Nonequilibrium Dynamics following a Quench to the Critical Point in a Semi-infinite System

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We study the nonequilibrium dynamics (purely dissipative and relaxational) in a semi-infinite system following a quench from the high temperature disordered phase to its critical temperature. We show that the local autocorrelation near the surface of a semi-infinite system decays algebraically in time with a new exponent which is different from the bulk. We calculate this new nonequilibrium surface exponent in several cases, both analytically and numerically.

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There has been a lot of current interest in understanding the growth of correlations in a system after being quenched from the high temperature disordered phase to or below its critical temperature (T_c) [1]. In either case the system exhibits dynamic scaling at late stage of the growth. The growth is characterized by a single time dependent length scale. For quench to below T_c, this length scale characterizes the linear size of the growing domains of competing broken symmetry phases. On the other hand, for quench to T_c, it characterizes the length scale over which equilibrium critical properties are established. A lot of theoretical and experimental efforts have been directed in determining the time dependence of this length scale and the scaling of the equal-time correlation functions. It was, however, realized later that even the two-time correlation functions have interesting dynamical scaling [2,3]. In particular, the autocorrelation function, measuring the memory of the initial conditions retained by the system after time t, decays algebraically with time [2]. This has been verified by exact calculations in a few cases [4–9], numerical simulations [10] and very recently experimentally [11] for quench to $T < T_c$, in a liquid crystal system using video microscopy.

In static critical phenomena, it is well known that the critical behavior near the boundary of a semi-infinite system is drastically different from the behavior deep inside the bulk [12–18]. It is therefore natural and important to know whether there are similar modifications in the dynamical behavior near the boundary. In this Letter we demonstrate, both analytically and numerically, that the temporal decay of the critical autocorrelations near the boundary of a semi-infinite system is characterized by new exponents different from that in the bulk.

We consider a semi-infinite $O(n)$ model in the space $[\vec{x} = (\vec{r}, z)]$ which extends over infinite space in $d - 1$ directions (denoted by $\vec{r}$) and over only positive half-space in one direction ($z \geq 0$). The system is assumed to be translationally invariant in the $d - 1$ directions, and this invariance is broken in the z direction due to the presence of a surface at $z = 0$. The model is described by an n component order parameter field $\vec{\phi} = [\phi_1, \ldots, \phi_n]$ and a coarse grained Landau-Ginzburg free energy functional with an additional surface contribution [15],

$$F(\vec{\phi}) = \frac{1}{2} \int d^d\vec{x}[(\nabla\vec{\phi})^2 + r_0\vec{\phi}^2 + \frac{g}{4}(\vec{\phi}^2)^2 + c\,\delta(z)\vec{\phi}^2], \qquad (1)$$

where the integration in Eq. (1) is over the half-space $z \geq 0$. The equilibrium properties of this model have been studied in detail [14,15]. Depending upon the value of c, different types of surface orderings take place. There exists a special value $c = c^*$ such that, for $c > c^*$, the surface orders along with the bulk at bulk T_c. This parasitical transition is called "ordinary" transition [14,15]. For $c < c^*$ and in high enough dimensions (such that a $d - 1$ dimensional surface can order), the surface orders first as the temperature is lowered, while the bulk is still disordered ("surface" transition) and then as the temperature is lowered further the bulk orders in presence of an ordered surface ("extraordinary" transition). The value $c = c^*$ is a special point where the critical exponents are different from the ordinary or surface transitions. This is called the "special" transition. Within mean field theory, $c^* = 0$ but becomes nonzero for $d < 4$ due to corrections arising from fluctuations [15]. The critical exponents associated with these different types of transitions are different from each other and from the bulk values [15].

