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On the surface critical behaviour in Ising strips: density-matrix renormalization-group study

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Abstract

Using the density-matrix renormalization-group method we study the surface critical behaviour of the magnetization in Ising strips in the subcritical region. Our results support the prediction that the surface magnetization in the two phases along the pseudo-coexistence curve also behaves as for the ordinary transition below the wetting temperature for finite values of the surface field.

1. Introduction

More than two decades of recent studies have yielded a fairly detailed understanding of the critical behaviour at surfaces [1, 2]. However, attempts to verify theoretical predictions, both in experiments and in model systems, often point out issues which need further clarifications. We came across such an issue in the recent work by Brovchenko *et al*, where the surface critical behaviour of a model water in slitlike and cylindrical pores [3], and of a Lennard-Jones fluid in slitlike pores [4], was studied by means of Monte Carlo simulations. In both cases fluid particles were assumed to interact with a wall via a (10–4) long-range potential and a parameter that measures the well depth of the wall–fluid potential was chosen to correspond to a weakly attractive surface. A one-component fluid like water or the Lennard-Jones fluid is expected to lie in the universality class of the *normal* surface transition of a semi-infinite Ising system. In magnetic language the normal transition is characterized by *two* relevant scaling fields, a surface scaling field $c > 0$ and a non-zero external surface field $|h_1| > 0$. c describes the enhancement of interactions in the surface layer. $c > 0$ corresponds to a reduced tendency to order in the surface, which is the generic case for fluid systems because the presence of a wall should decrease the net fluid–fluid attraction between a molecule and its nearest neighbours below the corresponding bulk value. On the other hand, the containing walls exert an effective potential on a fluid and in magnetic language this corresponds to some generally *nonzero* surface field h_1. There is a possibility to mimic the situation of vanishing surface field $h_1 = 0$, i.e., the so-called *ordinary* surface transition behaviour, by suitable tuning of wall–fluid interactions relative to fluid–fluid interactions. Due to the lack of Ising symmetry in a 'real' fluid, it is very unlikely to find a wall–fluid potential that corresponds exactly to $h_1 = 0$; however, one does find a wall–fluid potential which is 'neutral'. As was shown in [5] for $T \geqslant T_c$, this 'neutral' wall gives rise to the Gibbs adsorption $\Gamma \sim 0$ that is constant along the critical isochore and is characterized by a fluid density profile which, away from the walls where oscillations arise, is almost flat throughout the slit [5]. For the 'neutral' wall a parameter that measures the well depth of the wall–fluid potential corresponds to a weakly attractive surface. In [3, 4] even more weakly attractive substrates were considered. The authors focused on the subcritical regime and studied the temperature dependence of density profiles along the pore liquid–vapour coexistence curve. Recall that the normal transition is governed by the fixed point of the renormalization-group transformation $h_1 = \infty$, $c = \infty$ and should be equivalent to the extraordinary transition given by the fixed point $h_1 = 0$, $c = -\infty$ [6–8]. At these (equivalent) surface transitions, the order parameter (OP) at the surface layer m_1 should have a leading thermal singularity of the same form as the bulk free energy, i.e. $|T_c - T|^{2-\alpha}$, where T_c is the bulk critical temperature. More precisely, one expects for $\tau \to 0$ [6–8] the limiting behaviour

$$m_1 - (m_{1C} + A_1\tau + A_2\tau^2 + \cdots) \approx +A^{\pm}_{2-\alpha}|\tau|^{2-\alpha}, \tag{1}$$

where $\tau \equiv (T_c - T)/T_c$, and the contribution in parentheses is a regular background. For both model fluids Brovchenko *et al* [3, 4] defined the local OP as $\Delta\rho(z) \equiv (\rho_l(z) - \rho_v(z))/2$, where $\rho_l(z)$ and $\rho_v(z)$ are the density profiles of the coexisting liquid and vapour phases, respectively, and found that below the bulk critical temperature T_c this OP shows behaviour which is in accordance with the ordinary transition. In particular, near the surface a variation of $\Delta\rho$ with reduced temperature τ follows the scaling law with a value of the exponent close to the $\beta_1 \simeq 0.82$ of the ordinary transition in the Ising system in $d = 3$, i.e.

