

## Effect of bulk magnetic field on critical Ising films

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(Received 27 December 1999)

Two-dimensional Ising films  $L \times \infty$  in a nonvanishing bulk magnetic field  $H$  are studied at the bulk critical temperature  $T_c$  for two choices of surface fields (a)  $H_1 = H_L = 0$  (ordinary transition), and (b)  $H_1 = H_L = \infty$  (normal transition) by the density-matrix renormalization-group method. Universal scaling functions for magnetization profiles, the excess magnetization  $\Gamma$ , the longitudinal correlation length  $\xi_{\parallel}$ , and for the analog of the solvation force  $f_{solv}$  are found and discussed. When  $H_1 = 0$  the scaling function for  $f_{solv}$  has two symmetric minima at  $y = \text{sgn}(H)L|H|^{v/\Delta} \approx \pm 1$  with an amplitude at the minimum about 3.8 times the value at  $H = 0$ , the Casimir amplitude. For the normal transition the scaling function for  $f_{solv}$  has a single minimum near the continuation of the pseudocoexistence (capillary condensation) line, with an amplitude about 100 times the Casimir amplitude.

PACS number(s): 05.70.Jk, 64.60.Fr, 68.35.Rh, 68.15.+e

### I. INTRODUCTION

There are two relevant scaling fields for critical behavior in Ising magnets: the (reduced) deviation from the critical temperature,  $\tau \equiv (T - T_c)/T_c$  and the bulk magnetic field  $H$ . The Onsager exact solution of a two-dimensional (2D) Ising model helped significantly to understand the behavior of systems shifted away from the critical point at  $\tau = H = 0$  by a change of the temperature field  $\tau$  [1]. This solution served as a test of scaling properties of various thermodynamic quantities near criticality, but it was limited to the case of  $H = 0$ . Other techniques, such as series expansions, were developed to explore the behavior of Ising magnets at nonzero magnetic field. However, these methods were not always satisfactorily accurate and there was a general awareness of the reliability of different conjectures. The lack of the exact solution of the Ising model in nonzero magnetic field makes the properties of an Ising magnet along the critical isotherm  $\tau = 0$  not fully explored. The renormalization group theory predicts that the effect of a change of the scaling field  $H$  at  $\tau = 0$  on a critical system should be analogous to the effect of a change of  $\tau$  at  $H = 0$  (with different critical exponents). However, this prediction was not confirmed by explicit calculations and many important issues such as the size of the scaling region along the  $\tau = 0$  axis, or the shapes of scaling functions at  $\tau = 0$  were not studied.

Commonly, the notion of the bulk correlation length is identified with a ‘‘temperature’’ bulk correlation length  $\xi_{\tau} \equiv \xi(H = 0, \tau) \sim |\tau|^{-\nu}$  and for many critical phenomena only a role of  $\xi_{\tau}$  was studied. Consider a critical Ising magnet bounded by a surface or confined between two parallel plates. The effects of a surface should extend to a distance comparable to the bulk correlation length. Near the bulk critical point  $\xi$  gets macroscopically large and hence the boundary region affected by the surface becomes macroscopic. As a consequence the local densities such as the order-parameter (OP) profile become inhomogeneous on a scale of  $\xi$ . The detailed predictions for a spatial variation of the OP, depending on the type of a surface, and for the scaling of various thermodynamic quantities in a presence of a

surface were given by the theory of a surface critical phenomena [2,3]. However, these predictions were formulated and tested mainly for the case of  $\xi = \xi_{\tau}$ , i.e., for  $H = 0$ .

In confined systems the finite size, in addition to the surface effects, influences criticality leading to the rounding and/or the shift of the critical point [4]. It is expected from the theory of a finite-size scaling that the behavior of various thermodynamic quantities should depend sensitively on the ratio  $\xi/L$ , where  $L$  is a characteristic length of a confined system. Again, the finite-size scaling hypothesis was confirmed mostly for  $H = 0$ , i.e., when  $\xi = \xi_{\tau}$ , and the role of the ‘‘magnetic’’ bulk correlation length in a confined system was not studied.

Confined Ising magnets generate a force between the confining plates, a ‘‘magnetic’’ analog of the solvation force, sometimes called the disjoining pressure [5]. For fluids this is the excess pressure (over the bulk value fixed by the reservoir) arising from confinement and can be measured directly by the surface force apparatus or atomic-force microscopes [6]. In the critical confined system this force becomes long-ranged as a result of critical fluctuations, a phenomenon which is a direct analog of the well-known ‘‘Casimir’’ effect in electromagnetism [7,8]. Contrary to the usual dispersion forces, the critical solvation force (‘‘Casimir’’ force) is governed by *universal* scaling functions. At the critical point the scaling functions reduce to the universal Casimir amplitudes. Recently, it was shown that the solvation force has a rich variation as a function of  $\tau$  at  $H = 0$ . For films with identical surfaces the solvation force is negative (attractive force) and has a minimum as a function of  $\tau$  *not* at the critical point, but for  $\tau$  such that  $\xi_{\tau} \sim L$ , where  $L$  is the width of the film [9,10]. The magnitude of  $f_{solv}$  at this minimum is much bigger than at  $\tau = 0$ , the Casimir amplitude. The behavior of the solvation force as a function of  $H$  at  $\tau = 0$  has not been studied so far, but if the ‘‘magnetic’’ correlation length manifests itself in a similar way to the ‘‘temperature’’ correlation length, an analogous, rich variation of this force with  $H$  can be expected near criticality.

In this paper we address some of the above issues by explicit calculations of various thermodynamic quantities in

the 2D Ising film at  $\tau=0$  and nonzero magnetic field  $H$ . We use the recently developed, approximate density-matrix renormalization-group (DMRG) method [11]. Based on the transfer-matrix approach, the DMRG method provides a very efficient algorithm for the construction of effective transfer matrices for thick films (large  $L$ ) [12,13] and works equally well for vanishing as well as nonvanishing bulk fields. The accuracy of this method proved to be very good for 2D Ising films at  $\tau=0$ ,  $H=0$ , and various surface fields [14].

Specifically, we consider a 2D Ising magnet defined on the square lattice  $L \times M$ ,  $M \rightarrow \infty$ . The lattice consists of  $L$  rows at spacing  $a \equiv 1$ , so that the width of the film is  $La = L$ . At each site, labeled  $i, j, \dots$ , there is an Ising spin variable taking the value  $\sigma_i = \pm 1$ . We assume nearest-neighbor interactions of strength  $J$  and a Hamiltonian of the form:

$$\mathcal{H} = -J \left[ \sum_{\langle i,j \rangle} \sigma_i \sigma_j - H \sum_i \sigma_i - H_1 \sum_i^{(1)} \sigma_i - H_L \sum_i^{(L)} \sigma_i \right], \quad (1.1)$$

where the first sum runs over all nearest-neighbor pairs of sites, while the last two sums run, respectively, over the first and the  $L$ th row.  $H$  is the bulk magnetic field,  $H_1$  and  $H_L$  are the surface fields corresponding to direct, short-range (“contact”) interactions between the walls and the spins in the film.  $H$ ,  $H_1$ , and  $H_L$  are measured in units of  $J$ . We assume that  $H_1 = H_L > 0$ .

The system defined above can serve as a model of a uniaxial magnet or a binary mixture confined between identical parallel plates or walls, or a simple fluid in a slitlike pore; the local surface fields model the substrate-fluid interactions which give rise to adsorption phenomena. For fluids the bulk field  $H$  corresponds to the chemical potential difference

$$H \approx \mu - \mu_{co}(T), \quad (1.2)$$

where  $\mu$  is the chemical potential (or, for binary fluids, chemical potential difference) of the bulk reservoir with which the film is supposed to communicate, while  $\mu_{co}(T)$  is the bulk coexistence curve. A nonzero  $H$  corresponds to the situation when, for example, the density  $\rho$  of the bulk reservoir is slightly different than  $\rho_c$ , the critical density of a bulk fluid.

In this work we focus on two types of surfaces: (a)  $H_1 = 0$  and (b)  $H_1 = \infty$ , which for the 2D Ising model in the semi-infinite geometry define two surface universality classes (a) the ordinary transition, and (b) the normal transition, representing an unstable and stable fixed point of the renormalization-group flow, respectively [3]. These are the only two surface universality classes in this system, since the boundary is one-dimensional. Ordinary transition is relevant to magnets and alloys with free surfaces and occurs when the tendency to order in the surface is de-enhanced compared to the bulk at zero surface external field  $H_1$ . The normal transition is the most relevant to fluids surface transition and occurs when the surface orders as a result of a surface external field  $H_1$  but with de-enhanced surface interactions.

