

Off-equilibrium scaling behaviors across first-order transitionsHaralambos Panagopoulos¹ and Ettore Vicari²¹*Department of Physics, University of Cyprus, Lefkosia, CY-1678, Cyprus*²*Dipartimento di Fisica dell'Università di Pisa and INFN, Largo Pontecorvo 3, I-56127 Pisa, Italy*

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We study off-equilibrium behaviors at first-order transitions (FOTs) driven by a time dependence of the temperature across the transition point T_c , such as the linear behavior $T(t)/T_c = 1 \pm t/t_s$ where t_s is a time scale. In particular, we investigate the possibility of nontrivial off-equilibrium scaling behaviors in the regime of slow changes, corresponding to large t_s . We consider the two-dimensional Potts models, which provide an ideal theoretical laboratory to investigate issues related to FOTs driven by thermal fluctuations. We put forward general ansatzes for off-equilibrium scaling behaviors around the time $t = 0$ corresponding to T_c . Then we present numerical results for the $q = 10$ and 20 Potts models. We show that off-equilibrium scaling behaviors emerge at FOTs with relaxational dynamics, when appropriate boundary conditions are considered, such as mixed boundary conditions favoring different phases at the opposite sides of the system, which enforce an interface in the system.

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I. INTRODUCTION

Slow time variations of system parameters across continuous transitions inevitably lead to off-equilibrium behaviors, giving rise to the so-called Kibble-Zurek (KZ) mechanism [1,2]. A typical example is provided by a linear change of the temperature across its transition value T_c , such as $T(t)/T_c = 1 - t/t_s$ starting from $t = t_i < 0$ to $t = t_f > 0$, where t_s controls the speed of the temperature variation. The emergence of off-equilibrium phenomena is essentially related to the fact that continuous transitions develop correlations with diverging length scale, which cannot adapt themselves to the variations of the temperature, even in the regime of slow variations. However, in the limit of large t_s , the system develops an off-equilibrium scaling behavior involving t_s , which is controlled by the same critical exponents of the system at equilibrium [2–4]. This issue has been also extended to quantum transitions, obtaining analogous behaviors when quasiadiabatic changes of an external parameter go through continuous quantum transitions [5–7]. Several experiments have investigated these off-equilibrium phenomena, in particular checking the predictions for the abundance of residual defects arising from the off-equilibrium conditions across T_c , as predicted by the KZ mechanism; see, e.g., Refs. [8–30].

In this paper we investigate whether off-equilibrium scaling phenomena arise in systems undergoing first-order transitions (FOTs), characterized by a discontinuity of the energy density in the thermodynamic limit. Unlike continuous transitions, the length scale of the correlations in the thermodynamic limit (within each phase) remains finite when approaching T_c . Nevertheless, we show that off-equilibrium scaling behaviors may also arise at FOTs when slowly varying the temperature across T_c , in systems with appropriate boundary conditions favoring the presence of an interface.

Two-dimensional (2D) q -state Potts models provide an ideal theoretical laboratory to investigate issues related to FOTs driven by the temperature (when $q > 4$). We consider the off-equilibrium behavior arising from a relaxational dynamics with a time-dependent temperature T crossing T_c , such as $T(t)/T_c \approx 1 \pm t/t_s$. We show that, when slowly crossing the FOT, i.e., for large time scales t_s , the off-equilibrium behavior

turns out to be dependent on the geometry and boundary conditions. This is essentially related to the dependence of the equilibrium relaxational dynamics at FOTs on the boundary conditions. For symmetric boundary conditions, such as periodic boundary conditions (PBCs), systems of size L are characterized by an exponentially slow dynamics due to an exponentially large tunneling time $\tau \sim e^{\sigma L}$ between the coexisting phases. On the other hand, power-law behaviors characterize the slow dynamics when mixed boundary conditions (MBCs) are considered, i.e., when the boundary conditions at two opposite sides of the system are related to the different high- T and low- T phases, effectively generating an interface. We argue that the MBC settings lead to a power-law off-equilibrium scaling behavior involving the time scale t_s of the slow temperature variation across the FOT point. This is confirmed by a numerical analysis of Monte Carlo (MC) simulations.

We mention that off-equilibrium behaviors arising from sudden quenches below and at the FOT point have been discussed in several works; see, e.g., Refs. [31–37].

The paper is organized as follows. In Sec. II we present the 2D Potts model in which we develop and check the off-equilibrium scaling theory at FOTs. There we also define the protocol we consider for the time variation of the temperature across T_c , which leads to the off-equilibrium behavior. In Sec. III we develop an off-equilibrium scaling theory at FOTs, stressing the crucial dependence on the geometry and boundary conditions of the system undergoing the FOT. We essentially report results for the 2D Potts model, but the main features can be straightforwardly generalized to other systems. In Sec. IV we report a numerical analysis which provides support to the off-equilibrium scaling behavior put forward in Sec. III. Finally, we draw our conclusions in Sec. V. The appendices contain some details of our numerical study.

II. THE MODEL AND THE OFF-EQUILIBRIUM PROTOCOL**A. The 2D Potts model**

2D q -state Potts models provide a useful theoretical laboratory where to study issues related to FOTs driven by

thermal fluctuations. They are defined by the partition function

$$Z = \sum_{\{s_x\}} e^{-H/T}, \quad H = - \sum_{\langle xy \rangle} \delta(s_x, s_y), \quad (1)$$

where the sum in the Hamiltonian is meant over the nearest-neighbor sites of a square lattice, and s_x are integer variables $1 \leq s_x \leq q$, $\delta(a, b) = 1$ if $a = b$ and zero otherwise. The Potts model undergoes a phase transition [38,39] at

$$\beta_c = T_c^{-1} = \ln(1 + \sqrt{q}), \quad (2)$$

which is continuous for $q \leq 4$ and first order for $q > 4$. For $q = 2$ the Potts model becomes equivalent to the Ising model. FOTs for $q > 4$ become stronger and stronger with increasing q ; indeed, the latent heat grows with increasing q .

We consider 2D Potts models with two different geometries: square $L \times L$ lattices and anisotropic $L_\perp \times L_\parallel$ slablike lattices with $L_\parallel \gg L_\perp$. We also consider different boundary conditions: periodic boundary conditions (PBCs) and mixed boundary conditions (MBCs) where opposite boundary sides are related to the different high- T and low- T phases.

More precisely, in the MBC case we consider anisotropic $L_\perp \times L_\parallel$ lattices with $L_\perp = 2L + 1$, so that $-L \leq x_1 \leq L$ and $1 \leq x_2 \leq L_\parallel$. We take open boundary conditions along the $x_1 = L$ line, which corresponds to having $T = \infty$ bonds between the line s_{L, x_2} and a further fictitious line s_{L+1, x_2} . At the opposite side, in order to have boundary conditions corresponding to the ordered $T = 0$ phase, we add a fictitious $x_1 = -L - 1$ line where we fix $s_{-L-1, x_2} = 1$, and add the corresponding bond terms to the Hamiltonian. The boundary conditions are chosen periodic along the x_2 direction of size L_\parallel . Note that MBC breaks explicitly the q -state permutation symmetry of the Potts model.

