Universal Short-Time Behavior in Critical Dynamics
near Surfaces

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Abstract

We study the time evolution of classical spin systems with purely relaxational dynamics, quenched from \( T \gg T_c \) to the critical point, in the semi-infinite geometry. Shortly after the quench, like in the bulk, a nonequilibrium regime governed by universal power laws is also found near the surface. We show for ‘ordinary’ and ‘special’ transitions that the corresponding critical exponents differ from their bulk values, but can be expressed via scaling relations in terms of known bulk and surface exponents. To corroborate our scaling analysis, we present perturbative (\( \varepsilon \)-expansion) and Monte Carlo results.

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The dynamics of spin systems after quenches from a high-temperature initial state to or below a critical point has attracted a great deal of interest during recent years [1]. In particular, for quenches from \( T \gg T_c \) to the critical temperature Janssen et al. [2] found that in Ising-like systems with purely relaxational dynamics (model A) [3] a previously unknown regime shortly after the quench with unexpected features exists. In its most pronounced form the so-called universal short-time behavior (USTB) appears in the time dependence of the order parameter itself. Suppose the initial state carries some small magnetization \( m_0 \). Then, as Janssen et al. [2] showed, after the quench the magnetization will grow for a macroscopic time span, governed by the universal power law

\[
m(t) \sim m_0 t^\theta \quad \text{with} \quad \theta = \left( x_0 - \beta/\nu \right) / \zeta ,
\]

where \( x_0 \) is the scaling dimension of the initial field [4,5] (whereas the static exponents have their usual meaning, and \( \zeta \) denotes the dynamic exponent). Thus, technically spoken, USTB is caused by the influence of the scaling behavior of the initial field on (in macroscopic units) early stages of the relaxational process [3]. The corresponding operator dimension \( x_0 \) is a genuine new exponent. Especially for the \( n \)-vector model in \( 2 < d < 4 \) it turns out that \( x_0 > \beta/\nu \), and thus the magnetization really increases initially, up to a characteristic time \( t_0 \sim m_0^{-\zeta/x_0} \). After that it crosses over to the well-known algebraic decay \( m \sim t^{-\beta/\nu \zeta} \) [2,6].

Recently, the scenario developed in Ref. [2] was directly confirmed by means of Monte Carlo simulation [7], and, based on USTB, a procedure to determine static critical exponents was suggested [8].

Another quantity where the short-time exponent \( \theta \) enters is the autocorrelation function \( A(t) = \langle \phi(t) \phi(0) \rangle \sim t^{-\lambda/\zeta} \). It was shown by Janssen [9] that \( \lambda = d - \zeta \theta \), and it is this quantity where USTB was actually first seen in a numerical simulation [10].

Similar in many respects to initial conditions for time-dependent processes are boundary conditions at surfaces. It is well known that critical behavior is modified near surfaces; each bulk universality class splits up in three surface universality classes, depending on whether at bulk criticality the surface is disordered, ordered, or also critical. The corresponding universality classes are called ordinary, extraordinary, and special transition, respectively [11]. In this Letter we focus attention on the influence of ‘ordinary’ and ‘special’ surfaces on the time-dependence of \( m \) and \( A \). We show that close to the surface the USTB is modified depending on the surface universality class. Further, we show that the values of the ‘new’ exponents that govern the short-time dynamics near the surface can be expressed in terms of scaling relations between other known critical exponents. In a recent preprint, Majumdar and Sengupta [12] correctly determined the surface behavior of the autocorrelation function for the \( n \)-vector model, but the underlying scaling relation was not recognized.

In the framework of field theory the modification of critical behavior near surfaces is the result of additional primitive uv-divergences, which are located in the surface [11]. These divergences need additional \( Z \)-factors, which, in turn, give rise to independent surface exponents. As shown by Janssen et al. [2], the situation is largely analogous at the time ‘surface’ \( t = 0 \). That in general \( x_0 \neq \beta/\nu \) is the result of an additional logarithmic divergence at \( t = 0 \) in the upper critical dimension \( d^* = 4 \). What happens, if we have both initial and boundary conditions? It is well known that the degree of surface divergences is reduced at least by one compared with bulk divergences [11]. Since the bulk divergence at \( t = 0 \) is just logarithmic, it is immediately clear that no additional primitive divergence located at \( z = t = 0 \) exists,
and, thus, the USTB near surfaces must be governed by known bulk, bulk short-time, and surface exponents.

