Dynamic Off-Equilibrium Transition in Systems Slowly Driven across Thermal First-Order Phase Transitions

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We study the off-equilibrium behavior of systems with short-range interactions, slowly driven across a thermal first-order transition, where the equilibrium dynamics is exponentially slow. We consider a dynamics that starts in the high-T phase at time $t = t_i < 0$ and ends at $t = t_f > 0$ in the low-T phase, with a time-dependent temperature $T(t)/T_c \approx 1 - t/t_s$, where t_s is the protocol time scale. A general off-equilibrium scaling (OS) behavior emerges in the limit of large t_s. We check it at the first-order transition of the two-dimensional q-state Potts model with $q = 20$ and 10. The numerical results show evidence of a dynamic transition, where the OS functions show a spinodal-like singularity. Therefore, the general mean-field picture valid for systems with long-range interactions is qualitatively recovered, provided the time dependence is appropriately (logarithmically) rescaled.

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The dynamical behavior of statistical systems driven across phase transitions is a typical off-equilibrium phenomenon. Indeed, the large-scale modes present at the transition are unable to reach equilibrium as the system changes phase, even when the time scale t_s of the variation of the system parameters is very large. Such phenomena are of great interest in many different physical contexts [1–31]: One observes hysteresis and coarsening phenomena, the Kibble-Zurek defect production, etc. At continuous transitions, thermodynamic quantities obey general off-equilibrium scaling laws as a function of t_s, controlled by the universal static and dynamic exponents of the equilibrium transition [32,33]. Similar results hold along the *magnetic* first-order transition line of systems with continuous $\mathrm{O}(N)$ symmetries ($N > 1$) [34].

This Letter considers systems with short-range interactions undergoing a *thermal* first-order transition (FOT) driven by the temperature T. At the FOT temperature T_c, the energy density is discontinuous and any local dynamics is very slow, due to an exponentially large tunneling time between the two phases: $\tau(L) \sim \exp(\sigma L^{d-1})$ for a system of size L^d, where the constant σ is related to the interface free energy. We study the off-equilibrium behavior arising when T is slowly varied across $T_c \equiv \beta_c^{-1}$. We consider a linear time dependence

$$\delta(t) \equiv \beta(t)/\beta_c - 1 = t/t_s, \qquad \beta \equiv 1/T, \tag{1}$$

starting the dynamics at a time $t_i < 0$ in the high-T phase and ending it at $t_f > 0$ in the low-T phase. t_s is the time scale of the temperature variation. This protocol is general, since a generic time dependence can be approximated by a linear function around T_c.

In the mean-field approximation, which becomes exact for long-range interactions [3], after crossing T_c the system persists in a metastable state with an infinite mean lifetime, up to a spinodal-like point $T_{\rm sp} < T_c$ and, thus, up to a time $t > 0$ such that $\delta(t) = T_c/T_{\rm sp} - 1$, where a rapid transition to the low-T phase occurs. This picture requires a substantial revision in the case of short-range interactions, because metastable states may decay when $T(t) < T_c$, due to droplet formation [3].

We show that short-ranged systems at a thermal FOT show an off-equilibrium scaling (OS) behavior, which significantly differs from that obtained in the mean-field approximation. For finite t_s we observe a sharp transition to the low-temperature phase at a temperature $T(t_s) < T_c$, but the temperature $T(t_s)$ approaches (logarithmically) T_c as t_s becomes large. Moreover, the time dependence of the OS functions develops a singular behavior characterized by peculiar scaling properties.