In our study we consider observables related to the magnetization and energy density, i.e.,

$$m = \frac{1}{V} \sum_x \frac{q\delta(s_x, 1) - 1}{q - 1}, \quad (3)$$

$$e = \frac{1}{V} \sum_x \delta(s_{x_1, x_2}, s_{x_1, x_2+1}), \quad (4)$$

where V is the number of sites of the lattice. Their equilibrium values at the FOT point are known for any $q > 4$ [39]. In particular, approaching the transition point after the thermodynamic $L \rightarrow \infty$ limit, we have

$$e_c^- \equiv e(T_c^-) = 0.910342\dots, \quad e_c^+ \equiv e(T_c^+) = 0.313265\dots, \\ m_c \equiv m(T_c^-) = 0.9411759\dots, \quad \text{for } q = 20, \quad (5)$$

and

$$e_c^- = 0.832126\dots, \quad e_c^+ = 0.428553\dots, \\ m_c = 0.857106\dots, \quad \text{for } q = 10. \quad (6)$$

We also define the related renormalized quantities

$$m_r(t) \equiv \frac{m(t)}{m_c}, \quad e_r(t) \equiv \frac{e(t) - e_c^+}{e_c^- - e_c^+}, \quad (7)$$

so that, at equilibrium and in the thermodynamic limit, $m_r = e_r = 0$ for $T \rightarrow T_c^+$ and $m_r = e_r = 1$ for $T \rightarrow T_c^-$.

The correlation length related to the exponential decay of the two-point function in the limit $T \rightarrow T_c^+$ (after the

thermodynamic limit) is exactly known [40,41]. It decreases with increasing q , e.g., $\xi^+ = 2.6955\dots$ for $q = 20$ and $\xi^+ = 10.5595\dots$ for $q = 10$. Numerical results [42,43] support the hypothesis that the correlation length ξ^- for $T \rightarrow T_c^-$ equals ξ^+ .

B. Off-equilibrium protocol across the transition

The protocol that we consider for the off-equilibrium simulations across T_c is similar to that leading to the KZ mechanism [2,4] at continuous transitions. We vary the temperature across the transition point and study the resulting off-equilibrium behavior in the limit of slow time variations. More precisely, we vary the inverse temperature $\beta = 1/T$ so that

$$\delta(t) \equiv \beta(t)/\beta_c - 1 = \pm t/t_s, \quad (8)$$

where $t \in [t_i < 0, t_f > 0]$ is a time variable varying from a negative to a positive final value. The value $t = 0$ corresponds to $\delta(t) = 0$, i.e., $T(t) = T_c$. The parameter t_s provides the time scale of the temperature variation. We start our simulations from equilibrium configurations at $\beta = \beta_c[1 + \delta(t_i)]$. Then we make the system evolve under a purely relaxational dynamics (also known as model A in the context of critical dynamics [44]), which can be realized by standard Metropolis or heat bath updatings in MC simulations; see Appendix A. The \pm sign in Eq. (8) corresponds to crossing T_c starting from the high- T phase (sign $+$) or from the low- T phase (sign $-$). The unit time for t corresponds to a complete sweep of the whole lattice by heat bath or Metropolis updatings. The temperature is changed according to Eq. (8) every sweep, incrementing t by one. We stop the off-equilibrium relaxational dynamics when $t = t_f$. We repeat this procedure several times averaging the observables at fixed time t , thus the average is performed on the equilibrium Gibbs ensemble of the initial inverse temperature $\beta = \beta_c[1 + \delta(t_i)]$.

III. OFF-EQUILIBRIUM SCALING THEORY AT FIRST-ORDER TRANSITIONS

Analogously to the case of off-equilibrium slow dynamics at continuous transitions [2,4], we construct an off-equilibrium scaling theory in terms of the effective length-scale exponent ν describing the finite-size scaling (FSS) at equilibrium, and the dynamic exponent z associated with the equilibrium relaxational dynamics corresponding to the heat-bath or Metropolis updating algorithm. In the following we mainly focus on the FOTs of 2D Potts models, but most scaling arguments can be straightforwardly extended to other FOTs.

A. Equilibrium exponents

Before discussing the off-equilibrium behavior when varying the temperature across the FOT, we consider the equilibrium behavior of finite systems at FOTs and determine the equilibrium exponents describing the asymptotic behaviors in the large-size limit. These exponents will then enter the scaling ansatzes for the off-equilibrium behavior induced by slow changes of the temperature, as discussed in Sec. III B.

1. The length-scale exponent ν

In the case of FOTs the effective length-scale exponent ν controlling the FSS at T_c generally depends on the geometry of the lattice [45–48], i.e., whether it is square L^2 or slablike $L_\perp \times L_\parallel$ with $L_\parallel \gg L_\perp$, and on the boundary conditions [47–49].

In the case of square L^2 systems, the FSS around T_c is generally described by the effective length-scale exponent $\nu = 1/d = 1/2$ [45,50–54]. This length-scale exponent may be associated with a discontinuity fixed point in the renormalization-group framework [50]. It represents the limiting case of continuous transitions, leading to the energy discontinuity at T_c in the thermodynamic limit [51].

In the case of slablike geometries, the length-scale exponent controlling the FSS at T_c with respect to the finite size L_\perp may significantly change [45,47,48]. This is essentially due to the anisotropic behavior of the longitudinal length scale ξ_\parallel , which may show a nontrivial power-law (or exponential) dependence on L_\perp , such as $\xi_\parallel \sim L_\perp^\epsilon$. This may give rise to a change of the effective dimensions of the FSS in a slab at the FOT. Indeed, assuming that the free-energy density scales as the inverse of the relevant critical volume $V_c \sim L_\perp \times \xi_\parallel \sim L_\perp^{1+\epsilon}$, we obtain the effective dimension $d_{\text{eff}} = 1 + \epsilon$. Thus, in this anisotropic setting, the effective length-scale exponent controlling the FSS with respect to L_\perp turns out to be

$$\nu = \frac{1}{d_{\text{eff}}} = \frac{1}{1 + \epsilon}. \quad (9)$$

This value allows for the discontinuity of the energy density at T_c after taking the $L_\perp \rightarrow \infty$ limit. Equation (9) can be also obtained from the FSS of the corresponding one-dimensional quantum model at the first-order quantum transition [47,48], exploiting the quantum-to-classical mapping [55] which relates the gap Δ (energy difference of the lowest levels) of the quantum model to the inverse longitudinal correlation length ξ_\parallel of the 2D classical model in a slab geometry.

In a slab geometry with symmetric boundary conditions, such as PBC, the relevant configurations involve domain walls which divide the system into successive regions of high- T and low- T phases, whose length scale ξ_\parallel is expected to diverge exponentially with the transverse size L_\perp . This length scale is related to the interfacial tension σ , i.e., $\xi_\parallel \sim e^{\sigma L_\perp}$. An analogous scenario applies to 2D Ising models in a slab geometry, at their FOTs driven by the magnetic field in their low- T phase [45]. As a consequence, Eq. (9) leads to the extreme value $\nu \rightarrow 0$.

The situation changes in the case of MBC, for which ξ_\parallel increases as a power law of L_\perp . In particular, in the case of the FOTs of 2D Potts models we have $\xi_\parallel \sim L_\perp$, i.e., $\epsilon = 1$. This can be inferred from the behavior of the gap, $\Delta \sim 1/L$, of the one-dimensional quantum Potts model at the transition point, of size L with the corresponding MBC [48].

