Corrections to local scale invariance in the nonequilibrium dynamics of critical systems: Numerical evidences

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Local scale invariance (LSI) has been recently proposed as a possible extension of the dynamical scaling in systems at the critical point and during phase ordering. LSI has been applied *inter alia* to provide predictions for the scaling properties of the response function of nonequilibrium critical systems in the aging regime following a quench from the high-temperature phase to the critical point. These predictions have been confirmed by Monte Carlo simulations and analytical results for some specific models, but they are in disagreement with field-theoretical predictions. By means of Monte Carlo simulations of the critical two- and three-dimensional Ising model with Glauber dynamics, we study the intermediate integrated response, finding deviations from the corresponding LSI predictions that are in qualitative agreement with the field-theoretical computations. This result casts some doubts on the general applicability of LSI to critical dynamics.

I. INTRODUCTION

The nonequilibrium dynamics of systems at the critical point has been recently the subject of a renewed interest due to its similarities with the aging phenomena occurring in a variety of glassy materials (see Refs. 1–3 for reviews). In the typical scenario the system is prepared in the high-temperature equilibrium state. Then, at time $t=0$, it is quenched to the critical temperature T_c. Due to the critical dynamics, after this sudden thermal perturbation the system undergoes a neverending relaxation towards the equilibrium state. Interesting scaling properties of this evolution are revealed by two-time quantities such as the correlation function $C_{\mathbf{x}}(t,s) = \langle \phi_{\mathbf{x}}(t)\phi_{\mathbf{0}}(s) \rangle$ and the linear response function $R_{\mathbf{x}}(t,s) = \delta \langle \phi_{\mathbf{x}}(t) \rangle / \delta h_{\mathbf{0}}(s)|_{h=0}$, where $\phi_{\mathbf{x}}(t)$ is the order parameter at the point $\mathbf{x}$ and time t, and $h_{\mathbf{0}}(s)$ is the conjugated field at time $s < t$ and position $\mathbf{x}=\mathbf{0}$ (here translational invariance is assumed).

In thermal equilibrium C and R depend on $t-s$ and they are related by the fluctuation-dissipation theorem, whereas in the present case they are nontrivial functions of both times. This is the so-called aging regime.[1–3] In particular, in the dynamical scaling regime $s \gg \tau_{\text{micro}}$ and $t-s \gg \tau_{\text{micro}}$, where τ_{micro} is some microscopic time, the autoresponse function $R_{\mathbf{x}=\mathbf{0}}$ is expected to scale as[1,2]

$$R_{\mathbf{x}=\mathbf{0}}(t,s) = \mathcal{A}_R (t-s)^{-(a+1)}(t/s)^{\theta} \mathcal{F}_R(s/t). \quad (1)$$

The scaling function $\mathcal{F}_R(v)$ is universal in the sense that it depends only on the universality class of the statistical system, provided one fixes the nonuniversal constant $\mathcal{A}_R$ to have $\mathcal{F}_R(0)=1$. The exponent θ is related to the initial-slip exponent of the magnetization[4] (equivalently to the autocorrelation exponent[5] λ, as $\theta=1+a-\lambda/z$), whereas $a=2\beta/(\nu z)=(d-2+\eta)/z$. Here β, ν, and η are the usual static critical exponents, d is the number of space dimensions, and z is the dynamic critical exponent.

Equation (1) is basically obtained (for example within the renormalization-group approach)[3,4] by exploiting the fact that, at the critical point, the response function transforms covariantly under dilatations in space $\mathbf{x} \mapsto b\mathbf{x}$ and time $t \mapsto b^z t$. It is possible to *prove*, under quite general assumptions, that the covariance of static correlation functions (of suitable operators) under a scale transformation $\mathbf{x} \mapsto b\mathbf{x}$ extends to conformal transformations, resulting in strong constraints on the functional form of the associated scaling functions. It is then natural to address the question whether an analogous extension carries over to the case of dynamic scaling with $z \neq 1$, where the dilatation factors in space and time are different. (In strongly anisotropic systems the role of the time is formally played by a special direction in space.[6]) This possibility has been recently investigated, leading to the identification of a group of local scale transformations which generalize the dynamic scaling.[7,8] The covariance of the dynamic correlation functions (of suitable operators) under such a group is called Local scale invariance (LSI). The conditions under which the dynamical scaling implies LSI have not yet been established beyond the specific case[9] $z=2$. In the absence of such a general result one can heuristically *assume* LSI and then check whether its predictions are actually confirmed. For the response function in aging systems [see Eq. (1)] LSI yields[7,8,10]

