Critical wetting transitions in two-dimensional systems subject to long-ranged boundary fields

A. Drzewiński,¹ A. Maciołek,^{2,3,4} A. Barasiński,¹ and S. Dietrich^{2,3} ¹Institute of Physics, University of Zielona Góra, ul. Prof. Z. Szafrana 4a, 65-516 Zielona Góra, Poland

²Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, D-70569 Stuttgart, Germany

³Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, D-70569 Stuttgart, Germany

⁴Institute of Physical Chemistry, Polish Academy of Sciences, Department III, Kasprzaka 44/52, PL-01-224 Warsaw, Poland

(Received 19 January 2009; published 28 April 2009)

Using the quasiexact density-matrix renormalization-group method and ground-state analysis we study interface delocalization transitions in wide two-dimensional Ising strips subject to long-ranged boundary fields with opposite signs at the two surfaces. Based on this approach, our explicit calculations demonstrate that critical wetting transitions do exist for semi-infinite two-dimensional systems even if the corresponding effective interface potentials decay asymptotically for large ℓ as slow as $\ell^{-\delta}$ with $\delta < 2$, where ℓ is the distance of the mean interface position from the one-dimensional surface. This supersedes opposite claims by Kroll and Lipowsky [Phys. Rev. B 28, 5273 (1983)] and by Privman and Švrakić [Phys. Rev. B 37, 5974 (1988)] obtained within effective interface models. The corresponding wetting phase diagram is determined, including the cases $\delta = 2$ and $\delta = 49$ with the latter mimicking short-ranged surface fields. Our analysis highlights the limits of reliability of effective interface models.

DOI: 10.1103/PhysRevE.79.041144

PACS number(s): 05.50.+q, 68.35.Rh, 68.08.Bc

I. INTRODUCTION

Wetting phenomena are surface induced phase transitions at or close to two-phase coexistence in the bulk, the nature and characteristics of which depend *sensitively* on the range and strength of the underlying microscopic forces and on the spatial dimensionality of the system [1]. Using various models and techniques critical wetting (i.e., continuous surface phase transitions at bulk coexistence) in two dimensions (2D) has been studied intensively for systems in which both the intermolecular forces and the surface fields are purely short ranged. Exact solutions for the nearest-neighbor latticegas model [2,3], which is equivalent to the 2D Ising model, are in a perfect agreement with the predictions of reduced effective interface Hamiltonian models as far as the universal critical behavior is concerned [4]. These original effective Hamiltonian models, which are designed to describe the interfacial structures at length scales much larger than the bulk correlation length ξ , have been generalized to study also the relevant effects of long-ranged, i.e., algebraically decaying forces. Examples of such long-ranged forces are dispersion or van der Waals forces, dipolar forces, Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions, forces in charged systems, and elastic forces in solids. These effective models allow one to identify the universality classes and various so-called fluctuation regimes depending on the range of the underlying microscopic forces [5]. Such effective models are particularly useful and popular because the full lattice-gas model with long-ranged interactions allows only for approximate solution such as various mean-field approximations.

In this spirit the analysis of effects of long-ranged forces in 2D on the nature of critical wetting has been performed by Kroll and Lipowsky [6] using the simple local effective interface Hamiltonian of the form

$$\mathcal{H}[\ell] = \int dx \left\{ \frac{\Sigma}{2} \left(\frac{d\ell}{dx} \right)^2 + W(\ell(x)) \right\}.$$
(1)

Here $\ell(x) > 0$ is a collective coordinate representing the local distance (height) of the interface separating a bulk phase β from a second phase α which coexists in the bulk and which intrudes between the bulk and the wall. The statistical weight of a configuration $\ell(x)$ is proportional to $\exp[-\mathcal{H}[\ell]/(k_B T)]$. Σ is a stiffness coefficient which penalizes interface fluctuations. $W(\ell)$ is an effective interface potential which can contain both attractive and repulsive parts. Both may vary algebraically, i.e., $W(\ell) = -A\ell^{-\delta} + B\ell^{-q}$, or W may have a form appropriate for the combined presence of short-ranged and long-ranged forces, i.e., $W(\ell) = -A\ell^{-\delta} + B \exp(-\ell/\xi)$. We note that Eq. (1) is supposed to be a reliable, reduced description if the forces among the ordering degrees of freedom are short ranged with the boundary fields decaying algebraically or faster. 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 [7-9] 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 boundary 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. [6] effective interface potentials, which decay asymptotically as