In this paper, we consider the nonconserved dynamics of the order parameter field (model A as in [19]) in presence of a surface following a quench from the high temperature disordered ($T > T_c$) to the bulk critical point $T = T_c$ and ask whether the presence of the surface modifies the dynamics near the surface. Far from the surface one should recover the critical dynamics of a truly infinite system for which several results are known. For example, it is now well established [20,21] that the bulk equal-time correlation function, $G(\vec{x}, t) = \langle\phi(\vec{x}', t)\phi(\vec{x}' + \vec{x}, t)\rangle$, exhibits dynamic scaling, $G(\vec{x}, t) \sim x^{-(d-2+\eta)} g_c(x/\xi(t))$,

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where g_c is a universal scaling function and $\xi(t) \sim t^{1/Z}$ is the time-dependent correlation length. η and Z are the usual static and dynamic exponents and the $\langle\,\rangle$ denotes an average over all possible initial conditions (corresponding to the equilibrium distribution at the initial high temperature) and over the history of time evolution. The bulk two-time correlation function $C(\vec{x},t) = \langle\phi(\vec{x}',0)\phi(\vec{x}'+\vec{x},t)\rangle$, measuring the correlation with the initial condition, also exhibits dynamic scaling [12,13], $C(\vec{x},t) \sim [\xi(t)]^{-\lambda_c} f_c(x/\xi(t))$, where $f_c(0)$ is a constant of $O(1)$. The exponent λ_c, characterizing the decay of the bulk autocorrelation, $A_b(t) = \langle\phi(\vec{x},0)\phi(\vec{x},t)\rangle \sim [\xi(t)]^{-\lambda_c}$, is a new critical exponent [20,21] in the sense that no simple scaling relation has been found relating it to other static or dynamic critical exponents. For an infinite system, λ_c has been calculated analytically for the $O(n)$ model in the limit $n \to \infty$ and also within ϵ expansion where $\epsilon = 4 - d$ ($d = 4$ being the upper critical dimension) [21]. For the Ising model in $d = 2$ and 3, λ_c has been determined numerically [20].

The specific dynamical quantity that we calculate explicitly in this paper for the semi-infinite system, and show that it gets drastically modified due to the presence of the surface, is the decay of the autocorrelation $A(z,t) = \langle\phi(\vec{r},z,0)\phi(\vec{r},z,t)\rangle$ with time t. In the limit $z \to \infty$, we recover, as expected, the bulk results $A(\infty,t) \sim [\xi(t)]^{-\lambda_b}$, where we denote the bulk λ_c by λ_b. However, for small z near the surface, we find that the autocorrelator decays as $A_s(t) \sim [\xi(t)]^{-\lambda_s}$, where λ_s is a new dynamical surface exponent different from λ_b. Also, the value of λ_s depends explicitly on the type of the surface transition. In this paper, we calculate λ_s analytically within ϵ expansion and in the $n \to \infty$ limit for the ordinary and special transitions. Also, we determine the value of λ_s numerically for the two-dimensional Ising model.

The model-A dynamics of the order parameter is governed by the Langevin equation,

$$\partial\vec{\phi}/\partial t = -\delta F/\delta\vec{\phi} + \vec{\eta}\,, \tag{2}$$

where F is given by Eq. (1), and $\vec{\eta}(\vec{x},t)$ is a Gaussian noise with zero average and a correlator $\langle\eta_i(\vec{x},t)\eta_j(\vec{x}',t')\rangle = 2k_B T\delta_{i,j}\delta(\vec{x}-\vec{x}')\delta(t-t')$, where T is the temperature. We first consider the Gaussian theory where one neglects the interaction [set $u = 0$ in Eq. (1)] and which is valid for $d > 4$. We define the Fourier transformation $G(\vec{k},z,z',t) = \int d^{d-1}(\vec{r}-\vec{r}') \times G(\vec{r}-\vec{r}',z,z',t)\exp[i\vec{k}\cdot(\vec{r}-\vec{r}')]$, where $\vec{k}$ is a $(d-1)$-dimensional vector in the reciprocal space. Then from Eq. (2), at the critical point ($r_0 = 0$ and setting $k_B T_c = 1$), $G(\vec{k},z,z',t)$ evolves as

$$\partial_t G(\vec{k},z,z',t) = [-2k^2 + \partial_z^2 + \partial_{z'}^2]G(\vec{k},z,z',t) + 2\delta(z-z')\,, \tag{3}$$

