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UNIVERSALITY OF THE 2D WETTING TRANSITION WITH RESPECT TO LONG-RANGE FORCES

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Abstract. Effective Hamiltonian models predict non-universal critical singularities for two-dimensional wetting transitions with long-ranged forces. We verify these predictions by studying delocalization transitions in an infinitely long Ising strip, of width L (lattice spacings), with long-ranged surface fields that have opposite sign at each surface. The extrapolated asymptotic value for the exponent β_s does not confirm to the predicted non-universality but instead approaches the same universal value representative of systems with short-ranged forces. The crossover of the scaling behaviour of the transition lines is presented. Moreover, contrary to the existing predictions, the critical wetting transition for $p = 2$ has been found.

Introduction

The presence of marginal forces has a relatively minor influence on critical singularities at bulk phase transitions, but they are believed to influence fluctuation effects at wetting transitions [1]. These predictions arise from analysis of simple interfacial Hamiltonian models which are supposed to describe the relevant physics at length scales much greater than the bulk correlation length. The Ising model is ideally suited to verify it. Therefore we use density-matrix renormalization group (DMRG) technique [2] to numerically investigate a two-dimensional Ising model with long-ranged surface interactions. The DMRG generates very accurate numerical results for thermodynamic quantities for infinitely long strips with widths up to several hundred lattice spacings.

1. Model

A semi-infinite Ising model with the nearest-neighbour particle-particle interactions but with a particle-wall potential that contains a) a contact surface field h_1 at the wall b) a long-ranged tail decaying as $h_{LR}\, l^{-3}$, with l the distance from the surface, should generate the marginal interactions [3].

To extract a value for the critical exponent β_s we rely on finite-size scaling methods which are known to work well for systems with short-ranged forces. Consider a *2D* Ising strip with surfaces that preferentially adsorb different bulk phases. That is why the external potentials arising from each wall are of opposite sign. Further we suppose each semi-infinite surface exhibits a critical wetting transition at temperature (or equivalently surface field strength) T_w. In the confined geometry phase coexistence (or pseudo-phase coexistence) between net up-spin and down-spin phases is restricted to temperatures $T < T_d(L)$. Rather general finite-size scaling arguments suggest that the delocalization temperature is shifted below the semi-infinite wetting temperature by an amount [4]

$$T_w - T_d(L) \sim L^{-1/\beta s}$$

Alternatively at fixed T the same scaling holds for the shifted surface field $h_1(L)$ below its wetting value. The finite-size shift of the delocalization temperature (and the associated behavior of the transverse correlation length) has been well studied for short-ranged forces and allows one to identify the critical wetting critical exponent $\beta_{s.}$

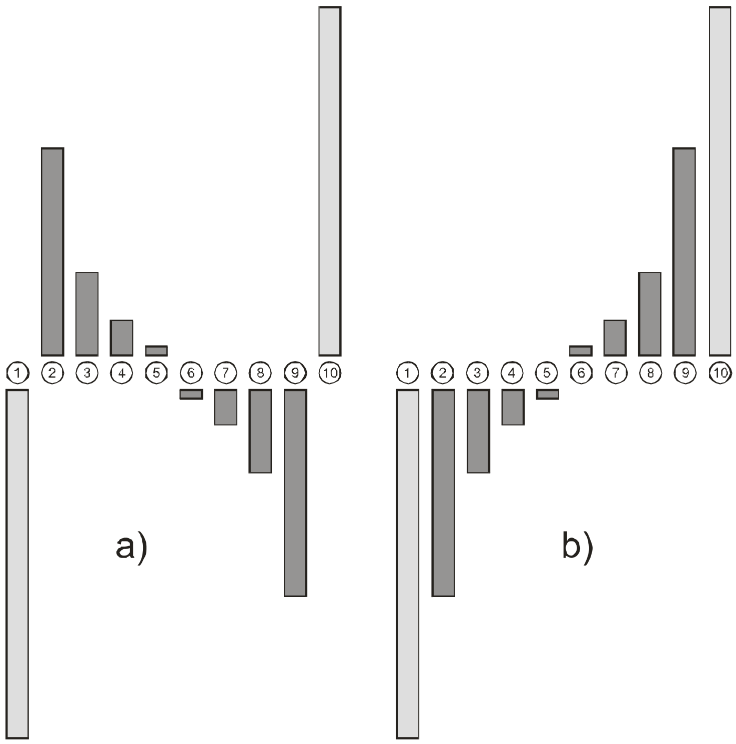

Fig. 1. Schematic drawing of both fields. Light gray columnes denote the short-ranged surface fields, whereas gray ones represent the long-ranged surface fields. There are two cases presented: a) $h_{LR} > 0$ and b) $h_{LR} < 0$