Note that $\epsilon = 1$ is not a general feature of MBC. For example, at the low- T coexistence line of 2D Ising models, where FOTs are driven by an external magnetic field coupled to the order parameter, we have $\xi_\parallel \sim L_\perp^2$ (thus $\epsilon = 2$) in the case of MBC favoring the two different magnetized phases (i.e., fixed and opposite boundary conditions for the order-parameter field) [47].

In conclusion, 2D Potts models in square geometries and slab geometries with MBC share the same length-scale exponent

$$\nu = 1/2. \quad (10)$$

2. The equilibrium dynamic exponent z of the purely relaxational dynamics

The equilibrium dynamic exponent z of the relaxational dynamics is related to the equilibrium large- L behavior of the autocorrelation time τ of observables at T_c , i.e., $\tau \sim L^z$. Again we expect that it depends on the boundary conditions at FOTs.

In the case of symmetric boundary conditions, such as PBC, the autocorrelation time at T_c is expected to exponentially increase with increasing lattice size, corresponding to $z \rightarrow \infty$. This is related to the exponential increase of the tunneling time between the coexisting phases at FOTs; indeed [56], $\tau \sim e^{\sigma L}$ (neglecting powers of L in the prefactor) where σ is the interfacial free energy per unit length. To overcome this exponential slow down at FOTs, multicanonical updating algorithms have been developed [56].

The behavior of the autocorrelation time drastically changes in the case of MBC. In this case the dynamics at T_c is essentially related to the interface enforced by MBC, which moves within the slab. Indeed, this gives rise to a power-law behavior: $\tau \sim L^z$.

We numerically estimate z by equilibrium MC simulations of the $q = 20$ Potts model at T_c for slablike geometries (in particular for anisotropic $L_\perp \times L_\parallel$ with $L_\perp = 2L + 1$ and $L_\parallel \gg L$), with MBC. Some details on the calculation of the autocorrelation time of the magnetization and energy are reported in Appendix B.

In Fig. 1 we show data for the integrated autocorrelation time τ of the magnetization (3), from $L = 12$ to 32 and $L_\parallel = 8L$ (as already discussed above, $L_\parallel \sim L$ is the correct scaling

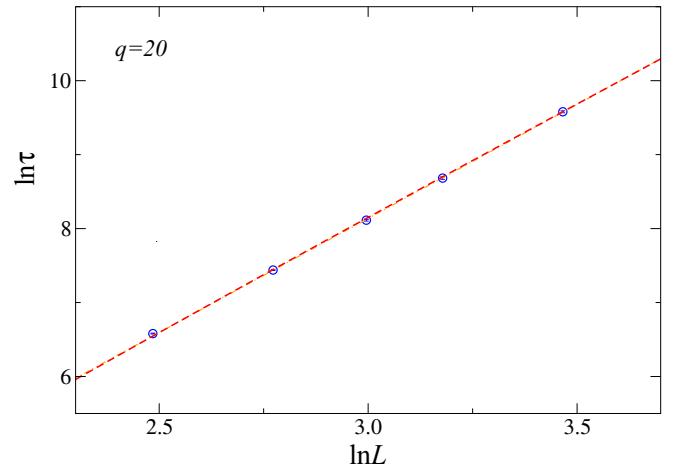


FIG. 1. (Color online) Log-log plot of the integrated autocorrelation time τ of the magnetization at T_c vs L , computed by equilibrium heat-bath MC simulations. The dotted and dashed lines show fits of the data for the lattice sizes $L \geq 16$, to the ansatzes $\tau = aL^3 + bL^2$, corresponding to $z = 3$ with the expected $O(1/L)$ corrections, and to $\tau = aL^z$. These fits are practically equivalent; indeed, the corresponding lines are hardly distinguishable (both of them give an acceptable $\chi^2/\text{d.o.f.} \approx 1$).

of the longitudinal size since $\xi_{\parallel} \sim L$). These results strongly support a power-law behavior, i.e., $\tau \sim L^z$. In order to estimate z , we fit the data to the ansatzes $\tau = aL^z$ [fitting the data for $L \geq 16$, it gives $z = 3.08(2)$ and $a = 0.33(2)$] and $\tau = aL^3 + bL^2$ corresponding to $z = 3$ with the expected $O(1/L)$ corrections [it gives $a \approx 0.46(1)$ and $b = -0.7(2)$]. These fits work equally well as shown in Fig. 1. We consider

$$z = 3.0(1) \tag{11}$$

as our final estimate (the central estimate $z = 3$ is also supported by the off-equilibrium simulations; see below). The integrated autocorrelation time of the energy density gives substantially equivalent results. The value of the dynamic exponent is expected to be independent of the aspect ratio of the lattice, i.e., of the ratio L_{\parallel}/L_{\perp} , including the limit $L_{\parallel}/L_{\perp} \rightarrow \infty$ (this is a standard FSS hypothesis).

Although this estimate of z is obtained for heat-bath MC simulations at $q = 20$, we expect that it holds for any $q > 4$. Indeed, the value of z should be intrinsically related to the interface dynamics, which is expected to be shared by all $q > 4$ at their FOTs. Moreover, it should extend to the whole class of purely relaxational dynamics, including also the Metropolis upgrading. Different classes of dynamics may lead to other values of the dynamic exponent z .

As already mentioned we argue (see also later) that the dynamic exponent z in the case of MBC is essentially related to the interface enforced by MBC, which fluctuates within the slab. This simple scenario may lead to the conjecture that z is a simple integer number, thus $z = 3$ exactly. However, we do not have a proof.

B. Off-equilibrium scaling ansatzes

A scaling theory for the off-equilibrium dynamics across T_c can be heuristically derived by scaling arguments, similar to those commonly used at continuous transitions.

Assuming the existence of a nontrivial scaling behavior around $t = 0$ corresponding to T_c , we may expect that it is controlled by two scaling variables, such as

$$r_1 = (t/t_s)^{-\nu}/L, \quad r_2 = t/L^z. \tag{12}$$

r_1 may be interpreted as the ratio between the equilibrium finite-size correlation length at the given $\beta(t)$ and L , while r_2 is the standard scaling variable of the equilibrium dynamics with the appropriate value of z . Equivalently we may consider the scaling variables

$$u \equiv t_s^{\kappa}/L, \quad \kappa = \nu/(1 + z\nu), \tag{13}$$

$$w \equiv t/t_s^{\kappa_t}, \quad \kappa_t = z\kappa, \tag{14}$$

which are combinations of r_1 and r_2 . The off-equilibrium scaling behavior arising from the protocol (8) is meant to describe the deviations of the statistical correlations from the equilibrium scaling behavior, when they cannot adapt themselves to the changes of the temperature across T_c . It is defined in the limit of large t_s and L keeping the scaling variables u and w fixed. An important feature of the off-equilibrium ansatz is that the expected equilibrium static finite-size scaling should be recovered in the appropriate limit, which is obtained when $u \rightarrow \infty$ keeping r_1 fixed.

We already note that the case of symmetric boundary conditions, such as PBC, appears problematic, due to the divergence of the dynamic exponent z . In particular, taking the $z \rightarrow \infty$ limit of the exponents κ and κ_t in the case of a square geometry, one would naively obtain $\kappa = 0$ and $\kappa_t = 1$. This may hint at the absence of a nontrivial scaling behavior around T_c ; i.e., we may not observe a nontrivial off-equilibrium scaling behavior around $t = 0$ in the off-equilibrium protocol (8). Alternatively, this may indicate a logarithmic scaling behavior, for example, with scaling variables $u \approx \ln(t_s)/L$ and $w \approx t/t_s$. As we shall see, numerical simulations favor a regular behavior around $t = 0$ extending to $t/t_s > 0$, which may be somehow related to a metastability phenomenon.

