Surface Criticality at a Dynamic Phase Transition

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[1]*Department of Physics, Virginia Tech, Blacksburg, VA 24060-0435, USA*

In order to elucidate the role of surfaces at nonequilibrium phase transitions we consider kinetic Ising models with surfaces subjected to a periodic oscillating magnetic field. Whereas the corresponding bulk system undergoes a continuous nonequilibrium phase transition characterized by the exponents of the equilibrium Ising model, we find that the nonequilibrium surface exponents do not coincide with those of the equilibrium critical surface. In addition, in three space dimensions the surface phase diagram of the nonequilibrium system differs markedly from that of the equilibrium system.

The ubiquity of nonequilibrium steady states in nature constitutes a permanent reminder of the challenges encountered when trying to understand interacting many-body systems far from equilibrium. Whereas in some instances, as for example paradigmatic transport models [1] or driven diffusive systems [2], notable progress has been achieved in understanding nonequilibrium steady states, a common theoretical framework remains elusive. This is especially true in cases where steady states are influenced by the presence of surfaces or interfaces, which can change properties even deep inside the bulk [3–17].

Nonequilibrium phase transitions form an interesting class of phenomena that share many commonalities with their equilibrium counterparts. For example, for continuous transitions different universality classes, characterized by different sets of critical exponents, have been identified. Well-known examples can be found in driven diffusive systems [2], at absorbing phase transitions [18, 19] or in magnetic systems subjected to a periodically oscillating external field [20, 21]. For some absorbing phase transitions, as for example directed percolation, the surface critical properties have been studied to some extent, see [6] and references therein.

Kinetic ferromagnets in a periodically oscillating magnetic field display as a function of the field frequency a nonequilibrium phase transition between a dynamically disordered phase at low frequencies and a dynamically ordered phase at high frequencies. Let us assume that the magnetization is aligned with the direction of the external field. If the field now reverses direction, the system becomes metastable and tries to reverse its magnetization through the nucleation of droplets that are aligned with the field. If the period of the field is large compared to the metastable lifetime, then the metastable state completely decays before the field reverses direction again, i.e. the ferromagnet is able to 'follow' the field, yielding a time-dependent magnetization that oscillates symmetrically about zero. The dynamically ordered phase is obtained when the period of the field is small compared to the metastable lifetime, thus that the system is not able to fully decay from the metastable state before the field changes direction again. The magnetization then oscillates about a non-zero value. This behavior has been studied theoretically in a large range of systems, as for example the Ising [22–24], Heisenberg [25, 26], or Blume-Emery-Griffiths [27] models, too name but a few. Possible experimental realizations have been discussed in Co films on Cu(001) [28] as well as in [Co/Pt]$_3$ magnetic multilayers [29]. Of special interest in the following is the kinetic Ising model in an oscillating field that is displaying critical exponents at a dynamic phase transition which are identical to those found at the phase transition of the equilibrium Ising model [24]. This surprising observation is consistent with a symmetry argument given in [30] and has been substantiated through the study of the time-dependent Ginzburg-Landau model in an oscillating field [31].

In the past very few studies have looked at the impact surfaces can have on this dynamic phase transition, thereby focusing mostly on rather general aspects. For example, the effects of boundaries on magnetization switching in kinetic Ising models were studied in [32]. In [25, 33] the dynamic phase transition was investigated in Heisenberg films with competing surface fields.

In this Letter we present the first study of the surface critical properties at a dynamic phase transition. Using large-scale numerical simulations, we study kinetic Ising models with free surfaces subjected to a square-wave oscillating field. Both in two and three space dimensions we obtain values for the surface critical exponents that differ markedly from the values of the equilibrium surface exponents, thus demonstrating that the dynamic surface universality class differs from that of the equilibrium system, even though the same universality class prevails for the corresponding bulk systems. In addition, we find that the kinetic surface phase diagram in three dimensions is remarkably simple and does not exhibit a special transition point, nor a surface or extraordinary transition, which are all present in the equilibrium surface phase diagram.