$$\Delta\rho_1(\tau) \approx \tau^{\beta_1}. \tag{2}$$

On the basis of these observations, made for the confined fluids, the authors put forward the hypothesis that the difference $\Delta\rho$ between the densities of coexisting phases near the surface should follow the behaviour (2) also near strongly attractive surfaces below the wetting temperature T_w. This is based on the assumption that the term $\sim\tau^{\beta_1}$ should always be present in both coexisting phases below T_w. The authors reconsider the surface critical behaviour of the semi-infinite Ising model, claiming that below the wetting temperature the surface magnetizations m_1^{I} and m_1^{II} in the two phases along the coexistence curve should have the following limiting behaviour for $\tau \to 0$:

$$m_1^{\mathrm{I}} = B_1\tau^{\beta_1} + m_{1C} + A_1'\tau + \cdots + A^{-}_{2-\alpha}|\tau|^{2-\alpha} \tag{3}$$

$$m_1^{\mathrm{II}} = -B_1\tau^{\beta_1} + m_{1C} + A_1'\tau + \cdots + A^{-}_{2-\alpha}|\tau|^{2-\alpha}. \tag{4}$$

The symmetric term $\sim\tau^{\beta_1}$, which describes the temperature dependence of the magnetization at $h_1 = 0$, accounts for the missing-neighbour effect and, as the authors claim, was overlooked in [7, 8]. Above the wetting temperature there exists a single phase which is expected to have surface magnetization of the form given by the above equation.

For the $d = 2$ semi-infinite Ising model there exist exact results for m_1 in the presence of the surface field. They were derived by McCoy and Wu and also by Au-Yang and Fisher using a Pffafian method [9, 10]. Specifically, let us consider a planar rectangular lattice with coordinates i (horizontal) and j (vertical) with spins $\sigma_{i,j} = \pm 1$ located at the sites of the lattice and interacting with nearest neighbours via the coupling $K = \beta J > 0$, $\beta = 1/k_B T$. Assume vanishing bulk magnetic field $h = 0$, a cycling boundary condition in the horizontal direction and a surface magnetic field h_1, measured in the units of the coupling constant J, interacting with one of the two horizontal boundary rows of spins. On the second boundary the spins are free. The configurational Hamiltonian is defined as

$$\mathcal{H} = -J\sum_{i,j}\sigma_{i,j}\sigma_{i,j+1} - J\sum_{i,j}\sigma_{i,j}\sigma_{i+1,j} - h_1\sum_{j}\sigma_{1,j}, \tag{5}$$

where the sums run over $1 \leqslant i \leqslant M$ and $1 \leqslant j \leqslant N$. The analytic expression for the free energy of this system was obtained as a sum [9]

$$MNF + 2N\mathcal{F}_0 + N\mathcal{F}. \tag{6}$$

The first term is the bulk free energy, and the terms $2N\mathcal{F}_0$ and $N\mathcal{F}$ are additional contributions coming from the existence of the free boundary which interacts with the surface magnetic field. The magnetization m_1 of the first row was calculated from

$$m_1 = -\frac{\partial\mathcal{F}}{\partial h_1} \tag{7}$$

and various limiting cases were discussed. In the case relevant for the ordinary transition, i.e. for $h_1 \to 0$, the boundary spontaneous magnetization exists only in the thermodynamic limit $M, N \to \infty$:

$$m_1(0^+) = \lim_{h_1\to 0} m_1(h_1) = \left[\frac{\cosh 2\beta J - \coth 2\beta J}{\cosh 2\beta J - 1}\right]^{1/2}. \tag{8}$$

This vanishes at the critical temperature as

$$m_1(0^+) \approx \left[\frac{2\ln(1+\sqrt{2})}{\sqrt{2}-1}\right]^{1/2} |\tau|^{1/2} \tag{9}$$

from which one can read off the value of the surface critical exponent β_1^{ord} for $d = 2$ Ising model, i.e. $\beta_1^{\mathrm{ord}} = 1/2$. The case when T is near T_{c} and h_1 is positive and *away* from zero is relevant for the normal transition. For this case the result is

$$m_1(h_1) = \text{Taylor ser. in} \quad \tau + \frac{(\sqrt{2}-1)(1-z_1^2)}{\pi z_1^2}\left(\frac{2J}{\beta_{\mathrm{c}}}\right)^2 \tau^2 \ln|\tau|, \tag{10}$$