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

were considered. We note that in 2D van der Waals interactions correspond to δ =3. By using transfer-matrix methods this interfacial model can be treated exactly by replacing the functional integration over $\ell(x)$ 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. From the analysis of this equation it follows that the character of the critical behavior depends on whether the exponents δ and q are larger or less than a marginal value given by 2. The conclusion of the analysis by Kroll and Lipowsky [6] has been 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. This conclusion has been drawn by providing upper and lower bounds for the ground-state energy E_0 of the aforementioned corresponding Schrödinger equation. Within this approach the occurrence of a bound state solution of the Schrödinger equation $(E_0 < 0)$ corresponds to a localized interface. When the bound state ceases to exist, $E_0 \nearrow 0$ signals a critical wetting transition. The construction of upper and lower bounds (based on using an exponentially decaying trial wave function) shows that the ground-state energy has a nonzero value (i.e., there is no transition) for a finite potential strength.

The case corresponding to δ =1 has been studied by Privman and Švrakić in Ref. [10] within the so-called restricted solid-on-solid (SOS) model in which the first term in Eq. (1) is replaced by the absolute value of limited height differences between neighboring lattice sites. They have argued that for attractive effective interface potentials decaying such as $1/\ell$ for large distances ℓ from the boundary the wetting transition is no longer sharp but rounded. This finding is consistent with the claim by Kroll and Lipowsky [6].

There are at least two reasons for trying to describe interfacial properties in terms of effective interface models. First, a reliable statistical mechanics treatment of fully microscopic models of inhomogeneous systems is either very challenging or even out of reach. Thus an effective interface model provides practical means to overcome these difficulties via a reduced description and thus reduced difficulties (which can still be very demanding). Second, if the reduced description turns out to work successfully, it provides deep insight into which degrees of freedom are the relevant driving forces for certain interfacial phenomena (such as wetting phenomena) and which degrees of freedom of a fully microscopic model are either irrelevant or of reduced importance.

Over the last 25 years intensive research on wetting transitions, as paradigmatic phenomena which lend themselves to resort to the concept of effective Hamiltonians, has demonstrated that utmost care is necessary for designing effective descriptions-in particular if non-Gaussian thermal fluctuations play a decisive role (a situation in which a reduced description happens to be most needed). In spatial dimension D=3 this is the case for critical wetting in systems with short-ranged forces [1]. After substantial efforts in describing these kinds of critical wetting transitions by effective interface models, large scale Monte Carlo (MC) simulations for a fully microscopic three-dimensional (3D) Ising model revealed qualitative shortcomings of the reduced descriptions [11,12]. It took several years of dedicated efforts, through various stages, to overcome these shortcomings and to reach a more satisfactory understanding in terms of improved effective models [13].

Whereas in D=3 for long-ranged forces the leading thermal singularities of continuous wetting transitions are captured correctly by mean-field theory [1], in D=2 non-Gaussian fluctuations remain relevant for critical wetting in systems with long-ranged forces [4]. Guided by the aforementioned experience in D=3, the natural question arises, whether and to which extent the effective interface models. used so far in D=2 for systems with long-ranged forces [Eqs. (1) and (2)], capture the actual behavior of the underlying microscopic model they are supposed to describe. In order to answer this question, one has to study appropriate microscopic models such as the 2D lattice-gas model. This has become possible only recently due to substantial progress in simulation and numerical techniques and computer capacities. In this context, as far as algebraically decaying boundary fields are concerned, for the full 2D lattice-gas model (i.e., Ising model) up to now only for the case $\delta = 2$ [Eq. (2)], which is marginal in the sense of Ref. [6], the critical wetting temperature T_w has been determined by the density-matrix renormalization-group (DMRG) approach [14] and by MC simulations [15,16]. These studies have shown that the presence of long-ranged tails in the decay of the boundary fields decreases the critical wetting temperature T_w relative to the one of the short-ranged boundary fields with the same strength. The observation of this trend is, at least in principle, compatible with the expectations raised in Ref. [6], provided T_w reaches zero for $\delta < 2$.