with the boundary condition $\partial_z G = cG$ at $z = 0$ and the initial condition $G(\vec{k},z,z',0) = \Delta\delta(z-z')$ [this "white noise" form of the initial condition corresponds to quench from the infinite temperature, where the field $\phi(\vec{x},t)$ is completely random and Δ controls the size of initial onsite fluctuations in ϕ]. Similarly, the symmetrized two-time correlation function $C_s(\vec{k},z,z',t)$ defined as the Fourier transform of $C_s(\vec{k},z,z',t) = \frac{1}{2}\langle(\phi(\vec{r}',z',0)\phi(\vec{r}'+\vec{r},z,t) + \phi(\vec{r}',z,0)\phi(\vec{r}'+\vec{r},z,t)\rangle$ evolves as

$$\partial_t C_s(\vec{k},z,z',t) = \frac{1}{2}[-2k^2 + \partial_z^2 + \partial_{z'}^2]C_s(\vec{k},z,z',t)\,, \tag{4}$$

with the same boundary and initial conditions. By choosing the basis function

$$\psi(u,z) = \frac{1}{\sqrt{2}}\left[\exp(iuz) - \frac{c-iu}{c+iu}\exp(-iuz)\right], \tag{5}$$

it is easy to see that the solutions to Eqs. (3) and (4) are given by $G(\vec{k},z,z',t) = \int_{-\infty}^{\infty} du\,\psi(u,z)\psi^*(u,z') \times f_1(k,u,t)$ and $C_s(\vec{k},z,z',t) = \int_{-\infty}^{\infty} du\,\psi(u,z)\psi^*(u,z') \times f_2(k,u,t)$, where

$$f_1(k,u,t) = \Delta\exp[-2(k^2+u^2)t] + \frac{1-\exp[-2(k^2+u^2)t}{k^2+u^2}\,, \tag{6}$$

$$f_2(k,u,t) = \Delta\exp[-(k^2+u^2)t]\,. \tag{7}$$

Therefore the autocorrelation $A(z,t) = \int C_s(\vec{k},z,z,t) \times d^{d-1}\vec{k}/(2\pi)^{d-1}$ is given by

$$A(z,t) \sim t^{-(d-1)/2}\int_0^\infty du\,\exp(-u^2 t) \times \frac{(c\sin uz + u\cos uz)^2}{c^2+u^2}\,. \tag{8}$$

It is clear from Eq. (8) that in the limit $z \to \infty$ we recover the bulk result: for large t, $A(\infty,t) \sim [\xi(t)]^{-d}$, where $\xi(t) \sim t^{1/2}$ ($Z = 2$ within Gaussian theory) and hence $\lambda_b = d$. On the other hand, for $z = 0$, we find that, for large t, $A(0,t) \sim [\xi(t)]^{-(d+2)}$ for $c > 0$ and $A(0,t) \sim [\xi(t)]^{-d}$ for $c = 0$. Thus we obtain the results that for the special transition ($c = 0$) $\lambda_{\rm sp} = d$ while for the ordinary transition ($c > 0$), $\lambda_{\rm or} = d + 2$ within the Gaussian theory. It is interesting to note that while λ_b satisfies the upper bound $\lambda_b \le d$ conjectured by Fisher and Huse [2], clearly $\lambda_{\rm or}$ violates this upper bound.

For $d < 4$, where the interaction term is no longer irrelevant, we evaluate the exponent λ_c in $\epsilon = 4 - d$ expansion. The two-time correlator (unsymmetrized) $C(\vec{x},\vec{x}',t) = \langle\phi(\vec{x}',0)\phi(\vec{x},t)\rangle$ in real space evolves as

$$\partial_t C(\vec{x},\vec{x}',t) = [-r_0 + \nabla^2]C(\vec{x},\vec{x}',t) - \frac{g}{n}\sum_{ij}\langle\phi_i(\vec{x}',0)\phi_i(\vec{x},t) \times \phi_j(\vec{x},t)\phi_j(\vec{x},t)\rangle\,. \tag{9}$$