where $z_1 = \tanh\beta h_1$. Thus the leading singularity of the boundary magnetization agrees with the prediction by Diehl [8] for the normal surface transition, i.e. m_1 has a leading thermal singularity of the same form $\tau^{2-\alpha}$ as the bulk free energy. $\alpha = 0$ in the $d = 2$ Ising model, which corresponds to the logarithmic behaviour. In [10] the first two terms of the Taylor series in τ were given explicitly

$$m_1(h_1) = m_{1,\mathrm{c}}(h_1) + D_1(z_1)\frac{2K_{\mathrm{c}}\tau}{z_1} + \mathrm{O}(\tau^2/z_1^3), \tag{11}$$

where

$$\tfrac{1}{2}\pi D_1(z_1) = 1 + (1+\sqrt{2})^2 z_1^2 \ln z_1^2 + (1+\sqrt{2})^2\left[\tfrac{1}{4}\pi + \sqrt{2} + \ln(1+1/\sqrt{2})\right]z_1^2. \tag{12}$$

On the other hand, if h_1 is nonzero but *small* then, for T near T_{c}, the limiting behaviour of m_1 is different:

$$m_1 \sim \frac{(1-\alpha)^{1/2}}{z^{1/2}} - \frac{2z_1}{\pi z}\ln(1-\alpha+z_1^2), \tag{13}$$

where $\alpha = (1-z)/z(1+z)$, $z = \tanh K$ and $\alpha = 1 - 4K_{\mathrm{c}}\tau + \mathrm{O}(\tau^2)$ for $\tau \to 0$. Thus, as $z_1 \to 0$, equation (13) agrees with equation (8) and exhibits the square-root behaviour of the ordinary transition. These exact results show explicitly that for strong surface field the prediction (3) is not true sufficiently close to the critical temperature. On the other hand

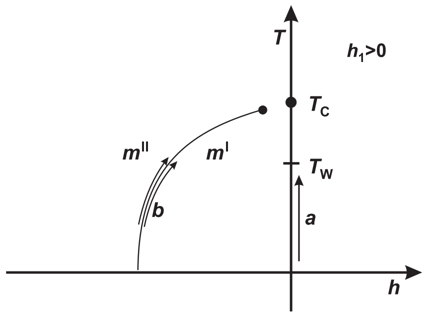

Figure 1. Schematic phase diagram for an Ising strip with positive surface fields. There are two thermodynamic paths presented: (a) along the bulk coexistence and (b) along the (pseudo-) coexistence of the confined system.

in view of equation (13) it is understandable why simulation results for weakly attracting substrates [3, 4] may show the ordinary transition behaviour. However, results described above concern the behaviour of the boundary magnetization only for one of the two possible bulk phases, and the temperature dependence of the *difference* between the magnetizations of both coexisting phases near the surface has not been studied. This is due to the fact that in the absence of the bulk magnetic field the choice of the sign of h_1 breaks the symmetry in the finite system, and, for example, the positive surface field yields (+) phase in the bulk in the thermodynamic limit. In order to calculate the boundary magnetization for the case of the (−) bulk phase in the presence of the positive boundary field, one would have to perform calculations in the presence of infinitesimally small negative bulk field and put $h \to 0^-$ after taking the thermodynamic limit or to solve the model with very sophisticated boundary conditions.

So far, the exact solution of the $d = 2$ Ising model at nonvanishing bulk magnetic field is not available; however, the recently developed density-matrix renormalization-group (DMRG) method [11] allows for very accurate numerical calculations in the presence of the *arbitrary* surface and bulk fields. The DMRG method, based on the transfer matrix approach for calculating the partition functions, includes the critical fluctuations and therefore is very suitable for studying the critical behaviour. In the following we will use this approach to calculate the magnetization profiles in the strip geometry, i.e. the geometry analogous to the one studied in [3, 4]. We assume identical surface fields $h_1 = h_2 > 0$ acting on the two boundaries separated by a finite distance L and consider two different thermodynamic paths: (i) along the bulk coexistence $h = 0$, and (ii) along the pseudo-coexistence of the confined system $h = h_{co}(T)$ (see figure 1). The first path is the one for which the exact results summarized above have been obtained. In this case we want to explore how the finite-size effects in the confined geometry influence the crossover from one type of the surface critical behaviour to another. The second path allows us to study the temperature dependence of the *difference* between the surface magnetizations of both pseudo-coexisting phases.

