Anomalous finite-size scaling at thermal first-order transitions in systems with disordered boundary conditions

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(Dated: May 14, 2018)

We investigate the equilibrium and off-equilibrium behaviors of systems at thermal first-order transitions (FOTs) when the boundary conditions favor one of the two phases. As a theoretical laboratory we consider the two-dimensional Potts model. We show that an anomalous finite-size scaling emerges in systems with open boundary conditions favoring the disordered phase, associated with a mixed regime where the two phases are spatially separated. Correspondingly, if the system is slowly heated across the transition, the characteristic times of the off-equilibrium dynamics scale with a power of the size. We argue that these features generally apply to systems at FOTs, when boundary conditions favor one of the two phases. In particular, they should be relevant for the experimental search of FOTs of the quark-gluon plasma in heavy-ion collisions.

Understanding finite-size effects at phase transitions is of great phenomenological importance, because it allows us to interpret correctly experiments and numerical investigations of finite-size systems close to the transition point, where thermodynamic quantities develop singularities in the infinite-volume limit. At continuous transitions finite-size scaling (FSS) [1,2] is characterized by universal power laws, with critical exponents that are independent of the geometry and of the boundary conditions, the latter affecting only FSS functions and amplitudes. In this respect first-order transitions (FOTs) are more complicated. Most theoretical studies, see, e.g., Refs. [3–7], have considered cubic $L^d$ systems with periodic boundary conditions (PBC), showing that finite-size effects are generally characterized by power laws related to the space dimension of the system; for instance, the correlation-length exponent is $\nu = 1/d$. However, as noted in Refs. [8,9], finite-size effects strongly depend on the geometry, differing significantly in cubic $L^d$ and anisotropic geometries. For instance, in $L^{d-1}\times M$ geometries with $M \gg L$, FSS in Ising systems is characterized by exponential laws in $L [8]$. Recent studies of quantum FOTs have also reported a significant dependence on the boundary conditions [10,11].

In this paper, we study the static and dynamic behavior at thermal FOTs in finite-size systems with boundary conditions favoring one of the two phases, in particular the disordered phase, such as open boundary conditions (OBC). We consider the two-dimensional (2D) Potts model, which is a standard theoretical laboratory to understand issues concerning the statistical behavior at a thermal FOT. We show, in the presence of OBC, the emergence of an anomalous equilibrium FSS (EFSS), which is characterized by scaling laws that differ from those that apply in the coexistence region with PBC. Boundary conditions have also a crucial influence when considering dynamic phenomena, for instance, when one considers a slow heating of the system, starting in the ordered phase and moving across the FOT. We show that disordered boundary conditions give rise to an off-equilibrium FSS (OFSS) characterized by a time scale increasing as a power of the size $\ell$, i.e. $\tau(\ell) \sim \ell^2$. We argue that these static and dynamic features are shared among generic thermal FOTs, when the boundary conditions favor one of the two phases.

Before presenting our results, we discuss the phenomenological relevance of our study. While PBC are not usually appropriate to describe realistic situations, OBC are appropriate whenever the disordered phase is somehow favored by the boundaries. Such a situation arises in many physical contexts. One notable example is provided by heavy-ion collision experiments, probing the phase diagram of hadronic matter. At finite temperature $(T)$, theoretical arguments [16] predict the existence of a high-$T$ quark-gluon phase and of a low-$T$ hadronic phase, separated by a FOT line at finite quark chemical potential, ending at an Ising-like transition point. Heavy-ion collision experiments are trying to find evidence for such FOT line [12–14]; see, in particular, the planned activities discussed in Ref. [15] and references therein. One major problem in identifying its signature is the presence of space-time inhomogeneities in the quark-gluon plasma generated in the collisions. The plasma is expected to be confined in a small region with a size of a few femtometers (fm), and to hadronize within a time interval of a few fm/$c$. In the appropriate region of the phase diagram, as the plasma cools down, the system is expected to cross the FOT line. However, as the size and time scales are finite, there must be a substantial rounding of the FOT singularities, which may conceal its presence. Therefore, for a correct interpretation of the experimental results, it is important to understand the effects of space-time inhomogeneities at FOTs. Since, for the hadronic transition, the high-$T$ and low-$T$ phases are the ordered and the disordered ones, respectively (such correspondence is the opposite of the usual one) [16], the quark-gluon plasma
dynamics corresponds to that of a finite-size statistical system, such as the Potts model, that is slowly heated across a FOT. Note also that hadron matter surrounds the quark-gluon plasma, hence the appropriate boundary conditions in the corresponding statistical system must favor the disordered phase, as is the case for the OBC. The dynamics across the FOT of a finite-size system with OBC should therefore capture some of the important features of the evolution of a confined quark-gluon plasma cooled down across the FOT toward the hadronic low-T phase. This may lead to a better understanding of the signatures of the FOT line in heavy-ion collisions [17].