Systems with MBC appear more promising to realize an off-equilibrium scaling behavior. Indeed, the corresponding values of the equilibrium exponents ν and z provide well-defined exponents κ and κ_t in Eqs. (13) and (14). In the case of the FOT of the 2D Potts model, for which $\nu = 1/2$ and $z = 3.0(1)$, we obtain $\kappa = 0.200(4)$ and $\kappa_t = 0.600(8)$, which lead to a nontrivial power-law dependence of the scaling variables. Therefore, observing an off-equilibrium scaling behavior around $t = 0$ is to be expected in this case.

Our main working hypothesis is that the slow dynamics across T_c presents a double scaling behavior in the large- L limit, in terms of the scaling variables u and w , i.e.,

$$m_r(t, t_s, L) \approx f_m(u, w), \tag{15}$$

$$e_r(t, t_s, L) \approx f_e(u, w). \tag{16}$$

We also expect that, if we start from the high- T phase [sign + in Eq. (8)], the following asymptotic limits apply:

$$\lim_{w \rightarrow -\infty} f_{\#}(u, w) = 0, \quad \lim_{w \rightarrow \infty} f_{\#}(u, w) = 1, \tag{17}$$

corresponding to the large- L equilibrium values at the two phases (the subscript # corresponds to both m and e). The limits are reversed if we start from the low- T phase [minus sign in Eq. (8)].

Summarizing, in the cases where an off-equilibrium scaling behavior is driven by slow variations across T_c , around $t = 0$ corresponding to $T(t) = T_c$, Eqs. (15) and (16) with the scaling variables (13) and (14) are expected to provide the asymptotic scaling behaviors, when L is much larger than any other length scale, thus when $L \gg \xi^{\pm}$ (see the end of Sec. II A). These asymptotic behaviors should be approached with power-law $O(L^{-\omega})$ suppressed corrections, presumably $\omega = 1$. Note that for observables depending on the spatial coordinates one may add the spatial scaling dependence on x/L .

In the case of MBC the off-equilibrium behavior is expected to be related to the dynamics of the interface enforced by the MBC. This scenario implies a close relation between the scaling functions f_m and f_e of the magnetization and energy density. Let us assume that the slowest modes, determining the off-equilibrium dynamics of the magnetization and energy density, are associated with the interface separating the spatial regions corresponding to the two different phases. If we define $x(t)$ as the location of the interface along the x_1 axis, separating the low- T from the high- T region, we expect that $m_r = e_r = 1$ for $x_1 < x(t)$ and $m_r = e_r = 0$ for $x_1 > x(t)$. Figure 2 shows a sketch of the space dependence of the time-dependent local

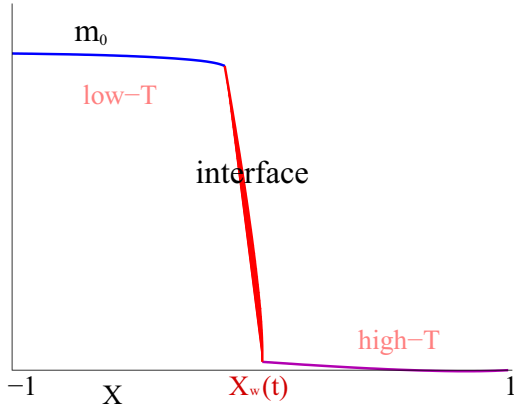


FIG. 2. (Color online) Sketch of the space dependence of the local magnetization at fixed time during the slow dynamics induced by the temperature variation in the case of MBC. The system shows both phases extending from the corresponding low- T and high- T boundaries, which are separated by an interface. The dynamics during the slow variation of the temperature across the FOT is essentially related to the movement of the interface from the low- T boundary to the high- T one, or vice versa.

magnetization within the slab at a fixed time t , as a function of $X = x_1/L$ (note that assuming translation invariance along x_2 , for example choosing periodic boundary conditions along x_2 and then sending $L_{\parallel} \rightarrow \infty$, the local magnetization must be independent of x_2). Thus, when the width of the domain wall becomes negligible, thus asymptotically for large L , we expect that

$$m_r(t) \approx e_r(t) \approx \frac{1}{2}[1 + X_w(t)], \quad (18)$$

where $X_w(t) = x(t)/L$ with $-1 \leq X_w(t) \leq 1$. As a trivial consequence, we would have

$$f_e(u, w) = f_m(u, w). \quad (19)$$

Therefore, $\mathcal{X}_w(u, w) \equiv 2f_m(u, w) - 1$ may be considered as an estimator of the average position of the interface in the large- L limit.

The off-equilibrium scaling behaviors (13)–(16) at FOTs are analogous to those expected at continuous transitions when slowly crossing the critical temperature, usually related to the KZ mechanism [2,4]. The main difference is related to the fact that at continuous transitions the critical exponents, such as ν and z , do not depend on the boundary conditions (only the scaling functions do). For example, in the case of the 2D Ising model corresponding to the $q = 2$ Potts model, the off-equilibrium dynamics of the magnetization (3) across the continuous transition is expected to be

$$m(t, t_s, L) = L^{-\eta/2} f_m(u, w), \quad (20)$$

where $\eta = 1/4$ and the scaling variables have the same form as those in Eqs. (13) and (14). The exponents κ and κ_t are obtained using the Ising exponents $\nu = 1$ and $z \approx 2.167$ associated with the purely relaxational dynamics (model A of the critical dynamics; see, e.g., Refs. [57–59] and references therein), i.e., $\kappa \approx 0.316$ and $\kappa_t \approx 0.684$. At the Ising critical point, different geometries and boundary conditions can change only the scaling function f_m .

We finally mention that similar scaling arguments have been also employed to study the effects of smooth spatial inhomogeneities at FOTs [60–62], for example, when we assume a spatially dependent temperature and look at the behavior of the system around the spatial region where the temperature takes the value at the transition point of the homogenous system. However, the off-equilibrium behaviors we study in this paper have not been investigated.

IV. MONTE CARLO SIMULATIONS

In order to check the predictions of the previous section, we present a numerical analysis of MC simulations following the off-equilibrium protocol (8), for various geometries, boundary conditions, lattice sizes, and time scales. We use the heat-bath upgrading (see Appendix A), varying the temperature according to Eq. (8), after each sweep which corresponds to a unit time.

A. Square systems with PBC

To begin, we present results for the square L^2 lattice with PBC, and the off-equilibrium protocol (8) starting from the high- T phase. In this case the magnetization vanishes by symmetry, as a consequence of the average on the initial Gibbs ensemble at $\beta(t_i) < \beta_c$. Therefore we look at the behavior of the energy density. Figure 3 shows some results for the renormalized energy density [cf. Eq. (7)] obtained by heat-bath MC simulations of the $q = 20$ Potts model for various L and time scales t_s .