In order to elucidate the influence of the range of boundary fields on 2D wetting phenomena we use the DMRG method [17–20] to numerically investigate the existence of critical wetting transitions in the 2D Ising model with longranged boundary fields corresponding to $\delta = 0.5, 1, 2$. For completeness and in order to test our numerical procedure we also consider the case $\delta = 49$, which is expected to exhibit a behavior which closely resembles that for the short-ranged potential corresponding to $p = \infty$. The DMRG method, which is based on the transfer-matrix approach, provides a numerically very efficient iterative truncation algorithm for constructing the effective transfer matrices for strips of fixed width and infinite length. At present, strips of widths up to L=700 lattice constants can be studied. The quantitative data for thermodynamic quantities and correlation functions obtained this way are very accurate and can be provided in a wide range of temperatures and in the presence of arbitrary boundary and bulk fields.

In order to locate critical wetting transitions we resort to finite-size scaling methods [21-23] which proved to work well for 2D systems with short-ranged forces [2,24] and were also used to locate critical wetting transitions for long-ranged forces with $\delta=2$ [15,16]. These methods amount to extrapolating the finite-size delocalization temperature of an interface, which forms in a 2D Ising strip with boundaries preferring different bulk phases, to the thermodynamic limit.

Locating critical wetting transitions for algebraically decaying boundary fields with various decay exponents is a prerequisite for investigating the crossover behavior between the complete wetting and critical adsorption regimes in the presence of long-ranged boundary fields. In our subsequent work [25] we study an interplay of complete wetting, critical adsorption, and capillary condensation for two-dimensional Ising ferromagnets in strip geometries subject to long-ranged boundary fields with $\delta = 0.5$, 1, 2, and 49. The present study shows that there exist continuous wetting transitions for δ < 2, although for this range of values of δ the simple effective interface model predicts incomplete wetting for all temperatures. Our subsequent study shows [25] that even if one enforces by fiat that the *full* effective interface potential $\overline{W}(\ell)$, i.e., the potential $W(\ell)$ renormalized by the interface fluctuations, exhibits complete wetting, the corresponding increase in the wetting film thickness for decreasing undersaturation as calculated from the full microscopic model does not agree with predictions based on $\overline{W}(\ell)$. Thus for $\delta < 2$ the concept of the effective interface model, at least in its presently available form, does not capture the essential features of the underlying microscopic model.

We introduce the model in Sec. II. In Sec. III we determine the wetting transition temperatures for different ranges of the boundary fields. Section IV contains our conclusions.

II. MICROSCOPIC MODEL

In this section we introduce the microscopic model for which we investigate quantitatively the existence of critical wetting. We consider Ising ferromagnets in slit geometries subject to the same boundary fields on both sides but of *opposite* sign. Contingent on the type of numerical approach we shall use, our results refer to D=2 strips defined on a square lattice of size $M \times L$, $M \rightarrow \infty$. The lattice consists of Lparallel rows at spacing a so that the width of the strip is La; in the following we set a=1. Successive rows are labeled by an index j. At each site, labeled (k,j), there is an Ising spin variable taking the value $\sigma_{k,j}=\pm 1$. The boundary surfaces are located in the rows j=1 and j=L, and periodic boundary conditions (PBCs) are assumed in the lateral x direction. Our model Hamiltonian for the strip with PBCs and $M\rightarrow\infty$ is given by

$$\mathcal{H} = -J\left(\sum_{\langle kj,k'j'\rangle} \sigma_{k,j}\sigma_{k',j'} + \sum_{j=1}^{L} V_{j,L}^{\text{ext}}\sum_{k} \sigma_{k,j} + H\sum_{k,j} \sigma_{k,j}\right),\tag{3}$$

where the first sum is over all nearest-neighbor pairs and the external potential is measured in units of J>0. $V_{j,L}^{\text{ext}}=V_j^s$ $-V_{L+1-j}^s$ is the total boundary field experienced by a spin in row *j*; it is the sum of the two independent wall contributions. The single-boundary field V_j^s is taken to have the form

$$V_j^s = \frac{h_1}{j^p},\tag{4}$$

with p > 0 and $h_1 > 0$. *H* is a bulk magnetic field. According to Eq. (3) h_1 and *H* are dimensionless.