$$\mathcal{F}_R^{(\text{LSI})}(v) \equiv 1. \quad (2)$$

This prediction has been found in excellent agreement with Monte Carlo simulations of two- and three-dimensional Ising models and the three-dimensional *XY* model, with Glauber dynamics, both at and below T_c (Refs. 7 and 11–13). In all these simulations the measured quantity has been either the autoresponse function $R_{\mathbf{x}=\mathbf{0}}(t,s)$ or some related integrated responses. Moreover the prediction (2) has been also confirmed by analytical results for spherical models with nonconserved order parameter[4,14] and for the two-

dimensional XY model in the spin-wave approximation.[15] These findings strongly support the idea that LSI is actually realized at the critical point, providing constrains on the form of scaling functions.

For the spatial dependence of the response function LSI predicts[8]

$$R_{\mathbf{x}}(t,s) = R_{\mathbf{x}=0}(t,s)\Phi(|\mathbf{x}|(t-s)^{-1/z}), \qquad (3)$$

where the function Φ satisfies a (fractional) differential equation whose general solution is reported in Ref. 8.

Instead of studying numerically local quantities, one can consider global ones such as the time-dependent total order parameter $M(t)=\int d^d x \phi_{\mathbf{x}}(t)=\phi_{\mathbf{q}=0}(t)$ (**q** is the wave vector). The linear response of $M(t)$ to a homogeneous field $H(s)$ applied at time $s<t$ is given by $\delta\langle M(t)\rangle/\delta H(s)|_{H=0}$ $=R_{\mathbf{q}=0}(t,s)\equiv\int d^d x R_{\mathbf{x}}(t,s)$. This quantity, for nonconserved dynamics, is expected to scale as[3]

$$R_{\mathbf{q}=0}(t,s) = \hat{\mathcal{A}}_R(t-s)^{-(a+1)+d/z}(t/s)^\theta\hat{\mathcal{F}}_R(s/t), \qquad (4)$$

where the nonuniversal constant $\hat{\mathcal{A}}_R$ is fixed requiring $\hat{\mathcal{F}}_R(0)=1$, and $\hat{\mathcal{F}}_R(v)$ is a universal scaling function. From Eq. (3) one can work out the prediction of LSI for this susceptibility, finding

$$\hat{\mathcal{F}}_R^{(\text{LSI})}(v) \equiv 1 \qquad (5)$$

and $\hat{\mathcal{A}}_R^{(\text{LSI})}=\mathcal{A}_R\int d^d x \Phi(\mathbf{x})$. In spite of the support to the LSI prediction Eq. (2) provided by the result of Monte Carlo simulations of some critical lattice models, recent field-theoretical (FT) computations[3,16] suggest the presence of corrections to Eq. (2). For the universality class of models in d dimensions with N-component order parameter, short-range interactions with $O(N)$ symmetry, and purely dissipative dynamics (model A of Ref. 17), it has been predicted

$$\hat{\mathcal{F}}_R^{(\text{FT})}(v) = 1 - \epsilon^2 c_N \Delta f(v) + O(\epsilon^3), \qquad (6)$$

