example, methods based on the structure factor or its statistical moments. However, the perimeter density ceases to be directly related to the size of the domains at high temperatures, because thermal fluctuations become appreciable. For this reason, we consider here an alternative method, and estimate the domain size from the energy density.

Consider a large system of linear dimension L in equilibrium such that $N = L^d$, where d is its spatial dimensionality. Consider also a flat interface of perimeter L^{d-1}

separating two coexisting phases. Clearly the internal energy density u is increased by the presence of this interface by a term proportional to the interface density $\rho = 1/L$. That is,

$$u = \tilde{u} + \epsilon\rho(L), \tag{7}$$

where $\tilde{u}$ is the internal energy density in the absence of the interface (bulk contribution), and ϵ is the excess surface internal energy density (per unit length). ϵ is related to the surface tension $\gamma(T)$ by the relation

$$\epsilon = \gamma - T\frac{\partial\gamma}{\partial T}, \tag{8}$$

where $-(\partial\gamma/\partial T)$ is the excess surface entropy.

During domain growth, local equilibrium is reached in a time scale small compared to the time scale of motion of the interfaces that separate the coexisting phases. For an Ising system, this means that the interface density $\rho(t)$ can be obtained directly from the internal energy except at very early times after the quench. At low temperatures, this approach is equivalent to obtaining the interface density from the perimeter density measured from the number of broken bonds. That is, as $T \to 0$, $\epsilon \to 2J$, in agreement with the definition of R from the number of broken bonds. We define the average domain size by

$$R(t,T) \equiv 1/\rho(t,T) = \frac{\epsilon(T)}{u(t,T) - \tilde{u}(T)}. \tag{9}$$

This is a convenient definition for us, since we directly obtain $u(t,T)$ from the numerical simulation, and the results for $\tilde{u}(T)$ and $\epsilon(T)$ follow from Onsager's solution of the two-dimensional Ising model.[31] In particular, from the equation of motion for the interface and the hypothesis of self-similarity[32] one can obtain the growth law for the average domain size,

$$R^2(t,T) = \left[\frac{\epsilon}{u(t) - \tilde{u}}\right]^2 = \ell^2(T) + \alpha(T)t, \tag{10}$$

where ℓ is a time-independent length. We will use this form and the simulation results to obtain $\alpha(T)$.

B. Anisotropy

It is well known that the surface tension of the Ising model $\gamma(T,\theta)$ is anisotropic, where θ is the relative orientation of an antiphase boundary with respect to the lattice. For the two-dimensional Ising model, the angular dependence of $\gamma(T,\theta)$ is well known.[33,34] Given this angular dependence, it is then possible to determine the equilibrium shape of a domain of fixed area by using Wulff's construction.[35] This will be useful to us in what follows.

The angular dependence of the interface internal energy, obtained from $\gamma(T,\theta)$, is approximately included in our analysis in the following way. We perform a weighted average to obtain an effective isotropic interface internal energy $\bar{\epsilon}$. If the interface of an *equilibrium* domain is parametrized by a contour variable s, then the average is

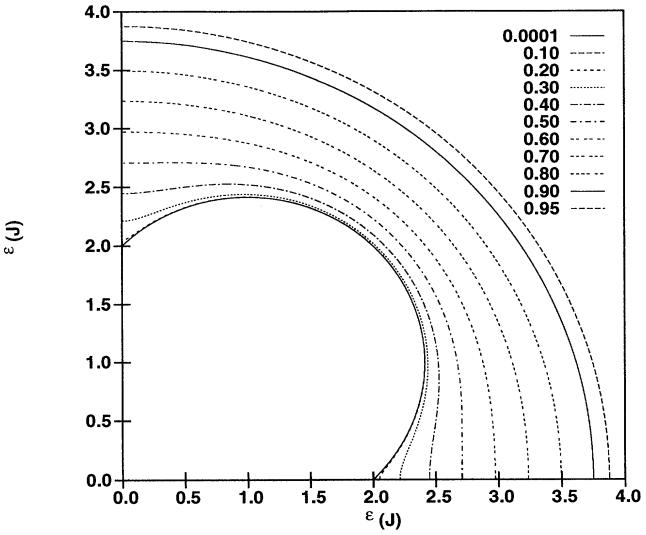

FIG. 1. Polar plot of the interface internal energy $\epsilon(\theta,T)$ for the indicated temperature values. Temperatures are in units of T_c and increase outwards.