This model can be viewed as being obtained from a 2D lattice gas model mimicking a two-dimensional onecomponent fluid with a short-ranged interaction potential between the fluid particles and either short-ranged or longranged substrate potentials. The equivalence between the lattice gas and the Ising model implies the following relationships (see, e.g., Ref. [26]): the bulk magnetic field Hin the former is proportional to the deviation $\Delta \mu$ of the chemical potential from the bulk phase boundary $\mu_0(T)$ in the latter, i.e., $H \sim \Delta \mu$. The lattice gas analog of the number density ρ in the fluid is related to the magnetization m by $\rho = (m+1)/2$ so that $\Delta \rho = \rho_l - \rho_g \sim 2m_b$, where m_b is the spontaneous magnetization and ρ_l and ρ_g are the number densities of the coexisting liquid and gas phases in the bulk, respectively. Finally 4J corresponds to the strength of the attractive pair potential between the fluid particles, taken to be short ranged so that in the lattice gas model it can be modeled by a nearest-neighbor interaction. V^{ext} is a combination of the substrate potential and the liquid-liquid interaction. These relationships can be extended to binary liquid mixtures [27].

The decay exponent p of the boundary field [Eq. (4)] is related to the decay exponent δ of the effective interface potential [Eq. (2)] according to

$$\delta = p - 1. \tag{5}$$

The strength h_1 of the boundary field can be related to the amplitude A of $W(\ell)$ in Eq. (2). This relation has been studied in Ref. [8] within the density-functional theory. The surface stiffness is known exactly for the 2D Ising model: $\Sigma/(k_BT) = \sinh 2(K - \frac{1}{2}\ln \coth K)$, where $K = J/(k_BT)$. The amplitude of the effective interface potential is given by $A = m_0 K h_1$, where m_0 is the spontaneous bulk magnetization.

III. DETERMINATION OF THE WETTING TRANSITION TEMPERATURE

For the finite systems we are studying, below the bulk critical temperature T_c the wetting transition temperature $T_w(h_1,p)$ as a function of h_1 for any range p of the boundary fields can be inferred from the so-called (weakly rounded in d=2) interface localization-delocalization (ILD) transition [21,23] which occurs in strips with antisymmetric boundary fields, i.e., for $V_{j,L}^{\text{ext}} = V_j^s - V_{L+1-j}^s$. This transition is the precursor of a wetting phase transition which occurs in the limit of infinite film thickness $(L \rightarrow \infty)$ at $T_w(h_1,p)$. For $T < T_w(h_1,p)[T > T_w(h_1,p)]$ such an interface is bound to (unbound from) the walls [21,23].

A. Ground-state analysis

First, we note that $T_w(h_1 \rightarrow 0, p) \rightarrow T_c$ for any p [see Eq. (4)]. On the other hand $h_{1w}(T=0,p)$, which is the solution of the implicit equation $T_w(h_1,p)=0$ and denotes the critical surface field strength beyond which the system is wet even at T=0, shifts toward lower values upon decreasing p. There is no reason to expect a nonmonotonic behavior of $T_w(h_1,p)$. Therefore, the gross features of the shape of the wetting transition line $T_w(h_1,p)$ for an arbitrary p>1 can be inferred from localizing the position of the wetting transition $h_{1w}(T=0,p)$ in the ground state. The ground-state energy of the system (in units of J) can be found directly from the Hamiltonian with a vanishing bulk field. Because the system is translationally invariant along a strip, it is sufficient to consider only the configurations of a single column.