To be more specific, let us consider the $t$- and $z$-dependent magnetization in the semi-infinite system. At the bulk critical point it follows from dimensional analysis and renormalization-group (RG) invariance that asymptotically

$$m(z, t, m_0) \sim t^{-\beta/\nu} F(z/t^{\eta/\zeta}, m_0 t^{x_0/\zeta}).$$

As usual all quantities are made dimensionless with the help of an appropriate power of the renormalization mass $\mu$, and we set $\mu = 1$ afterwards. Because of different scaling dimensions, $m_0$ is not the initial value of $m$. Instead, as close as possible to the naive expectation, one finds that $m \sim m_0$ for $t \ll t_0$ \[13\]. It follows that $F(x, y) \sim y$ for $x \to \infty$ and $y \to 0$, and we obtain the known bulk short-time behavior of Eqn. (1).

When do we expect modifications due to the surface? The surface will influence the dynamics of a spin when the nonequilibrium (growing) action length $\xi(t) \sim t^{1/\zeta}$ has become larger than the spin’s distance $z$ from the surface. This is analogous to the static situation, where surface critical behavior is observed if the equilibrium correlation length is larger than $z$ \[11\]. Now, if $z \ll \xi(t)$, the short-distance expansion (SDE) \[14,11\]

$$m(z, t, m_0) \sim z^{(\beta - \beta_1)/\nu} m_1(t, m_0),$$

should hold, where $\beta_1/\nu$ is the scaling dimension of the surface field \[14\] and $m_0$ homogeneous. Moreover, exploiting as before the RG-invariance leads to $m_1(t, m_0) \sim t^{-\beta_1/\nu} F_1(m_0 t^{x_0/\zeta})$. Demanding again that $m \sim m_0$ for $t \ll t_0$, it follows that $F_1(y) \sim y$ for $y \to 0$. As a result, the magnetization close to the surface ($z \ll \xi(t)$) takes the form

$$m(z, t, m_0) \sim m_0 z^{(\beta - \beta_1)/\nu} \theta_1,$$

with

$$\theta_1 = (x_0 - \beta_1/\nu)/\zeta = \theta + (\beta - \beta_1)/\nu\zeta.$$ 

In other words, the short-time exponent near the surface is determined by the difference between the scaling dimensions of the initial field and the surface field. Eqn. (4a) holds if $t \ll t_0$ and $z \ll \xi(t)$. If, on the other hand, $z \geq \xi(t_0)$ only bulk short-time behavior will be seen and eventually a crossover to the nonlinear surface behavior $m \sim t^{-\beta_1/\nu}$ \[16,17\].

Next we set $m_0 = 0$ and consider the autocorrelation function $A(z, t) := \langle \phi(r, t) \phi(r, 0) \rangle$. Because of the Dirichlet initial condition the asymptotic result for $A$ vanishes identically, and, as shown by Janssen \[9\], one has to consider the leading correction in an expansion in the inverse of the initial temperature $\tau_0^{-1}$:

$$A(z, t) = \tau_0^{-1} \langle \phi(r, t) \tilde{\phi}_0(r) \rangle.$$ 

$\tilde{\phi}_0$ is the initial response field with bulk scaling dimension $d - x_0$ \[3\].

For $z \ll \xi(t)$ both operators in (5) can be replaced by their SDE. The SDE of the order-parameter field can be read from Eqn. (3). The SDE of $\tilde{\phi}_0$ is obtained as follows: It is known from the equilibrium dynamics \[14,11\] that the response field $\tilde{\phi}$ needs an additional renormalization factor $Z_1^{1/2}$ at the surface, the same $Z$-factor that is required to renormalize
the order-parameter field at the surface. Utilizing our earlier result that there are no new primitive divergencies at $z = t = 0$, we conclude that an additional $Z_{1/2}^1$ also suffices to renormalize $\tilde{\phi}_0$ at the surface. As a consequence, $\tilde{\phi}_0$ has the same SDE as $\phi$, and the autocorrelation function takes the form

$$A(z, t) \sim z^{2(\beta_1 - \beta)/\nu} t^{-\lambda_1/\zeta},$$

with

$$\lambda_1 = d - \zeta \theta + 2(\beta_1 - \beta)/\nu.$$  \hspace{1cm} (6b)

Eqs. (4) and (6) are the essential results of this Letter. Numerical values for $\theta_1$ and $\lambda_1$, where we have used the literature values of the exponents involved, are given in Table 1 (together with other results discussed below).

