Near-Surface Long-Range Order at the Ordinary Transition

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Abstract

We study the spatial dependence of the order parameter near surfaces belonging to the universality class of the ordinary transition. Special attention is paid to the influence of a small surface magnetic field $h_1$ at and above the bulk critical temperature. A detailed scaling analysis (which is confirmed by a perturbative calculation) reveals that $h_1$ may give rise to an anomalous short-distance behavior of the order parameter. Close to the surface the magnetization increases with a power law $m \sim z^\kappa$ with $\kappa \equiv 1 - \eta_{\text{ord}}^\perp \simeq 0.23$ for the three-dimensional Ising model. These results are closely related to experimental findings where exponents of the ordinary transition were observed in Fe$_3$Al, while superstructure reflections revealed the existence of long-range order near the surface [X. Mailänder et al., Phys. Rev. Lett. 64, 2527 (1990)].

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A prototypical system to study critical phenomena in restricted geometries is the semi-infinite Ising model, terminated by a plane surface and extending infinitely in the direction perpendicular to the surface (z-direction) [1]. Spins located in the surface may experience interactions different from those in the bulk, for example due to missing neighbors at a free surface or due to a strong coupling to an adjacent medium. In the framework of continuum field theory such as the $\phi^4$ model the surface influence is taken into account by additional fields like the surface magnetic field $h_1$ and the local temperature perturbation $c_0$ at $z = 0$. The latter can be related to the surface enhancement of the spin-spin coupling in lattice models [2].

At the bulk critical temperature $T_b^c$ the tendency to order near the surface can be reduced ($c_0 > 0$) or increased ($c_0 < 0$), or, as a third possibility, the surface can be critical as well. As a result, each bulk universality class in general divides into several distinct surface universality classes, called ordinary ($c_0 \to \infty$), extraordinary ($c_0 \to -\infty$), and special transition ($c_0 = c_{sp}^*$).

Close to the surface, within the range of the bulk correlation length $\xi \sim |\tau|^{-\nu}$, the singular behavior of thermodynamic quantities is markedly changed compared to the bulk. For $z \ll \xi$ the magnetization behaves as $\sim |\tau|^{\beta}$ when $\tau = (T - T_b^c)/T_b^c \to 0$ from below, with $\beta_1$ assuming characteristic values for special and ordinary transition, which are in general different from the bulk exponent $\beta$. (At the extraordinary transition the surface is already ordered at $T_b^c$.) Further, the correlation functions near the surface are characteristically modified. The correlation function for points within a plane parallel to the surface is given by $C(\Delta r_{||}) \sim |\Delta r_{||}|^{-(d-2+\eta_1)}$, where the anomalous dimension $\eta_1$ is related to $\beta_1$ by $\beta_1 = (1/2)(d - 2 + \eta_1)$ [3]. Correlations in the z-direction (and all other directions except the parallel one) are governed by $C(z, z') \sim |z - z'|^{-(d-2+\eta_z)}$.

Some of the theoretical predictions [2,3] were found in excellent agreement with experiments carried out by Mailänder et al. [4,5]. In these experiments Fe$_3$Al was studied close to the DO$_3$-B$_2$ transition by scattering of evanescent waves generated by total reflection of x-rays at a [110] surface. The system was expected to belong to the universality class of the ordinary transition, and indeed the exponents measured were in remarkable agreement with theoretical predictions [3]. A somewhat disturbing feature was that superstructure reflections revealed the existence of unexpected long-range order (LRO) near the surface reminiscent to the situation at the extraordinary transition. In the sequel it was demonstrated by Schmid [3] that in a similar situation (at the A$_2$-B$_2$ transition in Fe$_3$Al) an effective ordering field $h_1$ at the surface can arise when the stoechiometry of the alloy is not ideal. Assuming that an $h_1$ is also present at the DO$_3$-B$_2$ transition, the observed LRO can be explained, leaving unanswered the question, however, why exponents of the ordinary transition were measured despite the LRO. In the following we show that a small $h_1$ may generate an universal power-law growth of the order parameter near the surface and, as a result, a LRO considerably (and, in fact, infinitely) larger than expected from mean-field (MF) approximations, while the correlation function is still governed by the exponents of the ordinary transition.

