LOCALIZATION OF THE WETTING TRANSITION FOR FINITE SYSTEMS WITH A LONG-RANGE WALL-FLUID POTENTIAL

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Abstract. The properties of a simple fluid, or Ising magnet, confined in an $L\times\infty$ geometry, are studied by means of numerical density-matrix renormalization-group techniques. We have proposed and have verified a few criterions to determine the wetting transition phase boundary with different ranges of surface forces.

Introduction

Wetting phenomena are ubiquitous in nature [1-3]; the most familiar situation being a liquid-vapour system in a contact with a solid wall. Usually one considers a semi-infinite geometry with a solid planar wall that preferentially adsorbs one of the phases of a system in thermodynamic equilibrium. Below the bulk critical temperature T_c, the adsorbed phase either forms isolated droplets or a thick macroscopic layer. The first case, known as partial wetting, occurs for temperatures below the wetting temperature T_w, while the second case occurs for $T_w \le T < T_c$ and it is referred to as complete wetting. Here, as a model system, the Ising model is considered in a two-dimensional (d = 2) geometry and both phases, a liquid one and a vapour one, correspond to two phases with opposite magnetization. The fact that a wall can favour one of the phases corresponds, in Ising language, to introducing a surface magnetic field h_1. In the d = 2 semi-infinite Ising model the wetting temperature is known exactly [4] and decreases monotonically with the surface field h_1.

For d = 2 Ising strips of a finite width L (with opposing surface fields $h_2 = -h_1$) a partial wetting is restricted to temperatures below the so-called interface delocalisation (ID) temperature $T_d(L)$. For the short-range boundary fields at fixed h_1, when L grows to infinity $T_d(L)$ scales to the wetting temperature T_w as $T_d(L) - T_w \approx L^{-1/\beta_s}$, where β_s is the exponent describing the divergence of the thickness of the wetting layer for a semi-infinite system [5, 6]. At fixed T there is an equivalent form $h_1^{(d)}(L) - h_1^{(w)} \approx L^{-1/\beta_s}$, where ($d$) and ($w$) denote the values of the surface magnetic field on the interface delocalisation line and the wetting transition line, respectively.

A long-standing problem in wetting is the existence or non-existence of universality for $d = 3$ systems with marginal short-ranged interactions. Ising model simulations do not reproduce the non-universality predicted by interfacial models. For
$d = 2$ the marginal interaction is long-ranged and again interfacial models predict non-universality [7]. We propose a study to investigate whether this non-universality is observed in a microscopic Ising system. In order to do it first we should be able to determine the wetting transition line for finite L with a high accuracy. The main goal of the paper is to propose and verify various criteria for doing this.

1. Model

In spite of the name, the density-matrix renormalization-group method (DMRG) has only some analogies with the traditional renormalization group being essentially a numerical, iterative basis, truncation method. It was proposed by White in 1992 as a new tool for the diagonalization of quantum chain spin Hamiltonians [8]. Later, it was adopted by Nishino for $d = 2$ classical systems at non-zero temperatures [9]. The DMRG method allows one to study much larger systems (up to $L = 500$ in this paper) than it is possible with standard exact diagonalization method (up to $L = 40\div50$ for Ising strips) and provides data with remarkable accuracy. In the application of the DMRG method for classical $d = 2$ spin systems, symmetric transfer matrices are used. Comparisons with exact results for the case of vanishing bulk magnetic field and boundary fields acting only on spins in the surface layers, show that this technique gives very accurate results in a wide range of temperatures [10]. Recently the method has been also applied to an Ising film subject to long-range boundary fields [6, 11].

Our results refer to the $d = 2$ strip defined on the square lattice of the size $M\times L$, $M\to\infty$. The lattice consists of L parallel columns at spacing $a = 1$, so that the width of the strip is $La = L$. We label successive columns by the index l. At each site, labeled (k,l), there is an Ising spin variable taking the value $\sigma_{kl} = \pm1$. We assume nearest-neighbour interactions of strength J and Hamiltonian of the form

$$\boldsymbol{H} = -J\left\{\sum_{<kl,k'l'>}\sigma_{kl}\sigma_{k'l'} - h_1\sum_k\sigma_{kl} + h_1\sum_k\sigma_{kL} + \sum_{l=2}^{L-1}H_l\sum_k\sigma_{kl}\right\} \tag{1}$$