where $c_N=3(N+2)/[8(N+8)^2]$ and $\epsilon=4-d>0$. $\Delta f(v) \equiv f(0)-f(v)>0(0\leq v\leq 1)$ is a monotonically increasing and regular function of order of unity, whose expression can be found in Ref. 16. In particular Eq. (6) with $N=1$ provides, in the dimensional expansion, an analytic prediction for the universal scaling function of the Ising model with Glauber dynamics. Note that $\hat{\mathcal{F}}_R^{(\text{FT})}=\hat{\mathcal{F}}_R^{(\text{LSI})}+O(\epsilon^2)$, i.e., the prediction of LSI coincides with the Gaussian approximation for the scaling function. This observation accounts for the agreement between LSI and the analytical results for spherical models with $2<d<4$, mentioned above. Indeed, apart from non-mean-field exponents, they typically display Gaussian universal scaling functions.

The discrepancy between $\hat{\mathcal{F}}_R^{(\text{FT})}$ and $\hat{\mathcal{F}}_R^{(\text{LSI})}$ casts some doubts on the effective realization of LSI at the critical point and calls for a more careful analysis of the results obtained by Monte Carlo simulations, given that no discrepancy is emerging from the data presented in the past.

II. THE INTERMEDIATE INTEGRATED RESPONSE

We consider the susceptibility $(s<t)$,

$$\chi(t,s) = \int_{s/2}^s du R_{\mathbf{q}=0}(t,u), \qquad (7)$$

which is the integrated linear response of the order parameter to a spatially homogeneous field switched on during the time interval $[s/2,s]$. This integrated response, corresponding to the intermediate protocol proposed in Ref. 11, presents some advantages over the more commonly studied thermoremanent susceptibility $\rho_{\text{TRM}}(t,s)=\int_0^s du R_{\mathbf{q}=0}(t,u)$ and zero-field-cooling susceptibility $\chi_{\text{ZFC}}(t,s)=\int_s^t du R_{\mathbf{q}=0}(t,u)$. As first noted in Ref. 18, ρ_{TRM} is in general hampered by the presence of a finite-time correction that originates from the response to a change in the initial condition. Indeed, at the lower integration limit the necessary conditions for the dynamical scaling regime are not fulfilled and the scaling function (4) cannot be used in that regime. As discussed in Ref. 19 a similar remark applies to χ_{ZFC} close to the upper integration limit, which contributes with a leading term that is independent of the waiting time s, the expected scaling part being only a subleading correction. These problems with the applicability of the scaling form (4) are not encountered for the intermediate integrated response (7).

The expected scaling behavior of $\chi(t,s)$ can be worked out from Eq. (4),

$$\chi(t,s) = \hat{\mathcal{A}}_\chi t^{-a+d/z}\left(\frac{s}{t}\right)^{1-\theta}\hat{\mathcal{F}}_\chi(s/t), \qquad (8)$$

where $\hat{\mathcal{A}}_\chi=\hat{\mathcal{A}}_R B_\theta$,

$$\hat{\mathcal{F}}_\chi(v) = B_\theta^{-1}\int_{1/2}^1 dw(1-vw)^{-(a+1)+d/z}w^{-\theta}\hat{\mathcal{F}}_R(vw), \qquad (9)$$

and $B_\theta\equiv(1-2^{\theta-1})/(1-\theta)$, so that $\hat{\mathcal{F}}_\chi(0)=1$. The prediction of LSI that follows from Eq. (5) is given by

$$\hat{\mathcal{F}}_\chi^{(\text{LSI})}(v) = \frac{B_\theta^{-1}}{1-\theta}[{}_2F_1(1-\theta,1+a-d/z,2-\theta;v)$$
$$- 2^{\theta-1}{}_2F_1(1-\theta,1+a-d/z,2-\theta;v/2)], \qquad (10)$$

whereas the FT prediction is obtained from Eq. (6), with $\theta=O(\epsilon)$, $z=2+O(\epsilon^2)$, and $\eta=O(\epsilon^2)$,

$$\frac{\hat{\mathcal{F}}_\chi^{(\text{FT})}(v)}{\hat{\mathcal{F}}_\chi^{(\text{LSI})}(v)} = 1 - \epsilon^2 c_N \frac{2}{v}\int_{v/2}^v du\Delta f(u) + O(\epsilon^3). \qquad (11)$$