When increasing t_s and L , the data approach the corresponding $L \rightarrow \infty$ equilibrium values up to $t = 0$, where e_r vanishes within errors (we recall that $e_r = 0$ is the $T \rightarrow T_c^+$ limit of the equilibrium value in the thermodynamic limit). Then they increase slowly up to $t/t_s = \tau^* > 0$ with $\tau^* \approx 0.005$, corresponding to $T(t) \approx 0.995 T_c$, remaining well below the equilibrium values of the low- T phase. Then the data show a sharp crossover to the values corresponding to the low- T phase. Note also that the lower panel of Fig. 3 reports data with $\ln(t_s)/L \approx \text{const}$, which do not support scaling with respect to the scaling variables $u \approx \ln(t_s)/L$ and $w \approx t/t_s$. Of course, we cannot exclude that an eventual logarithmic scaling behavior may set in for larger L and t_s .

The numerical results for medium-size $L = O(10^2)$ lattices and time scales $t_s = O(10^6)$ suggest a smooth nonsingular behavior around $t/t_s = 0$, without hinting at nontrivial off-equilibrium scaling behaviors around $t = 0$. This scenario was somehow anticipated in the previous section, as a consequence of the trivial values of the exponents κ and κ_t obtained using the scaling ansatzes (13) and (14). It may be related to some form of metastability developing in this slow cooling procedure, which likely requires another theoretical framework. This issue calls for further investigation.

We expect that analogous scenarios occur at the FOTs of any $q > 4$.

B. Results for slablike systems with MBC

We now present results for the 2D Potts models with $q = 10$ and $q = 20$, in anisotropic $L_{\perp} \times L_{\parallel}$ lattices (we set $L_{\perp} = 2L + 1$) with MBC, starting from the high- T and low- T phase.

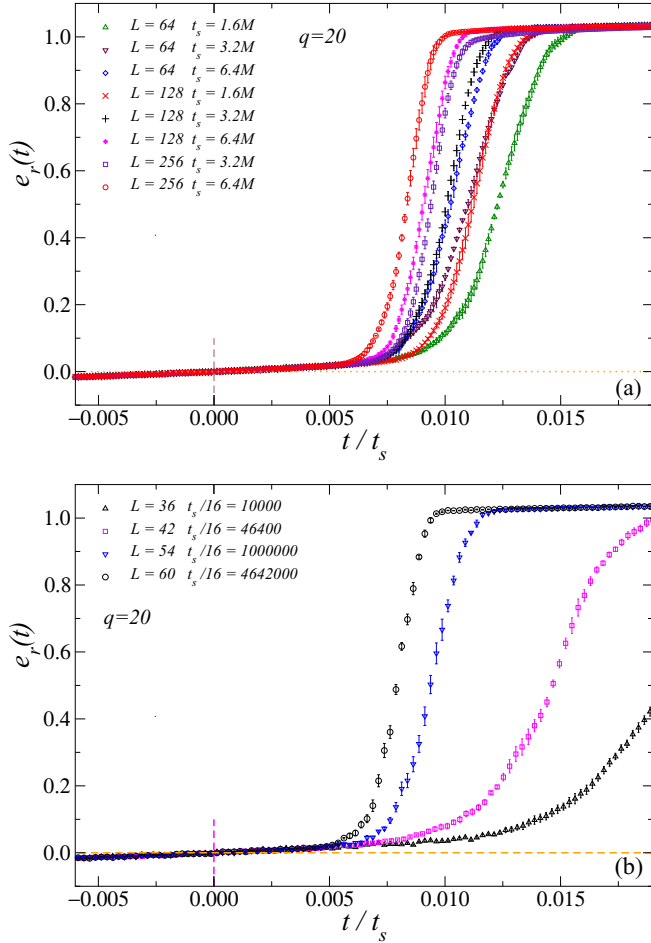


FIG. 3. (Color online) Data of $e_r(t)$ for the 2D $q = 20$ Potts model in square L^2 lattices with PBC, starting from the high- T phase. We show two sets of data: (a) data for large lattices with $t_s = O(10^6)$; and (b) data for smaller lattices, for which the ratio $\ln(t_s/16)/L \approx 0.2558$ is kept fixed (to check the possibility of a logarithmic scaling around $t = 0$). Both of them indicate a smooth behavior up to $t/t_s \approx 0.005$ and then a sharp relaxation toward the low- T values, without showing nontrivial scaling behaviors around $t = 0$.

We consider the slab limit $L_{\parallel} \gg L_{\perp}$, for which numerical results can be straightforwardly obtained by increasing the longitudinal size up to the point where the data appear stable within the errors. We checked that $L_{\parallel} = 8L$ turns out to be sufficiently large to effectively provide infinite- L_{\parallel} results within the errors (the linear scaling of L_{\parallel} with L takes into account that $\xi_{\parallel} \sim L_{\perp}$ for MBC). This is clearly shown by the numerical results for the time-dependent magnetization $m(t)$ reported in Fig. 4, where we compare data for $L_{\parallel}/L = 8$ and $L_{\parallel}/L = 16$ at the same $L = 24$ and time scale t_s with MBC. Analogous results are obtained for other values of L and t_s .

In our numerical simulations we choose $|\delta(t_i)| = |\delta(t_f)| = 1/32$. However, as we shall see, the emerging scaling behavior does not depend on these particular values, because it is essentially related to the behavior around $t = 0$ where $T(t) = T_c$.

In Fig. 5 we report some raw data during a slow variation of the temperature across T_c for the slab geometry with MBC. They are obtained starting from the high- T phase

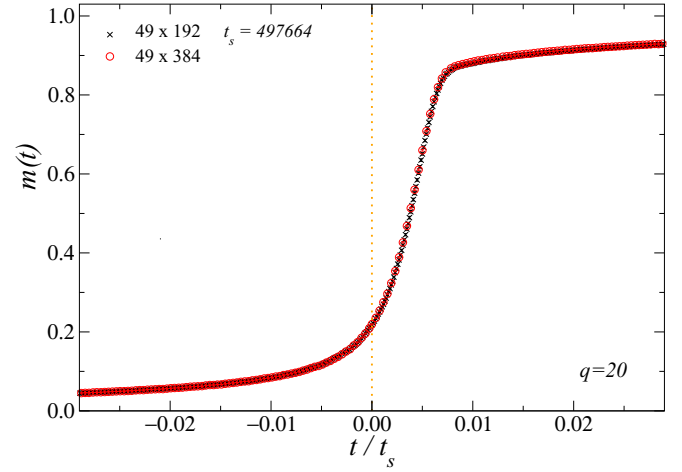


FIG. 4. (Color online) We check the effective $L_{\parallel} \rightarrow \infty$ limit of the numerical results by comparing data of the magnetization $m(t)$ of systems with MBC, for $L_{\parallel}/L = 8$ and $L_{\parallel}/L = 16$ at the same $L = 24$ (corresponding to $L_{\perp} = 49$) and t_s . The two sets of data appear practically indistinguishable within the accuracy of the data, showing that $L_{\parallel}/L = 8$ is sufficiently large to provide accurate estimates of the $L_{\parallel} \rightarrow \infty$ limit.