In order to study the surface critical behavior at the dynamic phase transition we consider square and cubic lattices with open boundary conditions in one direction, called z-direction in the following, whereas in the direc-

tion(s) perpendicular to the z-direction we have periodic boundary conditions [34]. In this way we have in a system of linear extend L two surfaces, located at $z = 1$ and $z = L$. Every lattice site $\mathbf{x}$ is characterized by an Ising spin $S_{\mathbf{x}} = \pm 1$. The Hamiltonian is given by

$$H = -J_b \sum_{\langle \mathbf{x}, \mathbf{y} \rangle} S_{\mathbf{x}} S_{\mathbf{y}} - J_s \sum_{\{\mathbf{x}, \mathbf{y}\}} S_{\mathbf{x}} S_{\mathbf{y}} - H(t) \sum_{\mathbf{x}} S_{\mathbf{x}} , \quad (1)$$

where $J_b > 0$ and $J_s > 0$ are ferromagnetic bulk and surface coupling constants. The first sum is over nearest neighbor sites where at most one of the sites is in a surface layer. The second sum, on the other hand, is over neighboring sites that are both in a surface layer. We thereby allow for different values of the coupling constants at the surface and inside the bulk. Finally, the last term is the magnetic field term where $H(t)$ is a spatially uniform field that oscillates in time. We follow [24] and use a square-wave field with amplitude H_0. Both temperature and magnetic field strength are chosen in such a way that the system is in the multidroplet regime [24]: $T = 0.8 T_c^{2d}$, $H_0 = 0.3 J_b$ for $d = 2$ and $T = 0.8 T_c^{3d}$, $H_0 = 0.4 J_b$ for $d = 3$. Here $T_c^{2d} = 2.269 \cdots J_b / k_B$ and $T_c^{3d} = 4.5115 J_b / k_B$ are the critical temperatures of the two- and three-dimensional equilibrium systems.

As the surfaces break spatial translation invariance, all quantities of interest depend on the distance to the surface. We therefore define local, i.e. layer-dependent, quantities. Thus we consider the layer magnetization averaged over one period of the external field ($t_{1/2}$ is the half-period of the oscillating field):

$$Q(z) = \frac{1}{2t_{1/2}} \oint m(t, z) dt , \quad (2)$$

with the time-dependent magnetization $m(t, z) = \frac{1}{L^{d-1}} \sum_{\mathbf{x}} S_{\mathbf{x}}(t)$ of layer z, the sum being taken over all spins in that $(d-1)$-dimensional layer. The local order parameter is then given by $\langle |Q(z)| \rangle$ where $\langle \cdots \rangle$ indicates both a time average (i.e. an average over many periods) and a thermal average (realized in the numerical simulations through multiple independent runs with different random number sequences), yielding typically a total of 50,000 periods over which the average is taken. In a similar way we define the layer Binder cumulant

$$U(z) = 1 - \frac{\langle (Q(z))^4 \rangle}{3 \langle (Q(z))^2 \rangle^2} \quad (3)$$

and the layer susceptibility

$$\chi(z) = L^{d-1} \left(\langle Q(z)^2 \rangle - \langle |Q(z)| \rangle^2 \right) . \quad (4)$$

In the following the surface quantities will be characterized by an index s, whereas an index b will be given to the quantities from the middle of the sample.

An important quantity in the study of the dynamic phase transition is the ratio

$$\Theta = \frac{t_{1/2}}{\langle \tau \rangle_b} \quad (5)$$

that quantifies the competition between the metastable state, characterized by the metastable lifetime $\langle \tau \rangle_b$, and the oscillating magnetic field. For small values of Θ we are in the dynamically ordered phase, whereas for large values the system is dynamically disordered. The quantity Θ therefore plays the same role as that played by temperature at an ordinary equilibrium phase transition. The metastable lifetime in our systems is again layer dependent, the value of $\langle \tau(z) \rangle$ being smaller in the surface layer than deep inside the bulk, as surface spins are coupled to fewer spins. As we are interested in the surface properties at the bulk phase transition, we define Θ with respect to the bulk quantity $\langle \tau \rangle_b$. The dynamic phase transition then takes place at the critical value $\Theta_c = 0.918$ in $d = 2$ [24] and $\Theta_c = 1.285$ in $d = 3$.

As shown in Figure 1 for the two-dimensional system with $J_s = J_b$, both the bulk and the surface order parameters decrease rapidly when approaching the critical point Θ_c from below. Concomitantly, the bulk and surface susceptibilities display peaks in the vicinity of Θ_c. Changing the system size yields system size dependencies (shifts of the positions of the maxima of the susceptibilities, increasing peak heights, $\cdots$) typical for a continuous phase transition.