To test the general OS ideas, we consider the 2D Potts model, which is an ideal theoretical laboratory to study thermal FOTs. Its Hamiltonian reads

$$H = -\sum_{\langle xy \rangle} \delta(s_x, s_y), \tag{2}$$

where the sum is over the nearest-neighbor sites of a square lattice, s_x (*color*) are integer variables $1 \le s_x \le q$, $\delta(a, b) = 1$ if $a = b$ and zero otherwise. It undergoes a phase transition [35,36] at $\beta_c = \ln(1 + \sqrt{q})$, between a disordered phase and an ordered phase with q equivalent *vacua*. The transition is of the first order for $q > 4$. We consider $L \times L$ square lattices with periodic boundary conditions (PBCs), which preserve the q-permutation symmetry. In an infinite volume, the energy density

$E = \langle H \rangle / L^2$ is discontinuous at T_c, with different [37] $E_c^\pm \equiv E(T_c^\pm)$. We define the *renormalized* energy density

$$E_r \equiv \Delta_e^{-1}(E - E_c^-), \qquad \Delta_e \equiv E_c^+ - E_c^-, \tag{3}$$

which satisfies $E_r = 0,\ 1$ for $T \to T_c^-$ and $T \to T_c^+$, respectively. The magnetization

$$M_k = \frac{1}{L^2}\left\langle \sum_x \mu_k(\boldsymbol{x}) \right\rangle, \qquad \mu_k(\boldsymbol{x}) \equiv \frac{q\delta(s_{\boldsymbol{x}}, k) - 1}{q-1}, \tag{4}$$

vanishes due to the q-state permutation symmetry, for any T. We consider the correlation function $G_{kp}(\boldsymbol{x},\boldsymbol{y}) \equiv \langle \mu_k(\boldsymbol{x})\mu_p(\boldsymbol{y})\rangle$ and, in particular, its space integral

$$I_G = L^{-2}\sum_{k=1}^{q}\sum_{\boldsymbol{x},\boldsymbol{y}} G_{kk}(\boldsymbol{x},\boldsymbol{y}). \tag{5}$$

Equilibrium finite-size scaling (EFSS) holds also at FOTs [38–44]. For cubiclike lattices, the relevant scaling variable is $r_1 = L^d\delta$, where $\delta \equiv \beta/\beta_c - 1$. The energy density and I_G scale correspondingly as

$$E_r(T,L) \approx \mathcal{E}_{\rm eq}(r_1), \qquad I_G(T,L) \approx L^d\mathcal{C}_{\rm eq}(r_1), \tag{6}$$

in the EFSS limit $L \to \infty$ keeping r_1 fixed [45].

The system is driven across the transition by the temperature protocol (1), starting from equilibrated configurations at $\beta = \beta_i = \beta(t_i) < \beta_c$. Observables, such as E_r and I_G, are averaged at fixed t over the starting configurations. We anticipate that the OS behavior across the FOT does not depend on the value of $\beta_i < \beta_c$.

To specify the OS laws that describe the dynamic behavior for $\beta(t) \approx \beta_c$, we must identify the correct scaling variables. First, we use the variable r_1, parametrizing the EFSS functions, as equilibrium should be recovered in the appropriate limit. To define a second scaling variable, we should identify the appropriate time scale. When the global symmetry is preserved by the boundary conditions or in the absence of boundaries such as PBCs, the slowest mode in the system is the tunneling between the two phases. This is expected to proceed via mixed-phase striplike configurations with two interfaces, whose probability is suppressed by a factor of $\exp(-\sigma L)$ [46,47], where $\sigma = 2\beta_c\kappa$ and κ is the interface tension (which is exactly known for 2D Potts models [37]). Thus, the relevant time is $\tau(L) = L^\alpha \exp(\sigma L)$, where α is an appropriate exponent. Therefore, the OS behavior is expected to be controlled by the scaling variables

$$r_1 = \delta(t)L^2 = (t/t_s)L^2, \qquad r_2 = t/\tau(L), \tag{7}$$

where t_s is the time scale of the protocol (1). The deviations from equilibrium are conveniently controlled by

$$s_1 = r_2/r_1 = t_s/[L^2\tau(L)]. \tag{8}$$

We expect $E_r(t, t_s, L)$ and $I_G(t, t_s, L)$, defined as in Eqs. (3) and (5) and averaged at fixed t, to scale as

$$E_r \approx \mathcal{E}_s(s_1, r_1), \qquad I_G \approx L^2\mathcal{C}_s(s_1, r_1), \tag{9}$$

in the OS limit $t, t_s, L \to \infty$ keeping r_1 and s_1 fixed, thereby extending the EFSS relations (6). EFSS should be recovered for $s_1 \to \infty$, where $\mathcal{E}_s(s_1, r_1)$ and $\mathcal{C}_s(s_1, r_1)$ converge to their equilibrium counterparts $\mathcal{E}_{\rm eq}(r_1)$ and $\mathcal{C}_{\rm eq}(r_1)$, respectively. These OS arguments are quite general and can be extended to any thermal FOT, in any dimension [48].