The 2D $q$-state Potts model provides a theoretical laboratory to study thermal FOTs. It is defined by

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

where $\beta \equiv 1/T$, the sum is over the nearest-neighbor sites of an $L \times L$ lattice, $s_x$ are integer variables $1 \leq s_x \leq q$, $\delta(a, b) = 1$ if $a = b$ and zero otherwise. It undergoes a phase transition [18, 19] at $\beta_c \equiv 1/T_c = \ln(1 + \sqrt{q})$, which is of first order for $q > 4$. At $T_c$ the infinite-volume energy density $E \equiv \langle H \rangle/L^2$ is discontinuous. We define

$$E_r = \Delta_e^{-1}(E - E_c^+), \quad \Delta_e = E_c^+ - E_c^- \quad (2)$$

where $E_c^\pm = E(T_c^\pm)$ [20], so that $E_r = 0, 1$ for $T \to T_c^+$ and $T \to T_c^-$, respectively. The magnetization $M_k$

$$M_k = \langle \mu_k \rangle, \quad \mu_k = \frac{1}{V} \sum_{x} \frac{q\delta(s_x, k) - 1}{q - 1}, \quad (3)$$

is also discontinuous, i.e. $\lim_{L \to \infty} M_k = m_0 > 0$ [21].

One can define an EFSS [3–10] also at FOTs, with scaling laws that are analogous to those holding at continuous transitions [1, 2]. This issue has been mostly investigated for cubic $L^d$ systems with PBC, finding that the finite-size coexistence region shows a scaling behavior in terms of the variable $u \propto \delta L^d$ with $\delta \equiv 1 - 1/\beta_c$. For instance, the energy density scales as $E_r(T, L) \approx \mathcal{E}(u)$. For the 2D Potts model $\mathcal{E}(u) = (1 + qe^{-u})^{-1}$ [21]. Systems with boundary conditions favoring the high-T phase, such as the OBC, show a more complex behavior, due to surface effects, which give rise to a shift $\delta^*(L) \sim 1/L$ of the transition temperature. Correspondingly the scaling variable to describe the coexistence regime is $u \propto \delta - \delta^*(L)L^2$ [22], whose check requires a precise determination of $\delta^*(L)$. However, as we shall see, other interesting EFSS properties emerge.

To investigate these issues, we have performed simulations with $q = 20$ (up to $L = 200$) and $q = 10$ (up to $L = 512$) using OBC [22]. Quite surprisingly, see Fig. 1 the results appear to scale as

$$E_r(\delta, L) \approx \mathcal{E}_c(w), \quad w = \delta L^\varepsilon, \quad (4)$$

where $\varepsilon \approx 3/2$ (the optimal collapse of the data suggest it with an accuracy on $\varepsilon$ of a few per cent). This nontrivial scaling is observed for $w < 0$ up to an $L$-dependent value $w^*(L)$. Since $E_r = 0$ in the $L \to \infty$ limit for $\delta = 0^-$, we expect $\mathcal{E}_c(w \to -\infty) \to 0$. Moreover, since for OBC the $L \to \infty$ limit at fixed $T$ is approached with $1/L$ corrections, we expect $\mathcal{E}_c(w) \approx |w|^{-1/\varepsilon}$ for $w \ll -1$. This is confirmed by the data for $w \lesssim w^*$, see the inset of Fig. 1. For $w > w^*(L)$, the scaling behavior is trivial as $\mathcal{E}_c(w) = 1$, the high-T value, with $1/L$ corrections. Analogous results are obtained for other observables and for $q = 10$ [24]. For $w = w^*(L)$ the energy has a two-peak structure, see Fig. 2 and the probabilities of the corresponding configurations are approximately equal. The value $w^*(L)$ is therefore related to the shift $\delta^*(L)$ of the transition [25]. Note that the scaling in terms of $w$ is not appropriate to describe coexistence, but only the low-T region $w < w^*$. Indeed, when expressed in terms of $w$, the EFSS functions are singular for $w = w^*$, and the scaling is trivial for $w > w^*$.