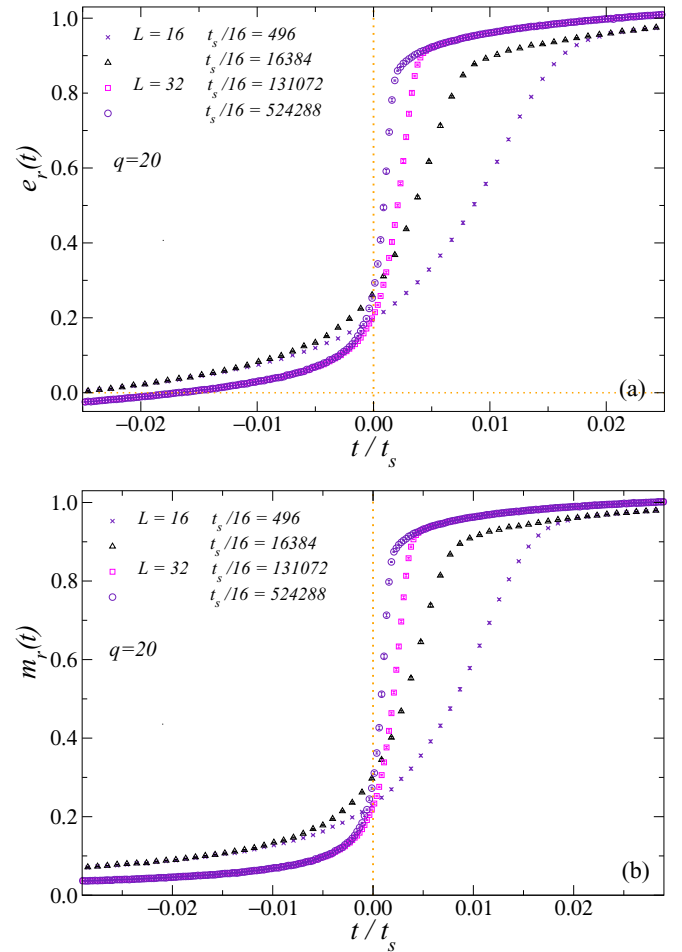


FIG. 5. (Color online) Data of $e_r(t)$ (a) and $m_r(t)$ (b) for the 2D $q = 20$ Potts model with MBC, in anisotropic $L_{\perp} \times L_{\parallel}$ lattices with $L_{\perp} = 2L + 1$ and $L_{\parallel} = 8L$, for $L = 16$ and $L = 32$, and various values of t_s .

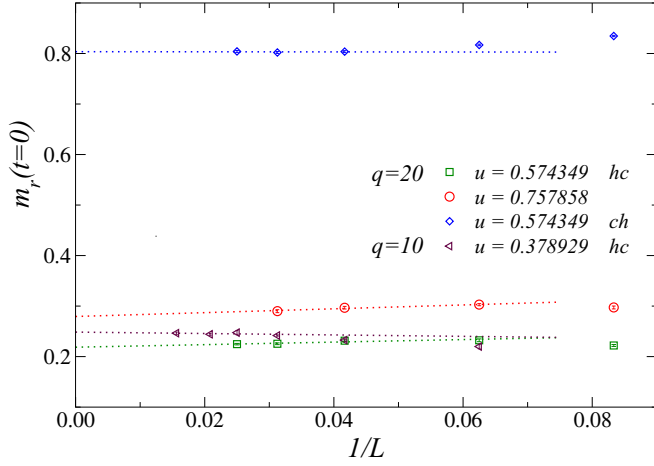


FIG. 6. (Color online) Data of $m_r(t=0)$ for $q=20$, starting from high- T (hc) and low- T (ch) phases and for various values of $u \equiv t_s^{0.2}/L$ (which is kept fixed when varying t_s and L) vs $1/L$. They appear to approach a constant value with increasing L , with corrections which approximately decay as $O(L^{-1})$, supporting the general scaling ansatz (15) with $\kappa = 0.2$. The dotted lines show linear fits to $a + b/L$ of the data for the largest available lattice sizes.

and show the behavior of the energy and the magnetization when the transition is crossed with different time scales t_s and lattice sizes L . The data show that the effective passage from one phase to the other occurs around $t/t_s = 0$. As we shall see, the dependence of the various curves on L and t_s can be cast in the off-equilibrium scaling behavior put forward in the previous section; cf. Eqs. (13)–(16).

In order to check the scaling in the variable $u = t_s^\kappa/L$, we first note that Eqs. (15) and (16) imply that at $t = 0$

$$m_r(0, t_s, L) \approx g_m(u), \quad e_r(0, t_s, L) \approx g_e(u). \quad (21)$$

Therefore, we expect that data at $t = 0$ and fixed $u = t_s^\kappa/L$ must converge to nontrivial u -dependent values with increasing L . Figure 6 shows data at some fixed values of u (using $\kappa = 0.2$ obtained taking the central value $z = 3$), for $q = 20$ and $q = 10$. They appear to converge to nontrivial values, supporting the above asymptotic behavior, with corrections which approximately decay as $O(L^{-1})$. Note that $O(1/L)$ corrections are generally expected due to fact that boundary conditions such as MBC break translation invariance. The data indicate that they are the leading corrections. We also note that with increasing u the $L \rightarrow \infty$ extrapolated values of m_r approach the value $1/2$, which is the expected equilibrium limit for $u \rightarrow \infty$.

Analogous results are obtained by slightly changing the value of z , according to the equilibrium estimate $z = 3.0(1)$, corresponding to $\kappa = 0.200(4)$. Actually, one may assume the off-equilibrium scaling (21) to independently estimate z from the off-equilibrium data. For example, by allowing for deviations from $z = 3$, i.e., $z = 3 + \delta z$, and interpreting the scaling corrections of the data of Fig. 6 as due to δz , we find again that the optimal value is $z = 3$ with a few percent of uncertainty (corrections to scaling have different sign in some cases, which cannot be explained by a unique shift of z , thus $z \approx 3$ appears as the optimal value).

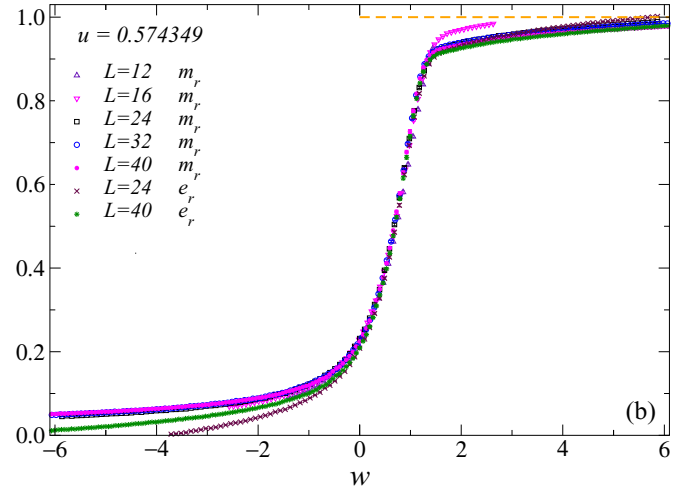
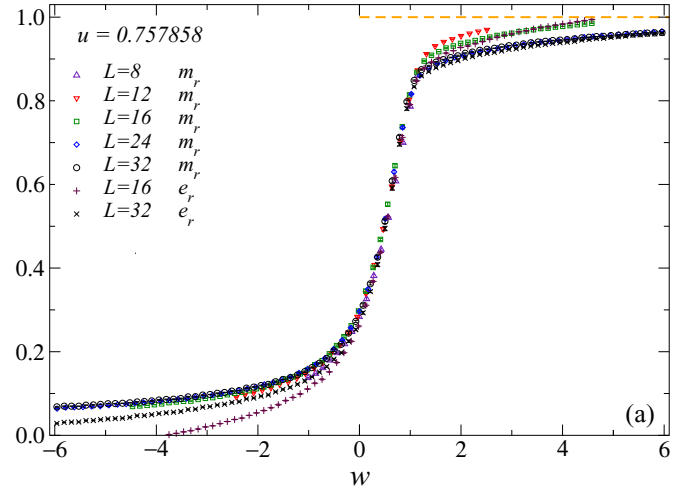


FIG. 7. (Color online) Data of $m_r(t)$ and $e_r(t)$ for $q=20$ starting from the high- T phase, i.e., $T > T_c$, for two values of $u = t_s^\kappa/L$ with $\kappa = 0.2$, i.e., $u \approx 0.7578$ (a) and $u \approx 0.5743$ (b). With increasing L , they approach asymptotic curves when plotted versus $w = t/t_s^{\kappa}$ with $\kappa_r = 0.6$, supporting the scaling ansatzes (15) and (16). Moreover, the data are consistent with the relation (19) predicting the same asymptotic curve for m_r and e_r .