where h_1 and H_l are in units of the coupling constant J. The first term in Eq. (1) is a sum over all nearest-neighbour pairs of sites, while in the next two terms h_1 is the surface (short-ranged) magnetic field acting on all sites in the first and in the last column. The opposing signs of these terms guarantee the presence of an interface below T_c, when $L\rightarrow\infty$. The value $H_1 = H_1^s - H_{L+1-l}^s$ is the total long-ranged boundary magnetic field experienced by a spin in the columns $1 < l < L$. The single long-ranged boundary field H_1^s is assumed to have a form $H_1^s = w/l^p$ with $p > 0$. It is worth noticing that if the wetting is universal with respect to the range of the wall-fluid potential β_s should be independent from w.

2. Criterions of localization

In order to determine a localization of the ID transition we have applied four criterions and then extrapolated results to infinity to recover the wetting transition line. Because we are interested in a low-temperature behaviour all calculations were performed at $T = 1.5$. In order to analyse the long-range case we perform our studies for $p = 2, 3, 4$. The $p = 3$ is a marginal case, where both energy and entropy of relevant degrees of freedom scale with L in the same way [2, 12-15]. There is no wetting transition for fields which drop off more slowly than $1/l^3$ so that in our studies of the force law with $p = 2$ we expect that the interface remains pinned to the wall at all finite temperature. For $p > 3$ the entropic contribution dominates and critical behaviour is the same as for the case of short-ranged forces characterising the so-called strong-fluctuation regime [2].

A. The straight profile criterion

Our first criterion is based on a shape of the profile. It is known [16] that for the short-range case for infinite Ising strips with opposing boundary fields at the ID transition the interface meanders in such a way that the magnetization gradient is constant over the whole width L. Therefore the magnetization profile is characterized by the scaling function of a linear form

$$m(l) = m_b\left(1 - \frac{2l}{L}\right) \tag{2}$$

We have adopted it for the long-range case. At fixed T, L, p, and w we changed h_1 measuring the deviations of the profile from a straight line. The ID transition was at the value of h_1, where the deviations were the smallest.

B. The profile scaling criterion

The second criterion is based on the scaling behaviour of a profile, which also occurs at the ID line [16]. In order to localize the ID transition $T_d(h_1;L)$ at a certain temperature T, boundary field scans can be performed for lengths L and L+2. The profiles are compared according to the quantity

$$d(l) = \left[\frac{1}{L} \sum_{l=1}^{L} \left(\frac{m(l)}{m_b} \right)^2 \right]^{1/2} \tag{3}$$

which measures a deviation from the bulk magnetization. To compare the data for L and L+2 we rescale l to value (l–1)/(L–1) which varies between 0 and 1. Then at the value of h_1, where $d(L)$ and $d(L+2)$ cross each other as functions of h_1, both profiles are the most similar. This optimal scaling corresponds to the ID transition. The procedure can be applied to the long-range case as well.

C. The pseudo magnetic susceptibility criterion

The singularity (or a maximum) of the magnetic susceptibility χ is one of the most popular criteria for localization of a phase transition (or a pseudophase directly from the fluctuations of the total magnetization and has been used extensively in Monte Carlo simulations [15]. This is less convenient for the DMRG method, where the free energy is calculated straightforwardly with very high accuracy. Therefore it is natural to use an alternative expression, known from thermodynamics [17], relating the magnetic susceptibility to the second derivative of the free energy f with respect to the bulk magnetic field h. In this case it is necessary to extend our Hamiltonian with a bulk field term acting on all spins in the same way.

Nevertheless our case is a bit special, because we want to determine the transition line at zero bulk field, where in the partial wetting regime there is a first order transition region. For infinite system there is a coexistence of phases with opposing magnetizations. So, there is a discontinuity of the first derivative of the free energy (a jump of the magnetization $m = -df/dh$), when the bulk magnetic field changes sign. That is the reason why, in order to calculate χ (a reaction of a system to a change of the bulk magnetic field) here, one should calculate the derivatives for small nonzero bulk fields and then let h go to zero. In the complete wetting regime the most likely are the configurations, where an interface meanders freely between walls and where there is no discontinuity of the free energy derivatives, when the $h = 0$ plane is crossed.