In order to confirm Eqs. (4) and (6), we present a first-order $\epsilon$-expansion (one-loop) for the equation of motion of the $n$-vector model $A$ \cite{3}. According to the above discussion, $m$ is small for $t \ll t_0$, and so we may consider a linear approximation (in $m$). It takes the form

$$\dot{m} + \Gamma \tau m - m'' + \frac{\Gamma g}{6} (n + 2) C(z, t) m = 0,$$

where $C(z, t)$ is the one-loop (tadpole) contribution. According to the standard procedure \cite{11} $C(z, t)$ can be separated in a bulk and a surface part, where the latter is determined by the bulk propagator at the image point:

$$C(z, t) = C_b(0, t) \pm C_b(2z, t).$$  \hspace{1cm} (8a)

In this equation ‘$+$’ stands for special and the ‘$-$’ for ordinary transition, and

$$C_b(z, t) = \frac{2\Gamma}{(2\pi)^d} \int d^d p \ e^{-2\Gamma(p_1^2 + p_2^2 + 4\tau_0)(t-t') + i2p_\perp z}.$$  \hspace{1cm} (8b)

The first term in (8a), the bulk contribution, contains the usual uv-divergence. Without going into technical details, we state that this divergence (after dimensional regularization) can be absorbed in the bare temperature by minimal subtraction as in the static calculation. The second term on the right-hand side of (8a) is the surface contribution, which is finite for any $z > 0$. So after renormalization we obtain a finite equation, and at the RG fixed point $g^* = 48\pi^2\epsilon/(n + 8)$ and $\tau = 0$ it takes the form

$$\dot{m} - m'' + \theta \left( -\frac{1}{t} \pm \frac{1}{z^2} e^{-z^2/t} \right) m = 0,$$  \hspace{1cm} (9)

where $\theta = \epsilon (n + 2)/(4n + 32)$ is the one-loop result for the bulk short-time exponent \cite{44} and with $\tilde{t} = 2\Gamma t$. It is straightforward to show that for uniform initial magnetization $m_0$ Eqn. (8) has solutions of the form $m(\tilde{t}, z) = m_0 U(\tilde{t}) V(z^2/\tilde{t})$. Let us first consider the bulk limit $z \gg \xi(\tilde{t})$ with $\xi \sim \tilde{t}^{1/2}$ ($\zeta = 2$ in one-loop). By straightforward analysis it follows that $U \sim \tilde{t}^0$ and $V \to \text{const.}$, and thus $m \sim t^\theta$. This is the bulk short-time behavior.

What happens if we move closer to the surface? For $z \ll \xi(\tilde{t})$ the function $V(x)$ behaves as a power of $x$, which now depends on the universality class of the surface. For the ordinary
transition one finds $V \sim x^{1/2-\theta}$. This means that $m \sim m_0 z^{1-2\theta} t^{-1/2+2\theta}$ and \(\theta^{\text{ord}}_1 = -1/2 + \epsilon (n + 2)/(2n + 16)\). For the special transition the result is $V \sim x^{-\theta}$ and $m \sim m_0 z^{-2\theta} t^{2\theta}$ such that \(\theta^{\text{sp}}_1 = \epsilon (n + 2)/(2n + 16)\). The one-loop values of \(\theta^{\text{ord}}_1\) and \(\theta^{\text{sp}}_1\) are consistent with (14). That in this simple approximation the surface exponents can effectively be expressed with the help of the bulk \(\theta\) is an artifact of the one-loop approximation.

We do not repeat the calculation of Ref. [12] for the autocorrelation function here. The one-loop results \(\lambda^{\text{ord}}_1 = 6 - \epsilon (5n + 22)/(2n + 16)\) and \(\lambda^{\text{sp}}_1 = 4 - \epsilon (5n + 22)/(2n + 16)\) derived in [12] are both consistent with the scaling relation (6b). The figures for \(n = \epsilon = 1\) are given in the Table.

From the one-loop results we can immediately read off the exact exponents for \(n \to \infty\). They are given by \(\theta^{\text{ord}}_1 = (3 - d)/2, \theta^{\text{sp}}_1 = (4 - d)/2, \lambda^{\text{ord}}_1 = (5d - 8)/2,\) and \(\lambda^{\text{sp}}_1 = (5d - 12)/2\). Numerical values for \(d = 3\) are displayed in the Table.