Most of the theoretical studies concerning inhomogenous systems concentrated on the behavior at the fixed points $c_0 = \pm \infty$ and $c_0 = c_{sp}^*$, respectively. At $T_b^c$ for both the ordinary and the special transition (for $h_1 = 0$) the order-parameter profiles are zero for all $z \geq 0$. At the extraordinary transition the surface is ordered and the order decays as $z^{-\beta/\nu}$ with increasing distance from the surface [7], where in the Ising-case $\beta/\nu \simeq 0.52$ [8]. Concerning
the effects of \( h_1 \) it was assumed for a long time \cite{9} and recently also shown by rigorous arguments \cite{10} that a strong \( h_1 \) at the ordinary transition (the so-called normal transition) is equivalent to the extraordinary transition. The special transition was studied by Brezin and Leibler \cite{11} and by Ciach and Diehl \cite{12}. It was found that at the fixed point the scaling field \( h_1 \) gives rise to a length scale \( l^{sp} \sim h_1^{-\nu/\beta_1^{sp}} \). For \( z \gg l^{sp} \) one finds that \( m \sim z^{-\beta/\nu} \) as at the extraordinary transition. In the opposite limit, \( z \ll l^{sp} \), the magnetization behaves as \( m \sim m_1 z^{(\beta_1^{sp}-\beta)/\nu} \). Since \( \beta_1^{sp} \leq \beta \), the order still decays, governed by a somewhat smaller exponent compared to large distances. For the Ising model \( (\beta_1^{sp} - \beta)/\nu \simeq -0.15 \) \cite{8}.

What can we expect if a small \( h_1 \) is applied in the presence of a large \( c_0 \), i.e. close to the fixed-point of the ordinary transition. In this situation the parameter \( c_0 \) is a so-called dangerous irrelevant variable \cite{2,13}, comparable to the \( \phi^4 \) coupling constant at and above the upper critical dimension \( d^* = 4 \), and in general must not be naively set to its fixed point value \( c_0 = \infty \). Setting the bulk magnetic field \( h = 0 \), the remaining linear scaling fields at the ordinary transition are \( \tau \) and \( h_1 \equiv h_1/c_0 \) \cite{2,13,14}. Hence, the behavior of the magnetization under rescaling of distances should be described by

\[
m(z, \tau, h_1) \sim b^{-\beta/\nu} m(z b^{-1}, \tau b^{1/\nu}, h_1 b^{x_1}),
\]

where the scaling dimension of \( h_1 \) is given by \( x_1 = (d - \eta_1^{ord})/2 \) \cite{3}.

Let us first discuss the profile for \( h_1 = 0 \). As mentioned above, for \( \tau > 0 \) we have \( m = 0 \) everywhere. For \( \tau < 0 \), on the other hand, the magnetization approaches its bulk value \( m_0 \sim |\tau|^{\beta/\nu} \) for \( z \rightarrow \infty \). Close to the surface \( (z \ll \xi) \) the magnetization increases with a power law \cite{13}. To see this from (1), we set \( h_1 = 0 \) and fix the arbitrary rescaling parameter \( b \) by setting it \( \sim z \). Then the magnetization takes the scaling form

\[
m(z, \tau) \sim z^{-\beta/\nu} M_\tau(z/\xi).
\]

Since we expect that \( m(z \rightarrow 0) \sim m_1 \) and know that \( m_1 \sim |\tau|^{\beta_{ord}} \), we conclude for the short-distance form of the scaling function \( M_\tau \sim \zeta^{\beta_{ord}/\nu} \) and, in turn, the behavior of \( m \) is given by \( m(z, \tau) \sim |\tau|^{\beta_{ord}} z^{(\beta_{ord} - \beta)/\nu} \) \cite{13}.

