THE WETTING LAYERS FOR LONG-RANGE WALL-PARTICLE POTENTIALS

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Abstract. The complete wetting in 2D Ising strips subject to identical surface fields decaying as $h_1 z^{-p}$ is studied by means of the density-matrix renormalization-group technique. Using different criteria the thickness of a layer is determined along some isotherms above the wetting temperature. It is found that magnetization profiles are characterized by wide interfacial regime.

Introduction

Wetting layers are relevant in many types of liquid coating processes, such as, lubrication, adhesion, microfluidics and nanoprinting. The simple model to mimic these phenomena is a liquid-vapour system in a semi-infinite system [1], where a solid planar wall preferentially adsorbs one of phases. Below the wetting critical temperature T_w, at bulk coexistence (see Fig. 1), the most likely are configurations where a whole system is filled with one phase apart from some isolated droplets of the second phase on the wall. When one moves along the coexistence line to higher temperatures, droplets grow, join each other and finally make a thick macroscopic layer at T_w. Continuous divergence of a layer thickness $l \approx (T_w - T)^{-\beta_s}$ defines, so called, the critical wetting transition. When one is off the coexistence line, the wetting layer is finite. But approach to bulk coexistence above the wetting temperature results in the complete wetting transition (see Fig. 1), where the thickness of a wetting layer is governed by $l \approx h^{-\beta_{co}}$.

Here, as a model system, the Ising model is studied that can be interpreted as the map of a two-dimensional (d = 2) lattice gas model mimicking a d = 2 fluid with short particle-particle interactions. In contrast to mean-field analysis thermal fluctuations are here properly taken into account. Our calculations have been done at the lower critical dimension where the effect of thermal fluctuations is the strongest. In the Ising model both phases, the liquid one and the vapour one, correspond to two phases with opposite magnetization. The fact that a wall can favour one of phases, in Ising language, corresponds to introducing surface magnetic field h_1. In the d = 2 Ising model the wetting temperature is known exactly [2] and decreases monotonically with the surface field h_1. The bulk magnetic field h refers to the chemical potential of the liquid-vapour system.

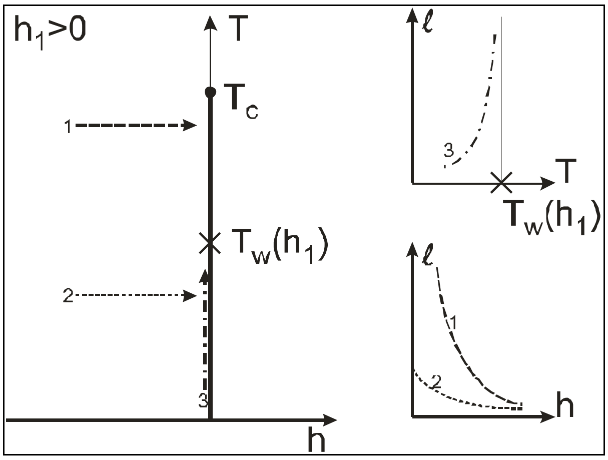

Fig. 1. Phase diagram of the Ising model for a semi-infinite system in the (h,T) plane, where the surface field is positive. The thermodynamical path (1) relates to the complete wetting, (3) to the critical wetting, whereas (2) to the first order transition with a finite l

The main scope of this paper is to verify numerically different ways of determining the thickness of a wetting layer. Contrary to the effective interfacial Hamiltonian approach there is no slab-like magnetization profiles that makes a proccedure unequivocal.

Moreover, the presence of walls makes the system a quasi one-dimensional and there is no longer any true phase transition for finite L. Nevertheless there is still a line of extremely weakly rounded first-order transitions $h_{ca}(T,L)$ ending at a pseudocritical point (Fig. 2) whose location in the plane (h,T) spanned by the bulk field and the temperature depends on the surface field [3]. This phenomenon is equivalent to capillary condensation, where the pseudo-phase coexistence between phases of spin up and spin down occurs along the line h_{ca}, which is given approximately by the analogue of the Kelvin equation [4]

$$h_{ca}(L,T) = \frac{\sigma(T)}{L m_b(T)}$$

where $\sigma(T)$ is the interfacial tension between the coexisting bulk phases and $m_b(T) > 0$ is the spontaneous bulk magnetization. These lines have been identified by localization of points, where the total magnetization of the k-th row vanishes, i.e., $\sum_{z=1}^{L} m_z = 0$, where $m_z = \langle \sigma_{k,z} \rangle$. Simultaneously those points corespond to the maximum of the free energy of a row.