The DMRG provides an efficient algorithm to construct the effective transfer matrix $\mathcal{T}_{\mathcal{L}}$ for large two-dimensional classical systems at finite temperatures [12]. Starting with a small system (e.g. $L = 4$ in our case), for which $\mathcal{T}_{\mathcal{L}}$ can be diagonalized exactly, one adds iteratively couples of spin columns until the allowed (in the computational sense) size of the effective matrices is reached. Then further addition of new spins forces one to discard simultaneously the least important states to keep the size of the effective transfer matrices fixed. This truncation is done through the construction of a reduced density matrix whose eigenstates provide the

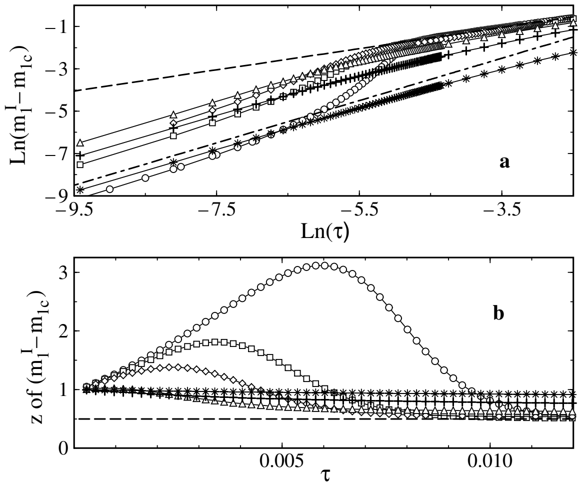

Figure 2. The difference $(m_1^{\rm I} - m_{1c}^{\rm I})$ as a function of τ at $L = 340$ for various surface fields (circles $h_1 = 0.001$, squares $h_1 = 0.005$, diamonds $h_1 = 0.01$, triangles $h_1 = 0.03$, crosses $h_1 = 0.1$, stars $h_1 = 0.5$): (a) the log–log plot, (b) the effective exponent. The dashed line denotes the slope 1/2 and the dotted–dashed line describes the slope 1.

optimal basis set m_λ. The size of the effective transfer matrix is then substantially smaller than the original dimensionality of the configurational space $(2m_\lambda)^2 \ll 2^L$. Generally, the larger is m_λ, the better accuracy is guaranteed. In the present case, we keep this parameter up to $m_\lambda = 40$. Typically, the truncation error was not larger than 10^{-12}. We estimate that the errors in the plots are smaller than the symbol size. The DMRG method allows us to study much larger systems (up to $L = 340$ in this paper) than is possible with the standard exact diagonalization method, which can handle systems up to several dozen columns for the Ising model. Comparisons with exact results for the case of vanishing bulk magnetic field show that this technique gives very accurate results in a wide range of temperatures [13].

2. Along the bulk coexistence $h = 0$

First we discuss results for $h = 0$. Recall that in a finite system with positive h_1 and $h = 0$, below T_c there exists only a (+) phase characterized by magnetization profiles $m^{\rm I}(z)$ which are positive across the strip [14]. In figure 2(a) we show the log–log plot of the difference $m_1^{\rm I} - m_{1c}^{\rm I}$ as a function of τ calculated for the strip of the width $L = 340$ and for the selection of the surface fields. For the weakest considered surface fields, i.e. for $h_1 = 0.001, 0.005, 0.01$, and 0.03, we find the square-root behaviour of the ordinary transition but only for temperatures $\tau > 0.01$. In agreement with the exact result (13) the amplitude of this leading decay does not depend on h_1. For smaller τ there is a crossover to the linear behaviour with the h_1-dependent amplitude. The range of temperatures in which the crossover takes place depends sensitively on the value of the surface field, the weaker h_1 the further away from T_c the crossover starts, but in any case the linear behaviour is observed for $\tau < 0.001$. This is very well illustrated in the plot of the *effective exponent* of $m_1^{\rm I} - m_{1c}^{\rm I}$ as a function of τ (figure 2(b)). The effective exponent, i.e. the quantity

$$z_i = \frac{\ln m_1(i+1) - \ln m_1(i)}{\ln \tau(i+1) - \ln \tau(i)}, \tag{14}$$