The paper is arranged as follows. Section II is devoted to the theory where the most relevant for our paper definitions

and results for the critical systems bounded by a surface at and near ( $\tau \ll 1$ ,  $H=0$ ) the ordinary and normal transitions are reviewed. On the basis of the scaling analysis the predictions concerning the behavior of the OP profile in the semi-infinite system near the normal transition at  $\tau=0$  and *nonzero*  $H$  are formulated. In this paper we concentrate on the behavior of films for weak  $H$  at  $\tau=0$ . Nevertheless, it is instructive for the discussion of the results to recall shortly critical behavior and the phase diagram of films with finite  $L$ . This is done in Sec. II B for (a)  $H_1=0$  and (b)  $H_1=\infty$ . Section II C reviews the finite-size scaling for the free energy, the magnetization profile and the adsorption (excess magnetization), the solvation force and the correlation length parallel to the walls suitable at  $\tau=0$  and *nonzero* bulk magnetic field  $H$ . The above quantities and their scaling functions were calculated using the DMRG method for the case of ordinary transition and normal transition, and the results are presented in Secs. III A and III B, respectively. A discussion of our results is given in Sec. IV.

## II. THEORY

The standard scaling expression for  $\xi$  near the critical point in nonzero magnetic field is (see, e.g., a review [15])

$$\xi(\tau, H) \approx |\tau|^{-\nu} \Xi_{\pm}(H|\tau|^{-\Delta}), \quad (2.1)$$

as  $\tau \rightarrow 0^{\pm}$  and  $H \rightarrow 0$ . We ignore here metric factors. The sign  $\approx$  indicates that corrections to scaling have been omitted.  $\Xi_{\pm}$  are certain scaling functions. As usual, in the above expression the  $+$  refer to  $\tau > 0$  and  $\tau < 0$ , respectively.  $\Delta = \beta + \gamma$  is the bulk gap exponent,  $\beta$  is the critical exponent describing the vanishing of the bulk OP and  $\gamma$  is the bulk susceptibility exponent. For the 2D Ising model  $\Delta = 15/8$ ,  $\gamma = 7/4$ , and  $\beta = 1/8$ . At  $H=0$  the scaling function reduces to the amplitude  $\Xi_{\pm}(0)$  and the bulk correlation length becomes, what we called in the Introduction, the “temperature” bulk correlation length:

$$\xi_{\tau} \equiv \xi(\tau, H=0) \approx \Xi_{\pm}(0) |\tau|^{-\nu}. \quad (2.2)$$

The amplitude  $\Xi_{\pm}(0)$  for the 2D Ising model is known exactly [16], i.e.,  $\Xi_{+}(0) = 1/[2 \ln(1 + \sqrt{2})]$  and  $\Xi_{-}(0) = 1/[4 \ln(1 + \sqrt{2})]$ .

In this paper we are concerned with the situation when  $\tau=0$  but  $H \neq 0$ . The suitable form of the scaling for  $\xi$  is then

$$\xi(\tau, H) \approx |H|^{-\nu/\Delta} \tilde{\Xi}_{\pm}(|H|^{-1/\Delta} \tau), \quad (2.3)$$

where  $\tilde{\Xi}_{\pm}$  is a new scaling function. At  $\tau=0$   $\xi$  reduces to the “magnetic” bulk correlation length

$$\xi_H \equiv \xi(0, H) \approx \tilde{\Xi}_{\pm}(0) |H|^{-\nu/\Delta}. \quad (2.4)$$

The amplitude  $\tilde{\Xi}_{\pm}(0)$  is known for the 2D Ising model only approximately. It was obtained from the power-series expansion of the spin-pair-correlation function  $G$  for the correlation length defined as the second moment of  $G$  [17]. It is equal to  $0.233 \pm 0.001$ . To our knowledge the ratio between the amplitude of the second moment correlation length and

the amplitude of the “true” correlation length, describing the exponential decay of the correlation function  $G$ , is not known for the 2D Ising model.

### A. Semi-infinite systems

In the critical regime thermodynamic quantities are described by homogeneous functions of the relevant scaling fields. For systems bounded by a surface in addition to the scaling fields  $\tau$  and  $H$  there exist relevant scaling fields pertaining to the surface. For the 2D Ising model defined in the Introduction there is a single such scaling field, the surface magnetic field  $H_1$  [3]. The scaling of the OP profile in the semi-infinite geometry reads (ignoring metric factors):

$$m(z) \approx |\tau|^\beta \mathcal{M}^\pm(z|\tau|^\nu, H|\tau|^{-\Delta}, H_1|\tau|^{-\Delta_1}), \quad (2.5)$$

where  $\beta$  is the critical exponent describing the vanishing of the bulk OP and  $\Delta_1 \equiv \Delta_1^{ord}$  is the surface gap exponent.  $\mathcal{M}^\pm$  are universal scaling functions. For the 2D Ising model  $\Delta_1 = 1/2$  and  $\beta = 1/8$ . The scaling variables taken to the appropriate power are proportional to the ratio of characteristic lengths in the system  $\xi_\tau$ ,  $\xi_H$ , and  $l_1 \sim |H_1|^{-\nu/\Delta_1}$ , the length related to the surface.

(a) *Ordinary transition.* At the critical point  $\tau = H = 0$  and  $H_1 = 0$  the OP (magnetization) profile is zero for any distance  $z \geq 0$  from the surface since the symmetry under the reversal  $\sigma_i \rightarrow -\sigma_i$  is not broken, neither in a bulk nor in the surface. Accordingly, the excess magnetization (adsorption)  $\Gamma$  defined as

$$\Gamma \equiv \int_0^\infty m(z) dz, \quad (2.6)$$

where  $z$  is the distance measured normal to the surface, located at  $z = 0$  is equal to zero.

(b) *Normal transition.* For  $H_1 = \infty$  the magnetization  $m(z)$  takes the value  $m_1 = 1$  at the surface and then decays to the bulk equilibrium value being zero for  $T \geq T_c$ . From the scaling law for the OP profile one can read off the form of this decay at criticality [18]. At  $H = 0$  and  $|\tau| \ll 1$  the general scaling form of the magnetization (2.5) reduces to

$$m(z) \approx \tau^\beta \mathcal{M}_0 \left( \frac{z}{\xi_\tau}, \xi_\tau / l_1 \right). \quad (2.7)$$

Accordingly,

$$\Gamma \approx \tau^\beta \xi_\tau \mathcal{G}_0(\xi_\tau / l_1). \quad (2.8)$$

These formulas refer to  $\tau > 0$ . At  $\tau = 0$  and  $H = 0$  the decay of the magnetization  $m(z)$  to the bulk equilibrium value  $m^* = 0$  is described by

$$m(z) \approx z^{-\beta/\nu} \mathcal{M}_{0c}(z/l_1) \quad (2.9)$$

with  $\mathcal{M}_{0c}(\zeta)$  approaching a constant for  $\zeta \rightarrow \infty$ . In the 2D Ising model  $\beta/\nu = 1/8$ . When  $\tau \neq 0$  and  $H = 0$  a crossover to the exponential decay

$$m(z) \sim \exp(-z/\xi_\tau) \quad (2.10)$$

takes place in a distance  $z \approx \xi_\tau$  from the surface. Such a behavior of the magnetization profile implies that the adsorption  $\Gamma$  diverges for  $\tau \rightarrow 0^+$  according to the universal power law [18]

$$\Gamma \sim \tau^{\beta-\nu}. \quad (2.11)$$

Consider the case of  $\tau = 0$  and  $H \neq 0$ . The scaling form of the OP profile more suitable for this case is

$$m(z) \approx |H|^{\beta/\Delta} \mathcal{N}^\pm(z|H|^{\nu/\Delta}, |H|^{-1/\Delta} \tau, H_1^{-1/\Delta_1} \tau), \quad (2.12)$$

where  $\mathcal{N}^\pm$  are scaling functions. At  $\tau = 0$  Eq. (2.12) reduces to

$$m(z) \approx |H|^{\beta/\Delta} \mathcal{N}_0^\pm \left( \frac{z}{\xi_H}, \xi_H / l_1 \right). \quad (2.13)$$

The arguments of the scaling functions  $\mathcal{N}_0^\pm$  are completely analogous to the arguments of the scaling function in Eq. (2.7) with  $\xi_\tau$  replaced by  $\xi_H$ . Thus, the same scaling analysis of the OP profile near the normal transition  $H_1 = \infty$  performed for  $H = 0$  and small  $\tau$  [18] should hold for  $\tau = 0$  and small  $H$ . However,  $H \neq 0$  explicitly breaks the symmetry contrary to  $\tau > 0$  and the shape of the scaling functions  $\mathcal{N}_0^\pm, \mathcal{M}_0$  can be different; for  $H < 0$  an interfacelike region between the near-surface positively magnetized region and  $m_b < 0$  for  $z \rightarrow \infty$  is formed.