At the Wilson-Fisher fixed point, $g = 8\pi^2\epsilon/(n+8)$ to leading order in ϵ [15]. This allows one to calculate the corrections to the two-point correlator pertubatively in g. To leading order in ϵ, the term proportional to g in Eq. (9) can be expressed, using Wick's theorem, in terms of the mean-field propagators as $-g(n+2)G_0(\vec{x},\vec{x},t)C_0(\vec{x}',\vec{x},t)$, where G_0 and C_0 denote the mean-field equal-time and two-time propagators, respectively. To leading order in ϵ, one can replace C_0 in this term by C, and then Eq. (9) becomes a linear evolution equation for the two-time correlator which is correct to $O(\epsilon)$. This evolution equation, for the symmetrized correlator $C_s(\vec{x},\vec{x}',t)$, reads

$$\partial_t C_s(\vec{x},\vec{x}',t) = \frac{1}{2}[-2\tilde{r}_0 + \nabla^2_{\vec{x}} + \nabla^2_{\vec{x}'} - V(z,t) - V(z',t)]C_s(\vec{x},\vec{x}',t), \qquad (10)$$

with $\tilde{r}_0 = r_0 + g(n+2)G_0(\infty,\infty,\infty)$, where $G_0(\vec{x},\vec{x}',t)$ denotes the mean-field equal-time propagator. The potential $V(z,t) = g(n+2)\int[G_0(\vec{k},z,z,t) - G_0(\vec{k},\infty,\infty,\infty)]d^3(\vec{k})/(2\pi)^3$ captures the corrections due to fluctuations for $d<4$ and can be calculated explicitly. For example, at the special ($c=0$) and the ordinary ($c=\infty$) fixed points, we get $V_{\rm sp}(x,x,t) = -g(n+2)[1+(2t/z^2)\exp(-z^2/2t)]/32\pi^2 t$ and $V_{\rm or}(z,z,t) = -g(n+2)[1-(2t/z^2)\exp(-z^2/2t)]/32\pi^2 t$ in the scaling regime where $z \gg \Lambda^{-1}$, Λ being the upper cutoff.

Equation (10) and the form of the potential $V(z,t)$ suggest a late time scaling ansatz for the Fourier transform $C_s(\vec{k},z,z',t) \approx t^{-\alpha}\exp(-k^2 t)f[z/\sqrt{t}, z'/\sqrt{t}]$. To determine the exponent α we first consider the bulk limit $z\to\infty, z'\to\infty$. Using $V(\infty,\infty,t) = -g(n+2)/32\pi^2 t$ and $g = 8\pi^2\epsilon/(n+8)$ in Eq. (10) we get $\alpha = \frac{1}{2} - (n+2)\epsilon/4(n+8)$ and $f(x,y) \sim e^{-(x-y)^2}$ as $x,y\to\infty$. It follows immediately that the bulk autocorrelation $A_b(t) \sim t^{-[d-(n+2)/(n+8)(\epsilon/2)]/2}$. Since the dynamic exponent $Z = 2 + O(\epsilon^2)$, we recover the bulk result $\lambda_b = d - \frac{n+2}{n+8}\frac{\epsilon}{2}$. For the surface autocorrelator, we need to know the small argument behavior of the scaling function $f(x,y)$. For small x,y, $f(x,y) \sim (xy)^s(a + bx^2 + cy^2 + \cdots)$ where $s(s-1) = \pm\frac{n+2}{n+8}\frac{\epsilon}{2}$ and $\pm$ corresponds to special and to ordinary transitions, respectively. Then the autocorrelator $A(x,t) = \int C_s(\vec{k},z,z,t)d^{d-1}k/(2\pi)^{d-1} \sim t^{-(d-1+2s+2\alpha)/2}$. We choose the root of s to match the $\epsilon\to 0$ limit and get $\lambda_{\rm sp} = d - \frac{n+2}{n+8}\frac{3\epsilon}{2}$ for special transition and $\lambda_{\rm or} = d + 2 - \frac{n+2}{n+8}\frac{3\epsilon}{2}$ for the ordinary one.