$$\bar{\epsilon}(T) = \frac{\oint \epsilon(T,\theta(s))ds}{\oint ds} \tag{11}$$

for each quench temperature. Figure 1 shows a polar plot of the interface internal energy $\epsilon(T,\theta)$, whereas Fig. 2 shows the equilibrium shape of a domain obtained from Wulff's construction. The observation of the evolution of the domains during the quenches supports this method; for quenches at very low temperature the domains tend

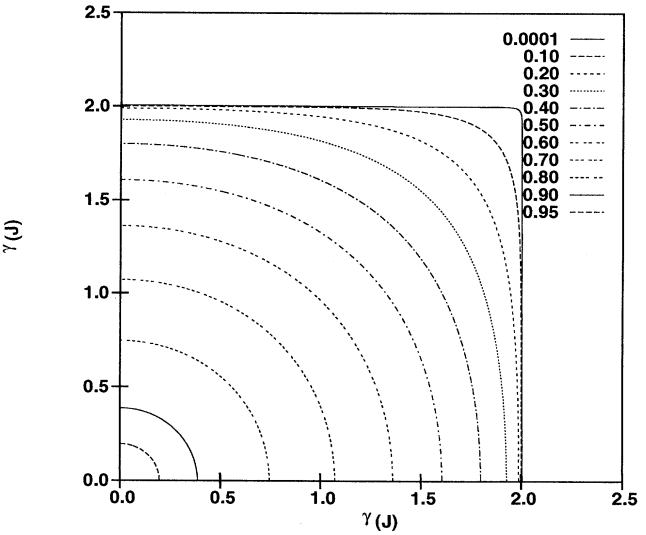

FIG. 2. Equilibrium shape of a two-dimensional domain as built from Wulff's theorem and Onsager's expression of the interface free energy. The scale on the axes represents the $\theta = 0, \pi/2$ values of the interface free energy $\gamma(\theta,T)$ in units of J. Temperatures are in units of T_c and increase inwards.

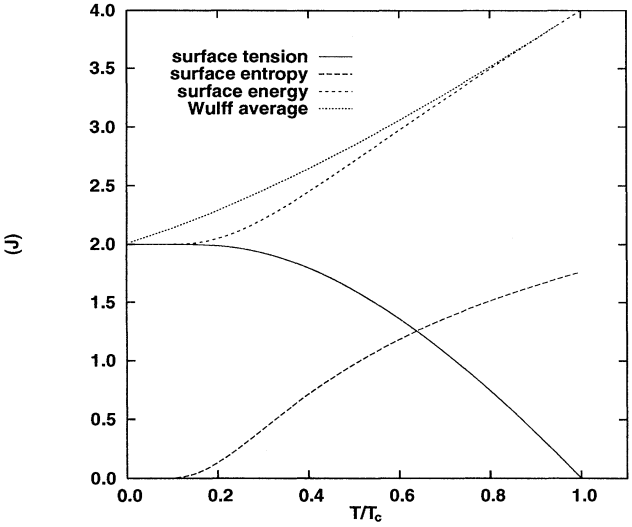

FIG. 3. Various interface characteristic quantities as extracted from the Onsager solution. These values are calculated along the direction of the lattice axes. The Wulff average represents the internal interface energy as corrected for the angular distribution found in the equilibrium construction of a droplet. Energy is in units of J.

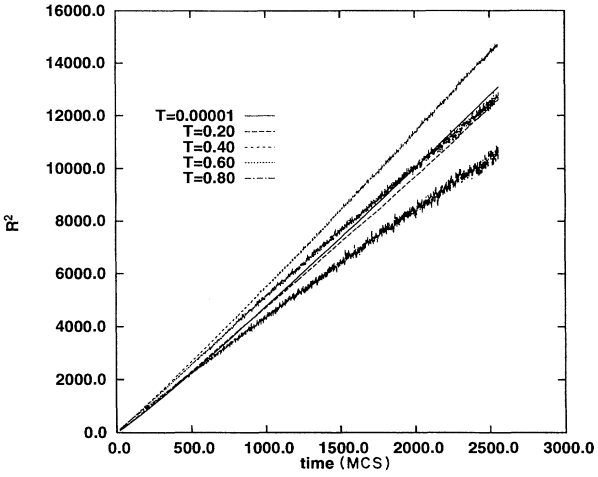

FIG. 4. Evolution of the interface density $R^2 = [\bar{\epsilon}/u(t) - \tilde{u}]^2$ for various quenches. R is measured in units of the lattice constant which is taken to be unity. The values of the quenching temperatures are 0.00 (10^{-5}), 0.20, 0.40, 0.60, and 0.80, in units of T_c. Results were averaged over 320 representations of the initial conditions, on a system of size 256^2. Time in Monte Carlo steps (MCS).

to be aligned along the lattice axes, whereas quenches at higher temperatures show smoother and more curved interfaces, in agreement with the shape given by the Wulff construction. Other methods to obtain an effective $\bar{\epsilon}$ may also be reasonable.