In the infinite system, the order parameter and the susceptibility show an algebraic behavior close to the critical point:

$$\langle |Q_b| \rangle \sim (\Theta_c - \Theta)^{\beta} \quad , \quad \chi_b \sim |\Theta_c - \Theta|^{-\gamma} . \quad (6)$$

Using finite-size scaling [35], the authors of [24] found in two dimensions the same values for the exponents as those obtained for the equilibrium Ising model, namely $\beta/\nu = 1/8$ and $\gamma/\nu = 7/4$, where ν is the critical exponent that governs the divergence of the correlation length.

Similarly, surface critical exponents are introduced to describe the behavior of surface quantities close to the bulk critical point (we use here the standard nomenclature of surface critical phenomena, see [34, 36, 37]):

$$\langle |Q_s| \rangle \sim (\Theta_c - \Theta)^{\beta_1} \quad , \quad \chi_s \sim |\Theta_c - \Theta|^{-\gamma_{11}} . \quad (7)$$

Close to a bulk critical point, finite-size scaling theory [34, 36, 37] provides us with scaling relations for our surface quantities:

$$\langle |Q_s| \rangle = L^{-\beta_1/\nu} F_{\pm}(\theta L^{1/\nu}) \quad (8)$$
$$\chi_s^Q = L^{\gamma_{11}/\nu} G_{\pm}(\theta L^{1/\nu}) \quad (9)$$

where $\theta = \frac{|\Theta - \Theta_c|}{\Theta_c}$, whereas $F_{\pm}$ and $G_{\pm}$ are scaling functions, where the $+$ $(-)$ sign corresponds to $\Theta > (<) \Theta_c$.
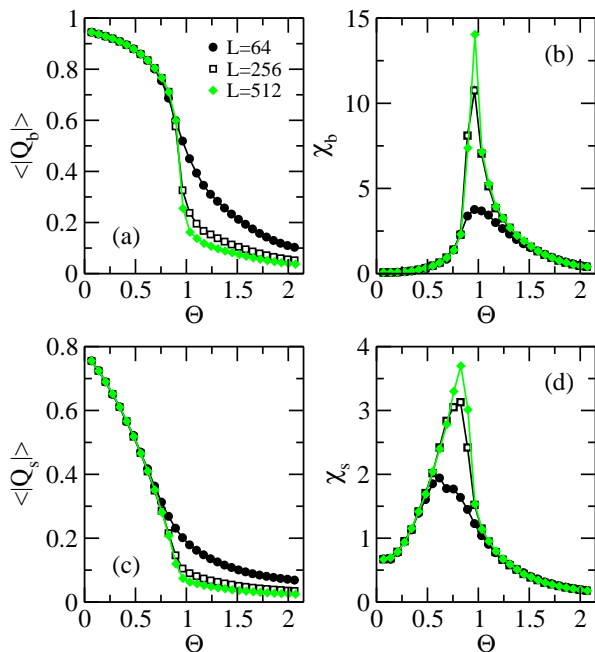
FIG. 1: (Color online) Bulk (a,b) and surface (c,d) quantities for the two-dimensional model, composed of $L \times L$ spins, with $J_s = J_b$. Close to the bulk critical point $\Theta_c = 0.918$, the local order parameters decrease rapidly and the local susceptibilities display pronounced maxima. Here and in the following error bars are smaller than the sizes of the symbols.

Choosing $\Theta = \Theta_c$, we therefore expect that our quantities depend algebraically on the linear system size. This is shown in Figure 2 for various values of the surface coupling J_s. For not too large values of J_s corrections to scaling are negligible, so that we can determine the values of the critical exponents from the slopes. We find $\beta_1/\nu = 0.43(1)$ and $\gamma_{11}/\nu = 0.18(1)$. We immediately remark that these values rather well fulfill the scaling relation $2\beta_1 + \gamma_{11} = d - 1$ that is expected to hold for surface critical exponents. We also note that our values differ strongly from the values of the surface exponents in the equilibrium critical Ising model: $\beta_1^e/\nu = 0.5$ and $\gamma_{11}^e/\nu = 0$ [34, 36, 37]. We therefore have the interesting situation that while the dynamic phase transition in the bulk belongs to the universality of the equilibrium Ising model, this is not true for the corresponding surface universality class.