In order to determine a localization of the delocalization transition we have tested four criterions [5]. The approach, we have found the best, is one involving the calculation of the two-point spin-spin correlation function $c_{L/2} = \langle\sigma_{i,L/2}\ \sigma_{i,L/2+1}\rangle$, where $\sigma_{i,j}$ is the usual Ising spin variable defined on a square lattice. This quantity is independent of the index i denoting the position along the strip, and measures the correlation between a nearest-neighboor pair centred at the middle and directed across the strip. In the pseudo-coexistence (partial wetting) regime $\sigma_{i,L/2}$ is large and positive since the two spins tend to align. On the other hand if an interface forms at the center of the strip the spins tend to have opposite sign and $\sigma_{i,L/2}$ is negative. We identify $T_d(L)$ as the maximum of the derivative $\partial\sigma_{i,L/2}/\partial h_1$ at fixed T, L and h_{LR}.

Our model Hamiltonian for the infinitely long strip has the form:

$$H = -J\left(\sum \sigma_{k,l}\sigma_{k',l'} - h_1\sum_k \sigma_{k,1} + h_1\sum_k \sigma_{k,L} + \sum_{l=2}^{L-1} V(l,L)\sum_k \sigma_{k,l}\right)$$

where the first sum is over all nearest-neighbor pairs and we have measured the surface field h_1 and particle-wall potential V in units of J. The walls are located in the l = 1 and l = L lines which are the source of the surface fields h_1 and the long-ranged potential $V(l,L)$. The latter is assumed to arise from the sum of the two independent wall contributions

$$V(l,L) = h_{LR}\left(\frac{1}{l^p} - \frac{1}{(L+1-l)^p}\right)$$

where p = 3 is chosen to generate a marginal long-ranged interaction in the binding potential (Fig. 1).

2. Results

To numerically determine the shifted delocalization temperature $T_d(L)$ in the finite-size strip we use the DMRG method. It was originally proposed by White as a new tool for diagonalization of quantum spin chains [6] and was later adapted to classical *2D* equilibrium statistical mechanics by Nishino [7]. The DMRG allows one to study much larger systems (up to L = 220 in the present paper) than is possible with standard exact diagonalization methods (typically L ~ 50) and provides data with remarkable accuracy. Comparison with exact results for case of vanishing bulk and contact boundary fields show this gives very accurate results in a wide range of temperatures.

Numerical results for various ranges of the surface fields are shown in Figure 2, where sections of the phase diagram separating the localized and delocalized regimes are presented. The temperature is fixed at $T = 1.5$ corresponding to a temperature far far below the critical temperature $T \approx 2.269$. The spontaneous magnetization m_0 is very close to unity at this temperature and the bulk correlation length ξ_b is of order a lattice spacing. This is the region where we anticipate the effective Hamiltonian accurately describes the interfacial physics at length scales much bigger than ξ_b.

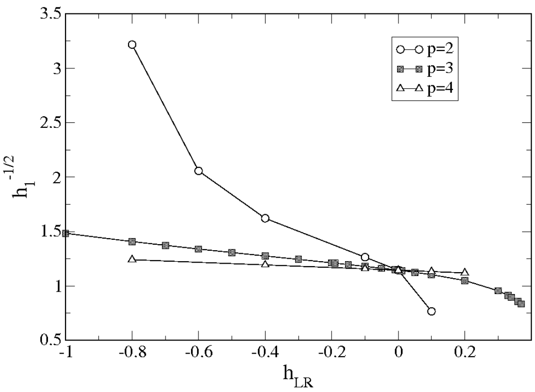

Fig. 2. The lines of pseudocritical points separating the localized and delocalized interfacial states for various ranges p at the $L\to\infty$ limit