### B. Critical behavior of films

The critical behavior of systems confined between parallel plates or walls is modified due to the *combined* effect of the finite thickness  $L$  of the film and the specific surface interactions. First, for the Ising film that is of infinite extent in  $d - 1$  dimensions, parallel to the walls, true criticality can occur provided  $d - 1 \geq 2$ —the lower critical dimension of the corresponding bulk system. Criticality for finite  $L$  lies in the universality class of the bulk  $d - 1$  system. Second, the location of the critical point crucially depends on the type of surfaces.

(a)  $H_1 = H_L = 0$ . In films with free boundaries the Ising symmetry requires two-phase coexistence to be at  $H = 0$  and it is known that for  $d \geq 3$  and large but finite  $L$ , a line of coexistence extends to the critical temperature  $T_c(L) < T_c$ . The expression for the shift follows from the finite-size scaling [4]:

$$\Delta T_c \equiv [T_c(L, H_1) - T_c] / T_c \approx -L^{-1/\nu} X_c(H_1 L^{\Delta_1/\nu}), \quad (2.14)$$

where the scaling function  $X_c(w)$  reduces to the amplitude  $X_c(0)$  for  $H_1 = 0$ .

(b)  $H_1 = H_L = \infty$ . For any  $H_1, H_L > 0$  the entire phase boundary in the  $(T, H)$  plane is displaced into the half-plane  $H < 0$  with a positive slope. The (capillary) critical point of the film lies below  $T_c$  and is shifted in  $H$  as well as in temperature. The expression for the temperature shift is given by Eq. (2.14) and the similar form holds for  $\Delta H_c \equiv H_c(L, H_1)$  [20]:

$$\Delta H_c \approx -L^{-\Delta/\nu} Y_c(H_1 L^{\Delta_1/\nu}). \quad (2.15)$$

The simple interpretation of the result (2.14) states that the growth of droplets within the film is determined by bulklike fluctuations until, at the shifted critical point  $T_c(L)$ , the droplet size is comparable with the smallest film dimension, i.e.,  $L \sim \xi \sim [T_c - T_c(L)]^{-\nu}$ . The analogous argument can be formulated to interpret the result (2.15) for the shift of the critical field.

For the 2D Ising film of finite  $L$  the situation is similar. Although there can be no true phase transition for finite  $L$  there is still a line of sharp (very weakly rounded) transitions (ending in a pseudocritical point) [21]. The thermodynamic quantities such as the free energy and the magnetization depend smoothly on temperature, surface, and bulk fields. The singularities of the free energy, specific heat, etc. are rounded forming maxima. For  $T < T_c$  the maximum of the free energy  $f(H)$  at fixed  $T$ ,  $L$ , and  $H_1$  can be identified with the pseudocoexistence field  $H_{co}(L)$ . The pseudocritical point  $(T_c(L), H_c(L))$  cannot be found from the maxima of the free energy as they are present even for  $T > T_c$  [22]. The pseudocritical point can be defined, for example, as a position of a maximum of a specific heat along the pseudocoexistence line. The scaling properties of the free-energy maximum at  $T = T_c$ ,  $H_{max}(T_c, L; H_1)$  for the model considered here were studied in Ref. [22]. It was found that  $H_{max}(T_c, L; H_1)$  scales in the same way as  $\Delta H_c$  in Eq. (2.15), and that the scaling function is, as expected, equal to 0 for  $H_1 = 0$  and saturates for large  $H_1$ .

### C. Finite-size scaling

In this paper we want to test the scaling properties of various thermodynamic quantities at  $\tau = 0$  and nonzero bulk field. For finite-size systems it has been recognized [4] that the system size  $L$  ‘‘scales’’ with the correlation length  $\xi(\tau, H)$  of the bulk system. Thus the scaling hypothesis for the singular part of the free energy per spin is

$$f_s(L; T, H, H_1) \approx L^{-d} W(L^{1/\nu} \tau, y, x), \quad (2.16)$$

(ignoring metric factors) where

$$y \equiv \text{sgn}(H)L|H|^{v/\Delta} \quad (2.17)$$

and

$$x \equiv L|H_1|^{v/\Delta_1}. \quad (2.18)$$

For  $H = 0$ , exact calculations for the 2D Ising model confirmed Eq. (2.16) for  $H_1 = 0$  [23] as well as for  $H_1 \neq 0$  [24]. We will evaluate the scaling function  $W_c(y, x) \equiv W(0, y, x)$  at  $\tau = 0$ .

We will be also concerned with the order-parameter profile  $m(z)$  and the excess magnetization  $\Gamma$ . For the model (1.1) the profile is defined as

$$m(z) \approx m_l \equiv \langle \sigma_l \rangle, \quad z \approx la \equiv l, \quad (2.19)$$

where  $\sigma_l$  denotes a typical spin in the  $l$ th row (with  $l = 1, 2, \dots, L$ ) corresponding to a perpendicular distance  $z$  ( $0 \leq z \leq L$ ) from the first wall. The profiles, likewise, obey scaling [18, 24]. We will be testing the form of the scaling suitable at  $\tau = 0$

$$m(z) \approx |H|^{\beta/\Delta} M_c^\pm(z|H|^{v/\Delta}; y, x). \quad (2.20)$$

For films the adsorption  $\Gamma$  is defined as in Eq. (2.6) but with the upper limit of an integration equal to  $L$ . The  $\tau$  dependence of the adsorption for films with nonzero  $H_1$  in zero bulk field differs from that in semi-infinite systems. Consider the case when the bulk critical temperature is approached from above. Then,  $\Gamma$  first increases but when  $\xi_\tau \sim L$  it starts to saturate at a positive value, which depends on the width of the film  $L$  and on the value of the surface field  $H_1$ . We will be investigating the  $H$  dependence of  $\Gamma$  at  $\tau = 0$ . In particular, we will be testing the scaling of  $\Gamma$  which follows from Eq. (2.20):

$$\Gamma \approx |H|^{(\beta-\nu)/\Delta} G(y, x) \approx L^{-\beta/\nu+1} G_L(y, x), \quad (2.21)$$

where  $G$  and  $G_L$  are scaling functions.

The transfer-matrix approach gives a way of defining the longitudinal spin-spin correlation length  $\xi_{\parallel}$  of a finite system. If we take the transfer matrix in the infinite dimension then

$$\xi_{\parallel}^{-1}(\tau, H; L, H_1) = -\ln[\Lambda_1/\Lambda_0]. \quad (2.22)$$

Here  $\Lambda_0$  and  $\Lambda_1$  are the largest and the second largest eigenvalues of the transfer matrix. For  $\xi_{\parallel}^{-1}$  a method similar to the free-energy scaling ansatz holds (ignoring metric factors)

$$L\xi_{\parallel}^{-1}(\tau, H; L, H_1) \approx K(L^{1/\nu} \tau, y, x) \quad (2.23)$$

with the appropriate universal scaling function  $K(L^{1/\nu} \tau, y, x)$ . When  $\tau = 0, H = 0$  the universal amplitude  $K(0, 0, x)$  is identified from the relation  $L\xi_{\parallel}^{-1}(0, 0; L, H_1) \approx K(0, 0, x)$ . The universal amplitudes established from the correlation length defined by the exponential decay of the spin-spin correlation function along  $L \times \infty$  strip are  $K(0, 0, 0) = \pi/2$  for free boundary conditions and  $K(0, 0, \infty) = 2\pi$  for fixed boundary conditions [16].