For the three-dimensional system, the bulk system undergoes again a dynamic phase transition characterized by the critical exponents of the three-dimensional equilibrium critical Ising model, as we verified. For the surface, however, the situation is more complicated. For not too small values of the surface coupling, the situation is similar to the two-dimensional case, see the example $J_s = 2J_b$ shown in the first row in Fig. 3: When reducing Θ the surface undergoes at the bulk transition value Θ_c a transition to a dynamically ordered phase. This transition is
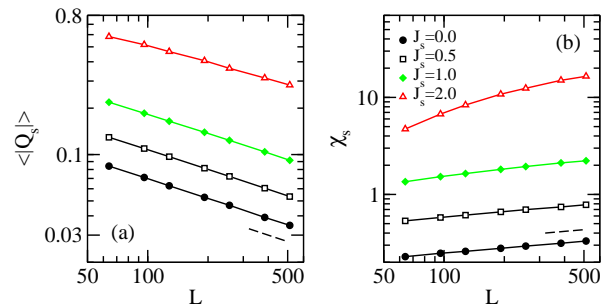

FIG. 2: (Color online) Log-log plot of (a) the surface order parameter and (b) the surface susceptibility as a function of the linear system size for the two-dimensional kinetic Ising model at $\Theta = \Theta_c$. The different curves correspond to different values of the surface coupling constant J_s (given in units of J_b). The dashed lines have slopes -0.43 (a) and 0.18 (b). For large values of J_s corrections to scaling become sizeable.

revealed by a characteristic peak in the surface susceptibility as well as by a crossing at Θ_c of the surface Binder cumulant computed for different system sizes. However, for values of $J_s < 1.5J_b$, see Fig. 3c, the surface spins do *not* order dynamically at Θ_c, but instead are still able of following the external field, even though this is no longer the case for the bulk spins. At lower values of Θ the surface order parameter of our finite systems deviates from zero, but this partial dynamical ordering is not related to a phase transition. This is also revealed by the presence of a non-critical peak (or, for very small values of J_s, by the complete absence of any peak) in the surface susceptibility (see Fig. 3d) as well as by the absence of the crossing of the surface Binder cumulants for different system sizes, as shown in the inset of Fig. 3b.

Based on our data, where we studied surface couplings from $J_s = 0$ to $J_s = 16J_b$, the surface phase diagram of the three-dimensional kinetic Ising model shown in Fig. 4b differs remarkably from the corresponding diagram of the equilibrium model [34, 36, 37], see Fig. 4a. Not only does the surface not order dynamically at the bulk critical point for $J_s < 1.5J_b$, as just discussed, the kinetic Ising model also does not exhibit a surface transition, where the surface orders alone, whereas the bulk remains disorder. Concomitantly, the special transition point, where both surface and bulk are critical, and the extraordinary transition, where the bulk orders in presence of an ordered surface, are also absent. In fact, whereas for the equilibrium system is it possible to shift the phase transition temperature of the two-dimensional surface $k_B T_c^{2d} = 2.269 \cdots J_s$ above the bulk transition temperature $k_B T_c^{3d} = 4.5115 J_b$ by sufficiently increasing the ratio J_s/J_b of the couplings, a similar mechanism does not exist in the kinetic Ising model.