Note also that, since the equilibrium average position of the interface at T_c is expected at equal distances from the boundaries in the large- L limit, leading to the asymptotic equilibrium values $m_r(T_c) = e_r(T_c) = 1/2$, we expect that $\lim_{u \rightarrow \infty} g_\#(u) = 1/2$.

The scaling with respect to w at fixed values of u is supported by the plots in Figs. 7, 8, and 9, respectively, for $q = 20$ with hot and cold starting point and $q = 10$ with hot start. In all cases the data approach an asymptotic function of the scaling variable w , as predicted by the scaling theory of Sec. III. Moreover, the data of $m_r(t)$ and $e_r(t)$ shown in Figs. 7 and 8 approach the same scaling curve, in agreement with the asymptotic relation (19), thus fully supporting the hypothesis that the off-equilibrium behavior is essentially controlled by the time-dependent position of the interface.

Finally, we check the universality of the off-equilibrium scaling behavior with respect to changes of the relaxational (a)

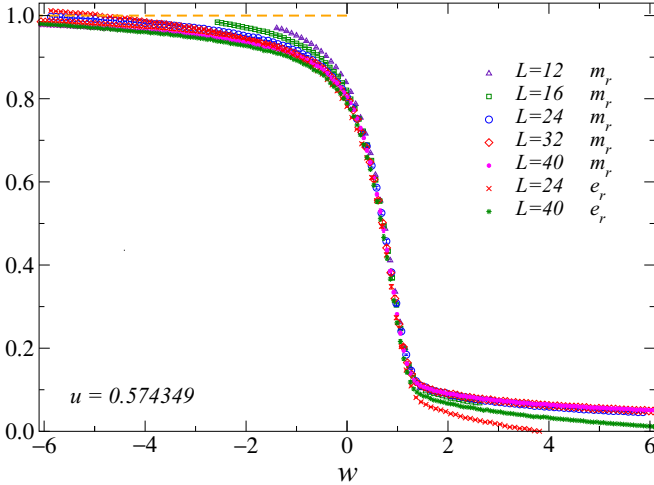


FIG. 8. (Color online) Data for $m_r(t)$ and $e_r(t)$ starting from the cold phase, i.e., $T < T_c$, keeping the scaling variable $u \approx 0.5743$ fixed. They approach a unique asymptotic curve with increasing L , when plotted vs $w = t/t_s^{\kappa_t}$, supporting the scaling ansatzes (15) and (16), and the interface relation (19).

dynamics. This is important to assess the degree of generality of the off-equilibrium scaling. In Fig. 10 we compare results obtained using the heat-bath algorithm with those obtained by a standard Metropolis algorithm with only one trial per site; see Appendix A. The curves match after a trivial rescaling of the scaling variables u and w , supporting the expected universality with respect to the type of relaxational dynamics.

We conclude that our numerical analysis for slab geometries with MBC supports the off-equilibrium scaling behaviors of the magnetization and energy density put forward in Sec. III B; cf. Eqs. (13)–(19).

V. CONCLUSIONS

We investigate off-equilibrium behaviors at FOTs driven by a time dependence of the temperature across the

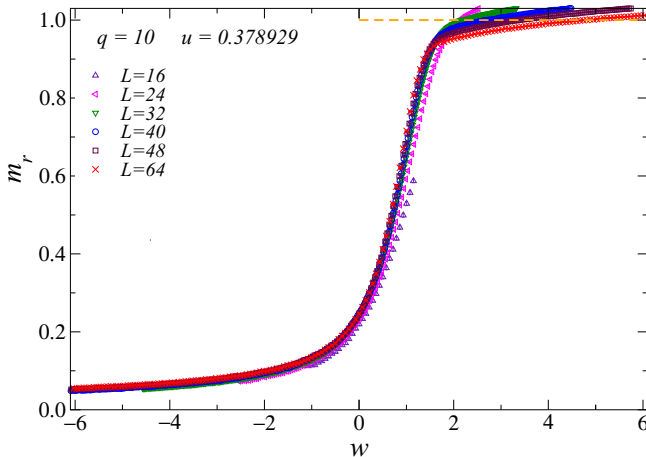


FIG. 9. (Color online) Data of $m_r(t)$ for $q = 10$ vs $w = t/t_s^{\kappa_t}$ at a fixed value of $u = t_s^{\kappa_s}/L \approx 0.3789$ (with $\kappa_t = 0.6$ and $\kappa_s = 0.2$), starting from the high- T phase. They approach an asymptotic scaling curve, in agreement with Eq. (15).

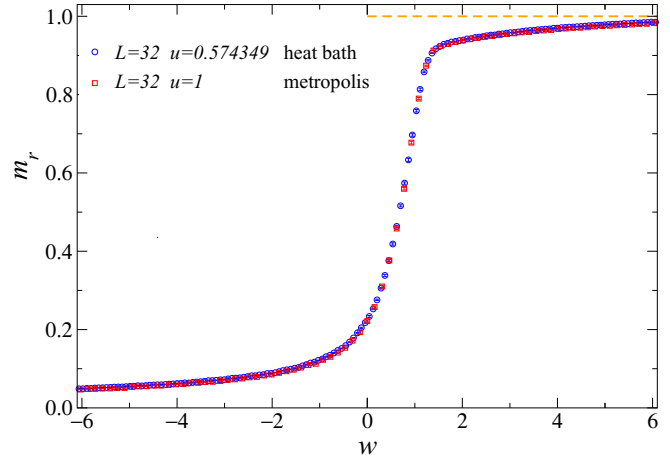


FIG. 10. (Color online) Check of universality between the heat-bath and Metropolis dynamics. The scaling curves coincide after a rescaling of the scaling variables u and w of the Metropolis data. In particular, the rescaling of the variable u can be fixed by looking for data with equal $m_r(0)$ (we obtain that $u \approx 0.5743$ of the heat-bath dynamics approximately corresponds to $u = 1$ of the Metropolis dynamics).

transition point T_c , for example, linearly as $T(t)/T_c \approx 1 - t/t_s$. Usually, off-equilibrium behaviors at FOTs are associated with phenomena of metastability and hysteresis [53]. We focus on the possibility of nontrivial off-equilibrium scaling behaviors driven by slow changes of the temperature, similar to those arising at continuous transitions [2–4], leading to the KZ mechanism. We show that off-equilibrium scaling phenomena emerge also at FOTs with appropriate boundary conditions inducing the presence of an interface.