The above OS theory is checked by a numerical analysis of Monte Carlo (MC) simulations of the 2D Potts model (2) for $q = 20$ and $q = 10$. We mostly present results for $q = 20$. The dynamics is provided by the heat-bath algorithm [49], which is a representative of a purely relaxational dynamics. The time unit is a sweep of the whole lattice. The temperature is changed according to Eq. (1) every sweep, incrementing t by one.

We first consider data at $t = 0$, i.e., $r_1 = 0$, as a function of s_1; see Fig. 1. Their optimal scaling is obtained when the power of the prefactor of $\tau(L)$ is $\alpha \approx 2$ [50]. We also verify the OS of E_r and I_G (and other observables) with respect to r_1 [cf. Eq. (9)]; see [51]. Note that the approach to the OS curves requires the necessary condition $L \gg \xi_\pm$, where $\xi_\pm$ are the correlation lengths of the pure phases at $T_c^\pm$ ($\xi_- \approx \xi_+ = 2.695$ for $q = 20$ [37]).

We now show that an interesting off-equilibrium behavior develops in the infinite-volume limit, corresponding to $s_1 \to 0$. As shown by Fig. 2, data at fixed t_s have a well-defined large-L limit; see the inset in Fig. 2. This is rapidly approached for small values of $\delta(t) \equiv t/t_s$, e.g., $\delta(t) \lesssim 0.02$

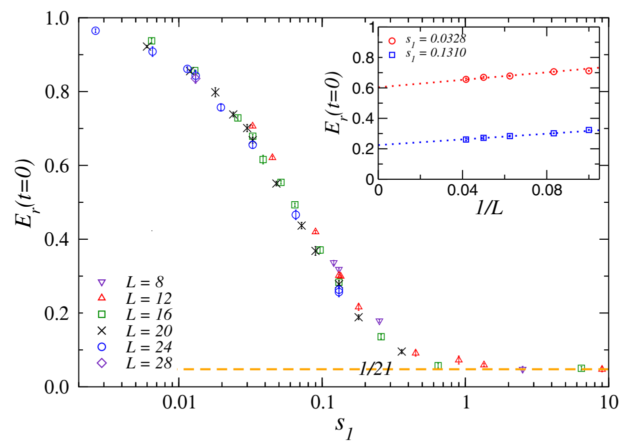

FIG. 1. MC data of E_r for $q = 20$ at $t = 0$ versus $s_1 = t_s/(L^{2+\alpha}e^{\sigma L})$, using the optimal value $\alpha = 2$ [57]. For $s_1 \to \infty$, the data converge to $\mathcal{E}_{\rm eq}(0) = 1/(1+q)$ (dashed line), since equilibrium is approached for $t_s \gg \tau(L)$. The inset shows the approach to the large-L limit at fixed s_1.

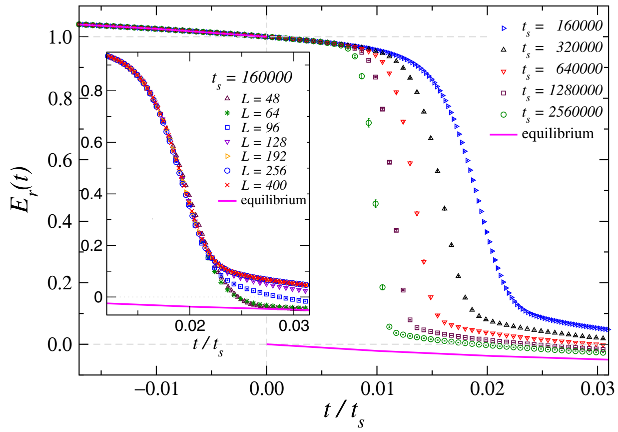

FIG. 2. MC data of $E_r(t)$ for $q = 20$ for some values of t_s, in the $L \to \infty$ limit. The large-L convergence (within errors) is checked by increasing L at fixed t_s, analogously to the case shown in the inset. The full lines show the equilibrium energy density at $\beta = \beta_c(1 + t/t_s)$.

