Non-equilibrium Dynamics Following a Quench to the Critical Point in a Semi-infinite System

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Abstract

We study the non-equilibrium 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 non-equilibrium 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 auto-correlation 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 [14] 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 behaviour near the boundary of a semi-infinite system is drastically different from the behaviour deep inside the bulk [14–18]. It is therefore natural and important to know whether there are similar modifications in the dynamical behaviour near the boundary. For the critical dynamics following a quench to $T_c$, it has been argued that even the semi-infinite system is characterized by a single time dependent length scale $\xi(t)$ which has the same growth law as the infinite system [20,21]. However, in this letter we demonstrate, both analytically and numerically, that the temporal decay of the critical auto-correlations 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 [16],

$$F(\vec{\phi}) = \frac{1}{2} \int d^d x [(\nabla \vec{\phi})^2 + r_0 \vec{\phi}^2 + \frac{u}{4} (\vec{\phi}_0^2)^2 + c \delta(z) \vec{\phi}^2],$$

(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 [15,16]. 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 [13,16]. 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 [16]. The critical exponents associated with these different types of transitions are different from each
other and from the bulk values \([14]\). For example, an exact calculation exists \([19]\) for the 2-d semi-infinite Ising model (where the surface undergoes an “ordinary” transition at the bulk \(T_c\) \([10]\) which shows that the two-point correlator between two-points on the surface (separated by \(r\)) decays faster as \(r^{-1}\) for large \(r\) than the bulk correlator that decays as \(r^{-1/4}\).

In this paper, we consider the non-conserved dynamics of the order parameter field 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 \([13,12]\) 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, \(G(\vec{x}, t) \sim x^{-(d-2+\eta)}g_c(x/\xi(t))\) where \(g_c\) is a universal scaling function and \(\xi(t) \sim t^{1/2}\) is the time-dependent correlation length. \(\eta\) 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 \([13,12]\), \(C(\vec{x}, t) \sim [\xi(t)]^{-\lambda_c}f_c(x/\xi(t))\) where \(f_c(0)\) is a constant of \(O(1)\). The exponent \(\lambda_c\), characterizing the decay of the bulk autocorrelation, \(A_0(t) = \langle \phi(\vec{x}', 0)\phi(\vec{x}', t) \rangle \sim [\xi(t)]^{-\lambda_c}\), is a new critical exponent \([12,13]\) in the sense that no simple scaling relation has been found relating it to other static or dynamic critical exponents. For an infinite system, \(\lambda_c\) has been calculated analytically for the \(O(n)\) model in the limit \(n \to \infty\) and also within \(\epsilon\)-expansion where \(\epsilon = 4 - d\) (\(d = 4\) being the upper critical dimension) \([13]\). For Ising model in \(d = 2\) and \(3\), \(\lambda_c\) has been determined numerically \([12]\).

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 auto-correlation \(A(z, t) = \langle \phi(\vec{r}, z, 0)\phi(\vec{r}, z, t) \rangle\) 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 \(\lambda_c\) by \(\lambda_b\). However, for small \(z\) near the surface, we find that the autocorrelator decays as \(A_s(t) \sim [\xi(t)]^{-\lambda_s}\) where \(\lambda_s\) is a new dynamical surface exponent different from \(\lambda_b\). Also, the value of \(\lambda_s\) depends explicitly on the type of the surface transition. In this paper, we calculate \(\lambda_s\) analytically within \(\epsilon\)-expansion and in the \(n \to \infty\) limit for the “ordinary” and “special” transition. Also, we determine the value of \(\lambda_s\) numerically for the two-dimensional Ising model.

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

\[
\frac{\partial \vec{\phi}}{\partial t} = -\frac{\delta F}{\delta \vec{\phi}} + \vec{\eta}
\]

(2)

where \(\vec{F}\) is given by Eq. \([1]\) and \(\vec{\eta}(\vec{x}, t)\) is a Gaussian noise with zero average and a correlator \(\langle \eta_i(\vec{x}, t)\eta_j(\vec{x}', t') \rangle = 2k_BT\delta_{ij}\delta(\vec{x} - \vec{x}')\delta(t - t')\), 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 transform, \(G(\vec{k}, z, z', t) = \int d^{d-1}(\vec{r} - \vec{r}')G(\vec{r} - \vec{r}', z, z', t) \exp[i\vec{k} \cdot (\vec{r} - \vec{r}')]\) 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 \(k_BT_c = 1\), \(G(\vec{k}, z, z', t)\) evolves as,
\[ \partial_t G(\vec{k}, z, z', t) = [-2k^2 + \partial_z^2 + \partial_{z'}^2]G(\vec{k}, z, z', t) + 2\delta(z - z') \]  