We consider the 2D Potts models, which provide an ideal testing ground to investigate issues related to FOTs. In our discussion we consider a purely relaxational dynamics such as that obtained by heat-bath and Metropolis upgrading in MC simulations. We study the off-equilibrium behavior in the case of a time-dependent temperature crossing the FOT. In particular, we consider a linear dependence of the inverse temperature $\beta(t) = \beta_c(1 \pm t/t_s)$, starting from the high- T or low- T phase.

We point out that off-equilibrium behaviors at FOTs are extremely sensitive to the geometry and boundary conditions of the system. This peculiar dependence is essentially related to the equilibrium relaxational dynamics at T_c . For symmetric boundary conditions, such as PBC, we expect an exponentially slow dynamics due to an exponentially large tunneling time $\tau \sim e^{\sigma L}$. On the other hand, a power-law slowing down $\tau \sim L^z$ with $z \approx 3$ is found when considering MBC, i.e., when the boundary conditions at two opposite sides of the system are related to the different high- T and low- T phases, effectively generating an interface separating the coexisting phases. We argue that an off-equilibrium scaling behavior around $t = 0$ (i.e., the time corresponding to T_c) is realized for MBC. This is controlled by the corresponding equilibrium length-scale and dynamic exponents. We argue that this scaling behavior is essentially related to the dynamics of the interface enforced by MBC.

In the case of slablike geometries with MBC, the numerical results for the $q = 10$ and $q = 20$ Potts model support the emergence of an off-equilibrium scaling picture characterized by power-law behaviors, analogous to those observed at continuous transitions.

On the other hand, symmetric boundary conditions do not apparently lead to nonanalytic scaling behaviors at $t = 0$, but rather to a delayed sharp relaxation to the other phase at $t/t_s \gtrsim \tau^*$ with $\tau^* > 0$, which may be related to a metastability phenomenon arising from the slow dynamics across the FOT. This point deserves further investigation to physically understand it. Further checks of the observed asymptotic behavior may also be called for. Indeed, we cannot exclude the possibility that a different (logarithmic) asymptotic behavior sets in for sizes and time scales larger than those considered in our numerical analysis, which are $L = O(10^2)$ and $t_s = O(10^6)$.

Our scaling arguments are quite general, therefore they should also apply to higher-dimensional systems, such as the 3D Potts models that undergo FOTs. Such an extension may generally depend on the geometry of the system, e.g., cubiclike L^3 , slablike $L_\perp \times L_\parallel^2$ and tubelike $L_\perp^2 \times L_\parallel$ (with $L_\parallel \gg L_\perp$) geometries, as well as on the boundary conditions. In particular, we again expect that geometries and boundary conditions favoring the emergence of an interface should give rise to off-critical scaling behaviors. This issue calls for further investigation.

Off-equilibrium scaling behaviors may also appear at FOTs driven by magnetic fields. For example, one may consider $O(N)$ -symmetric spin models in the low- T ordered phase, where FOTs are driven by an external magnetic field coupled to the spin variables. Then, one may consider the off-equilibrium dynamics driven by a time-dependent magnetic field $h(t) = t/t_s$ across the transition point $h = 0$. We expect that in the case of Ising models ($N = 1$) an off-equilibrium scaling behavior may emerge in systems with boundary conditions enforcing the presence of an interface, analogously to what is observed at the thermal FOTs of the 2D Potts models. In the case of a continuous symmetry ($N > 2$), off-equilibrium scaling behavior may emerge from the spin-wave dynamics [Goldstone modes related to the broken $O(N)$ symmetry] [46]. We believe that these issues are worth being further investigated.

Off-equilibrium behaviors at FOTs are quite general, they should be observable in many physical contexts where the FOTs are approached by varying the system parameters. The off-equilibrium protocol investigated in this paper may be exploited to probe the main features of systems at the FOT. Moreover, our results may turn out useful in understanding more complicated off-equilibrium phenomena at FOTs. For example, as a case of physical interest we mention the effects of the intrinsic space-time inhomogeneity of the quark-gluon plasma formation in heavy-ion collisions [63], whose equilibrium T - μ (μ is the chemical potential) phase diagram is expected to have a FOT line [64] which may be crossed during heavy-ion collisions. Another interesting context is that of the universe cosmology, which was the original ground of the Kibble proposal [1] to understand the effects of an expanding universe through a continuous transition. From analogous studies of off-equilibrium behaviors at FOTs we

may learn the effects of an expanding and cooling universe that passes through a FOT.

Analogous off-equilibrium phenomena should be also observable in quantum many-body systems, at first-order quantum transitions. Some issues arising from slow (quasi-adiabatic) passages through quantum FOTs have been recently discussed, in particular for some one-dimensional quantum chains [49,65,66], including issues related to adiabatic evolutions in quantum computations [49,67–69].

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APPENDIX A: METROPOLIS AND HEAT-BATH UPDATINGS OF THE POTTS MODELS

A heat-bath updating of a single site variable consists in the change $s_x \rightarrow s'_x$ with probability $\sim e^{-H(s'_x)/T}$ independent of the original spin s_x .

The Metropolis updating of a single spin s_x is performed by (i) proposing a new spin $s'_x \neq s_x$ by taking one of the other $q - 1$ states with equal probability and (ii) accepting the change with probability $\text{Min}[e^{[H(s_x) - H(s'_x)]/T}, 1]$.

The heat-bath updating is generally more effective than a single Metropolis updating, because the new variable is not correlated with the previous one. The Metropolis updating tends to be equivalent to the heat-bath one when a large number of trials are performed.

Both updating procedures give rise to a purely relaxational dynamics, usually named model A [44] in the context of critical dynamics, whose class also includes configuration updatings by Langevin equations with white noise. The time unit during the relaxational dynamics is generally associated with a complete sweep of the lattice variables.

APPENDIX B: COMPUTATION OF THE EQUILIBRIUM AUTOCORRELATION TIME

The integrated autocorrelation time of a given quantity Q is defined as

$$\tau \equiv \frac{1}{2} \sum_{t=-\infty}^{t=+\infty} \frac{C(t)}{C(0)}, \quad (\text{B1})$$

where $C(t) = \langle (Q(t) - \langle Q \rangle)(Q(0) - \langle Q \rangle) \rangle$ is the autocorrelation function of Q (t is the discrete Monte Carlo time, where a time unit is given by a sweep, i.e., a heat-bath update of all lattice variables). Averages are taken at equilibrium. Estimates of the corresponding integrated autocorrelation time τ can be obtained by the binning method (see, e.g., Refs. [70,71] for discussions of this method and its systematic errors), using the estimator

$$\tau = \frac{E^2}{2E_0^2}, \quad (\text{B2})$$

where E_0 is the naive error calculated without taking into account the autocorrelations, and E is the correct error found

after binning, i.e., when the error estimate becomes stable with respect to increasing of the block size b . The statistical error $\Delta\tau$ is just given by $\Delta\tau/\tau = \sqrt{2/n_b}$ where n_b is the number of blocks corresponding to the estimate of E . As discussed in Ref. [70] this procedure leads to a systematic error of $O(\tau/b)$. In our cases the ratio τ/b will always be much smaller than the statistical error, so we will neglect it. Equation (B2) can

be easily extended to the case the quantity Q is measured every n_m sweeps, i.e., $\tau = n_m E^2 / (2E_0^2)$, which is of course meaningful only if $n_m \ll \tau$.

Of course, τ depends on the quantity Q considered. However, barring unlikely exceptions, all quantities lead to the same asymptotic power-law behavior $\tau \sim L^z$.

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