The free energy per site of the 2D Ising film with two surface fields  $H_1 = H_L$  can be written for large  $L$  as

$$f(L, T, H_1) = f_b + 2f_w/L + f^*(L)/L, \quad (2.24)$$

where  $f_b$  is the bulk free energy,  $f_w$  is the  $L$ -independent surface contribution from each wall, and  $f^*$  is the finite-size correction to the free energy. The latter vanishes for  $L \rightarrow \infty$ . Such a term gives rise to the generalized force, which is analogous to the solvation force between the plates in confined fluids [5]

$$f_{solv} = -(\partial f^*/\partial L)_{H, T, H_1}. \quad (2.25)$$

For films with identical surface fields  $H_1 = H_L$   $f_{solv}(L) < 0$ , i.e., the net force between the confining plates is attractive. From the general theory of critical finite-size scaling [4] it follows that the solvation force should scale as

$$f_{solv} \approx L^{-2} F(L^{1/\nu} \tau, y, x). \quad (2.26)$$

At fixed points  $\tau = 0, H = 0$  and  $H_1 = 0$  or  $H_1 = \infty$  the scaling function  $F$  reduces to  $F(0, 0, 0) = \mathcal{A}_0 k_B T_c$  or  $F(0, 0, \infty) = \mathcal{A}_\infty k_B T_c$ , where  $\mathcal{A}_0$  and  $\mathcal{A}_\infty$  are universal, the so-called, Casimir amplitudes. For the 2D Ising model  $\mathcal{A}_\infty = \mathcal{A}_0 =$



$-\pi/48$ .  $f_{solv}$  and its scaling function were evaluated and analyzed in a wide range of the variable  $L^{1/\nu}\tau$  for  $x=0, \infty$  and  $y=0$  in Ref. [10]. For  $x=\infty$  and for a given  $L$  the solvation force has its minimum *above* the critical temperature. The amplitude of the force at the minimum is about 6.6 times the Casimir amplitude. The minimum of the scaling function  $F(L^{1/\nu}\tau, 0, \infty)$  occurs when the film width  $L \approx 2.2$  times the bulk correlation length  $\xi_\tau$ . It was also found that  $F(L^{1/\nu}\tau, 0, \infty) = F(-L^{1/\nu}\tau, 0, 0)$  which confirms that the Casimir amplitudes for free boundaries is the same as for  $H_1 = \infty$ . However, the minimum of the solvation force for the case of free boundaries occurs *below*  $T_c$ .

Scaling of the free energy, magnetization profile and adsorption, solvation force, and the correlation length will be tested at  $\tau=0$  in two cases (a)  $H_1=0$ , i.e.,  $x=0$  and (b)  $H_1$  large so that the scaling variable  $x \gg 1$ .

### III. DMRG RESULTS

In our calculations we have used the finite-system version of the DMRG algorithm designed to perform accurate studies for finite-size systems [12]. For more details see Ref. [13].

Calculations were performed for films of width  $L$  between 24 and 200 at the bulk critical temperature  $\tau=0$  and for bulk magnetic field ranging from  $H=0$  to 1. We consider two cases of surface fields  $H_1=H_L$ :

#### A. $H_1=H_L=0$

For free boundary conditions the Ising symmetry holds at  $H=0$  thus the sign of the applied bulk field is not relevant for the behavior of the system. In our calculations we have chosen  $H < 0$ . After switching on the negative bulk magnetic field at  $\tau=0$  the OP, vanishing everywhere in the system at  $\tau=0$  and  $H=0$ , becomes negative and inhomogeneous across the film. One can distinguish three characteristic regimes of behavior:

##### 1. Surface-governed regime (linear response)

For the weakest  $H$  such that  $\xi_H \gg L$  the magnetization responds linearly to the applied field in *the whole* system. This can be seen from the log-log plot of the modulus of the magnetization at the surface  $|m_1|$  and the modulus of the magnetization at the midpoint  $|m_{L/2}|$  as a function of  $|H|$  calculated for fixed  $L=200$  (see Fig. 1). For  $|H| < 5 \times 10^{-5}$  the straight line in Fig. 1 with a high accuracy has a slope equal to 1. Magnetization profiles in this regime are almost flat with a slight difference between the value of magnetization at the surface and in the middle part of the film. The adsorption  $\Gamma$  is small and negative but its absolute value increases fairly rapidly with  $|H|$ . The linear dependence of the magnetization profile on  $H$  implies the linear dependence of the adsorption on  $H$ . Such behavior can be read off from the scaling function  $G(y, 0)$  of  $\Gamma$  for  $|y| \ll 1$ . Figure 2 shows that the scaling given by Eq. (2.21) is excellent up to  $|y| \sim 100$ . This log-log plot of  $|G(y, 0)|$  is a straight line for  $|y| < 0.8$ . We checked that with a good accuracy the slope of this line is equal to  $1 + (\Delta - \beta)/\nu = 2.75$ , hence  $\Gamma \approx \text{sgn}(H)|H|^{(\beta - \nu)/\Delta}|y|^{1 + (\Delta - \beta)/\nu} \sim H$ .

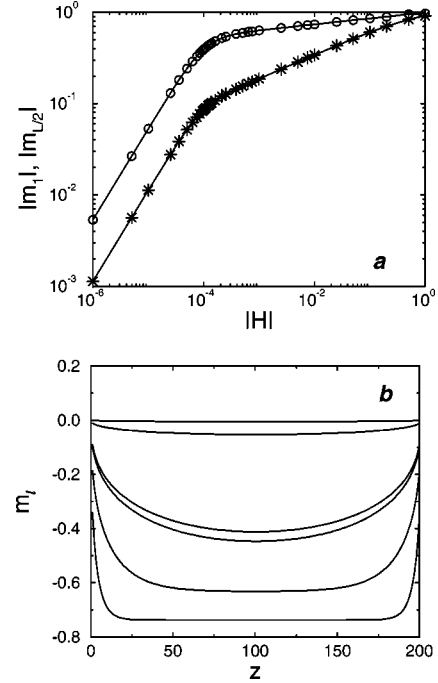


FIG. 1. (a) Log-log plot of the modulus of the surface magnetization  $|m_1|$  (stars) and the modulus of the magnetization in the center of the film  $|m_{L/2}|$  (circles) versus the modulus of the bulk magnetic field  $H$  for the 2D Ising film of width  $L=200$  at the critical temperature  $T=T_c$  and  $H_1=0$ . (b) Magnetization profiles  $m_i$  for the 2D Ising film of width  $L=200$  at  $T=T_c$ ,  $H_1=H_L=0$  and several values of the bulk field: the top profile corresponds to  $H = -10^{-6}$ , then subsequently from the next to the top to the bottom profile:  $H = -10^{-5}$ ,  $-1.1 \times 10^{-4}$ ,  $-1.3 \times 10^{-4}$ ,  $-0.001$ ,  $-0.01$ .  $H$  is in units of the coupling constant  $J$ ,  $z$  is in units of the lattice constant, the magnetization is dimensionless.

From the behavior of the scaling function of the inverse of the longitudinal correlation length  $\xi_{\parallel}$  shown in Fig. 3, it follows that in this regime  $\xi_{\parallel}$  is proportional to the width of a film  $L$  and does not depend on  $H$ . The scaling function  $K(0, y, 0) \approx K(0, 0, 0) = \pi/2$  for  $|y| < 0.8$ , in agreement with the results from the conformal invariance [16].

##### 2. Crossover regime

For stronger values of  $H$  such that  $\xi_H \sim L$  the adsorption  $\Gamma$  and  $\xi_{\parallel}$  exhibit a crossover to a different behavior. In this

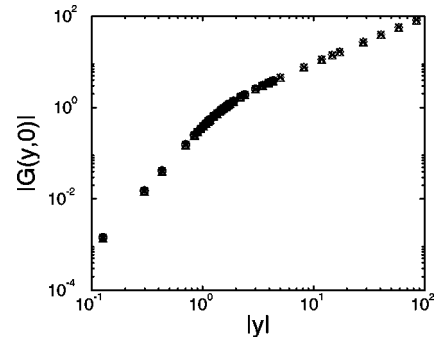


FIG. 2. Log-log plot of the modulus of the scaling function  $|G(y, 0)|$  [obtained using Eq. (2.21)] of the adsorption  $\Gamma$  calculated for 2D Ising films at  $T=T_c$ ,  $H_1=H_L=0$ , and several widths:  $L = 100$  (circles),  $124$  (squares),  $150$  (diamonds).