(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 \( \Delta \) controls the size of initial onsite fluctuations in \( \phi \)). Similarly, the symmetrized two-time correlation function \( C_s(\vec{k}, z, z', t) \) defined as the Fourier transform of \( C_s(\vec{r}, z, z', t) = \frac{1}{2}\langle(\phi(\vec{r}', z', 0)\phi(\vec{r} + \vec{r}', z, t) + \phi(\vec{r}', z, 0)\phi(\vec{r} + \vec{r}', z', t)) \rangle \) evolves as

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

(4)

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

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

(5)

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

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

(6)

and

\[ f_2(k, u, t) = \Delta \exp[-(k^2 + u^2)t]. \]

(7)

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

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

(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 \( (c = 0) \lambda_{sp} = d \) while for the "ordinary" transition \( (c > 0) \lambda_{or} = d + 2 \) within the Gaussian theory. It is interesting to note that while \( \lambda_b \) satisfies the upper bound \( \lambda_b \leq d \) conjectured by Fisher and Huse [2], clearly \( \lambda_{or} \) violates this upper bound.

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

\[ \partial_t C(\vec{x}, \vec{x}', t) = [-r_0 + \nabla^2]C(\vec{x}, \vec{x}', t) - \frac{u_0}{n} \sum_{ij} \langle\phi_i(\vec{x}', 0)\phi_j(\vec{x}, t)\phi_j(\vec{x}, t)\phi_j(\vec{x}, t)\rangle. \]

(9)

At the Wilson-Fisher fixed point, \( u_0 = 8\pi^2\epsilon/(n + 8) \) to leading order in \( \epsilon \). This allows one to calculate the corrections to the two-point correlator perturbatively in \( u_0 \). To leading order in \( \epsilon \), the term proportional to \( u_0 \) in Eq. (9) can be expressed, using Wick’s theorem,
in terms of the mean field propagators as \(-u_0(n+2)G_0(\vec{x}, \vec{x}'; t)C_0(\vec{x}', \vec{x}, t)\) where \(G_0\) and \(C_0\) denote the mean field equal-time and two-time propagators respectively. To leading order in \(\epsilon\), 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

\[
\partial_tC_s(\vec{x}, \vec{x}', t) = \frac{1}{2}[-2\vec{r}_0 + \nabla_{\vec{x}}^2 + \nabla_{\vec{x}'}^2 - V(z, t) - V(z', t)]C_s(\vec{x}, \vec{x}', t)
\]  

(10)

with \(\vec{r}_0 = r_0 + u_0(n+2)G_0(\infty, \infty, \infty)\) where \(G_0(\vec{x}, \vec{x}, t)\) denotes the mean-field equal-time propagator. The potential \(V(z) = u_0(n+2)\int[G_0(\vec{k}, z, z, t) - G_0(\vec{k}, \infty, \infty, \infty)]d^3(\vec{k})/(2\pi)^3\) 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, \(V_{sp}(z, t) = -u_0(n+2)[1 + (2t/z^2)\exp(-z^2/2t)]/32\pi^2 t\) and \(V_{or}(z, t) = -u_0(n+2)[1 - (2t/z^2)\exp(-z^2/2t)]/32\pi^2 t\) in the scaling regime where \(z >> \lambda^{-1}\), \(\lambda\) being the upper cutoff.