We now turn to the case \( \tau = 0 \) and \( h_1 \neq 0 \). This is the situation we are actually interested in and which is important for understanding the experimental results of Ref. \cite{3}. In this case the scaling form derived from (1) is

\[
m(z, h_1) \sim z^{-\beta/\nu} M_{h_1}(z h_1^{1/x_1}).
\]

First of all we notice from (3) that the scaling field \( h_1 \) gives rise to a length scale \( l^{ord} \sim h_1^{-1/x_1} \) quite comparable to the situation near the special transition discussed above. In order to find the short-distance behavior of \( M_{h_1}(\zeta) \) we have to recall that the surface is paramagnetic at the ordinary transition. Thus \( m_1 \) will respond linearly to \( h_1 \) \cite{16}. Arguing again that \( m(z \rightarrow 0) \sim m_1 \), we now find that \( M_{h_1} \sim \zeta^{x_1} \) for \( \zeta \ll 1 \), and, in turn, with the scaling relation \( \eta_\perp = (\eta_\parallel + \eta)/2 \) \cite{3}, the short-distance behavior is given by

\[
m(z, h_1) \sim h_1 z^\kappa \quad \text{with} \quad \kappa \equiv 1 - \eta_\perp^{ord}.
\]

In the opposite limit, \( z \gg l^{ord} \), the magnetization approaches the bulk equilibrium value zero as \( \sim z^{-\beta/\nu} \).
Eq. (4) is the central result of this Letter. It states that the magnetization even at (or slightly above) $T_b^c$ in the presence of a surface field $h_1$ shows a power-law increase reminiscent of the situation below $T_b^c$. The short-distance exponent $\kappa$ defined in (4) is zero in MF theory. Below $d^*$, however, as for the Ising system in $d = 3$, it is nonzero and positive. Taking the literature values for the surface exponents from Ref. [2], one obtains $\kappa \simeq 0.23$, which implies a rapid growth of LR0 with increasing $z$.

The spatial variation of the magnetization discussed above strongly resembles the time dependence of the magnetization in relaxational processes at the critical point. If a system with nonconserved order parameter (model A) is quenched from a high-temperature initial state to the critical point, with a small initial magnetization $m(i)$, the order parameter behaves as $m \sim m(i) t^\theta$ [17], where the short-time exponent $\theta$ is governed by the difference between the scaling dimensions of initial and equilibrium magnetization [18]. Like the exponent $\kappa$ in (4), the exponent $\theta$ vanishes in MF theory, but becomes positive below $d^*$.

There is also a heuristic argument for the growth of LRO near the surface. As said above, $h_1$ generates a surface magnetization $m_1 \sim h_1$. Regions (on macroscopic scales) close to the surface will respond to this magnetization by ordering as well. How strong this influence is depends on two factors. First, it is proportional to the correlated area in a plane parallel to the surface in a distance $z$. While in the surface correlations are suppressed, close to the surface the correlation length in directions parallel to the surface, $\xi_\parallel$, grows as $\sim z$ [12]. Second, for small $h_1$ (and thus small surface magnetization) it depends linearly on the probability that a given spin orientation “survives” in a distance $z$ from the surface. The latter is governed by the perpendicular correlation function $C(z) \sim z^{-(d-2+\eta_{\perp}^{ord})}$. Taking the factors together, we obtain

$$m(z) \sim h_1 C(z) \xi_\parallel^{d-1} = h_1 z^{1-\eta_{\perp}^{ord}}.$$  

(5)

Qualitatively speaking, the surface when carrying a small $m_1$ induces a much larger magnetization in the adjacent layers, which are much more susceptible and respond with a magnetization $m(z) \gg m_1$. This effect is not observed on the MF level since there the increase of the correlated surface area is exactly compensated by the decay of the perpendicular correlations.