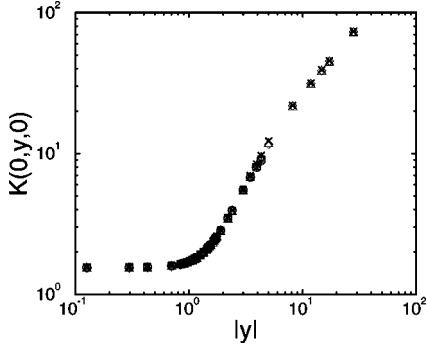


FIG. 3. Log-log plot of the scaling function  $K(0,y,0)$  [obtained using Eq. (2.23)] of the inverse of the longitudinal spin-spin correlation length of finite system  $\xi_{\parallel}$  calculated for 2D Ising films at  $T = T_c$ ,  $H_1 = H_L = 0$ , and several widths:  $L = 100$  (circles), 124 (squares), 150 (diamonds).

crossover regime profiles become highly inhomogeneous across the film [see middle two profiles in Fig. 1(b)].

### 3. Bulk field-governed regime

For even stronger  $H$  such that  $\xi_H \leq L$ , the OP profiles become flat in the middle part of a film. The magnetization of a bulklike phase formed inside the film satisfies the bulk critical isotherm relation, i.e.,  $m \sim \text{sgn}(H)|H|^{1/\delta}$  with  $\delta = 15$  for the 2D Ising model. Indeed, the log-log plot of  $|m_{L/2}|(|H|)$  in Fig. 1(a) is a straight line with a slope equal to  $1/15$  for  $|H| > 3 \times 10^{-4}$ . From the log-log plot of  $|m_1|(|H|)$  in the same figure it is seen that the magnetization at the surface  $m_1$  behaves in this regime as predicted from the theory of the surface critical phenomena for the semi-infinite system, i.e.,  $m_1 \sim \text{sgn}(H)|H|^{1/\delta_1}$ ,  $\tau = 0, H_1 = 0, H \rightarrow 0$  with  $\delta_1 = \Delta/\beta_1 = 15/4$  for the 2D Ising model [2]. To our knowledge this is the first confirmation of this prediction for systems of 2D Ising universality class. The scaling function of the adsorption  $\Gamma$  is a linear function of  $|y|$  for  $|y| \geq 3$  (see Fig. 2). This means that  $\Gamma \approx |H|^{(\beta - \nu)/\Delta} y \sim \text{sgn}(H)|H|^{\beta/\Delta} L$  so that a good estimate for the adsorption in this regime is  $\Gamma \approx m(H)L$ , where  $m(H) \sim \text{sgn}(H)|H|^{\beta/\Delta}$  is the magnetization in the middle part of a film. Also  $L/\xi_{\parallel}$  becomes a linear function of  $|y|$  for  $|y| \geq 8$ , which means that  $L/\xi_{\parallel} \sim L/\xi_H$ . If we identify  $\xi_{\parallel}$  with  $\xi_H$  in this regime we can estimate the amplitude  $\tilde{\xi}_{-}(0)$  of the ‘‘magnetic’’ correlation length  $\xi_H$  [see Eq. (2.4)]. Our rough estimate is  $\tilde{\xi}_{-}(0) \approx 0.388(7)$ .

We checked that the scaling of profiles as defined by Eq. (2.20) is excellent in all three regimes. In Fig. 4 we present scaling functions of typical profiles in the crossover and critical behavior regimes. To check the scaling of the singular part of the free energy we have to subtract the nonsingular part  $f_{ns}$  from the free energy of the whole system. We assume following Privman [19] that  $f_{ns}$  does not depend on the bulk field  $H$  and hence it should be the same as in the case of the 2D Ising film in zero bulk magnetic field. The exact formulas for the free energy per spin of the 2D Ising film with two arbitrary surface fields  $H_1, H_L$  ( $H_1 H_L > 0$ ) at  $H = 0$  were given in the Appendix of Ref. [24] [formulas (A14)–(A17)]. These formulas consist of parts which are explicitly nonsingular and integrals. We set  $T = T_c$  and  $H_1 = H_L = 0$  in explicitly nonsingular parts and subtract them

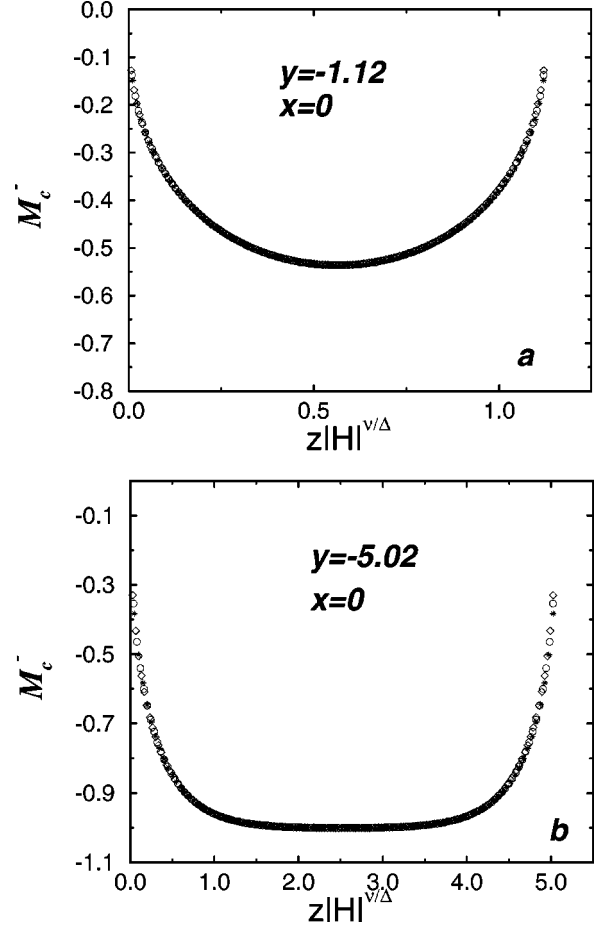


FIG. 4. Scaling functions of typical magnetization profiles in the (a) crossover regime for the scaling variable  $y = \text{sgn}(H)L|H|^{\nu/\Delta} = -1.12$  and in the (b) ‘‘critical behavior’’ regime for  $y = -5.02$  for 2D Ising films at  $T = T_c$ , surface fields  $H_1 = H_L = 0$ , and several widths:  $L = 100$  (circles), 124 (squares), 150 (diamonds).

from  $f(L)$  calculated from the leading eigenvalue of the effective transfer matrix. To obtain a perfect scaling of our data we had to subtract in addition the term  $1.3232(5) + 0.59472(5)/L$ , which probably is the nonsingular term ‘‘hidden’’ in integrals. The scaling function  $W_c(y,0)$  has, as expected, a maximum at  $y = 0$ .

In order to find the solvation force at  $T = T_c$  we first calculate the excess free energy per unit area  $f^{ex}(L) \equiv [f(L) - f_b]L$  [see Eq. (2.24)], where  $f(L)$  is the free energy per spin of the whole system and  $f_b$  is the bulk free energy per spin. Again,  $f_b$  is not known exactly for the 2D Ising model at  $T = T_c$  and the nonzero bulk field so we have to evaluate it numerically. We perform calculations of the free energy for films with widths up to  $L = 300$ . Next we extrapolate the bulk free energy using a powerful extrapolation technique, the Bulirsch and Stoer method and for  $L \rightarrow \infty$  we obtain the value  $f_b$  for each  $H$ . As a test of the correctness of the result we check the  $H$  dependence of the obtained  $f_b$ . At  $T = T_c$   $m_b(H) \sim \text{sgn}(H)|H|^{1/\delta}$  for  $H \rightarrow 0$ . As  $\partial f_b(T, H)/\partial H = m_b$  it follows that  $f_b(H, T_c) = f_0 + \mathcal{A}/(1/\delta + 1)|H|^{1/\delta + 1}$  for  $H \rightarrow 0$ , where  $f_0$  is a free energy per spin for bulk system in vanishing  $H$ . Our result for  $f_b$  shows a very good agreement with the above equation with  $\mathcal{A} = -0.9399(1)$  for  $|H| \geq 5 \times 10^{-4}$ . The deviation from the power function of  $H$  takes

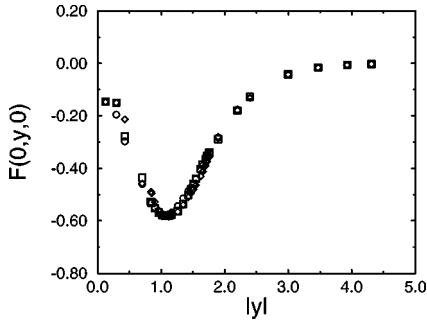


FIG. 5. Scaling function of the solvation force  $F(0,y,0)$  [Eq. (2.26)] calculated for 2D Ising films at  $T=T_c$ , surface fields  $H_1=H_L=0$ , and several widths:  $L=100$  (circles),  $124$  (squares),  $150$  (diamonds).

place in the linear-response regime where  $\xi_H \gg L$ . It is clear then that to obtain the bulklike behavior in this regime one has to go to much wider films. As the accuracy of  $f_b$  is the worst in this regime we expect the lowest accuracy of the results for the solvation force in this regime.