For numerical calculations (as for the DMRG method) the necessity of performing an extra limit ($h \to 0$ in this case) is troublesome. Therefore we decided to use another quantity χ_0 instead of χ, which is also the second derivative of the free energy at fixed T and h_1, but calculated in a symmetrical way with respect to the $h = 0$ plane (by means of the free energy values taken for five equidistance points: $-2\Delta h$, $-\Delta h$, 0, Δh or $2\Delta h$ - we used $\Delta h = 10^{-5}$ typically). Because our calculations are always carried out for finite L, there is no longer a discontinuity of the magnetization in the partial wetting regime. They are replaced by rounded, but very steep, functions when the $h = 0$ plane is crossed.

In order to determine the ID transition we scan the phase diagram at fixed *L*, *T*, *p*, and *w*. The higher the temperature, the less steep are magnetizations and the values of their derivative χ_0 are smaller. But, of course, at $T = 1.5$ the slope is very steep. At fixed *L*, the ID transition can be indicated by the maximal slope of the χ_0 or the minimum of its derivative with respect to the surface field. Although all derivatives have been performed in a numerical way, the accuracy of the DMRG method yielding very precise results.

D. The central correlation criterion

In this case we have localized $T_d(h_1;L)$ using the correlation function between two neighbouring spins at the center of the strip

$$c_{L/2} = \left\langle \sigma_{L/2,j}\sigma_{L/2+1,j} \right\rangle \quad (4)$$

In the partial wetting regime where there is pseudo-phase coexistence $c_{L/2}$ is large and positive since the two spins are preferably aligned. If an interface is present, $c_{L/2}$ drops to smaller values, since in many configurations when the interface is located at the center of the strip the two spins tend to have opposite values. We identify $T_d(h_1;L)$ as the maximum of the surface field derivative of $c_{L/2}$ at fixed *T*, *L*, *p* and *w*.

3. Discussion

The comparison of the wetting transition lines obtained using the above criteria is presented in Figure 1. The agreement is very good for negative *w*, where the fields (both short- and long-ranged) act in a similar way.

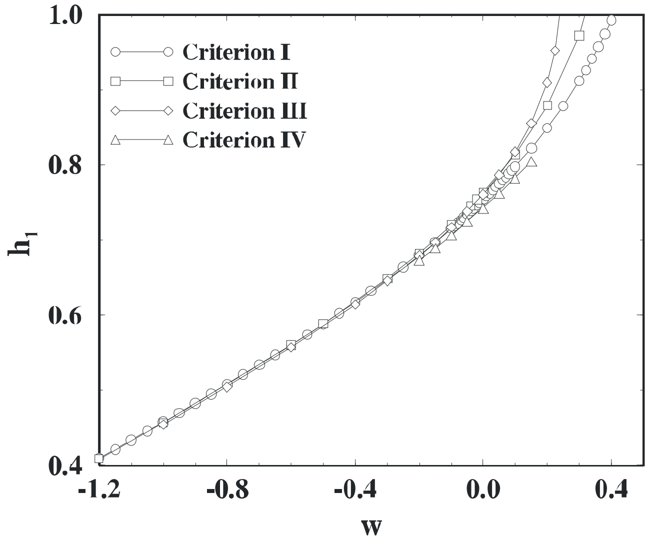

Fig. 1. The wetting transition lines for $L = 60$

As one can see in Eq. (1) here both field terms of the hamiltonian are negative (positive) on the same side of a strip. Due to this both fields induce the same interface. For positive *w* 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 (and critical behaviour). Moreover for large, positive *w* the wetting transition disappears altogether.

Figure 2 presents the extrapolated curves ($L\to\infty$) for different *p*. When *p* grows (the range of the *w* field is smaller with respect to the marginal case) the transition line become more flat. It means that the influence of the long-ranged field is smaller here. In the limit of the short-ranged field ($p\to\infty$) it would be a constant line at the value given by Abraham's curve [4]. When *p* goes down (the range of the *w* field is larger with respect to the marginal case) the transition line become more steep. It seems that contrary to the case with only one long-ranged field acting from the first to the last column (it would be then the following term in the hamiltonian: $\sum_{l=1}^{L} H_l \sum_k \sigma_{kl}$) there is a narrow window where the wetting transition occurs also below $p = 3$.

