Wedge filling and interface delocalization in finite Ising lattices with antisymmetric surface fields

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Theoretical predictions by Parry *et al.* for wetting phenomena in a wedge geometry are tested by Monte Carlo simulations. Simple cubic $L\times L\times L_y$ Ising lattices with nearest neighbor ferromagnetic exchange and four free $L\times L_y$ surfaces, at which antisymmetric surface fields $\pm H_s$ act, are studied for a wide range of linear dimensions ($4\leqslant L\leqslant 320$, $30\leqslant L_y\leqslant 1000$), in an attempt to clarify finite size effects on the wedge filling transition in this "double-wedge" geometry. Interpreting the Ising model as a lattice gas, the problem is equivalent to a liquid-gas transition in a pore with quadratic cross section, where two walls favor the liquid and the other two walls favor the gas. For temperatures T below the bulk critical temperature T_c this boundary condition (where periodic boundary conditions are used in the y direction along the wedges) leads to the formation of two domains with oppositely oriented magnetization and separated by an interface. For $L,L_y\to\infty$ and T larger than the filling transition temperature $T_f(H_s)$, this interface runs from the one wedge where the surface planes with a different sign of the surface field meet (on average) straight to the opposite wedge, so that the average magnetization of the system is zero. For $T<T_f(H_s)$, however, this interface is bound either to the wedge where the two surfaces with field $-H_s$ meet (then the total magnetization m of the system is positive) or to the opposite wedge (then $m<0$). The distance l_0 of the interface midpoint from the wedges is studied as $T\to T_f(H_s)$ from below, as is the corresponding behavior of the magnetization and its moments. We consider the variation of l_0 for $T>T_f(H_s)$ as a function of a bulk field and find that the associated exponents agree with theoretical predictions. The correlation length ξ_y in the y direction along the wedges is also studied, and we find no transition for finite L and $L_y\to\infty$. For $L\to\infty$ the prediction $l_0\propto(H_{sc}-H_s)^{-1/4}$ is verified, where $H_{sc}(T)$ is the inverse function of $T_f(H_s)$ and $\xi_y\propto(H_{sc}-H_s)^{-3/4}$, respectively. We also find that m vanishes discontinuously at the filling transition. When the corresponding wetting transition is first order we also obtain a first-order filling transition.

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I. INTRODUCTION

Recently the problem of wetting of fluids in a wedge geometry provided by a suitably prepared solid surface has found increasing attention, both in the context of applications, e.g., microfluidics, and because of its interest for the theory of inhomogeneous fluids [1–8]. Of particular interest is the striking finding that under conditions where the fluid does not yet wet the walls forming a wedge, i.e., where the contact angle Θ characterizing the wettability properties of planar substrates [9–14] is still nonzero, a phase transition occurs. There the liquid that has condensed in the wedge from the (saturated) gas, to which the substrate is exposed, starts to fill the wedge, i.e., the height ℓ_0 (Fig. 1) of the interface right above the wedge diverges to infinity when the transition temperature T_f of this "filling transition" is approached. In fact, considering a situation where the wetting transition [10–14] on a planar substrate can be brought about by a variation of temperature, one finds [1–4] that ℓ_0 is finite as long as $\Theta(T)>\alpha$, α being the opening angle of the wedge (Fig. 1), while the filling transition is reached for $\Theta(T_f)=\alpha$, and then ℓ_0 becomes of macroscopic size, $\ell_0\to\infty$.

While second-order wetting transitions at planar surfaces are a rather rare phenomenon [15], it has been predicted that continuous filling transitions in wedge geometries are possible even for wedges made from substrates exhibiting first-order wetting transitions, and hence critical phenomena associated with second-order filling transitions should be readily observable [6,7]. In addition, it has been predicted for systems with short-range forces between the wall atoms and the fluid molecules that the effect of interface fluctuations should be very strong and lead to the following divergences of the height ℓ_0 and the associated correlation lengths $\xi_\perp$, ξ_x, and ξ_y as one approaches the filling transition temperature T_f from below [6,7]:

$$\ell_0\propto(T_f-T)^{-\beta_s},\quad \xi_\perp\propto(T_f-T)^{-\nu_\perp},$$
$$\xi_x\propto(T_f-T)^{-\nu_x},\quad \xi_y\propto(T_f-T)^{-\nu_y}\qquad(1)$$

with the exponents

$$\beta_s=\nu_\perp=\nu_x=1/4,\quad \nu_y=3/4.\qquad(2)$$

Here $\xi_\perp$ describes the interface roughness in z direction, perpendicular to the interface (Fig. 1), while ξ_x, ξ_y measure correlations of interface height fluctuations $\ell(x,y)-\langle\ell(x,y)\rangle$ parallel to the interface in the x direction normal to the direction of the wedge and in the y direction along the wedge, respectively. Furthermore, the approach to the filled wedge at $T=T_f$ as a function of the chemical potential difference $\Delta\mu$, i.e., of the field conjugate to the order parameter in the bulk (the density difference between liquid and saturated gas), has been predicted as [6,7]