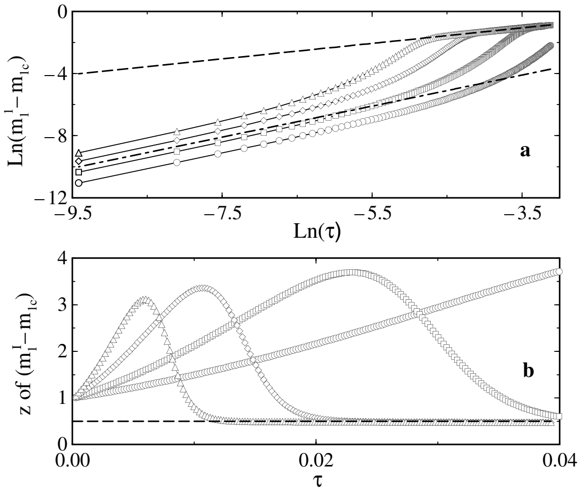

Figure 3. The difference $(m_1^{\rm I} - m_{1c}^{\rm I})$ as a function of τ at $h_1 = 0.001$ for various strip widths L (circles $L = 50$, squares $L = 100$, diamonds $L = 200$, triangles $L = 340$): (a) the log–log plot, (b) the effective exponent. The dotted–dashed line denotes the slope 1, whereas the dashed line describes the slope 1/2.

is the discrete derivative of the data in the log–log scale plot. Such a quantity probes the local slope (at a given reduced temperature $\tau(i)$), providing a better estimate of the leading exponent than a log–log plot. The calculation of z_i requires very accurate data, that can be guaranteed by DMRG data.

The crossover region is associated with the formation of the maximum of the local exponent; it shrinks as the surface field becomes stronger and disappears altogether for $h_1 = 0.1$. For the strongest considered h_1, i.e. for $h_1 = 0.5$, we find a linear behaviour for $\tau < 0.005$; again, the amplitude of this leading decay depends on the surface field. Our findings are consistent with the exact results (10), (13), $h_1 \approx 0.1$ being the approximate value of the surface field for which one type of limiting behaviour crosses over to another. We are not able to decide whether the crossover to the linear behaviour observed for weak surface field is connected with entering the supercritical region above the pseudocritical temperature $T_{c,L}$. Recall that the shift of the critical point due to the finite wall separation and the symmetry-breaking boundary conditions is given by (ignoring nonuniversal metric factors) $\Delta T_c \equiv T_{c,L} - T_c \sim -L^{-1/\nu} X_c(h_1 L^{\Delta_1/\nu})$, $\Delta h_c \sim -L^{-\Delta/\nu} Y_c(h_1 L^{\Delta_1/\nu})$ with $\nu = 1$, $\Delta = 1/15$ and $\Delta_1 = 1/2$ for the $d = 2$ Ising model [14]. X_c and Y_c are universal scaling functions. Mean-field analysis shows that the scaling function X_c is of the order O(1) for small arguments and very weakly depends on the value of h_1 [14]. Thus in the mean field $\Delta T_c \approx -0.001$, but the scaling function $X_c(\zeta)$, where $\zeta = h_1 L^{\Delta_1/\nu}$, is not known for the $d = 2$ Ising magnet. In principle it can vary strongly with the argument. Although the crossover depends sensitively on the value of the surface field, it is not connected with the wetting because $\tau_w \equiv (T_c - T_w(h_1))/T_c \simeq 8 \times 10^{-7}$ for $h_1 = 0.001$, $\simeq 10^{-5}$ for $h_1 = 0.005$, $\simeq 5 \times 10^{-5}$ for $h_1 = 0.01$, $\simeq 5 \times 10^{-4}$ for $h_1 = 0.03$.

Figures 3(a) and (b) show the influence of the finite width of the strip on the critical behaviour of $m_1^{\rm I} - m_{1c}^{\rm I}$ for the weak surface field, i.e. for $h_1 = 0.001$. For larger L the crossover region from the square-root to the linear behaviour is narrow and located closer to T_c. Notice that for small systems (see the curve for $L = 50$ in figure 3(b)) the finite-size effects are so strong that the ordinary transition behaviour is attained only very far from T_c.

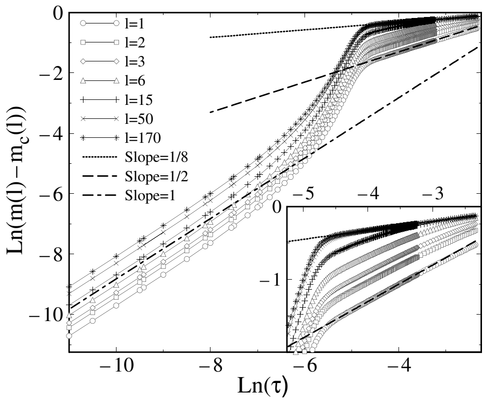

Figure 4. The magnetization as a function of τ at $L = 340$ for various strip layers. The inset presents the enlargement of the large-tau part.