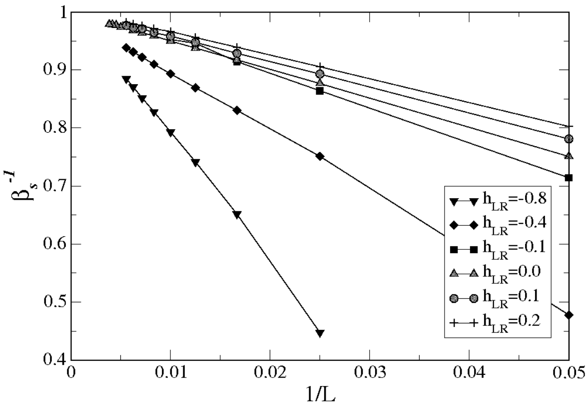

Fig. 3. The effective critical exponents (p = 4) for various values of h_{LR}

Figures 3-5 show the numerical results obtained for the critical exponent $1/\beta_s$ using the finite-size scaling law as applied to the surface field $h_1(L)$. The effective exponent $1/\beta_s^{eff}$ is defined using the usual logarithmic derivative and should converge to the asymptotic results as $L\to\infty$. For short-ranged forces $h_{LR} = 0$ the exponent can be indeed seen to converge to the exact value $\beta_s = 1$ as L increases.

Figure 3 presents the case for fast decaying long-ranged forces, where critical exponent β_s should belong to the universality class of the short-ranged particle-

-wall potentials. The data are completely consistent with this anticipated behaviour. Regardless of the sign of the surface forces, the effective exponent rapidly converges to the universal value $L\to\infty$.

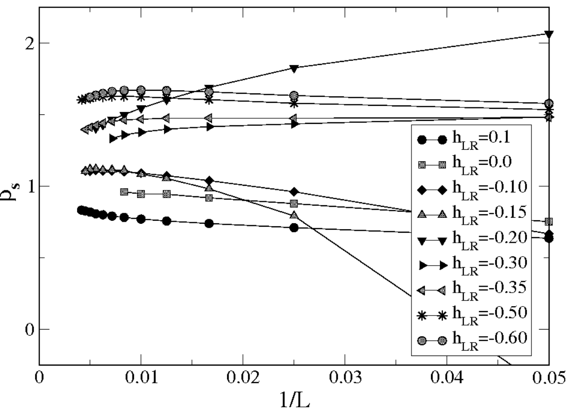

Fig. 4. The effective critical exponents (p = 3) for various values of h_{LR}

Then for the marginal case p = 3 (Fig. 4), if one had access only to strips with widths up to 100, one might reasonably conclude that the effective Hamiltonian predictions of non-universality are well founded. But, it is clear that at larger values of L, the graphs of $1/\beta_s^{eff}$ each show crossover behaviour such that the asymptotic, extrapolated value is close to unity, regardless of the strength of the interaction h_{LR} [8].

But plots for p = 2 (Fig. 5) have occurred to be even more surprising. In contrast to Kroll and Lipowsky [9] results obtained within the continuum one-dimensional solid-on-solid model there is the wetting transition for a field decaying slower than $1/l^3$.

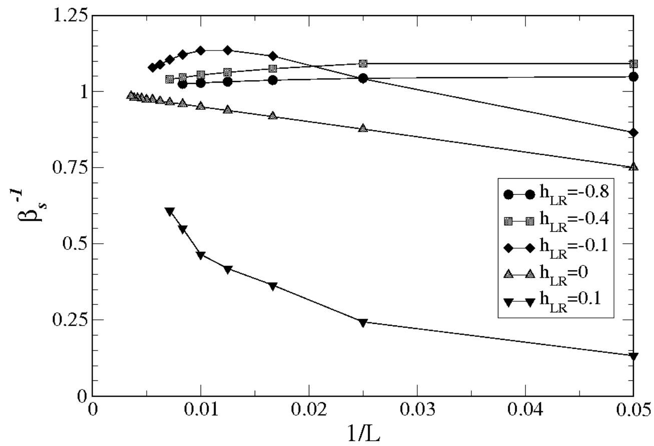

Fig. 5 The effective critical exponents (p = 2) for various values of h_{LR}

For negative h_{LR}, where the fields (both short- and long-ranged) act in a similar way inducing the same interface (see Fig. 1). For positive h_{LR} on the other hand the situation is considerably more involved with all four fields in the surface forces inducing frustration. This results in a rather different transition line for different p and, moreover for large, positive h_{LR} the wetting transition disappears altogether.