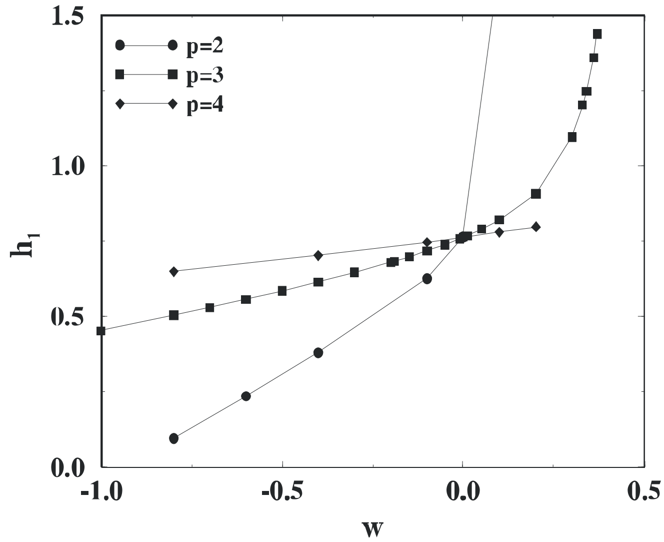

Fig. 2. The wetting transition lines at various *p* for the limit $L \to \infty$. Here, and in the following figures, results based on the central correlation criterion are presented

As far as the problem of scaling of the transition lines is considered there are always two regimes. It is shown in Figure 3 for $p = 3$, where the $L \to \infty$ curve is the bottom (upper) limit on the left (right) to a certain value of w. This crossover value $w_{crossover}$ can be found in the $L \to \infty$ limit, as it is presented in Figure 4. It is worth stressing that when p grows $w_{crossover}$ goes to more negative values of w, whereas when p goes down the position of $w_{crossover}$ moves towards zero.

The problem of universality of the wetting with respect to the range of the wall-fluid potential will be studied elsewhere.

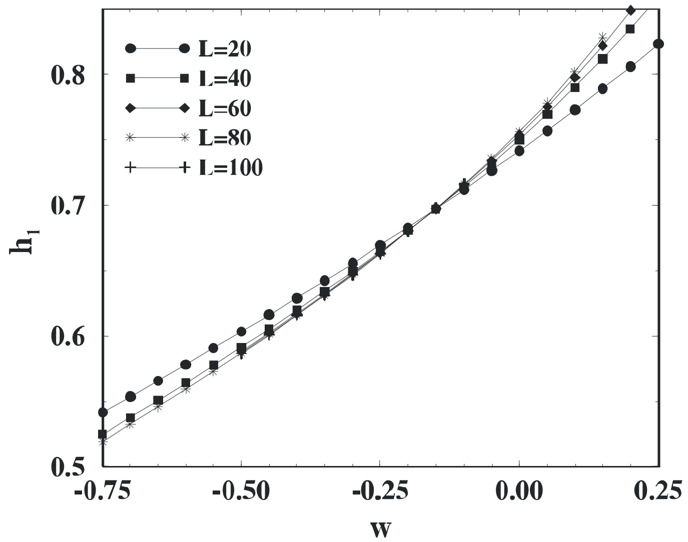

Fig. 3. The wetting transition lines for various *L* at *p* = 3

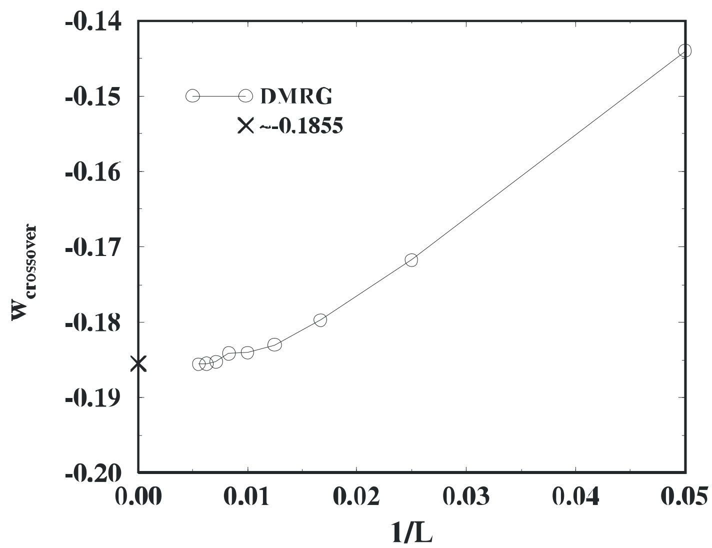

Fig. 4. The scaling of the crossover point at *p* = 3

This work was partially funded by the grant of the Ministry of Science and Higher Education No 1 P03B 061 30.

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