In order to corroborate our scaling analysis and the heuristic arguments from above, we carried out a one-loop calculation for the $\phi^4$-model employing the $\epsilon$ expansion. Expanded in powers of the coupling constant, the magnetization can be written in the form $m = m^{(0)} + gm^{(1)} + O(g^2)$, where $m^{(0)}$ is the well known MF solution [8,19] and $m^{(1)}$ is the 1-loop term. The latter was calculated exactly for arbitrary $c_0$ and $h_1$ in Refs. [11,12]. However, the renormalization of uv-divergences and the following improvement with the help of the renormalization group where done at (or in the vicinity of) the special transition in these references. As a consequence, the anomalous short-distance behavior at the ordinary transition was missed.

The MF solution that satisfies the boundary condition $\partial_z m - cm|_{z=0} = h_1$ at the surface is given by

$$m^{(0)}(z) = \sqrt{\frac{12}{g}} \left( \frac{1}{z} \right)^{\frac{1}{2}}.$$  

(6a)

with
\[ \tilde{z} \equiv z + z_+ \quad \text{and} \quad z_+^{-1} = \frac{(c_0^2 + 4h_1 \sqrt{g/12})^{1/2} - c_0}{2}, \]

which holds for general \( c_0 \) and \( h_1 \). Close to the ordinary transition (large \( c_0 \)) the mean field length scale becomes \( z_+ \simeq l^{\text{ord}} = (12/g)^{1/2} c_0 / h_1 \). As expected from \([4]\), there is no anomalous short-distance behavior on the MF level. The profile has its maximum value at \( \tilde{z} = 0 \), and for \( z \gg l^{\text{ord}} \) the profile decays as \( \sim z^{-\beta/\nu} \) with the MF value \( \beta/\nu = 1 \).

The one-loop term \( m^{(1)} \) is given by \([12,13]\)

\[ m^{(1)}(z) = -\frac{1}{2} \int_0^\infty \! dz' C(0; z, z') m^{(0)}(z') \int_p C(p; z', z'), \tag{7} \]

where \( m^{(0)}(z) \) is the zero-loop (MF) profile \([5]\) and \( f_p \equiv (2\pi)^{1-d} \int d^{d-1} p \). The propagator \( C(p; z, z') \) is Fourier-transformed with respect to the spatial coordinates parallel to surface. It can be calculated exactly \([11,12]\), and the somewhat lengthy results will be omitted here. The integrations in \((7)\) necessary to obtain the full scaling function \( M_{h_1} \) are complicated and can only be carried out numerically. However, it is straightforward to extract the divergent terms, poles \( \sim 1/\epsilon \) in dimensional regularization, and the short-distance singularities \( \sim \log z \), which, when exponentiated, give rise to power laws modified compared to the MF theory. Collecting these terms, \( m^{(1)} \) is given by \((7)\) with

\[ \int_p C(p; z, z) = \frac{K_{d-1}}{2} \tilde{z}^{-2+\epsilon} \int_1^\infty \! dy \, y^{1-\epsilon} \left[ e^{-2y \left( 2y l^{\text{ord}} / \tilde{z} - 1 \right) \left( 1 + \frac{3}{y} + \frac{3}{y^2} \right)^2} - \frac{3}{y^2} \right] + \text{finite} \tag{8} \]

where \( K_d \equiv 2 / \left( (4\pi)^{d/2} \Gamma(d/2) \right) \) and “finite” stands for terms which are finite for \( \epsilon \to 0 \) and \( z \to 0 \). Terms of \( \mathcal{O}(1/c_0) \) are also omitted in \((8)\). The zero-momentum propagator \( C(0, z, z') \) appearing in \((8)\) (for \( c_0 \to \infty \)) takes the simple form

\[ C(0, z, z') = \frac{1}{5} \frac{1}{\tilde{z}_-^{2} \tilde{z}_+^{5}} \left( \tilde{z}_-^{5} - \tilde{z}_+^{5} \right), \tag{9} \]

where \( \prec \succ \) denotes the smaller (larger) of \( \tilde{z} \) and \( \tilde{z}' \).