Having values  $f^{ex}(L_0+2)$  and  $f^{ex}(L_0)$  we approximate the derivative in Eq. (2.25) by a finite difference

$$f_{solv} = -(1/2)[f^{ex}(L_0+2) - f^{ex}(L_0)]. \quad (3.1)$$

We calculated  $f_{solv}$  as a function of  $H$  for various  $L$ . The solvation force is attractive for all values of  $H$  we studied. For given  $L$ ,  $f_{solv}/k_B T_c$  approaches the value  $-(\pi/48)L^{-2}$  as  $H \rightarrow 0$ , where  $-\pi/48$  is the Casimir amplitude. When  $|H|$  grows,  $f_{solv}$  exhibits a sharp minimum located at a small (less than 0.01),  $L$ -dependent value of  $H$  and then rapidly increases to zero. We restricted our calculations to the set  $L=24,50,74,100,124,150$  as for wider films the most interesting behavior of  $f_{solv}$ , i.e., the region around the minimum, is located at  $H$  for which the accuracy of our calculation is the worst. In Fig. 5 we plot  $L^2 \times f_{solv}$  as a function of the scaling variable  $|y|$ . Generally, scaling is very good. Only in the linear-response regime,  $|y| \ll 1$ , can one see slight deviations from the common curve which can be explained by the not sufficient accuracy of our calculations. The minimum of the solvation force is located in the crossover regime. It is reached for the scaling variable  $|y| \approx 1.12$ , i.e., when  $L \approx 2.88\xi_H \approx 1.8\xi_{||}$  [assuming the amplitude  $\tilde{\Xi}_-(0)$  of the ‘‘magnetic’’ correlation length  $\xi_H$  is approximately equal to  $\approx 0.388(7)$ ]. At the minimum the absolute value of  $F(0,y,0)/k_B T_c$ , where  $F$  is the scaling function of the solvation force is approximately 3.8 times the Casimir amplitude  $\mathcal{A}_0 = F(0,0,0)/k_B T_c$ . We found that, as expected,  $F(0,y,0)$  is an even function of  $y$ . This means that the solvation force has two symmetric minima—one located at some  $H_{\min} > 0$  and the second at  $-H_{\min}$ .

### B. $H_1=H_L=\infty$

Our DMRG calculations were performed for films of widths between 100 and 200 and for various  $H_1$ , such that the scaling variable  $x \sim L/l_1 = L|H_1|^{v/\Delta_1} \approx 20\,000$ . From our previous studies of 2D Ising films at vanishing bulk magnetic field it follows that for the above value of  $x$  the magnetization profile is almost saturated and coincides very well with

the exact profile of the limiting case  $x \rightarrow \infty$  [14]. To obtain scaling of the singular part of the free energy per spin  $f_s$  we proceeded in the same way as for the  $H_1=0$  case, but this time for each  $L$  we put into exact formulas of Ref. [24] a suitable value of  $H_1$  such that the scaling variable  $x$  was equal to 20 000. Again a perfect scaling of our data is found after subtracting from the free energy of the whole system the nonsingular part, as in the case of the ordinary transition, with an additional term  $1.3232(5) + 2.8397(0)/L$ .

The case of the normal transition is more complicated due to the shift of the phase coexistence from the  $H=0$  line. The presence of surface fields  $H_1=H_L$  breaks the symmetry and leads to the nonvanishing OP profile even at  $\tau=0, H=0$ . The OP profile, positive everywhere at  $\tau=0$  and  $H=0$ , is driven towards negative values by negative, decreasing bulk magnetic field. Contrary to the case of free boundary conditions the magnetization at the surface  $m_1$  remains equal to 1 for all studied values of  $H$  between 0 and -1. The shapes of the magnetization profiles for various  $H$ , and the  $H$  dependence of  $\Gamma/L$  at  $T=T_c$  for  $H_1=H_L=0.8$  and  $L=98$  were presented in Ref. [25] where the ‘‘critical depletion’’ phenomenon was studied. Our results for different  $L$  and  $H_1$  agree with the findings of Ref. [25], hence we present here only the scaling functions for the profiles and the adsorption. Again we can distinguish three regimes of behavior.

#### 1. Surface-governed regime (positive adsorption)

For the weak  $H$ , such that  $|y| < 2$ , the OP is positive throughout the film. Except near the walls the profiles are almost flat, similarly to the case of  $H_1=0$ . The adsorption  $\Gamma$  is positive and its value decreases as  $H$  becomes more negative. We found that although  $m_{L/2}$  changes linearly with  $H$  in this regime,  $m_1$  and the magnetization at a few other points near the surfaces do not change at all. Consequently, the  $\Gamma$  does not depend on  $H$  linearly, contrary to the case of free boundary conditions. The scaling function of the adsorption  $G(y, \infty) \sim y$  for  $|y| < 2$ , which means that the adsorption is a linear function of the width of the film  $L$  and very weakly depends on  $H$ , i.e.,  $\Gamma \sim \text{sgn}(H)L|H|^{-1/15}$ . This saturation is seen in a plot of the modulus of the scaling function  $G_L(y, 20\,000)$  in Fig. 6. Notice that the saturation regime is wider than the linear-response regime of the case  $H_1=0$ . The saturation regime extends up to  $|y| \approx 2$  whereas the linear-response regime ends at  $|y| \approx 0.8$ . Similarly to the case of free boundary conditions the scaling function of  $1/\xi_{||}$  saturates as  $y \rightarrow 0$ .  $K(0,y, 20\,000)$  becomes almost constant for  $|y| < 0.3$  which means that the longitudinal correlation length  $\xi_{||}$  of finite system is proportional to  $L$  in this regime and does not depend on  $H$ . We checked that with a good accuracy the amplitude  $K(0,0, 20\,000)$  is equal to  $2\pi$ , the value at  $x = \infty$  [16].

#### 2. Crossover regime

The behavior of studied quantities in this regime is far more rich for the normal transition than for the ordinary transition. Just like for the  $H_1=0$  case the crossover regime is characterized by highly inhomogeneous profiles across the film. Shapes of profiles and accordingly the adsorption  $\Gamma$  change very rapidly in a narrow interval of  $H$ . At  $|y| \approx 4.2$  the adsorption  $\Gamma=0$  and for greater  $|y|$  it becomes negative.

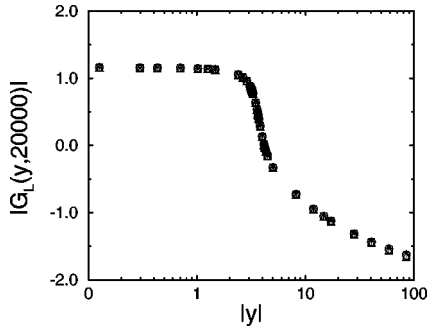


FIG. 6. Modulus of the scaling function  $G_L(y, 20\,000)$  [obtained using Eq. (2.21)] of the adsorption  $\Gamma$  calculated for 2D Ising films at  $T=T_c$  and different widths:  $L=100$  (stars), 124 (circles), 150 (squares), 174 (diamonds), and 200 (triangles). Calculations for each  $L$  were performed at the suitable value of surface fields  $H_1=H_L$  to meet the condition  $x=L|H_1|^{\nu/\Delta_1}=20\,000$ . The logarithmic scale is used to expose the saturation of  $|G_L(y, 20\,000)|$  for small values of  $y$ .