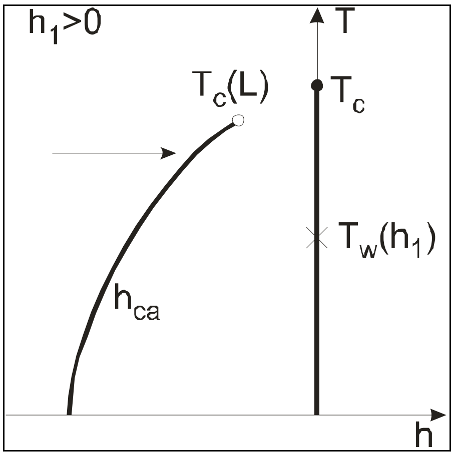

Fig. 2. The coexistence lines for the bulk system (h = 0) and the strip system with the width $L(h_{ca})$ are denoted by a thick line. The dashed arrow presents a typical termodynamical path employed in the present paper

It is worth noticing that following an arrow in Figure 2 the asymptotic complete wetting regime is always preempted by capillary condensation. Therefore we cannot expect divergence of the layer thickness as for a semi-infinite system (the path 1 in Fig. 1).

1. Model

We consider an Ising model in a slit geometry subject to identical surface fields. Our results refer to the d = 2 strip defined on the square lattice of the size $M\times L$, $M\rightarrow\infty$. 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 z. At each site, labeled (w,z), there is an Ising spin variable taking the value $\sigma_{wz} = \pm 1$. We assume nearest-neighbour interactions of strength J and Hamiltonian of the form

$$H = -J\left\{ \sum_{\langle wz,w'z'\rangle} \sigma_{wz}\sigma_{w'z'} + h\sum_{wz}\sigma_{wz} + \sum_{z=1}^{L} H_z \sum_{w}\sigma_{wz} \right\}$$

where h and H_z are in units of the coupling constant J. The first term in (3) is a sum over all nearest-neighbour pairs of sites, while in the second term h is the bulk magnetic field. The value $H_z = H_z^s + H_{L+1-z}^s$ is the total surface magnetic field experienced by a spin in column z. The single-surface field H_z^s is assumed to have a form $H_z^s = h_1 / z^p$ with $p > 0$, and the reduced amplitude of the surface field $h_1 \rightarrow 0$.

In the present paper we use the density-matrix renormalization group (DMRG) technique to study a two-dimensional Ising model with short-ranged as well as long-ranged wall-particle forces. In spite of the name, the DMRG has only some analogies with the traditional renormalization group being essentially the numerical, iterative basis, truncation method. It was proposed by White in 1992 as a new tool for the diagonalization of quantum chain spin Hamiltonians [5]. Later, it was adopted by Nishino for $d = 2$ classical systems at non-zero temperatures [6], where symmetric transfer matrices are considered. Presently this numerical variational technique has become one of the most effective methods in the statistical physics [7].

2. Results

Introducing the long-ranged particle-wall forces shifts the pseudo-coexistence line (it is localized slightly further away for the bulk coexistence line) [8], but this effect is not relevant for our problem. As well the position of the wetting temperature is shifted [9], but our selected isotherms always lie above the corresponding wetting temperature.

We have performed calculations of the magnetization profiles for a strip of width $L = 300$ for various ranges p of the surface field. They are characterized by pronounced interfacial region where a profile varies linearly with the distance from the wall and possesses a large tail. Upon approaching the pseudo-coexistence line this interfacial region thickenss and the decay length of the tail of the profile increases.