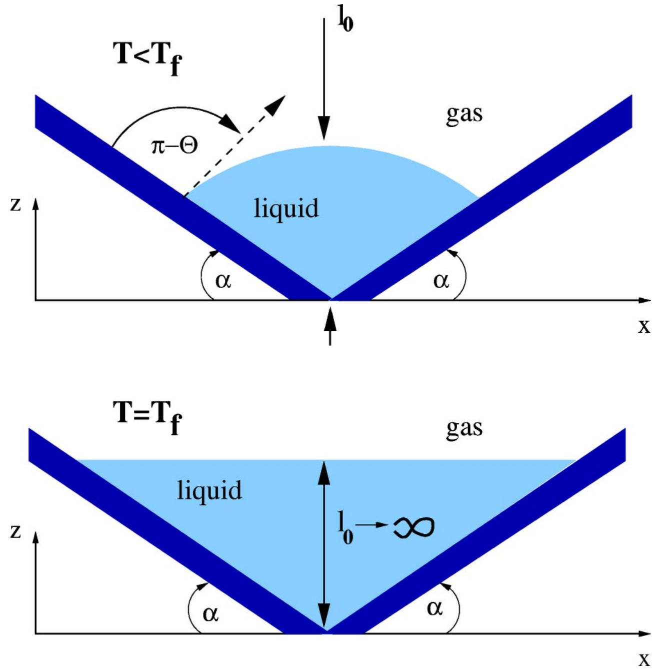

FIG. 1. Schematic view of the wedge geometry in which a liquid condenses from a gas held at the coexistence pressure $p_{\mathrm{coex}}(T)$ of the liquid-gas transition. The wedge is symmetric around the z axis ($\pi-2\alpha$ is the opening angle of the wedge) and the center of the wedge runs along the y axis. The liquid-gas interface (treated as a sharp kink) has the local position $\ell(x,y)$ above the wedge, while ℓ_0 denotes its midpoint position (for $x=0$). The situation where the contact angle Θ [of a macroscopic amount of fluid in the wedge, where ℓ_0 is much larger than all atomistic distances and line tension effects on $\Theta(T)$ can be neglected] exceeds α corresponds to $T<T_f$, while the filling transition temperature T_f, where then $\ell_0\to\infty$, is reached for $\Theta(T=T_f)=\alpha$. Note that the state shown in the upper part of the picture, where $\Theta>\alpha$ but ℓ_0 has a macroscopic value, can only be realized in an ensemble constrained such that there is a macroscopic amount of fluid in the wedge [5]. In an ensemble where the pressure p is fixed at $p_{\mathrm{coex}}(T)$, in the nonfilling situation ℓ_0 is still a microscopic length, and hence larger than the thickness of the film coating all the walls of the wedge by a finite factor only.

$$\ell_0 \propto (\Delta\mu)^{-1/5}. \quad (3)$$

In contrast, for $T>T_f$ one expects another power law, which is denoted as ‘‘complete filling’’ because of the analogy with ‘‘complete wetting’’ [11–14], namely [16],

$$\ell_0 \propto (\Delta\mu)^{-1}. \quad (4)$$

Unlike the related case of corner wetting in the two-dimensional Ising model [17–20], where one believes that the corresponding exponents ($\beta_s=\nu_\perp=1$, $\nu_x=2$) are known exactly, the results Eqs. (2) and (3) are based on a treatment that involves several approximations [6,7].

(i) The interface is treated in the framework of the simple capillary wave Hamiltonian.

(ii) Assuming small values of α in Fig. 1, only the interaction between the interface and that plane of the wedge surface which is geometrically closer to the interface than the other plane is taken into account.

(iii) It is assumed that the fluctuations of the height $\ell_0(y)=\ell(x=0,y)$ at the midpoint of the wedge dominate the critical behavior.