To interpret the scaling in terms of $w$, we note that, for $w < w^*(L)$, typical configurations are characterized by a central ordered region surrounded by a disordered ring of volume $V_\perp$, stabilized by the boundary conditions, see the right panel of Fig. 2 Thus, the size of the disordered region can be related to $E_r$, by $E_r \approx V_\perp/L^2$. At fixed $w$, the energy $E_r$ is fixed, implying that the scaling limit we consider is appropriate to describe low-T configurations characterized by the simultaneous presence of disordered and ordered regions. One should not confuse this mixed regime with thermodynamic coexistence: for $w < w^*(L)$ the free energy has only one minimum (thermodynamically it represents a low-T state), except in a small interval of $w$ around $w^*$, which shrinks as $L$ increases. Therefore, the scaling [3] is appropriate to

![FIG. 1: Equilibrium data for the renormalized energy density $E_r$, cf. Eq. (2), for systems with OBC around the FOT point, versus $w = \delta L^\varepsilon$ with $\varepsilon = 3/2$. By increasing the size of the system, the data appear to approach a nontrivial FSS curve (dashed line). The inset shows the data of the low-T region, versus $w^{-1/\varepsilon} = \delta^{-1/\varepsilon}L^{-\varepsilon};$ the dashed line is a fit to $E_r(w) \approx a_1|w|^{-1/\varepsilon} + a_2|w|^{-2/\varepsilon}$ ($a_1 \approx 0.6$ and $a_2 \approx 0.9$).](image-url)
describe the low-T side of the transition, in an interval \( \delta \sim L^{-s} \) where a significant part of the volume is disordered. Note that, since \(|w^*(L)|\) increases with \( L \), the region of the scaling \( \delta \) is restricted to larger and larger values of \(|w|\) with increasing \( L \). Since boundary effects cannot extend beyond a length scale \( \xi, V_+ \) is limited by \( L\xi \), and \( E_\beta(w^*) \) decreases as \( L \) increases. Nevertheless, this regime turns out to be relevant for the dynamic behavior across the FOT, see below.

We have checked that analogous EFSS behaviors are observed for different geometries and boundary conditions, for example when we consider OBC in the first direction and PBC in the second one, and in the case of fixed boundary conditions in which all spins are equal on the boundary, thus favoring the ordered phase.

We now discuss the dynamical behavior of the system, assuming that it is slowly heated across the FOT, starting from the low-T phase. We consider the linear protocol

\[
\delta(t) \equiv 1 - \beta(t) / \beta_c = t / \tau_s \tag{5}
\]

where \( t \in [t_0, t_f > 0] \) is a time variable varying from a negative to a positive value, and \( \tau_s \) is the time scale of the process. The value \( t = 0 \) corresponds to \( \beta(t) = \beta_c \). The dynamics starts from an ordered configuration with \( M_1 \approx m_0 \), cf. Eq. (3), at \( \beta_i = \beta_c[1 - \delta(t_i)] > \beta_c \), so that \( \delta(t_i) < \delta^*(L) \). Then, the system evolves under a heat-bath MC dynamics \( \delta(\tau) \), which corresponds to a purely relaxational dynamics \( \tau \). The time unit is a heat-bath sweep of the whole lattice. The temperature is changed according to Eq. (5) every sweep, incrementing \( t \) by one. We repeat this procedure several times averaging the observables, such as the energy density \( E(t, t_s, L) = (\mathcal{H})_t / V \) and magnetization \( M_1(t, t_s, L) = (\mu_1)_t \), over the ensemble of configurations obtained by the off-equilibrium protocol at time \( t \).