In figure 4 we show that the magnetization in the inside layers of the wide strip ($L = 340$) subject to the weak surface fields $h_1 = 0.001$ decays as $\sim\tau^{\beta}$ with $\beta = 1/8$, i.e., as the spontaneous magnetization, and then crosses over to the linear dependence. Similar behaviour for the variation of the local order parameter was presented by Brovchenko *et al* [4]. It is striking that the crossover to the linear behaviour takes place in approximately the same temperature range, around $\sim$0.01 for all layers.

3. Along the pseudo-coexistence

Now we consider the path along the pseudo-coexistence of the confined system $h = h_{\mathrm{co}}(T; L, h_1)$. When the Ising system is confined between parallel walls subject to identical surface fields h_1, there is a shift of the bulk first-order transition to a finite value of the bulk magnetic field. In order to restore the coexistence the sign of the bulk magnetic field h has to be opposite to the sign of h_1. In $d = 2$ for the system with finite L there is no unambiguous way to determine the pseudo-coexistence line. One can use several criteria, for example maxima of the specific heat, minima of the inverse correlation length or inflection points of the solvation force [15]. However, above some characteristic temperature, which corresponds to the (pseudo-) capillary critical point, the curves based on different criteria separate because they are governed by a different critical exponent. Here we adapt a very natural criterion of the zero total magnetization; i.e., for the fixed value of h one calculates the total magnetization $\Gamma \equiv \sum_{l=1}^{L} m_l$, where m_l is the magnetization in the l-layer corresponding to a perpendicular distance from the first wall, for different temperatures, and identifies $h = h_{\mathrm{co}}(T, h_1)$ at the temperature at which $\Gamma = 0$. This method works very well away from the immediate neighbourhood of the critical point, where the difference between two phases vanishes and it is difficult to locate the point corresponding to $\Gamma = 0$. In the end we are not able to determine the difference $\Delta m_1 \equiv m_1^{\mathrm{I}} - m_1^{\mathrm{II}}$ too close to the bulk critical temperature (in the limit of $\tau \to 0$).

We have performed calculations for the strip of width $L = 340$ and three different surface fields $h_1 = 0.01, 0.5, 0.8$. The temperature dependences of the surface magnetizations of the two coexisting phases m_1^{I} and m_1^{II} calculated along the line $h = h_{\mathrm{co}}(T, h_1)$ for $h_1 = 0.01$ and 0.5 are shown in figure 5. For the strongest field one can see the asymmetry due to the positive surface field. The temperature at which these two curves coincide may be identified with $T_{\mathrm{c},L}$.

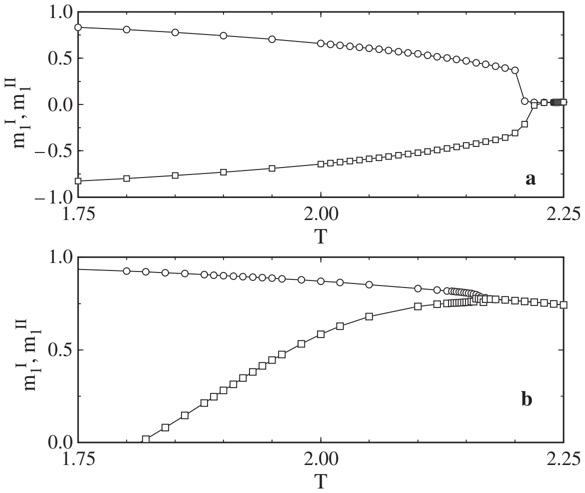

Figure 5. The temperature dependence of the surface magnetizations of the two coexisting phases calculated along the (pseudo-) coexistence lines: (a) $h_1 = 0.01$; (b) $h_1 = 0.5$.