We study the intermediate integrated response (7) by simulating Ising models on square and on cubic lattices. The systems are thereby prepared in a completely uncorrelated initial state and then quenched at time $t=0$ to the critical point. The temporal evolution is realized using the standard heat-bath algorithm. At time $t=s/2$ a spatially constant field with strength $H=0.05J$ (J being the strength of the nearest-neighbor couplings) is applied. This external field is switched off at $t=s$. We checked that for this field strength
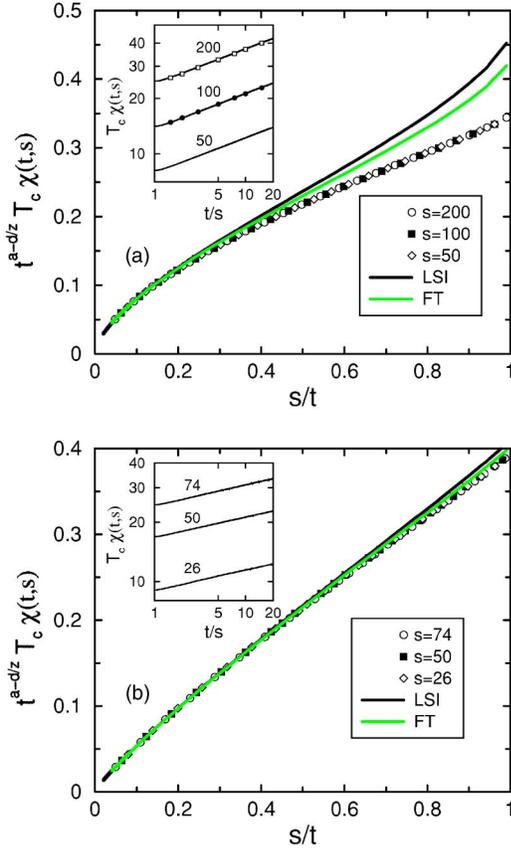
FIG. 1. Rescaled intermediate integrated response vs s/t for different waiting times s computed in the critical Ising model in (a) two and (b) three dimensions. In both cases a perfect data collapse is observed. The LSI prediction lies systematically above the numerical data for larger values of s/t, whereas the two-loop correction shifts the theoretical curve closer to the data. Error bars are smaller than the sizes of the symbols. The insets display the power-law increase of χ as a function of t/s for fixed values of s. In the inset of (a) we also probe the linear-response regime. Solid lines have been obtained with the field strength $H=0.05J$, whereas the symbols for $s=200$ and $s=100$ result from simulations with $H=0.025J$ and $H=0.1J$, respectively. The measured susceptibility does not depend on H, showing that we are well within the linear-response regime.

we are well within the linear-response regime, as shown in the inset of Fig. 1(a). The data discussed in the following are free from any finite-size effects and have been obtained for systems consisting of 450×450 spins in two dimensions and $80 \times 80 \times 80$ spins in three dimensions. Typically, we averaged over 50 000 different runs with different realizations of the thermal noise.

The temporal evolution of the integrated response

$$\chi(t,s) = \frac{1}{nH} \left\langle \sum_{i=1}^{n} S_i(t) \right\rangle, \quad t > s \qquad (12)$$