j

In a partial wetting regime with antisymmetric surface fields there are only two coexisting states (all spins up or all spins down) with the energy (per the number M of columns),

$$E_{pw}^{\pm} = -J(L-1) \mp h_1 J \left(1 - \frac{1}{L^p} + \frac{1}{2^p} - \frac{1}{(L-1)^p} + \frac{1}{(L-1)^p} - \frac{1}{2^p} + \frac{1}{L^p} - 1 \right)$$

= $-J(L-1).$ (6)

In a wet regime at least one interface between spin up and spin down configurations has to be present. For even L the lowest-energy configuration is that for the state with the interface located in the middle of the strip. For $p \rightarrow \infty$ (shortranged case) L-1 degenerate states emerge with a single interface positioned at any of the rows but the ones closest to the surfaces. In general, the energy of a single column with an interface in the middle of a strip (spin up for j=1,...,L/2 and spin down for j=L/2+1,...,L) is

$$E_{\text{wet}} = -J(L-3) - h_1 J \left(1 - \frac{1}{L^p} + \frac{1}{2^p} - \frac{1}{(L-1)^p} + \frac{1}{(L/2)^p} - \frac{1}{(L/2+1)^p} - \frac{1}{(L/2+1)^p} + \frac{1}{(L/2)^p} + \frac{1}{(L-1)^p} + \frac{1}{2^p} - \frac{1}{L^p} + 1 \right).$$
(7)

In the ground state and at the ILD transition the energies E_{pw} and E_{wet} are equal. For a particular *L* this determines the critical strength $h_{1w}^{\text{ILD}}(L)$,

$$h_{1w}^{\text{ILD}}(L) = 1/\left(1 + \frac{1}{2^p} + \frac{1}{3^p} + \dots + \frac{1}{(L/2)^p} - \frac{1}{(L/2+1)^p} - \dots - \frac{1}{(L-1)^p} - \frac{1}{L^p}\right)$$
$$= \left\{\sum_{n=0}^{\infty} \frac{1}{n^p} - 2\sum_{n=L/2+1}^{\infty} \frac{1}{n^p} + \sum_{n=L+1}^{\infty} \frac{1}{n^p}\right\}^{-1}.$$
 (8)

In order to find the critical wetting field $h_{1w} = h_{1w}^{\text{ILD}}(L \to \infty)$ we take the limit $L \to \infty$. According to the second line in Eq. (8) this leads to

$$h_{1w} = 1 \left/ \sum_{n=0}^{\infty} \frac{1}{n^p} = 1/\zeta(p),$$
 (9)

where $\zeta(p)$ is the Riemann zeta function (see Fig. 1). Its values are known analytically only for certain even values: $\zeta(p=2)=\pi^2/6$ and $\zeta(p=4)=\pi^4/90$ which gives $h_{1w}(p=2) \approx 0.6079$ and $h_{1w}(p=4) \approx 0.9239$. Other values can be found in tables of special functions, e.g., $\zeta(p=3) \approx 1.2021$ giving $h_{1w}(p=3) \approx 0.8319$. In the short-ranged limit $(p \to \infty)$ the Riemann zeta function approaches 1, confirming Abraham's solution at T=0 [2]. Even more interesting is the opposite limit $\zeta(p\to 1)\to\infty$ which results in $h_{1w}(p\to 1)\to 0$. This means that at T=0 the wetting transition does not exist for $p \le 1$. Thus there is a continuous wetting transition at T=0



FIG. 1. Onset strength $h_{1w}(p)$ [Eq. (9)] for critical wetting at T=0 as function of the decay exponent p of the boundary fields. Only for $0 < h_1 < h_{1w}(p)$ there is a temperature range $0 < T < T_w(h,p)$ within which the system is nonwet at bulk coexistence H=0. For the asymptotic behavior one has $h_{1w}(p \rightarrow 1^+)=p-1$ and $h_{1w}(p \rightarrow \infty)=1-2^{-p}=1-\exp(-p \ln 2)$.

for all values $\delta > 0$. [For $p \le 1$, $\sum_{j=1}^{L} h_1/j^p$ diverges for $L \to \infty$ which renders $W(\ell)$ as ill defined.]