The Eq. (10) and the form of the potential \(V(z, t)\) suggest a late time scaling ansatz for the Fourier transform \(C_s(\vec{k}, z, z', t) \approx t^{-\alpha} \exp(-|\vec{k}|^2 t f(z/\sqrt{t}, z'/\sqrt{t})\). To determine the exponent \(\alpha\) we first consider the bulk limit \(z \to \infty, z' \to \infty\). Using \(V(\infty, \infty, t) = -u_0(n+2)/32\pi^2 t\) and \(u_0 = 8\pi^2 \epsilon/(n+8)\) in Eq. (10) we get \(\alpha = 1/2 - (n+2)\epsilon/4(n+8)\) and \(f(x, y) \sim e^{-(x-y)^2/2}\) as \(t, y \to \infty\). It follows immediately that the bulk autocorrelation \(A_b(t) \sim t^{-(d-n+2)/2}\). Since the dynamic exponent \(Z = 2 + O(\epsilon^2)\), we recover the bulk result \(\lambda_b = d - \frac{n+2}{n+8}\). For the surface autocorrelator, we need to know the small argument behaviour of the scaling function \(f(x, y)\). For small \(x, y, f(x, y) \sim (xy)^s(a + bx^2 + cy^2 + \cdots)\) where \(s(s-1) = \pm \frac{n+2}{n+8}\) and \(+\) corresponds to “special” and to “ordinary” transitions respectively. Then the autocorrelator \(A(z, t) = \int C_s(\vec{k}, z, z, t)d^{d-1}k/(2\pi)^{d-1} \sim t^{-(d-1+2s+2\alpha)/2}\). We choose the root of \(s\) to match the \(\epsilon \to 0\) limit and get \(\lambda_{sp} = d - \frac{n+2}{n+8}\) for “special” transition and \(\lambda_{or} = d + 2 - \frac{n+2}{n+8}\) for the “ordinary” one.

We next calculate \(\lambda_{c}\) 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 \(V(z, t) = \frac{u_0(n+2)}{32\pi^2 t} \int G(\vec{k}, z, z, t) - G(\vec{k}, \infty, \infty, \infty)]d^{d-1}k/(2\pi)^{d-1}\). where the equal-time propagator \(G(\vec{k}, z, z', t)\) satisfies:

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

(11)

In analogy with epsilon expansion, we make the ansatz \(V(z, t) = a/2t + \mu^2 z^2 g[z/\sqrt{t}]\) where \(g(x) \to 1\) as \(x \to 0\) and \(g(x) \to 0\) as \(x \to \infty\). The values of \(a\) and \(\mu\) are determined respectively from the limits \(z \to \infty\) (bulk dynamics) and \(t \to \infty\) (static limit) and are already known to be \(a = (d-4)/2\) [13], \(\mu_{sp} = (d-5)/2\) and \(\mu_{or} = (d-3)/2\) [16]. 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 \(\lambda_s\), it is sufficient to know that \(g(0) = 1\). We then proceed identically as in the case of \(\epsilon\) 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 \(\lambda_{sp} = (5d - 12)/2\) and \(\lambda_{or} = (5d - 8)/2\). 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 $\epsilon$ 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 spin-flip 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) \cite{14,16}. 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 $r$ \cite{13}, 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 transition) \cite{14–16}. Since at $T_c$, the system is free of vortices and therefore, the dynamics of the phases is trivially that of damped independent spin waves. However, as shown by Rutenberg and Bray \cite{9}, the bulk auto-correlation decays algebraically with time and the corresponding exponent $\lambda_b$ depends continuously on temperature. It is straightforward to extend their calculations to systems with edges and corners. For example, we have found that $\lambda_{\text{corner}} = 2\lambda_{\text{edge}} = 4\lambda_b$. Details of these calculations will be published elsewhere \cite{22}.

A two-dimensional system where these boundary auto-correlation exponents can be calculated exactly is the dynamics of the X-Y model following a quench from one temperature to another, both temperatures being below the Kosterlitz-Thouless temperature. In this case, the system is free of vortices and therefore, the dynamics of the phases is trivially that of damped independent spin waves. However, as shown by Rutenberg and Bray \cite{9}, the bulk auto-correlation decays algebraically with time and the corresponding exponent $\lambda_b$ depends continuously on temperature. It is straightforward to extend their calculations to systems with edges and corners. For example, we have found that $\lambda_{\text{corner}} = 2\lambda_{\text{edge}} = 4\lambda_b$. Details of these calculations will be published elsewhere \cite{22}.

It is clear from the results presented in this paper that for quench to $T = T_c$, the surface autocorrelation exponents are quite different from their bulk counterparts. It is an interesting question to ask whether the same happens for quench to the ordered phase ($T < T_c$). From our preliminary $T = 0$ simulations of the 2d Ising model, $\lambda_s$ does not seem to be different from $\lambda_b$ at $T = 0$. This seems to be the case also for the exact $T = 0$ Glauber dynamics of the semi-infinite Ising chain. Interpretation of these results and further studies are relegated to a future publication \cite{22}.
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FIGURES

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

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