Further analysis shows that the uv-divergences can be absorbed in the standard fashion by renormalization of the coupling constant \( K_{d} g_0 = u \, (1 + 3u/2 + \mathcal{O}(u^2)) \) and of the scaling field \( h_{1,0} = h_1 (1 - u/4\epsilon + \mathcal{O}(u^2)) \) \([3]\). After this the coupling constant is set to its fixed point value \( u^* = 2\epsilon/3 \). Eventually, after exponentiation of logarithms we find the asymptotic power laws

\[ m(z, h_1) \sim \begin{cases} z^{-1+\epsilon/2} & \text{for } z \gg l^{\text{ord}} \\ h_1 \, z^{\epsilon/6} & \text{for } z \ll l^{\text{ord}}. \end{cases} \tag{10} \]

As expected the decay of the profile for \( z \gg l^{\text{ord}} \) is governed by the one-loop result \( \beta/\nu = 1 - \epsilon/2 \). The short-distance behavior is consistent with our scaling analysis; in first-order \( \epsilon \) expansion \( \kappa = 1 - \eta^{\text{ord}}_\perp = \epsilon/6 \) \([2]\).
Fig. 1: Qualitative shape of the scaling function $\tilde{\mathcal{M}}_{h_1}(\zeta) = \zeta^{-\beta/\nu} \mathcal{M}_{h_1}(\zeta)$ of the magnetization. More details are described in the text.

A more detailed account concerning the behavior of the magnetization in between the asymptotic regimes of Eq. (10) will be given elsewhere [21]. A qualitative preview on the form of the scaling function $\tilde{\mathcal{M}}_{h_1}(\zeta) \equiv \zeta^{-\beta/\nu} \mathcal{M}_{h_1}(\zeta)$ (see Eq. (3)) is shown in Fig. 1, where the asymptotic power laws are quantitatively correct but the crossover is described by a simple substitute for the scaling function. Regarding the crossover between ordinary ($h_1 = 0$) and the extraordinary (or normal) transition ($h_1 = \infty$) the following scenario should hold. While at the ordinary transition $m(z)$ vanishes everywhere, for $h_1 \neq 0$ the magnetization increases as $\sim z^\kappa$ up to $z \simeq l^{ord} \sim h_1^{-1/x_1} \approx 1.33$ for the Ising model and thereafter crosses over to the long-distance form given in (10). When $h_1$ becomes larger, the short-distance increase is steeper and $l^{ord}$ shrinks. For $h_1 \to \infty$ we have $l^{ord} \to 0$, and one finds $m \sim z^{-\beta/\nu}$ for all (macroscopic) distances, the result at the extraordinary transition. Largely analogous results—monotonous behavior at the fixed points and profiles with one extremum in the crossover regime—were found by Mikheev and Fisher for the energy density of the two-dimensional Ising model [22].

In conclusion, we studied the effects of a small surface magnetic field at the ordinary transition at or above $T_{c_0}^b$. We found order-parameter exhibits anomalous short-distance behavior in form of a power-law increase $m \sim h_1 z^{1-\eta^{ord}_z}$ near the surface implying a much more pronounced long-range order than could be expected from mean-field theory. For $z$ smaller than $l^{ord}$ and $\xi$, the magnetization increases, while the correlation function (and thus the structure function) is governed by the asymptotic form of the ordinary transition up to correction of $\mathcal{O}(1/c_0)$ [23]. Assuming that there exists a small ordering field $h_1$ in the system studied by Mailänder et al. [4], our scenario gives a plausible explanation for the experimental findings.

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