B. DMRG results

In order to determine the location of a quasi-ILD transition between T=0 and $T=T_c$ various criteria can be applied. For example, for p=3 in Refs. [15,16] the intersection points for various L of the fourth-order cumulant and of the total magnetization as a function of temperature, as well as the maximum of the susceptibility and the peak of the surface susceptibility, were used. The peaks of total and surface susceptibilities have been extrapolated to the thermodynamic limit $L \rightarrow \infty$ using the finite-size scaling behavior predicted for p=3. These different criteria led to a slight spread of the estimates for $T_w(h_1, p=3)$, probably because the linear dimensions L were not yet large enough for the asymptotic power laws to hold. Here we have adopted the approach involving the magnetic susceptibility χ [14]. The singularity (or a maximum) of the magnetic susceptibility χ is one of the most useful criteria for the localization of a phase transition (or of a pseudophase transition for a finite system). The magnetic susceptibility can be calculated as the second derivative of the free energy f with respect to the bulk magnetic field H. This method is very convenient for the DMRG approach because the latter provides the free energy with a very high accuracy.

Nevertheless the present case is somewhat special because we want to determine $T_w(p,h_1)$ at H=0, where in the partial wetting regime, i.e., for $T < T_w$, there is a first-order bulk transition. In the thermodynamic limit there is coexistence of phases with opposite magnetizations. Thus there is a discontinuity of the first derivative of the free energy f (a jump of the magnetization $m=-\partial f/\partial H$) upon changing the sign of the bulk magnetic field. Accordingly, in order to calculate χ there, one has to calculate the derivatives for small nonzero bulk fields and then to consider the limit $H\rightarrow 0$. In the complete wetting regime, i.e., $T>T_w$, or equivalently



FIG. 2. Illustration of the generic behavior of χ_0 as a function of temperature. χ_0 is a second derivative of the free energy with respect to the bulk field *H*, calculated symmetrically around *H*=0 and evaluated at *H*=0. The data shown here have been obtained for a film of thickness *L*=100 and boundary fields of strength h_1 =0.6 and with decay exponents *p*=3 and *p*=50 [Eq. (4)]. The peak of the derivative χ'_0 of χ_0 with respect to temperature (see inset) has been used to determine the quasi-interface localization-delocalization transition (see main text).

above the ILD transition, the finite system exhibits only a single phase with an interface meandering freely between the boundaries so that there is no discontinuity of the free-energy derivatives upon crossing H=0.

For numerical calculations such as the ones within the DMRG method the necessity of performing an extra limiting procedure $(H \rightarrow 0$ in this case) is cumbersome. Therefore, instead of χ , we have focused on another quantity χ_0 , which also corresponds to the second derivative of the free energy at fixed *T* and h_1 , but is calculated numerically in a symmetrical way with respect to H=0 by taking the free-energy values at five equidistant points: $-2\Delta H$, $-\Delta H$, 0, ΔH , or $2\Delta H$; we typically used $\Delta H=10^{-5}$. Because our calculations are always carried out for finite *L*, there is no discontinuity of the magnetization in the partial wetting regime. These discontinuities are replaced by functions which are rounded but steeply vary at H=0.

In order to determine the ILD transition we have scanned the phase diagram at fixed h_1 . The higher the temperature, the less steeply the magnetizations vary and the values of their derivative χ_0 are smaller. Above the wetting temperature, where there is no discontinuity, $\chi_0(H=0,T)$ saturates for increasing *T*; here χ_0 is equivalent to χ . Therefore, at fixed *L*, the ILD transition can be identified by the maximal slope of χ_0 or the minimum of its derivative with respect to temperature. Although all derivatives have been performed numerically, the high accuracy of the DMRG method guarantees very precise results. An example for the typical behavior of χ_0 and of its derivative $\chi'_0 \equiv \partial \chi_0 / \partial T$ as a function of temperature is shown in Fig. 2 for *L*=100, *h*₁=0.6, and *p*=3,50.

