WETTING FOR SYSTEMS WITH AN ATTRACTIVE EFFECTIVE INTERFACE POTENTIAL

***Andrzej Drzewiński*[1], *Katarzyna Szota*[2]**

[1] *Institute of Physics, University of Zielona Góra, Poland*
[2] *Institute of Mathematics, Czestochowa University of Technology, Poland*

Abstract. Effective Hamiltonian models for systems with attractive potentials predict the absence of the wetting transition for $p < 3$ (long-ranged wall-particle fields). Our numerical results based on the DMRG method that does not neglect the thermal fluctuations suggest more complex scenario.

Introduction

Wetting phenomena are surface induced phase transitions at or close to two-phase coexistence in the bulk [1]. The analysis of effects of long-ranged forces in 2D on the nature of critical wetting has been performed by Kroll and Lipowsky [2] using the simple local effective interface Hamiltonian of the form

$$H(l) = \int dx \left\{ \frac{\Sigma}{2} \left(\frac{dl}{dx} \right)^2 + W\big(l(x)\big) \right\} \tag{1}$$

Here $l(x) > 0$ is a collective coordinate representing the local distance of the interface separating a bulk phase from a second phase which coexists in the bulk and which intrudes between the bulk and the wall. The statistical weight of a configuration $l(x)$ is proportional to $\exp[-H(l)/(k_B T)]$. The symbol Σ is a stiffness coefficient which penalizes interface fluctuations. $W(l)$ is an effective interface potential which can contain both attractive and repulsive parts. If the forces between the ordering degrees of freedom are also long ranged, one faces the additional challenge to approximate an actually nonlocal effective interface Hamiltonian by the local version given by Eq. (1). In order to avoid this additional complication and in order to keep the full model system still treatable, in the following we consider the wall-particle fields to be the only ones which decay algebraically. The wetting transition refers to the unbinding of the interface from the boundary as the temperature T or the strength of the effective interface potential is varied. In Ref. 2 effective interface potentials, which decay asymptotically as

$$W(l \to \infty) = -Al^{-\delta}, \ \ A > 0 \tag{2}$$

were considered. We note that in 2D van der Waals interactions correspond to $\delta = 3$. By using transfer-matrix methods this interfacial model can be treated exactly by replacing the functional integration over $l(x)$ by an eigenvalue problem, which in the limit of infinite momentum cutoff in the Fourier space reduces to a Schrödinger-type equation for the eigenvectors of the transfer matrix.

Kroll and Lipowsky have concluded that there is no wetting transition for $\delta < 2$ whereas for the marginal value $\delta = 2$ it exists but the associated thermodynamic singularities are of a different nature than for $\delta > 2$. Their prediction is that for $\delta < 2$ the interface remains pinned to the boundary at all finite temperatures.

We have decided to verify the above predictions using non mean-field approach, especially that in two-dimensional systems non-Gaussian fluctuations remain relevant for critical wetting in systems with long-ranged forces [3].

1. Model

In order to determine a localization of the delocalization transition $T_d(L)$ we have tested four criterions [4]. The approach, we have found the best, is one involving the calculation of the two-point spin-spin correlation function $c_{L/2} = <\sigma_{i,L/2}\ \sigma_{i,L/2+1}>$, 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-neighbor 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} (the long-ranged surface field).

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

$$H = -J\sum \sigma_{k,l}\sigma_{k'l'} - h_1\sum_k \sigma_{k,l} + h_1\sum \sigma_{k,l} + \sum_{l=2}^{L-1} V(l,L)\sum_k \sigma_{k,l} \tag{3}$$

where the first sum is over all nearest-neighbor pairs and we have measured the surface field h_1 and wall-particle 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

$$V(l,L) = h_{LR}\left\{\frac{1}{l^p} - \frac{1}{(L+1-l)^p}\right\} \tag{4}$$

where $p > 1$ generates a marginal long-ranged interaction in the binding potential. The long-ranged fields amplitude must be positive to quarantee the attractive character of the potential for large l [5].