To summarize these results, at the ‘special’ surface in \(2 < d < 4\) the order grows always faster than in the bulk, and the autocorrelations decay slower. For ‘ordinary’ surfaces, the USTB for the Ising universality class is drastically different from bulk behavior; the order starts to decay from the beginning. On the other hand, for \(n \to \infty\) we find \(\theta^{\text{ord}}_1 > 0\) for \(d < 3\). Autocorrelations generally decay faster at ‘ordinary’ surfaces.

|          | bulk | surface | \(\theta_1\) | \(\lambda_1/\zeta\) |
|----------|------|---------|-------------|----------------|
| 1-loop   |      |         | \(\theta = 0.08\) | -0.33          |
| \(n = 1\)|      |         | \(\lambda/\zeta = 1.42\) | 2.25           |
| MC       |      |         | \(\theta^{\text{ord}}\) | -0.274(13)     |
| (Ising)  |      |         | \(\lambda^{\text{ord}}_1 = (5d - 8)/2\) | 1.94(16)       |
| Lit.     |      |         | \(\theta^{\text{sp}}_1 = (4 - d)/2\) | 0.17(7)        |
| (Ising)  |      |         | \(\lambda^{\text{sp}}_1 = (5d - 12)/2\) | 1.12(7)        |
| \(n \to \infty\) |      |         | \(\theta^{\text{ord}}_1 = (3 - d)/2\) | 0     |
| (exact)  |      |         | \(\theta^{\text{sp}}_1 = (4 - d)/2\) | 7/2           |
|          |      |         | \(\lambda^{\text{ord}}_1 = (5d - 8)/2\) | 1/2           |
|          |      |         | \(\lambda^{\text{sp}}_1 = (5d - 12)/2\) | 3/2           |

**Table 1:** Dynamic surface exponents \(\theta_1\) and \(\lambda_1/\zeta\) for the \(d=3\) Ising model \((n = 1)\) for ‘ordinary’ and ‘special’ surfaces. For comparison some bulk results are also displayed. The one-loop approximation has been extrapolated to \(\epsilon = 1\). In section ‘MC’ our Monte Carlo estimates are displayed. In ‘Lit.’ results obtained with [13] and [14] in combination with the best known literature values for the exponents involved are shown. The latter are taken from Refs. [11,20,21]. In the last section the exact exponents of the \(n \to \infty\) limit in \(d = 3\) are displayed.

Finally, we present a Monte Carlo simulation of the \(d = 3\) Ising model. We have used the heat-bath algorithm for nonconserved spins and the usual time-dependent interpretation of our data [18]. The simulations were carried out on a lattice of size \(20^2 \times 40\), where we have implemented the nontrivial boundary conditions on the surfaces perpendicular to the long axis and periodic boundary conditions in the remaining directions. The high-temperature initial configuration was generated as in Ref. [1] by randomly selecting and flipping \(1/2 - m_0/2\) of the spins in an initially completely (in +direction) ordered configuration. To determine the exponent \(\theta\) from the order-parameter profiles, we started from an initial state with nonzero \(m_0\); for the data displayed in Fig. 1 we chose \(m_0 = 0.04\). For system size tending to infinity,
$m_0$ would scale to zero \cite{4}. For $A(t)$ a disordered initial state (with $m_0 = 0$) was prepared. All simulations have been carried out at the bulk critical value $J/k_B T_c = 0.2216$ \cite{21}. The Monte Carlo results for $\theta_1$ and $\lambda_1$ were obtained by averaging over 200,000 independent histories. To estimate the errors of the exponents, we have divided the data into 20 runs. To simulate the special transition, the result of Ruge et al. \cite{21} for the critical surface coupling $J_1/J = 1.5004$ was adopted. In the case of the ordinary transition we chose a value somewhat lower than the bulk coupling \cite{19}.

\begin{figure}
\centering
\includegraphics[width=0.5\textwidth]{fig1.png}
\caption{Monte-Carlo results from $20^2 \times 40$ lattice for the order parameter for special (solid curves) and ordinary (dashed curves) transition. The distances from the surface are $z = 0, 1, 2, 3, 5, 10, 20$. The behavior at the surface ($z = 0$) is given by the uppermost curve in the case of special and by the lowest curve in the case of ordinary transition.}
\end{figure}

Results for the order parameter for special and ordinary transition are shown in Fig. 1 for different values of $z$. As expected from the above discussion, all curves for points off the surface start with bulk USTB. Close to the surface the profiles show a crossover to the respective surface USTB. Far off the surface this crossover does not occur within the period of initial increase. For later times all curves show the ‘linear’ bulk behavior \cite{3,4}; the nonlinear decay could only be seen in larger systems \cite{7}. The values for $\theta_1$, determined from our data, are displayed in Table 1. Taking into account the errors, they are consistent with the expectation from \cite{41}. The situation is very similar for the autocorrelation function. The results for $\lambda_1$ are also displayed in the Table.