Finally we have extrapolated $T_w(p,h_1;L)$ to the limit $L \rightarrow \infty$ in order to obtain the wetting temperatures $T_w(h_1,p)$. The obtained wetting phase diagram in the (T,h_1) plane is



FIG. 3. Phase diagram at bulk coexistence H=0 for continuous wetting transitions in the d=2 Ising ferromagnet for [Eqs. (4) and (5)] p=1.5, p=2, p=3, and p=50 (quasi-short-ranged boundary field) obtained within the DMRG approach. These values correspond to $\delta=0.5$, 1, 2, and 49, respectively [Eqs. (2) and (5)]. For p>1 the values in the limit $T \rightarrow 0$ are known exactly for semi-infinite systems. The dashed line is the analytically known exact result for $p=\infty$ and for semi-infinite systems [2]. Filled squares indicate estimates from the Monte Carlo simulations for p=3 [16]. $T_w^*=k_BT_w/J$ and $T_w^*(h_1\rightarrow 0,p)=T_c^*=2.269J/k_B$.

shown in Fig. 3 for p=1.5, 2, 3, and 50. The dashed line is the exact result by Abraham for $p=\infty$ as follows [2]:

$$\exp(2K)[\cosh(2K) - \cosh(2h_{1c})] = \sinh(2K), \quad (10)$$

where $h_{1c}(T)$ is the critical surface field [the inverse function of the wetting temperature $T_w(p=\infty,h_1)$]. The close agreement of our data for p=50 with this exact result generates confidence in our numerical procedures. Our results for p=3 are in a very good agreement with the Monte Carlo results of Ref. [16]. We observe that the presence of the longranged tails in the surface fields leads to a reduction in the value of the critical wetting temperature as compared to that for short-ranged surface fields.

IV. CONCLUSIONS

Our results show that, contrary to the claim by Kroll and Lipowsky [6] and by Privman and Švrakić [10], in 2D semiinfinite Ising models with boundary fields varying as h_1/j^p [Eq. (4)] as function of the distance *j* from the boundary, there are continuous wetting transitions at two-phase coexistence in the bulk for all decay exponents p > 1. The corresponding wetting transition temperatures $T_w(h_1, p)$ can be well localized as a function of the field strength h_1 and the decay exponent *p*, either numerically for $T_w > 0$ or even analytically for $T_w = 0$ (Figs. 3 and 1, respectively).

As discussed in the Introduction, the claim by Kroll and Lipowsky [6] is based on studying an effective interface model [Eq. (1)] which resembles the continuum version of so-called solid-on-solid (SOS) models. Privman and Švrakić [10] studied the SOS model itself for p=2. By focusing on the fluctuations of the local interface height only, such SOS

models ignore bulklike fluctuations such as the occurrence of bubbles and of "overhangs" of the line separating oppositely magnetized domains. Moreover, the continuum description captures only the long-wavelength fluctuations of the interface, expected to play the crucial role for wetting transitions.

In the present case of the 2D Ising model the bulk fluctuations are particularly strong even far below the bulk critical point T_c , giving rise to a rather diffuse intrinsic interface profile which is further broadened significantly by capillary wavelike fluctuations such that the interface is rough for all temperatures, i.e., its width scales $\sim \sqrt{M}$ for a lateral system size M and $L=\infty$. Since the latter fluctuations *are* captured by the effective interface model in Eq. (1), the missing types of fluctuations mentioned above have to be natural candidates for providing the mechanisms for the unbinding of the interface from the boundary even for 1 , although thelong-wavelength interfacial fluctuations are strongly suppressed by such long-ranged boundary fields. Thus we conclude, in accordance with the corresponding discussion inSec. I, that as in the case for critical wetting transitions in 3D