Unlike in the  $H_1=0$  case, the scaling function of  $1/\xi_{\parallel}$ ,  $K(0, y, 20\,000)$ , and the scaling function of the singular part of the free energy per spin  $f_s$ ,  $W_c(y, 20\,000)$ , show a non-trivial variation in this regime.  $K(0, y, 20\,000)$ , presented in Fig. 7, exhibits a minimum at  $|y| \approx 3.6$ .  $W_c(y, 20\,000)$  has a maximum at  $y \approx 4.2$ . As described in Sec. II B the maxima of the free energy for temperatures below  $T_c$  can be identified with the pseudocoexistence line of two pseudo phases. Thus the maximum of  $W_c(y, 20\,000)$  at  $T=T_c$  lies at the continuation of this line beyond the pseudocritical point. Notice that at the same value of  $y$  the adsorption  $\Gamma$  is equal to zero. This is consistent with the thermodynamics as the derivative of the free energy of the whole system with respect to  $H$  at fixed temperature is equal to a mean magnetization  $\tilde{m}$  in a system and  $\Gamma=L\tilde{m}$ .

### 3. Bulk field-governed regime (negative adsorption)

For sufficiently strong bulk magnetic field a bulklike phase forms inside the film and the OP profiles become flat in the middle part of the film. We found that for  $|y| > 10$  the

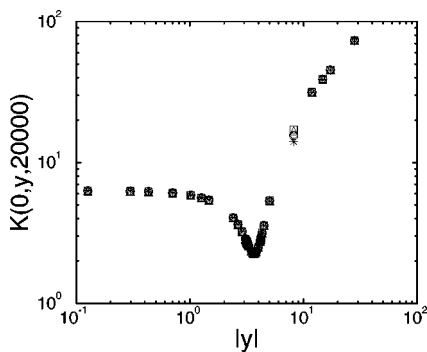


FIG. 7. Log-log plot of the scaling function  $K(0, y, 20\,000)$  [obtained using Eq. (2.23)] of the inverse of the longitudinal spin-spin correlation length of finite system  $\xi_{\parallel}$  calculated for 2D Ising films at  $T=T_c$  and several widths:  $L=100$  (stars), 124 (circles), 150 (squares), 174 (diamonds), and 200 (triangles). Calculations for each  $L$  were performed at the suitable value of surface fields  $H_1=H_L$  to meet the condition  $x=L|H_1|^{\nu/\Delta_1}=20\,000$ .

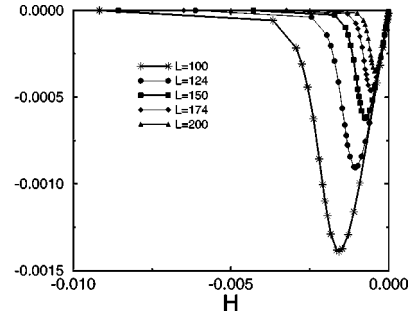


FIG. 8. Solvation force (in units of the coupling constant  $J$ ) as a function of the bulk magnetic field  $H$  (in units of  $J$ ) for the critical ( $T=T_c$ ) 2D Ising films of widths  $L$  between 100 and 200. Calculations for each  $L$  were performed at the suitable value of surface fields  $H_1=H_L$  to meet the condition  $x=L|H_1|^{\nu/\Delta_1}=20\,000$ .

magnetization in the middle of the film satisfies the bulk critical relation:  $m_{L/2} \sim \text{sgn}(H)|H|^{1/\delta}$ .  $L/\xi_{\parallel}$  becomes a linear function of  $y$  for  $|y| \geq 10$  with the same slope as in the case of  $H_1=0$ . This confirms our identification of  $\xi_{\parallel}$  with  $\xi_H$  in this regime.

The solvation force was calculated in the same way as for the case of free boundary conditions. Results for films with different  $L$  are presented in Fig. 8.  $f_{solv}$  is negative for all studied values of  $H$  and varies with the bulk magnetic field similarly to the case of  $H_1=0$ , i.e., it decreases rapidly when  $H$  decreases below zero, takes on a minimum value at some  $H_{min}(L)$  and then increases to zero. The striking feature of the behavior of the solvation force is that the minimum for the case of the normal transition is approximately two orders of magnitude deeper than for the case of the ordinary transition. For example, for  $L=100$  the value of  $f_{solv}$  at the minimum is for the ordinary transition approximately equal to  $-5.8 \times 10^{-5}$  whereas for the normal transition it is  $\approx -1.4 \times 10^{-3}$ . Also for the case of strong surface fields the location of the minimum  $H_{min}(L)$  for fixed  $L$  is further away from zero than for the case of  $H_1=0$ . Thus, for the current case of  $x=20\,000$  we could perform calculations with a good accuracy for wider films (up to  $L=200$ ) than for the case of  $x=0$ . From Fig. 8 it follows that for weak  $H$  corresponding to the saturation regime the solvation force is a linear function of the bulk magnetic field. Moreover, results for different  $L$  form a common straight line as though the solvation force would not depend on the width of the film in this range of  $H$ . Indeed, the scaling form of the solvation force implies that if  $f_{solv} \sim H$  then the scaling function  $F(0, y, 20\,000)$  should behave as  $\sim |y|^{\Delta/\nu}$  and the  $L$  dependence of the solvation force is  $f_{solv} \sim L^{-d+\Delta/\nu}$ . For 2D this is a very weak dependence as the exponent is equal to  $-0.125$ . In Fig. 9 we plot  $L^2 \times f_{solv}$  as a function of the scaling variable  $|y|$  and obtain an excellent scaling. The minimum of the solvation force is located in the crossover regime, close to the extrema of the free energy and the longitudinal correlation length. It is reached for the scaling variable  $|y| \approx 3.2$ . Due to the broken symmetry by the surface fields there is no symmetric minimum of the solvation force for the positive  $H$ . At the minimum  $F(0, y, 20\,000)/k_B T_c$  is approximately 100 times the Casimir amplitude  $\mathcal{A}_{\infty}$ .

The location of the minimum of the solvation force seems to be governed by  $\xi_{\parallel}$  since at the minimum  $L \approx 2.7\xi_{\parallel}$ . Recall



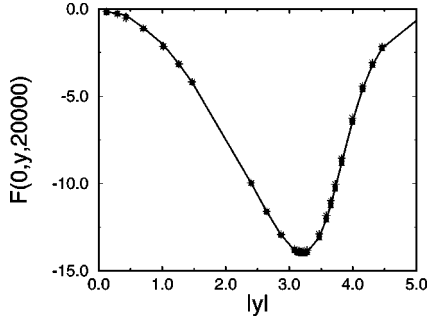


FIG. 9. Scaling function of the solvation force  $F(0,y,20000)$  [Eq. (2.26)] calculated for 2D Ising films at  $T=T_c$  of widths  $L=100$  (stars), 124 (circles), 150 (squares), 174 (diamonds), and 200 (triangles). Calculations for each  $L$  were performed at the suitable value of surface fields  $H_1=H_L$  to meet the condition  $x=L|H_1|^{\nu/\Delta_1}=20000$ .

that in the crossover regime  $\xi_{\parallel}$  differs significantly from  $\xi_H$ . Similarly to the case of free boundary conditions the minimum of the solvation force is associated with highly inhomogeneous profile (see Fig. 10).

$\xi_{\parallel}(H)$  for  $H$  around its maximum is much bigger than the corresponding bulk magnetic correlation length due to a presence of broad interfaces between thin layers of a liquid-like phase near walls and a gaslike phase in the middle of the film in a crossover regime. As is visible in Fig. 10, the scaling functions of the magnetization profile are linear in the region of the interface.

From the above analysis it follows that in our finite system one cannot check predictions described in Sec. II A concerning the universal behavior of the profile and of the adsorption in the semi-infinite system moved away from the bulk critical point by the bulk field  $H$ . Recall that in films at  $H=0$  and nonzero  $\tau$  when one can find a temperature regime such that  $\xi_{\tau} \ll L$  and  $\Gamma$  behaves as in the semi-infinite system, i.e., according to the universal Fisher de Gennes power law (2.11) [26]. For the present case when  $H$  becomes strong enough to meet the condition  $\xi_H \ll L$ , the vicinity of the pseudocoexistence manifests itself and the OP profile is modified. Thus for films the scaling fields  $\tau$  and  $H$  are not thermodynamically equivalent in the critical regime.

#### IV. DISCUSSION

In this paper we have undertaken the investigation of the effect of the bulk magnetic field on the ordinary and normal transitions in two-dimensional Ising films. Our results are restricted to the bulk critical temperature  $T_c$  to study the dependence of physical quantities on  $H$  and to explore the equivalence of the scaling fields  $H$  and  $\tau$ . Our results confirm general finite-size scaling predictions in the case when the bulk magnetic correlation length  $\xi_H$  sets the length scale. For quantities such as the adsorption  $\Gamma$  or the longitudinal correlation length  $\xi_{\parallel}$  the scaling region is very broad, up to  $y=\text{sgn}(H)L|H|^{\nu/\Delta} \approx -100$ .