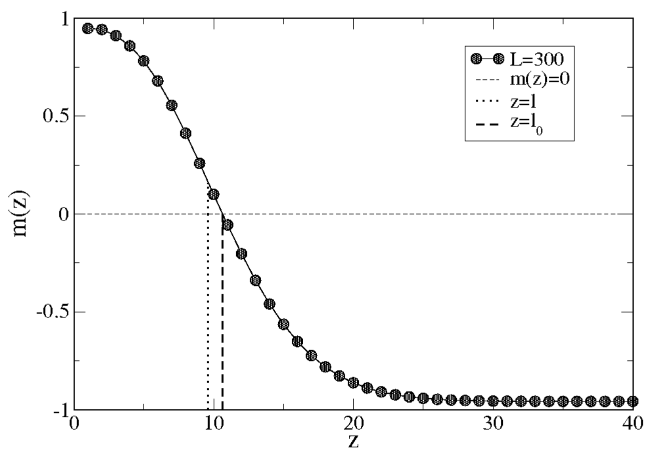

Fig. 3. An exemplary magnetization profiles for $T = 1.8$, $h_1 = 0.8$, $h = -0.0033$ and $p = 3$

In order to infer thickness of the wetting layers from the magnetization profiles we have chosen two criteria. The first one bases on the curvature of the profile: we have assigned to a wetting layer a thickness which corresponds to the distance l at which the profile exhibits its inflection point. The second criterion points out the layer thickness according to the distance l_0 at which the magnetization vanishes $m(l_0) = 0$.

As one can see in Figure 3 the values l and l_0 are somewhat mutually shifted. Since the temperature is relatively low a magnetization profile decay to the bulk value is here fast and as a result the wetting layer is thin (l, $l_0 \ll L$). Collecting those positions for various values of the bulk field the layer thickness can be presented as a function of the distance to the coexistence line. In accordance with expectations we have found a gradual increase of l (or l_0) upon approaching the capillary condensation line; the larger L the closer to the bulk coexistence line.

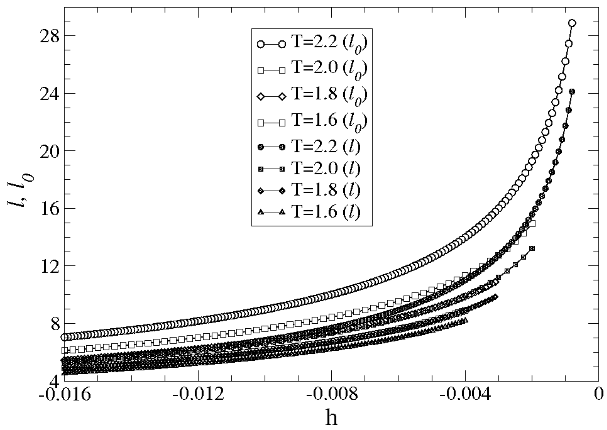

Fig. 4. The wetting layers for $L = 300$, $h_1 = 0.8$ and $p = 3$ for several temperatures

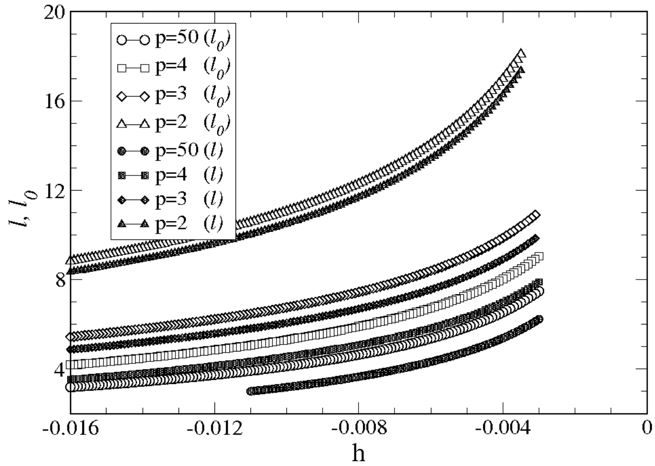

Fig. 5. The wetting layers for $L = 300$, $T = 1.8$ and $h_1 = 0.8$ for several p

Figures 4 and 5 show that both criteria of determining of a layer thickness can be used for different values of system parameters.

Conclusions

In this paper we have analysed the influence of a long-range wall-particle potential on the thermodynamics of an Ising model in a strip geometry. We have found that the magnetization profiles along the isotherms are not slab-like exhibiting a wide interfacial region. The width of the interfacial region growth uppon approaching the pseudo-coexistence line which corresponds to the complete wetting transition. Both applied criteria of determining the position of the wetting layer thickness bring on the same behaviour.

The critical exponents of the complete wetting transitions for long-range wall-particle potentials will be studied elsewhere.

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References

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