We next calculate λ_c exactly in the large n limit. In this limit, $C_s(\vec{x},\vec{x}',t)$ satisfies Eq. (10) exactly except that the potential $V(z,t)$ is determined self-consistently from $V(z,t) = g(n+2)\int[G(\vec{k},z,z,t) - G(\vec{k},\infty,\infty,\infty)]d^{d-1}(\vec{k})/(2\pi)^{d-1}$, where the equal-time propagator of $G(\vec{k},z,z',t)$ satisfies

$$\partial_t G(\vec{k},z,z',t) = [-2k^2 + \partial_z^2 + \partial_{z'}^2 - V(z,t) - V(z',t)]G(\vec{k},z,z',t) + 2\delta(z-z'). \qquad (11)$$

In analogy with epsilon expansion, we make the ansatz $V(z,t) = \frac{a}{2t} + \frac{(\mu^2-1/4)}{z^2}g[z/\sqrt{t}]$, where $g(x)\to 1$ as $x\to 0$ and $g(x)\to 0$ as $x\to\infty$. The values of a and μ are determined, respectively, from the limits $z\to\infty$ (bulk dynamics) and $t\to\infty$ (static limit) and are already known to be $a = (d-4)/2$ [11], $\mu_{\rm sp} = (d-5)/2$ and $\mu_{\rm or} = (d-3)/2$ [15]. The full form of the scaling function $g(x)$ is to be determined from a complicated self-consistent equation. However, for the purpose of determining the surface exponent λ_s, it is sufficient to know that $g(0)=1$. We then proceed identically as in the case of ϵ expansion by assuming a scaling ansatz for $C_s(\vec{k},z,z',t)$. We find $\alpha = (1+a)/2$ and $s(s-1) = \mu^2 - 1/4$. Using the fact that $Z=2$ in the large n limit, we obtain $\lambda_{{\rm sp}=(5d-12)/2}$ and $\lambda_{{\rm or}=(5d-8)/2}$. Note that in the limit $z\to\infty$ we recover the bulk result $\lambda_b = (3d-4)/2$. These results are consistent with those obtained from ϵ expansion after taking $n\to\infty$ limit and also with the mean field results in $d=4$.

We have also carried out a direct numerical simulation of the two-dimensional Ising model with open boundary conditions at the bulk critical temperature using a spin-flop Metropolis algorithm. We measure boundary spin correlations and compare them with the corresponding bulk measurements done with periodic boundary conditions. In the static limit, it is well known that the boundary spins order only due to the ordering of the bulk spins (ordinary transition) [13–15]. Since at T_c in the static limit, the boundary correlator falls off with distance r as $1/r$ (as opposed to the bulk decay $r^{-1/4}$) for large r [22], it is natural to assume a dynamic scaling form for the equal-time boundary correlator $G_s(r,t) \sim r^{-1}\gamma(r/\xi(t))$ at late times. It is believed that even in the presence of a boundary there is still only a single time-dependent correlation length $\xi(t) \sim t^{1/Z}$ with $Z \approx 2.15$ numerically [23,24]. The quantity $\chi_s(t) = \langle(M_s(t))^2\rangle$ [$M_s(t)$ being the total boundary magnetization at time t] is the integral of the correlation function $\int_s drG_s(r,t)$ on the boundary. From the scaling form of $G_s(r,t)$, $\chi_s(t)$ would then grow logarithmically with $\xi(t)$ (and hence logarithmically with t). In contrast, the corresponding quantity in the bulk,