As we have mentioned, for all considered p (2, 3, 4) the $L\to\infty$ limit for β_s is one, but $\beta_s^{eff}(L)$ curves for p = 2, 3 differ substantially from the p = 4 plots. Therefore it is worth studying the scaling of the transition lines. We have found that there are always two regimes. It is shown in Figure 6 for p = 3, where the $L\to\infty$ curve is the bottom (upper) limit on the left (right) to a certain value of h_{LR}. This crossover value $h_{LR}^{crossover}$ can be found in the $L\to\infty$ limit, as it is presented in Figure 7. It is worth stressing that when p grows $h_{LR}^{crossover}$ goes to more negative values of h_{LR}, whereas when p goes down the position of $h_{LR}^{crossover}$ moves towards zero.

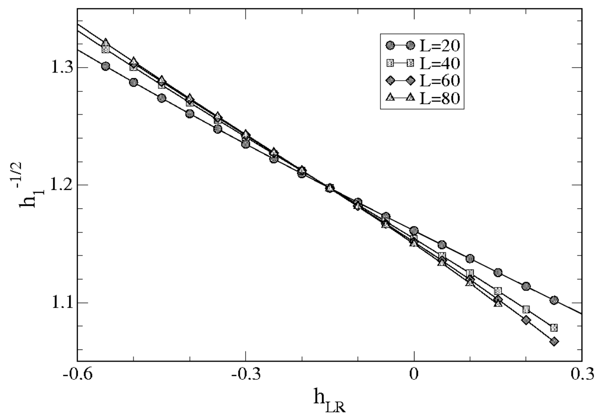

Fig. 6. Exemplary lines of pseudocritical points for various L(p = 3)

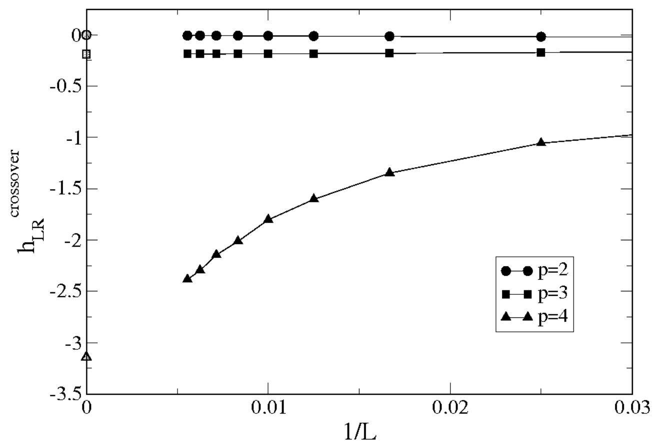

Fig. 7. The behaviour of crossover value $h_{LR}^{crossover}$ for several p

The problem of scaling of the wetting transition lines, especially for $p \leq 3$ will be studied elsewhere.

3. Discussion

We have investigated predictions of non-universality for 2*D* critical wetting in an Ising model with marginal long-ranged interactions. Our results have not supported them since the extrapolated asymptotic values for the critical exponent converge to the universal value. Moreover we have determined the critical wetting transition for $p = 2$ contrary to the existing predictions.

References

[1] Dietrich S. et al., Phase Transitions and Critical Phenomena, eds. C. Domb, J.L. Lebowitz, Academic, London 1988, vol. 12, 1-187.

[2] Schollwoeck U., Rev. Mod. Phys. 2005, 77, 259-315.

[3] Forgacs G., Lipowsky R., Nieuwenhuizen Th.M., (in:) Phase Transitions and Critical Phenomena, eds. C. Domb, J.L. Lebowitz, Academic, London, 1991, vol. 14, 135-367.

[4] Parry A.O., Evans R., Phys. Rev. Lett. 1990, 64, 439-442.

[5] Drzewiński A., Parry A.O., Szota K., Scientific Research of the Institute of Mathematics and Computer Science 2006, 1(5), 15-22.

[6] White S.R., Phys. Rev. Lett. 1992, 69, 2863; S.R. White, Phys. Rev. 1993, B 48, 10345-10356.

[7] Nishino T., J. Phys. Soc. Japan 1995, 64, 3598-3601.

[8] Drzewiński A., Parry A.O., Szota K., Phys. Rev. 2007, E 75, 041110-1-041110-6.

[9] Kroll D.M., Lipowsky R., Phys. Rev. 1983, B 28, 5273-5280.