The decay exponent p of the boundary field is related to the decay exponent δ of the effective interface potential Eq. (2) according to the relation $\delta = p - 1$. The strength h_1 of the boundary field can be related to amplitude A of $W(l)$ in Eq. (2). This relation has been studied in Ref. 6 within the density-functional theory.

2. Results

In order to numerically find the shifted delocalization temperature $T_d(L)$ in the finite-size strip we use the DMRG method [7] allowing us to study systems up to $L = 120$. To determine the ID transition we scan the phase diagram at fixed temperature and fixed p.

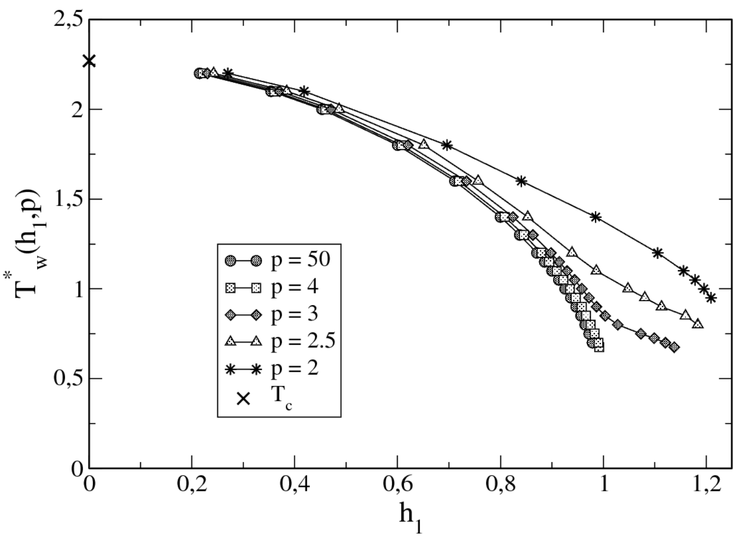

Fig. 1. The lines of points separating the localized and delocalized interfacial states for various ranges p at $L = 120$ and $h_{LR} = 0.05$

Since the $p = 50$ case corresponds to the short-range potential the circles follow practicaly the Abraham's line [8] that is expected to be reached when $L \to \infty$. The $p = 4$ case belongs to the same universality class, so the behaviour should be the same qualitatively. In turn the lines corresponding to long-ranged wall-particle potentials have another behaviour. According to them one can expect that for $p < 3$ there is still the wetting transition providing that temperature is not too low.

3. Discussion

The predictions of the mean-field effective Hamiltonian theory about the absence of the wetting transition for $p < 3$ when the effective interface potentials are attractive for large l was verified. The results for finite systems demonstrate the presence of pseudo-phase wetting transition also for $p < 3$. To clarify it farther considerations are necessary, especially for larger systems.

References

[1] Dietrich S., in Phase Transitions and Critical Phenomena, ed. C. Domb, J.L. Lebowitz, Academic, London 1988, vol. 12, p. 1.

[2] Kroll D.M., Lipowsky R., Phys. Rev. 1983, B 28, 5273.

[3] Forgacs G., Lipowsky R., Nieuwenhuizen Th.M., in Phase Transitions and Critical Phenomena, ed. C. Domb, J.L. Lebowitz, Academic, London 1991, vol. 14, p. 135, and references therein.

[4] Drzewiński A., Parry A.O., Szota K., Phys. Rev. 2007, E 75, 056110.

[5] Drzewiński A., Maciołek A., Barasiński A., Dietrich S., Phys. Rev. 2009, E 80, 019901E.

[6] Dietrich S., Napiórkowski M., Phys. Rev. 1989, A 43, 1861.

[7] Schollwoeck U., Rev. Mod. Phys. 2005, 77, 259.

[8] Abraham D.B., Phys. Rev. Lett. 1980, 44, 1165.