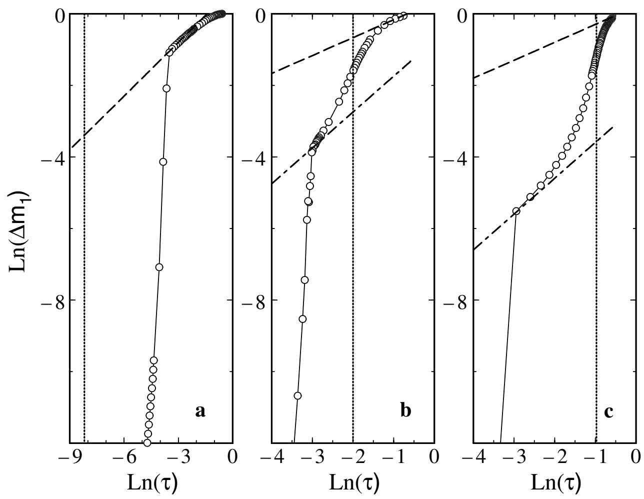

Figure 6. The log–log plots of Δm_1 as a function of τ at $L = 340$ for various surface fields: (a) $h_1 = 0.01$; (b) $h_1 = 0.5$; (c) $h_1 = 0.8$. The vertical dotted lines denote wetting temperatures, the dashed line presents the slope 1/2 and the dotted–dashed line the slope 1.

Note that the pseudo-coexistence temperature is located approximately at the same temperature at which the numerical errors become relevant, i.e. for $h_1 = 0.01$ at ≈2.22 and for $h_1 = 0.5$ at ≈2.165 ($T_c \approx 2.269\,19$ for the $d = 2$ Ising model). The appearance of the numerical errors is connected with large fluctuations near $T_{c,L}$.

The log–log plots of the difference $\Delta m_1 \equiv m_1^{\mathrm{I}} - m_1^{\mathrm{II}}$ versus τ for $h_1 = 0.01$, $h_1 = 0.5$ and $h_1 = 0.8$ are shown in figures 6(a), (b) and (c), respectively, and the effective exponent is presented in figure 7. We also mark the wetting temperature $T_w(h_1)$. The general behaviour which can be read off from these plots is that below $T_w(h_1)$ the difference $\Delta m_1 \equiv m_1^{\mathrm{I}} - m_1^{\mathrm{II}}$ decays approximately like $\tau^{1/2}$, then there is a crossover regime connected with the wetting

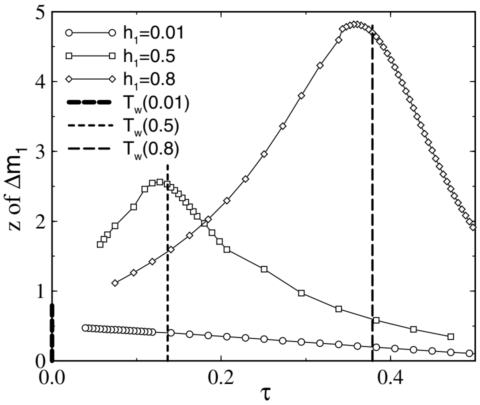

Figure 7. The effective exponent of Δm_1 for various surface fields.

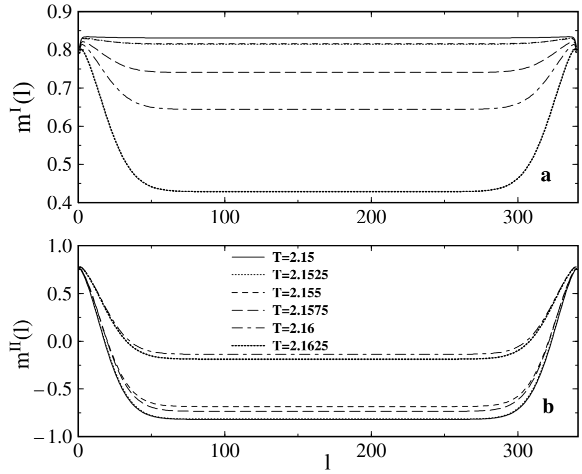

Figure 8. The magnetization profiles near the (pseudo-) critical point calculated along the zero-magnetization line: (a) m^{I}; (b) m^{II}.

transition, closer to T_{c} the linear behaviour dominates and finally there is a rapid decay due to the proximity of the pseudo-critical point. For $h_1 = 0.8$ the approximate square-root behaviour takes place in a very narrow range of temperatures, because T_{w} lies quite far away from T_{c} ($(T_{\mathrm{c}} - T_{\mathrm{w}})/T_{\mathrm{w}} \approx 0.38$). For $h_1 = 0.01$ the linear behaviour is not reached since $T_{\mathrm{w}}(0.01) \approx 2.269\,06$.