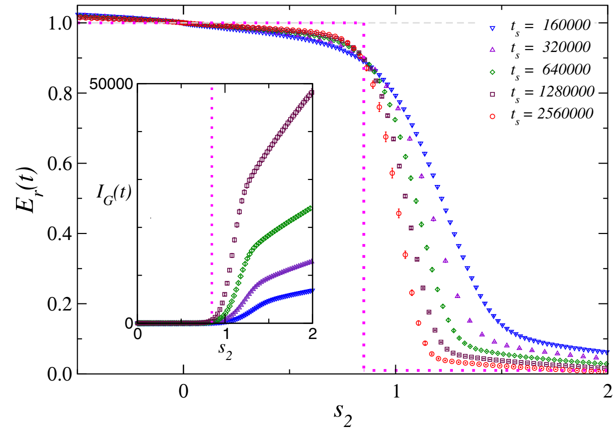

FIG. 3. The infinite-volume E_r and I_G (inset) for $q = 20$ versus s_2. The dotted lines show the conjectured singular large-t_s limit; see the text.

at $t_s \approx 10^5$, while significantly larger lattices are required for larger $\delta(t)$. The energy density does not converge to its equilibrium value as $L \to \infty$ due to the fact that the system settles in a metastable state with large coexisting droplets of different colors.

The infinite-volume energy density (see Fig. 2) takes the equilibrium high-T value $E_r(t = 0) = 1$ at $t = 0$ for any t_s and then shows a sharp decrease at a point $\delta^*(t_s)$, which decreases with increasing t_s. The system develops a nontrivial OS behavior close to $\delta^*(t_s)$. For large L, the system behaves as a gas of droplets of size R (evidence for this behavior is provided in Ref. [51]). The relevant scaling variables are expected to be analogous to r_1 and r_2 [cf. Eq. (7)], with R replacing the size L. The relevant time scale is that of the formation of droplets of size R. As the time τ_d to create a droplet of size R increases exponentially with R, $\ln \tau_d \sim R$, we expect $R \sim \ln t$. Thus, the analogue of the scaling variable r_1 becomes ($t > 0$)

$$s_2 = (t/t_s) \ln^2 t. \tag{10}$$

In Fig. 3, we report the infinite-volume energy density and I_G for $q = 20$ versus s_2. We note a crossing point of the energy curves for different values of t_s at approximately $s_2^* \approx 0.85$ with $E_r^* \approx 0.89$. At the same value of s_2, I_G shows a sharp change of behavior. These results suggest that, in the limit $t_s \to \infty$, the OS functions develop a singular behavior for $s_2 = s_2^*$. In particular, the infinite-volume energy density takes the high-T value $\mathcal{E}_\infty(s_2) = e_+ = 1$ for $s_2 < s_2^*$, while we expect $\mathcal{E}_\infty(s_2) = e_- \ll 1$ for $s_2 > s_2^*$. Note that, for large t_s, $(t \ln^2 t)/t_s = s_2^*$ implies $t/t_s \approx s_2^*/(\ln t_s)^2$, so that the value β_d of β at which the sharp change occurs converges to β_c as t_s increases.