Finally, for $J_s > 1.5J_b$ we can again measure the surface critical exponents through a finite-size scaling analysis. As shown in Fig. 5 corrections to scaling
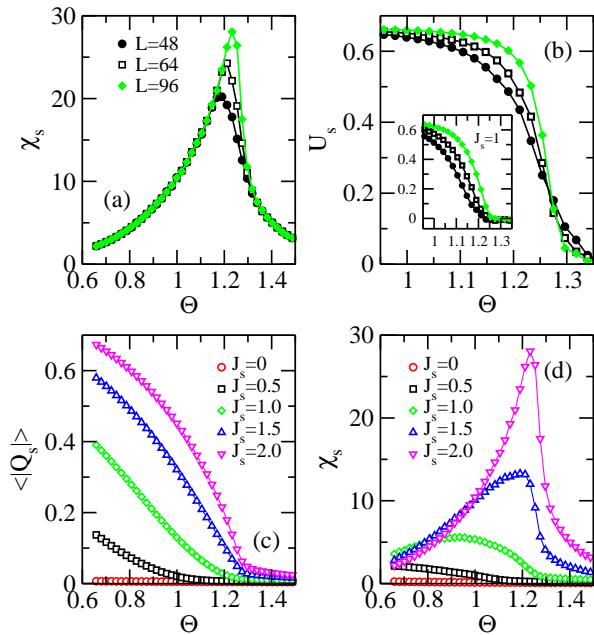
FIG. 3: (Color online) Surface susceptibility (a) and surface Binder cumulant (b) for the three-dimensional kinetic Ising model with $J_s = 2J_b$. For small values of J_s, the surface does not order dynamically at the bulk critical point, as shown by (c) the surface order parameter and (d) the surface susceptibility. All surface coupling constants are expressed in units of J_b. The inset in (b) shows that for $J_s = J_b$ the surface Binder cumulants do not cross at a common value of Θ.
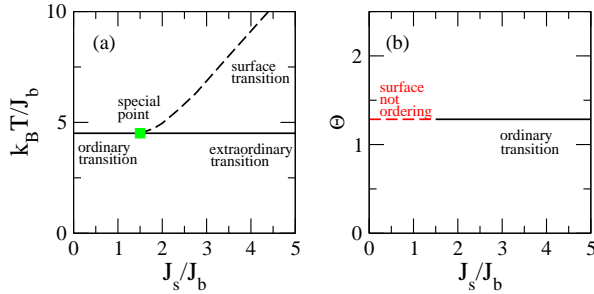

FIG. 4: (Color online) Surface phase diagram of (a) the equilibrium three-dimensional Ising model and (b) the nonequilibrium three-dimensional kinetic Ising model.

are much more important in three than in two dimensions. Based on our data, we obtain $\beta_1/\nu = 0.88(3)$ and $\gamma_{11}/\nu = 0.29(3)$. These values again differ markedly from the known values $\beta_1^e/\nu = 1.27$ and $\gamma_{11}^e = -0.40$ of the corresponding surface critical exponents [38]. Most notably, whereas in the equilibrium system the surface susceptibility displays a cusp singularity characterized by a negative critical exponent, in our system the surface susceptibility diverges with a positive critical exponent.

As we mentioned in the introductory remarks, a symmetry argument put forward in [30] states that continuous transitions with up-down symmetry and noncon-
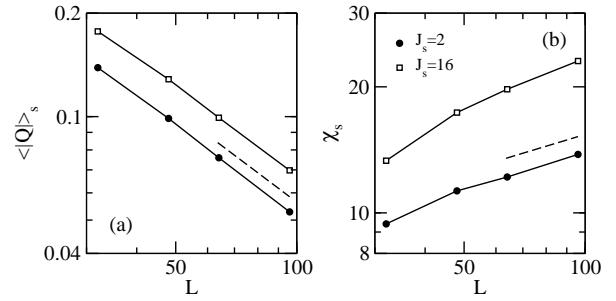

FIG. 5: (a) Surface order parameter and (b) surface susceptibility as a function of system size at the bulk critical point of the three-dimensional kinetic Ising model. The dashed lines have slopes -0.88 (a) and 0.29 (b).

served order parameter should fall into the university class of the ordinary Ising model. This indeed agrees with our own results (as well as with previous results [24, 31]) that the bulk critical exponents at the dynamic phase transition are the same as that of the equilibrium Ising model, and this both in two and three dimensions. However, once surfaces are introduced, the lattice symmetry is broken close to the surfaces, and one of the assumptions underlying the argument of [30] is no longer fulfilled. Indeed, our results show that the dynamic surface exponents differ from the surface exponents of the equilibrium model, yielding new nonequilibrium surface universality classes. Using field-theoretical methods similar to those developed for equilibrium critical surfaces [37, 38], it should be possible to compute these new exponents and to classify the possible dynamic surface universality classes.

It follows from our work that our understanding of the role played by surfaces in nonequilibrium systems, and more specifically at nonequilibrium phase transitions, is far from being complete. Surfaces break lattice symmetries, and this can have many surprising and unexpected effects out of equilibrium, as exemplified in our study of surface critical behavior at a dynamic phase transition. Based on our results we expect that future in-depth studies of the role of surfaces far from equilibrium will reveal additional new and unexpected phenomena.

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