To conclude, we have investigated the critical dynamics, especially the short-time behavior, of the $n$-vector model A near ‘ordinary’ and ‘special’ surfaces. By general scaling analysis combined with a short-distance expansion, we have related the surface short-time exponents to other known exponents. The corresponding scaling relations are given in Eqs. (4b) and (6b). In a one-loop calculation these scaling relation were verified, and numerical estimates for the surface exponents were determined by Monte Carlo simulation. We think that with the help of universal short-time behavior, along the lines suggested recently by Li et al. \cite{8} for the bulk, it should also be possible to determine static surface exponents more precisely. Further, we believe that short-time dynamics near surfaces could also be an attractive field for experimental studies.

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REFERENCES

[1] A. J. Bray, Advances in Physics, 43, 357 (1994).
[2] H. K. Janssen, B. Schaub, and B. Schmittmann, Z. Phys. B 73, 539 (1989).
[3] P. C. Hohenberg and B. I. Halperin, Rev. Mod. Phys. 49:435 (1977).
[4] The short-time exponent $\theta$ was denoted by $\theta'$ in Ref. [2]. But since the original $\theta$
 of [2] does not appear in the present work, we have dropped the prime. Further, in
 order to avoid confusion with the spatial coordinate $z$, we throughout call the dynamic
 equilibrium exponent $\zeta$.
[5] H. W. Diehl and U. Ritschel, J. Stat. Phys. 73, 1 (1993).
[6] U. Ritschel and H. W. Diehl, Phys. Rev. E 51, 5392 (1995).
[7] Z.-B. Li, U. Ritschel and B. Zheng, J. Phys. A: Math. Gen. 27, L837 (1994).
[8] Z.-B. Li, L. Schülke, B. Zheng, Phys. Rev. Lett. 74, 3396 (1995); L. Schülke and B.
 Zheng, The Short-Time Dynamics of the Critical Potts Model, preprint Si-95-2.
[9] H. K. Janssen, in From Phase Transitions to Chaos — Topics in Modern Statistical
 Physics, edited by G. Györgyi, I. Kondor, L. Sasvári, and T. Tel (World Scientific,
 Singapore, 1992).
[10] D. A. Huse, Phys. Rev. B 40, 304 (1989).
[11] H. W. Diehl, in Phase Transitions and Critical Phenomena, Vol. 10, C. Domb and J.
 L. Lebowitz, eds. (London, Academic Press, 1986).
[12] S. N. Majumdar and A. M. Sengupta, Non-equilibrium Dynamics Following a Quench
 to the Critical Point in a Semi-Infinite System, Preprint.
[13] For a more rigorous treatment we refer to Ref. [13].
[14] K. Symanzyk, Nucl. Phys. B 190 [FS3], 1 (1981);
 H. W. Diehl and S. Dietrich, Z. Phys. B 42, 65 (1981).
[15] These results hold for both surface transitions discussed here. For more details concern-
ing the definition of static surface exponents and scaling relations among them we refer
 to Ref. [15].
[16] H. W. Diehl and S. Dietrich, Z. Phys. B 50, 117 (1983);
 H. Riecke, S. Dietrich, and H. Wagner, Phys. Rev. Lett. 55, 3010 (1985).
[17] M. Kikuchi and Y. Okabe, Phys. Rev. Lett. 55, 1220 (1985).
[18] K. Binder and D. W. Heermann, Monte Carlo Simulation in Statistical Physics,
 (Springer Verlag, Berlin, 1988).
[19] Since the ‘special’ point is an unstable fixed-point of the renormalization-group flow,
 one should observe for all surface couplings $J_1$ lower than the multicritical value the
 ‘ordinary’ behavior provided the system is large enough.
[20] P. Grassberger, Physica A 214, 547 (1995).
[21] C. Ruge, S. Dunkelmann, and F. Wagner, Phys. Rev. Lett. 69, 2465 (1992).