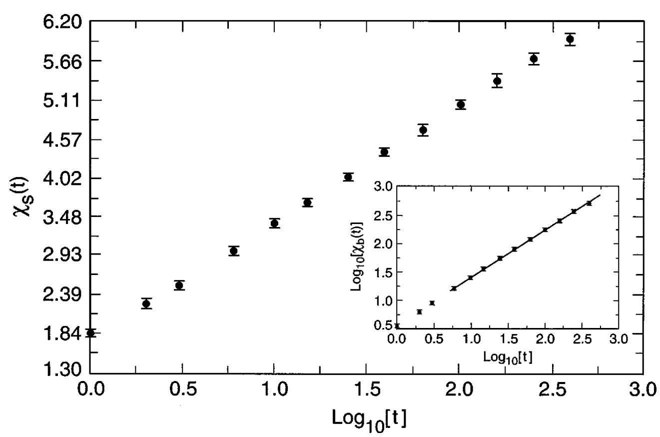

FIG. 1. $\chi_s(t)$ is plotted against $\log(t)$. The logarithmic dependence is pretty evident. The inset shows a log-log plot of $\chi_b(t)$ vs t, which is consistent with a power law.

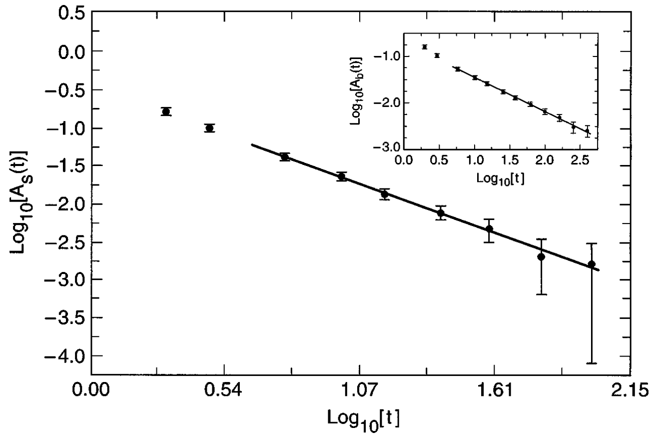

FIG. 2. The autocorrelation on the boundary, $A_s(t)$ vs time t in a log-log plot. From the slope we estimate the boundary exponent ratio $\lambda_{\rm or}/Z = 1.2 \pm 0.1$. The corresponding ratio in the bulk is estimated to be $\lambda_b/Z = 0.74 \pm 0.02$. Bulk data are shown in the inset.

$\chi_b(t) = \langle (M_b(t))^2 \rangle$ (M_b being the total bulk magnetization), grows algebraically as $[\xi(t)]^{7/4}$. In Fig. 1 we plot $\chi_s(t)$ and $\chi_b(t)$ against $\log(t)$ and, in the inset, show a log-log plot of $\chi_b(t)$ vs t. Next we compute the autocorrelation on the boundary of the open system and the periodic bulk system. The two results are contrasted in Fig. 2. The autocorrelation on the boundary decays much faster, as expected. From the slope of the log-log plot in Fig. 2 we estimate the boundary exponent ratio $\lambda_{\rm or}/Z = 1.2 \pm 0.1$. The corresponding ratio in the bulk is estimated to be $\lambda_b/Z = 0.74 \pm 0.02$ in agreement with the previous simulation [20]. Using $Z \approx 2.15$ (assuming Z retains its bulk value in the boundary as argued in [23,24]), we estimate $\lambda_{\rm or} \approx 2.58 \pm 0.1$ to be contrasted with $\lambda_b \approx 1.59 \pm 0.02$.

We calculate, as a simple extension of [9], these boundary autocorrelation exponents exactly, for the dynamics of the X-Y model in two dimensions, following a quench from one temperature to another, both temperatures being below the Kosterlitz-Thouless temperature. We also have some preliminary results on coarsening in the ordered phase of the Ising model in one and two dimensions which seem to indicate $\lambda_s = \lambda_b$ at zero temperature. These and other calculations will be published elsewhere [25].

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Note added.—Since this work was submitted, Ritscel and Czerner [26] pointed out the scaling relation $\lambda_s = \lambda_b + 2(\beta_s - \beta_b)/\nu$, where β and ν refer to the usual static exponents, and the subscripts "s" and "b" refer to surface and bulk, respectively.

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