The behavior around s_2^* turns out to be described by an additional scaling *Ansatz*. As shown in Fig. 4, the energy density $\mathcal{E}_\infty(s_2, t_s) \equiv E_r(t, t_s, L \to \infty)$ scales as

$$\mathcal{E}_\infty(s_2, t_s) \approx f_e(\tilde{s}_2), \qquad \tilde{s}_2 = (s_2 - s_2^*) t_s^\theta \tag{11}$$

with [50] $\theta = 1/3$. We stress that scaling is observed only when using the variable s_2. The estimate $\theta = 1/3$ is reasonably accurate (10% accuracy). Also $I_G(s_2, t_s)$ shows a scaling behavior, provided we multiply it by an additional power of t_s. Phenomenologically, we observe $I_G(t) \approx (\ln t_s)^2 t_s^{2/3} f_G(\tilde{s}_2)$; see the inset in Fig. 4 (the exponents of t_s and $\ln t_s$ in the prefactor are an educated guess). A similar analysis can be performed for $q = 10$; see [51]. The estimate of s_2^* changes ($s_2^* \approx 0.2$ for $q = 10$), but all other conclusions hold. In particular, the MC data are again consistent with $\theta = 1/3$. This singular behavior resembles that at the mean-field spinodal point [3] or, more generally, the power-law scaling at equilibrium continuous transitions. However, here the location β_d of the dynamic transition converges to β_c as $t_s \to \infty$: $\beta_d - \beta_c \sim (\ln t_s)^{-2} \to 0$ [58].

To understand the behavior of the system for $s_2 \approx s_2^*$, one may consider the evolution of the size of the clusters formed by spins of the same color. A typical case is

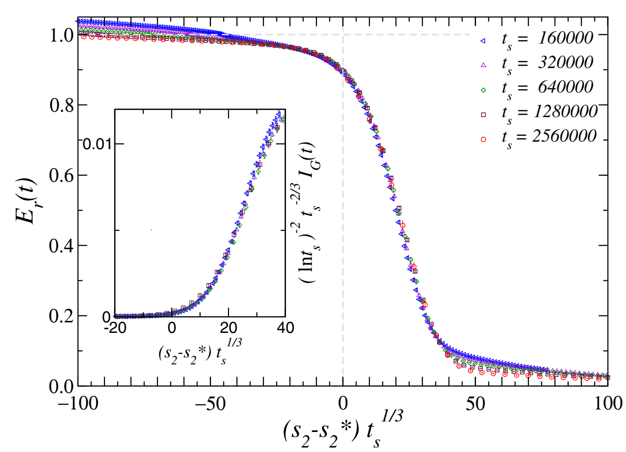

FIG. 4. Scaling of the infinite-volume E_r and I_G (inset) around s_2^*.

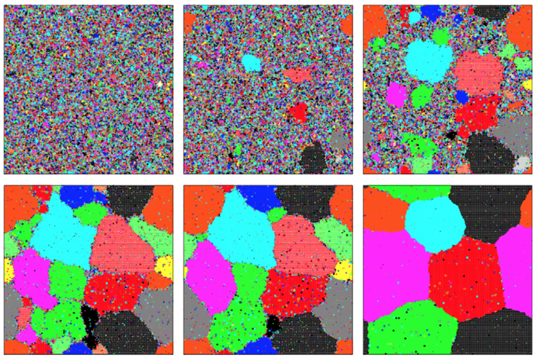

FIG. 5. Snapshots of a system of size $L = 512$ for $\tilde{s}_2 = (s_2 - s_2^*)t_s^{1/3} = -20, 0, 20, 40, 100, 1500$ (from left to right, top to bottom). Here $q = 20$ and $t_s = 640000$. We use different colors for each value of s_x. The range of $\tilde{s}_2$ covers the region where E_r significantly changes; see Fig. 4.

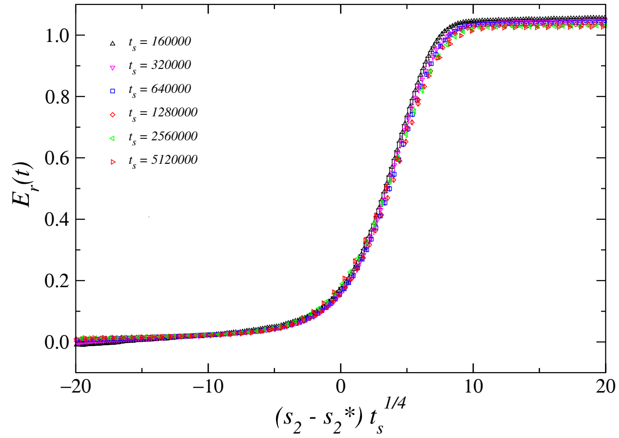

FIG. 6. Scaling of the infinite-volume E_r for the reversed protocol, in which the dynamics starts from an ordered configuration at $\beta_i > \beta_c$ and $\beta(t) = \beta_c(1 - t/t_s)$. The optimal collapse is obtained for $s_2^* \approx 0.85$ and $\theta \approx 1/4$ [the accuracy of the data does not exclude the value $\theta \approx 1/3$ obtained for protocol (1)]; see [51].