In systems with OBC the transition from the low-T to the high-T phase occurs through a mixed-phase regime, which is related to the dynamics of a closed domain wall, with a relatively small (negligible in the large-\( L \) limit) thickness, that spatially separates the two coexisting phases, see Fig. 2 For \( w \ll w^* \), such a domain wall is localized at the boundaries, thus \( E_r \approx 0 \). With increasing \( w \), it moves toward the center of the lattice, until the whole volume is in the high-T phase, thus \( E_r \approx 1 \). The transition occurs through a free-energy barrier, hence we expect the system to be out of equilibrium as one moves from one phase to the other.

To identify a scaling regime that describes the dynamic behavior, we must specify appropriate scaling variables. First, we wish to recover the EFSS defined in Eq. (4) in the appropriate limit, see below. Thus, the corresponding dynamic scaling limit should be defined at fixed \( r_1 = \delta(t)L^s = tL^s / \tau_s \). The second scaling variable must be \( t / \tau(L) \), where \( \tau(L) \) is the time scale of the dynamics. The identification of \( \tau(L) \) is strictly dependent on the choice of the EFSS variable. At fixed \( r_1 \), the transition region in which the free energy shows a double-peak structure shrinks as \( L \to \infty \). Therefore, the mixed-disordered coexistence region at \( \delta^* \) is not relevant for the scaling described here. The time interval \( \Delta t \) that the system spends in this region is vanishingly small compared to the relevant time scales: \( \Delta t L^s / \tau_s \to 0 \) in the scaling limit. The transition from the ordered to the disordered phase occurs for \( r_1 > w^* \), i.e., when the free energy has

\[\text{FIG. 2: (Left) Distribution of } E_r \text{ for various values of } L \text{ at } w = w^*, \text{ which is where the specific heat has a maximum (this is very close to the value where the areas below the two peaks are equal). Here } q = 10. \text{ (Right) A typical "low-temperature" configuration with } L = 192 \text{ at } w = w^*: \text{ the same color and symbol corresponds to the same value of the spin.}\]
only the high-\(T\) minimum. Under these conditions, we expect \(\tau(L) \sim L^z\) with \(z = 2\), which is the expected behavior of the time scale for the shrinking of an ordered domain surrounded by the more stable disordered phase under a purely relaxational dynamics \cite{Nienhuis}. Therefore, the relevant scaling variables are \(r_1 = (t/t_s)L^z\) and \(r_2 = t/L^z\), or their combinations

\[
s_1 = t_s/L^{z+z}, \quad s_2 = t/t_s^{z+1}(z+z).
\]

(6)

OFSS develops in the limit \(t, t_s, L \to \infty\) keeping \(s_1\) and \(s_2\) fixed. For example, we expect

\[
E_s(t, t_s, L) \equiv E(t, t_s, L) - E_s^- \approx E_o(s_1, s_2).
\]

(7)

Analogously \(m_r \equiv M_1(t, t_s, L)/m_0 \approx M_o(s_1, s_2)\). The EFSS of Eq. \(\ref{eq:EFSS} \) must be recovered for large values of \(s_1\) keeping \(r_1\) fixed, where \(E_o(s_1, s_1^{7/2}/z) \approx E_s(r_1)\). The MC results fully support the above OFSS. In particular, Fig. \(\ref{fig:scaling} \) shows that the data at \(t = 0\), thus \(s_2 = 0\), approach a function of \(s_1 = t_s/L^{7/2}\), and the data at fixed \(s_1 \approx 0.12\) approach a function of \(s_2 = t/t_s^{7/4}\) (analogous results are obtained for other values of \(s_1\)).

It is important to stress the difference between the types of scaling reported above and those discussed in the literature. For instance, for PBC the relevant time scale scales exponentially \cite{Nienhuis}, \(\tau(L) \sim \exp(\sigma L)\), as it is related to the tunneling time between the two phases. This occurs by means of the generation of strip-like configurations with two interfaces, whose probability is suppressed by a factor \(\exp(-\sigma L)\), where \(\sigma = 2\beta\kappa\) and \(\kappa\) is the interface tension \cite{Nienhuis}. The different behavior observed here has been made manifest by the particular choice of the static scaling variable, which allows us to focus on an emergent mixed regime in systems with OBC. If we were considering an EFSS appropriate to describe the coexistence region, we would also obtain an exponential behavior \(\tau(L) \sim e^{\alpha L}\), where \(\alpha\) is related to the height of the free-energy barrier present at coexistence. These different scalings can be rephrased by considering \(t_s\). In the OBC case, two different regimes appear. There is an intermediate regime in which \(t_s\) scales as \(L^{z+z} = L^{7/2}\) and we observe scaling in terms of \(s_1\) and \(s_2\). On the other hand, for \(t_s\) much larger, \(t_s \sim L^\epsilon e^{\alpha L}\), one should observe a different scaling appropriate to the dynamics in the coexistence region.