- S. Dietrich, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1988), Vol. 12, p. 1.
- [2] D. B. Abraham, Phys. Rev. Lett. 44, 1165 (1980).
- [3] L.-F. Ko and D. B. Abraham, Phys. Rev. B 39, 12341 (1989).
- [4] G. Forgacs, R. Lipowsky, and Th. M. Nieuwenhuizen, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1991), Vol. 14, p. 135, and references therein.
- [5] R. Lipowsky and M. E. Fisher, Phys. Rev. B 36, 2126 (1987).
- [6] D. M. Kroll and R. Lipowsky, Phys. Rev. B 28, 5273 (1983).
- [7] M. Napiorkowski and S. Dietrich, Europhys. Lett. 9, 361 (1989); Z. Phys. B: Condens. Matter 89, 263 (1992); Phys. Rev. E 47, 1836 (1993).
- [8] S. Dietrich and M. Napiórkowski, Phys. Rev. A 43, 1861 (1991); Physica A 177, 437 (1991).
- [9] K. R. Mecke and S. Dietrich, Phys. Rev. E 59, 6766 (1999).
- [10] V. Privman and N. M. Švrakić, Phys. Rev. B 37, 5974 (1988).
- [11] K. Binder, D. P. Landau, and D. M. Kroll Phys. Rev. Lett. 56, 2272 (1986); K. Binder, D. P. Landau, and S. Wansleben, Phys. Rev. B 40, 6971 (1989).
- [12] A. O. Parry, R. Evans, and K. Binder, Phys. Rev. B 43, 11535 (1991).
- [13] A. O. Parry, C. Rascón, N. R. Bernardino, and J. M. Romero-Enrique, Phys. Rev. Lett. **100**, 136105 (2008); **100**, 259902 (2008).

Ising models with short-ranged forces, critical wetting transitions in 2D Ising models with particularly long-ranged boundary fields (p < 2) represent another type of phenomena for which simple effective interface models such as the one given in Eq. (1) are insufficient to capture correctly the critical wetting phenomena of the actual underlying microscopic models.

Further examples for shortcomings of effective interface models in describing fluctuations in the underlying 2D microscopic models have been reported within the DMRG studies of the nonuniversal critical singularities for wetting transitions in the presence of marginal long-ranged forces (p=3) [28] and of corrections to the Kelvin equation at complete wetting in slab geometries [29]. In the latter case it was shown that the apparent discrepancies between predictions based on coarse-grained arguments and the results of microscopic calculations are due to the fact that even for very wide slabs the wetting layers are still rather thin and the singular part of the surface free energy is thus dominated by the contacts with the boundaries.

- [14] A. Drzewiński and K. Szota, Phys. Rev. E 71, 056110 (2005).
- [15] E. V. Albano, K. Binder, and W. Paul, J. Phys.: Condens. Matter 12, 2701 (2000).
- [16] A. De Virgiliis, E. V. Albano, M. Müller, and K. Binder, J. Phys.: Condens. Matter 17, 4579 (2005).
- [17] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); S. R. White, Phys. Rev. B **48**, 10345 (1993).
- [18] T. Nishino, J. Phys. Soc. Jpn. 64, 3598 (1995).
- [19] L. Notes, in *Physics*, edited by I. Peschel, X. Wang, M. Kaulke, and K. Hallberg (Springer, Berlin, 1999), Vol. 528.
- [20] U. Schollwöck, Rev. Mod. Phys. 77, 259 (2005).
- [21] A. O. Parry and R. Evans, Phys. Rev. Lett. 64, 439 (1990).
- [22] A. O. Parry and R. Evans, Physica A 181, 250 (1992).
- [23] K. Binder, Annu. Rev. Mater. Res. 38, 123 (2008).
- [24] E. V. Albano, K. Binder, D. W. Heermann, and W. Paul, Surf. Sci. 223, 151 (1989); Z. Phys. B: Condens. Matter 77, 445 (1989).
- [25] A. Drzewiński, A. Maciołek, A. Barasiński, and S. Dietrich, following paper, Phys. Rev. E 79, 041145 (2009).
- [26] R. Pandit, M. Schick, and M. Wortis, Phys. Rev. B 26, 5112 (1982).
- [27] T. Getta and S. Dietrich, Phys. Rev. E 47, 1856 (1993).
- [28] A. Drzewiński, A. O. Parry, and K. Szota, Phys. Rev. E 75, 041110 (2007).
- [29] E. Carlon, A. Drzewiński, and J. Rogiers, Phys. Rev. B 58, 5070 (1998).