reported in Fig. 5. For $s_2 \lesssim s_2^*$, the system is disordered and all clusters are small: Their typical size ℓ_d satisfies $\ell_d \lesssim \xi_+$, where ξ_+ is the correlation length of the pure disordered phase [37]. For $s_2 \approx s_2^*$, clusters start growing. There is a short coarsening interval [5,8,33], in which E_r decreases almost linearly. Then, the system settles into a metastable state characterized by many coexisting large clusters. Details are reported in Ref. [51].

One may also consider the dynamics induced by the reverse linear protocol across β_c, starting from an ordered configuration (equal spins) at $\beta_i > \beta_c$ and decreasing β across the FOT, $\beta(t) = \beta_c(1 - t/t_s)$, up to $\beta_f < \beta_c$. In this case, the q-permutation symmetry is broken by the initial condition. MC results show an analogous OS behavior. In the infinite-volume limit, the system persists in the ordered state up to a temperature $T(t_s) > T_c$, where it transits to the disordered state. For $T \approx T(t_s)$, one observes analogous OS laws. Equation (11) holds with a corresponding s_2^* and exponent θ, which may differ from those of protocol (1); see Fig. 6 and Ref. [51].

The OS theory can be applied to hysteresis phenomena that occur when T is first decreased below T_c and then increased above T_c. We mention that external periodically varying fields have been already considered at magnetic FOTs, where they give rise to a singular dynamic behavior of the magnetization hysteresis [59,60].

In conclusion, we have developed an OS theory to describe the off-equilibrium behavior of statistical systems when their temperature is slowly varied across a thermal FOT. We consider the linear protocol (1) and the reversed one [61]. Our numerical study of the Potts model confirms the general OS theory. In particular, in the infinite-volume limit it shows two dynamic regimes, separated by a spinodal-like transition point where the OS functions are singular. Such a transition occurs at a time $t_d > 0$ scaling as $t_d \sim t_s(\ln t_s)^{-2}$ in the large-t_s limit. Therefore, a spinodal-like behavior emerges dynamically in short-range models without assuming long-range interactions as in the mean-field theory [3]. The OS behavior arises from the interplay between the exponentially large tunneling times at T_c and the droplet formation. We expect that analogous dynamic scaling behaviors emerge at any thermal FOT characterized by these two features. Further investigations are needed to clarify its degree of universality and to develop a theory which is able to predict the exponent θ entering the OS laws, such as Eq. (11).

Our results provide an effective framework to interpret experimental data in many physical contexts, when thermal FOTs are crossed by slowly varying T. For example, we mention the formation of the quark-gluon plasma in heavy-ion collisions [62], whose intrinsic space-time inhomogeneities complicate the study of the hadronic phase diagram, and, in particular, the expected thermal FOT line at a nonzero baryon chemical potential [63]. Another issue concerns the Universe evolution. Kibble [1] made the first analysis of the behavior of a system going across a continuous transition, to study the defect production during the Universe expansion. Analogous studies at FOTs may shed some light on the behavior of an expanding and cooling Universe going across a FOT [64].

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[49] A heat-bath updating of a single site variable consists in the change $s_{\boldsymbol{x}} \to s_{\boldsymbol{x}}'$ with probability $\sim e^{-H(s_{\boldsymbol{x}}')/T}$ independent of the original spin $s_{\boldsymbol{x}}$.
[50] We are biased by the idea that simple integer or fractional exponents enter the various off-equilibrium scaling Ansätze at FOTs, likely arising from geometric reasons.
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