is shown in the insets of Fig. 1 in two and three dimensions. Here $S_i(t) \in \{-1, +1\}$ is the value of the Ising spin located at the lattice site i at time t. The sum in (12) is over all n sites and $\langle \cdots \rangle$ indicates the average over the thermal noise. A simi-
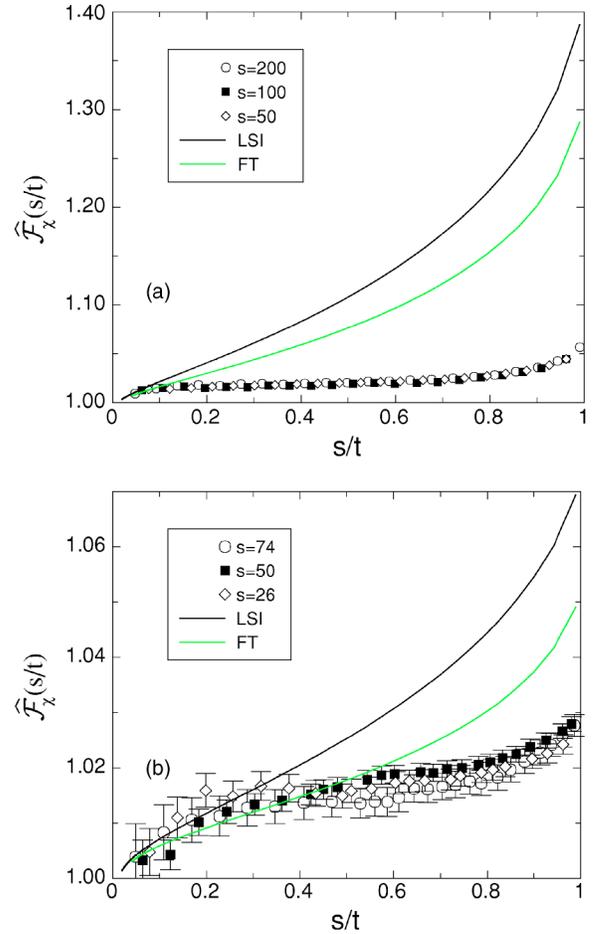

FIG. 2. Comparison of the numerically obtained scaling functions $\hat{\mathcal{F}}_\chi$ with the theoretical predictions in (a) two and (b) three dimensions. Corrections to LSI are clearly observed for this quantity in both cases. In (a) error bars are comparable to the symbol sizes.

lar behavior is observed in two and three dimensions: for a fixed value of the waiting time s the susceptibility rapidly displays a power-law increase as a function of t/s, with exponent $(d-\lambda)/z$ [see Eq. (8)]. Its measured values in two and three dimensions [0.186(2) and 0.108(2), respectively] are in excellent agreement with the expected values 0.185 and 0.108, obtained by using the known values of $\lambda(d=2:1.60, d=3:2.78)$ and $z(d=2:2.17, d=3:2.04)$.[3,7]

The scaling behavior (8) is tested in the main images of Fig. 1. Plotting $t^{a-d/z}\chi$ as a function of s/t yields a remarkable data collapse. The scaling functions so obtained can be compared with the available analytical predictions. In particular, assuming the well-known values of the critical exponents appearing in Eq. (8) (Refs. 3 and 7), one determines the nonuniversal constant $\hat{\mathcal{A}}_\chi$ from the small s/t behavior of $t^{a-d/z}\chi$. Then the prediction of LSI and FT are given by $\hat{\mathcal{A}}_\chi (s/t)^{1-\theta} \hat{\mathcal{F}}_\chi^{(LSI),(FT)}$, where $\hat{\mathcal{F}}_\chi^{(LSI)}$ is provided in Eq. (10) with $\theta=0.38$, $a=0.115$ in $d=2$ and $\theta=0.14$, $a=0.506$ in $d=3$. The numerical estimate of $\hat{\mathcal{F}}_\chi^{(FT)}$ is obtained through Eq. (11) with $N=1$, $\epsilon=2$ and 1 in two and three dimensions, respectively, corresponding to its Padé approximant [2,0],

which does not differ significantly from the approximant [0,2]. The comparison shows that the LSI curves (black lines) systematically lie above the numerical data for larger values of s/t. Including the two-loop correction coming from field theory shifts the theoretical curves (gray lines) closer to the data. This provides a numerical evidence for the existence of corrections to LSI in critical nonequilibrium systems.