We found that for the ordinary transition at  $\tau=0$  and  $H < 0$  a dominant length in the system is  $\xi_H$ , equivalently to  $\xi_{\tau}$  in the case of  $H=0$  and  $\tau > 0$ . The case of the normal transition is very different due to the proximity of the quasi-first-order capillary condensation phase transition below  $T_c$  which

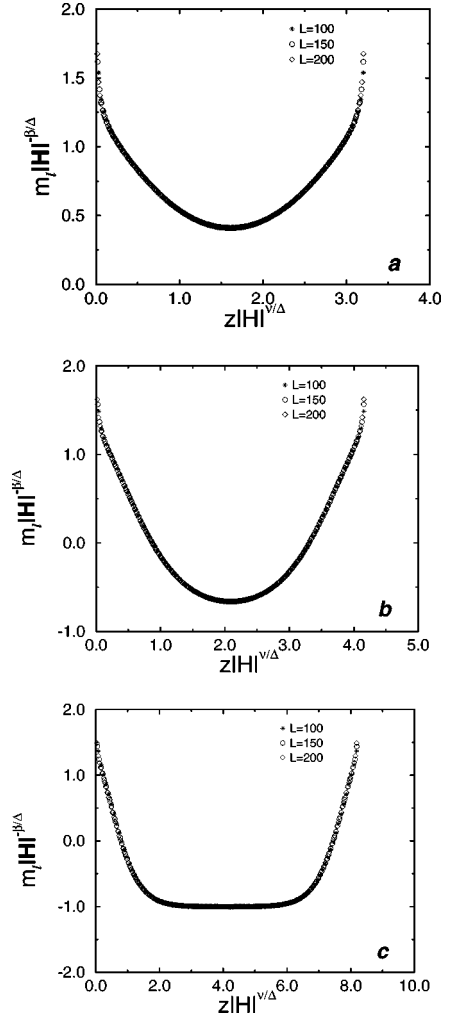


FIG. 10. Scaling functions of typical magnetization profiles for 2D Ising films at  $T=T_c$  in the crossover regime for the scaling variable (a)  $y=\text{sgn}(H)L|H|^{\nu/\Delta}=-3.2$ , i.e., at the minimum of the solvation force, (b)  $y=-4.2$ , at the maximum of the free energy of the film and in the (c) ‘‘bulk field-governed’’ regime, for  $y=-8.02$ . Calculations for each  $L$  were performed at the suitable value of surface fields  $H_1=H_L$  to meet the condition  $x=L|H_1|^{\nu/\Delta_1}=20000$ .

influences strongly the system even at  $T_c$ . For both the ordinary and the normal transitions we observe the crossover between the surface-governed behavior and the bulk field-governed behavior as  $H$  becomes more negative. The crossover in the case of the ordinary transition occurs when the bulk correlation length  $\xi_H \sim |H|^{-\nu/\Delta} \sim L$ , whereas for the normal transition it occurs when  $\xi_{\parallel} \sim L$ , which is near the continuation of the pseudocoexistence line beyond the capillary condensation pseudocritical point  $T_c(L)$ . In the case of the ordinary transition the surface-governed behavior resembles the behavior of the disordered phase, since the whole OP profile responds linearly to the bulk field  $H$ . In the case of the normal transition the strong surface field  $H_1$  breaks the symmetry and the surface-governed behavior resembles the behavior of the positively magnetized pseudophase with  $\Gamma > 0$ . In both cases the strong  $H$  in the bulk field-governed regime stabilizes the negatively magnetized pseudophase in the central part of the film with  $\Gamma < 0$  and  $m(L/2) \sim \text{sgn}(H)|H|^{1/\delta}$ .

We observed that in the crossover region the physical quantities exhibit extrema, as for example the solvation force, or inflection points, as for example, adsorption. Also the OP profile is highly nonuniform everywhere across the film. In other systems with the relevant length scales determined by  $\tau$  or by the surface field  $H_1$ ,  $\xi_\tau \sim |\tau|^{-\nu}$  or  $l_1 \sim |H_1|^{-\nu/\Delta_1}$ , respectively, similar crossover behavior characterized by nonuniform OP and extrema or inflection points of physical quantities was observed when  $\xi_\tau \sim L$  or  $l_1 \sim L$  [10,14].

The striking result of our work concerns the behavior of the solvation force for the case of the normal transition. The scaling function of  $f_{sol}$  has a minimum where the magni-

tude of the force (in units of  $k_B T_c$ ) is approximately 100 times the Casimir amplitude. The minimum of the solvation force lies close to the continuation of the pseudocoexistence line beyond the capillary condensation pseudocritical point  $T_c(L)$ , hence, we connect this strong effect with the proximity of the quasi-first-order capillary condensation phase transition below  $T_c$ .

#### ACKNOWLEDGMENTS

We are grateful to R. Evans for comments. This work was partially funded by KBN through Grant Nos. 2P03B10616 and 3T09A07316.

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- [1] For review see, for example, *The Critical Point* by C. Domb (Taylor and Francis, London, 1996).
- [2] For a general review of critical behavior at surfaces, see K. Binder, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1983), Vol. 8, p. 1.
- [3] H. W. Diehl, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1986), Vol. 10, p. 75, and references therein.
- [4] M. N. Barber, in *Phase Transitions and Critical Phenomena* (Ref. [2]), p. 1.
- [5] R. Evans, *J. Phys.: Condens. Matter* **2**, 8989 (1990), and references therein.
- [6] J. N. Israelachvili and P. M. McGuggian, *Science* **241**, 795 (1988).
- [7] L. Spruch, *Science* **272**, 1452 (1996).
- [8] M. Krech, *The Casimir Effect in Critical System* (World Scientific, Singapore, 1994), and references therein.
- [9] A. O. Parry and R. Evans, *Physica A* **181**, 250 (1992).
- [10] R. Evans and J. Stecki, *Phys. Rev. B* **49**, 8842 (1993), and references therein.
- [11] T. Nishino, *J. Phys. Soc. Jpn.* **64**, 3598 (1995).
- [12] S. R. White, *Phys. Rev. B* **48**, 10 345 (1993).
- [13] *Lectures Notes in Physics*, Vol. 528, edited by I. Peschel, X. Wang, M. Kaulke, and K. Hallberg (Springer, Berlin, 1999).
- [14] A. Maciołek, A. Ciach, and A. Drzewiński, *Phys. Rev. E* **60**, 2887 (1999).
- [15] M. E. Fisher, *Rev. Mod. Phys.* **46**, 597 (1974).
- [16] V. Privman, P. C. Hohenberg, and A. Aharony, *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1991), Vol. 11, p. 1.
- [17] H. B. Tarko and M. E. Fisher, *Phys. Rev. B* **11**, 1217 (1975).
- [18] M. E. Fisher and P. de Gennes, *C. R. Seances Acad. Sci., Ser. B* **287**, 207 (1978).
- [19] V. Privman, in *Finite Size Scaling and Numerical Simulation of Statistical Systems*, edited by V. Privman (World Scientific, Singapore, 1990).
- [20] M. E. Fisher and H. Nakanishi, *J. Chem. Phys.* **75**, 5857 (1981); H. Nakanishi and M. E. Fisher, *ibid.* **78**, 3279 (1983).
- [21] See, e.g., E. V. Albano, K. Binder, D. W. Heerman, and W. Paul, *J. Chem. Phys.* **91**, 3700 (1989).
- [22] E. Carlon, A. Drzewiński, and J. Rogiers, *Phys. Rev. B* **58**, 5070 (1998).
- [23] A. E. Ferdinand and M. E. Fisher, *Phys. Rev.* **185**, 832 (1969).
- [24] M. E. Fisher and H. Au-Yang, *Physica (Utrecht)* **101**, 255 (1980); H. Au-Yang and M. E. Fisher, *Phys. Rev. B* **21**, 3956 (1980).
- [25] A. Drzewiński, A. Ciach, and A. Maciołek, *Eur. Phys. J. B* **5**, 825 (1998).
- [26] A. Maciołek, A. Ciach, and R. Evans, *J. Chem. Phys.* **108**, 9765 (1998); A. Maciołek, R. Evans, and N. B. Wilding, *Phys. Rev. E* **60**, 7105 (1999).