Figure 3 shows a plot of the temperature dependence of the various equilibrium interface quantities for an interface normal to the $\theta = 0$ direction (i.e., aligned with the square lattice). It can be seen from this figure that corrections to the excess internal energy are largest at low temperatures (cf. Ref. 33).

III. RESULTS

The temporal evolution of the internal energy density u for various quenches at different temperatures is shown in Fig. 4. The data have been fitted to Eq. (10) both for $\bar{\epsilon}$ (Wulff corrected) or ϵ (noncorrected). The fitted values of $u(t \to \infty)$ agree with the exact equilibrium values $\tilde{u}$ within the accuracy of our study. Therefore, late-time metastable states, commonly observed at low temperatures in the form of stripes across the system,[20] and that are attributed to finite-size effects due to the periodic boundary conditions, do not seem to have any influence on our results. In general, finite-size effects have been argued to be significant for $R \gtrsim 0.4L$.[20] The time range used in our study is well below this approximate limit.

The estimated value of α at various quench temperatures is shown in Fig. 5. We see no evidence of activated processes as $T \to 0$ or evidence of slowing down in the temperature range we consider, $T \leq 0.95T_c$. Neither result is surprising: At low temperatures, we expect that the Ising ferromagnet with spin-flip dynamics does not require activated spin-flip processes for domain growth; and we are not sufficiently close to T_c to see critical slowing down. At intermediate temperatures, where roughening should be relevant, the shape of the curve is not consistent with the theoretical expression obtained by Grant and Gunton. Contrary to the predicted behavior at low temperatures, our data show that α increases with tem-

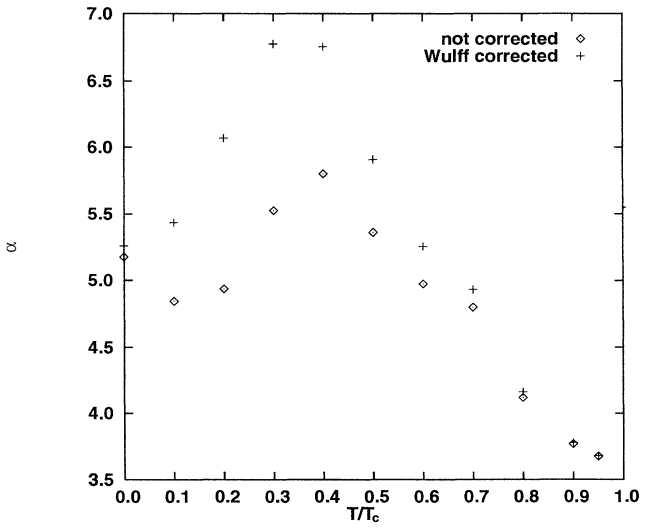

FIG. 5. Temperature dependence of the growth coefficient $\alpha(T)$, with and without anisotropy averaged from the Wulff construction. Note that even at $T = 0.95T_c$, α is well above zero, indicating that critical slowing down is not affecting its behavior.

perature. The form of the Wulff-corrected data serves to give a possible explanation for the discrepancy with theory. We note that the Wulff-corrected and noncorrected values of $\alpha(T)$ agree for $T \gtrsim 0.7T_c$, implying that anisotropy is irrelevant in that range. This is also the regime where the nonmonotonic behavior of $\alpha(T)$ ceases. Hence, it appears the ingredient necessary to explain our observations is anisotropy. Furthermore, we expect this effect to be more pronounced in three dimensions, since anisotropy can cause a roughening transition to occur in $d = 3$.

Therefore, in conclusion, we have shown that the linear scale of the domains during growth can be extracted from the internal energy for arbitrary temperatures. By using this method, we found at low temperatures a nonmonotonic dependence of the growth rate α on temperature, which we attribute to anisotropy.

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