Finally, we show in Figs. 2(a) and 2(b) the scaling function $\hat{\mathcal{F}}_\chi(s/t)$ obtained from the data of Fig. 1 after a multiplication by $(s/t)^{\theta-1}$ and a proper normalization. Corrections to the LSI predictions are clearly revealed in this quantity both in two and three dimensions. Analyzing the scaling function $\hat{\mathcal{F}}_\chi(s/t)$ seems therefore to be the appropriate way to highlight differences between the theoretical predictions and the numerical data. In the more common approach, where the rescaled susceptibility $s^{a-d/z}\chi$ is plotted against t/s, corrections are hardly detectable in three dimensions.

III. CONCLUSIONS

Local scale invariance proposes to generalize dynamical scaling to local space- and time-dependent scale transformations, leading to several predictions for dynamical correlation and response functions. Some of these predictions have been verified in the past through exact solutions of soluble models and through numerical simulations of nonsoluble ones. In this paper we have focused on the scaling functions of the dynamic response function in nonequilibrium critical Ising models. Previous numerical studies did not reveal any systematic deviations from the LSI prediction when computing local quantities. Recent field-theoretical calculations, however, yielded a two-loop correction to the LSI prediction. In the present work we have studied the nonequilibrium response of the total order parameter to an homogeneous external field, i.e., we have investigated a global quantity. It has been realized recently that in the usually studied integrated responses, the thermoremanent susceptibility, and the zero-field-cooling susceptibility, additional terms appear that make the study of the dynamical scaling part (i.e., the aging part) notoriously difficult. We therefore propose to study the intermediate integrated response where the field is only switched on during a time interval $[s/2,s]$, with $0<s<t$, t being the time at which the resulting magnetization is measured, and 0 the time at which the quench to the critical point occurs. Looking at this quantity we have indeed identified corrections to the LSI prediction. In addition, we observe that the field-theoretical two-loop correction brings the theoretical curve closer to the numerical data.

[1] L. F. Cugliandolo, in *Slow Relaxation and NonEquilibrium Dynamics in Condensed Matter*, edited by J.-L. Barrat, J. Dalibard, J. Kurchan, and M. V. Feigel'man, Proceedings of the Les Houches Session 77 July 2002 (Springer, New York, 2003).

[2] C. Godrèche and J.-M. Luck, J. Phys.: Condens. Matter **14**, 1589 (2002).

[3] P. Calabrese and A. Gambassi, cond-mat/0410357; J. Phys. A (to be published).

[4] H. K. Janssen, B. Schaub, and B. Schmittmann, Z. Phys. B: Condens. Matter **73**, 539 (1989).

[5] D. A. Huse, Phys. Rev. B **40**, 304 (1989).

[6] M. Pleimling and M. Henkel, Phys. Rev. Lett. **87**, 125702 (2001).

[7] M. Henkel, M. Pleimling, C. Godrèche, and J.-M. Luck, Phys. Rev. Lett. **87**, 265701 (2001).

[8] M. Henkel, Nucl. Phys. B **641**, 405 (2002).

[9] M. Henkel and J. Unterberger, Nucl. Phys. B **660**, 407 (2003).

[10] Note that LSI does not fix the values of the critical exponents appearing in Eq. (1).

[11] M. Henkel, M. Paeßens, and M. Pleimling, Europhys. Lett. **62**, 664 (2003); Phys. Rev. E **69**, 056109 (2004).

[12] M. Henkel and M. Pleimling, Phys. Rev. E **68**, 065101(R) (2003).

[13] S. Abriet and D. Karevski, Eur. Phys. J. B **41**, 79 (2004).

[14] C. Godrèche and J. M. Luck, J. Phys. A **33**, 9141 (2000).

[15] A. Picone and M. Henkel, Nucl. Phys. B **688**, 217 (2004).

[16] P. Calabrese and A. Gambassi, Phys. Rev. E **65**, 066120 (2002); **66**, 066101 (2002).

[17] P. C. Hohenberg and B. I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).

[18] W. Zippold, R. Kühn, and H. Horner, Eur. Phys. J. B **13**, 531 (2000).

[19] M. Pleimling, Phys. Rev. E **70**, 018101 (2004).