It is instructive to see the near surface behaviour of the magnetization profiles in both phases for different temperatures (see figures 8(a), (b)). In the phase opposite to the one that is favoured by walls, i.e. in the negatively magnetized phase m^{II}, the wetting transition manifests itself by a change in $\mathrm{d}m^{\mathrm{II}}(l)/\mathrm{d}l$ from a monotonic function of the distance from the surface l to one exhibiting a minimum (see figure 9).

In conclusion, our DMRG results for the case of vanishing bulk field are in agreement with the exact results and show two different types of the asymptotic behaviour of the surface magnetization. For weak surface fields we see the square-root τ-dependence characteristic of the ordinary surface universality class which crosses over to the linear behaviour sufficiently

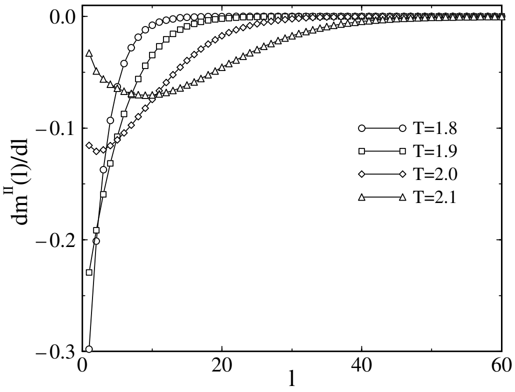

Figure 9. The first derivative of the m^{II} profiles with respect to the distance from the surface at $h_1 = 0.5$. The strip width is $L = 340$. The wetting temperature for this surface field is $T_{\mathrm{w}} \sim 1.96$.

close to T_{c}. This crossover is not connected with the wetting. For $h_1 > 0.1$ we find the linear behaviour which dominates over the singular $\tau^{2-\alpha}$, characteristic of the normal universality class. Results along $h_{\mathrm{co}}(T)$ suggest that $\Delta m_1 \sim \tau^{1/2}$ below the wetting transition but $\Delta m_1 \sim \tau$ above it. However, in order to clear out this issue exact calculations of Δm_1 in the *semiinfinite* system are needed. Because for very weak surface field the wetting temperature lies very close to T_{c} one may in such a case observe only the square-root behaviour as in the simulation of references [3, 4].

References

[1] For a general review of critical behaviour at surfaces, see Binder K 1983 *Phase Transitions and Critical Phenomena* vol 8, ed C Domb and J L Lebowitz (London: Academic) p 1
[2] Diehl H W 1986 *Phase Transitions and Critical Phenomena* vol 10, ed C Domb and J L Lebowitz (London: Academic) p 75 and references therein
[3] Brovchenko I, Geiger A and Oleinikova A 2004 *J. Phys.: Condens. Matter* **16** S5345
[4] Brovchenko I, Geiger A and Oleinikova A 2005 *Eur. Phys. J.* B **44** 345
[5] Maciołek A, Evans R and Wilding N B 2003 *J. Chem. Phys.* **119** 8663
[6] Bray A J and Moore M A 1977 *J. Phys. A: Math. Gen.* **10** 1927
[7] Burkhard T W and Diehl H W 1994 *Phys. Rev.* B **90** 3894
[8] Diehl H W 1994 *Ber. Bunsenges. Phys. Chem.* **98** 466
[9] McCoy B M and Wu T T 1967 *Phys. Rev.* **162** 436
[10] Au-Yang H and Fisher M E 1980 *Phys. Rev.* B **21** 3956
[11] Nishino T 1995 *J. Phys. Soc. Japan* **64** 3598
[12] Peschel I, Wang X, Kaulke M and Hallberg K (ed) 1999 *Lectures Notes in Physics* vol 528 (Berlin: Springer)
Schollwoeck U 2005 *Rev. Mod. Phys.* **77** 259
[13] Maciołek A, Ciach A and Drzewiński A 1999 *Phys. Rev.* E **60** 2887
[14] Fisher M E and Nakanishi H 1981 *J. Chem. Phys.* **75** 5857
Fisher M E and Nakanishi H 1982 *J. Chem. Phys.* **78** 3279
[15] Maciołek A, Drzewiński A and Evans R 2001 *Phys. Rev.* E **64** 056137