Although the numerical data strongly support the existence of the anomalous EFSS, with corresponding OFSS, some open questions still remain, calling for additional studies. In particular, we are not able to predict the exponent \(\epsilon\), which is likely related to the dynamics of the domain wall separating the ordered and disordered phase regions, and its dependence on the spatial dimension.

Our results show that the behavior of mixed phases at FOTs strongly depend on the boundary conditions. In particular, in systems with boundary conditions that favor one of the two phases there exists a scaling regime characterized by the physical coexistence of both phases: the thermodynamically favored phase coexists with the unfavored one, which is stabilized by the boundary conditions. In this scaling regime, in which \(\delta L^\gamma\) is the appropriate scaling variable, if one slowly heats the system across the transition, one may define a dynamical scaling with a characteristic time \(\tau(L)\) that scales as \(L^\gamma\). We expect the main features observed in the Potts model with OBC to be generally shared by systems at thermal FOTs when boundary conditions favor one of the two phases. Moreover, we expect that the main properties of the off-equilibrium behavior across the FOT also hold for other types of dynamics, for example in the presence of conservation laws. We note that power-law OFSS are generally observed at continuous transitions \cite{Nienhuis,Nienhuis2}. Our study shows that the main distinguishing feature of the OFSS across a FOT is related to the existence of a mixed regime, where the two phases are spatially separated.

Unlike PBC, boundary favoring one of the two phases are of experimental interest. Their EFSS and OFSS may be exploited to gain evidence of a FOT in experiments with finite-size systems in off-equilibrium conditions. For example, they are relevant for heavy-ion experiments \cite{Nienhuis3} searching for evidences of FOTs in the hadron-matter phase diagram \cite{Nienhuis4}. According to our results, when the quark-gluon plasma cools down across the FOT line, a scaling behavior can be observed on time scales \(\tau \sim L^\ell\), where \(\ell\) is the size of quark-gluon plasma, expected to be a few fm. Note that, since the cooling is relatively fast—typical times should be of the order of a few fm/c—this is probably the only scaling behavior that can be observed in practice. As already noted, power-law OFSS behaviors also characterize continuous transitions; however, the key feature of the crossing of a FOT line should be that it occurs through a mixed regime, where the hadronic and quark-gluon phases are spatially separated.

We finally mention that anomalous EFSS, and corresponding OFSS, are expected to also arise at quantum FOT of many-body systems whose boundary conditions favor one of the two phases. The recent great progress in the control of isolated small quantum systems \cite{Nienhuis5,Nienhuis6} may allow their experimental investigations.

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[24] Numerical results for q = 10 show an analogous behavior (they will be reported elsewhere). However, its convergence to the large-L behavior appears slower. This is not unexpected, since EFSS requires $L \gg \xi$ at the FOT, where $\xi$ are the correlation lengths of the pure phases at $T_c^\pm$, which are $\xi^\pm \approx 2.7$ for q = 20 and $\xi^\pm \approx 10.5$ for q = 10 (see A. Klümper, A. Schadschneider, and J. Zittartz, Z. Phys. B 76, 247 (1989); E. Buddenhoir and S. Wallon, J. Phys. A 26, 3045 (1993); F. Iglói and E. Carlon, Phys. Rev. B 59, 3783 (1999); W. Janke and S. Kappler, Europhys. Lett. 31, 345 (1995)).

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[26] The resulting asymptotic OFSS around $\delta(t) = 0$ does not depend on the initial finite value of $\delta_i < 0$, because it develops in a narrow range around $\delta(t) \approx 0$. It does not depend on the final value $\delta_f > 0$ either.