In view of these uncertainties about the validity of these assumptions, it is desirable to test them by a Monte Carlo study of the filling transition, and this is the goal of the present paper. Recall that Monte Carlo tests of critical wetting with short-range forces [21–23] have called the corresponding theory [24] into question [25].

In Sec. II we define the model that is studied here. For technical reasons we study a double wedge of cross section $L\times L$ and hence $\alpha=\pi/4$, i.e., α is *not* small, since this allows us to study also the present model within the framework of a nearest neighbor Ising model on the simple cubic lattice; a double wedge is used, since in computer simulations necessarily all linear dimensions are finite, and hence a wedge that is open and infinitely extended, as sketched in Fig. 1, cannot be simulated. Also in Sec. II we recall what is known about the wedge filling transition in more detail and discuss our finite size scaling concepts used to analyze our results in Sec. III Finally, Sec. IV gives a summary and outlook on future work.

In the present paper we complement the information provided in abbreviated form [26]. Specifically, we extend the previous study in the following points.

(i) We locate the filling transition by calculating the contact angle on a planar substrate via Young’s equation. We compare this result to the finite size scaling analysis [26], the dependence of the height ℓ_0 in the middle of the wedge, and a naive analysis of profiles of the wedge’s cross section.

(ii) We study complete filling.

(iii) We elucidate the role of the length of the wedge L_y and provide evidence for the absence of a transition in the limit $L_y\to\infty$ at fixed cross section.

(iv) We change the model as to consider surfaces which exhibit second-order and first-order wetting transitions in planar geometry.

II. THE MODEL AND SOME THEORETICAL BACKGROUND

A. The problem

Throughout this paper we consider a nearest neighbor Ising ferromagnet on a simple cubic lattice with linear dimensions $L\times L\times L_y$, with periodic boundary conditions applied only in the third direction (the y direction, where the linear size is L_y). In the first two directions (the x and z directions of the lattice), we have free boundary conditions (i.e., missing spins across the boundary), but we also apply surface fields $+H_s$ at the two upper $L\times L_y$ surfaces (for clarity, Fig. 2 shows a schematic cross section through our system to define the notation) and surface fields $-H_s$ at the two lower surfaces.

The Ising model in this antisymmetric double-wedge geometry is described by the following Hamiltonian:

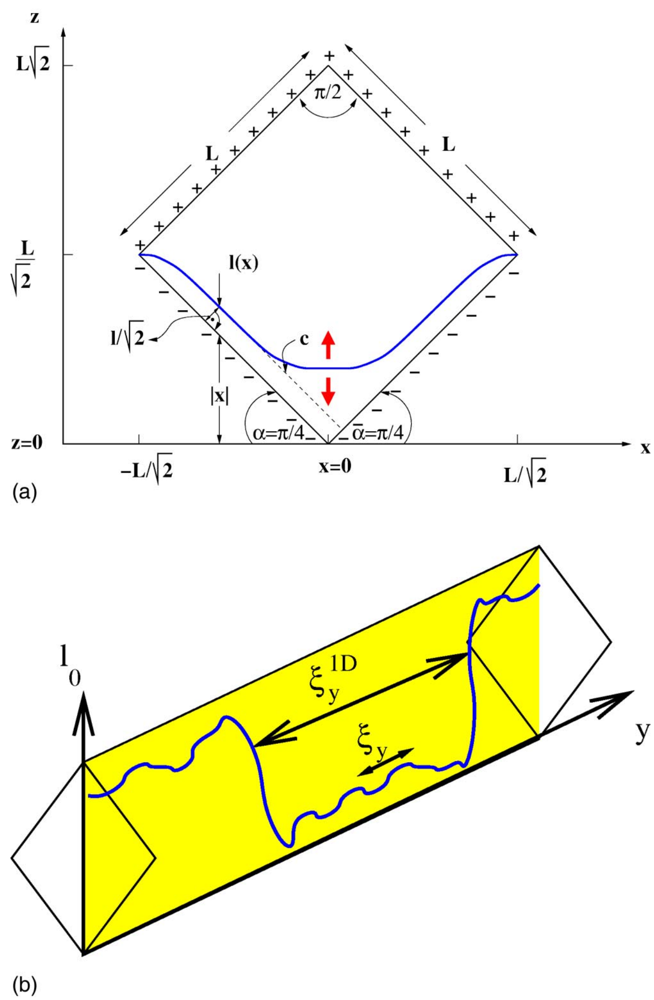

FIG. 2. (a) Cross section through the double-wedge geometry of the simulated $L\times L\times L_y$ Ising lattice. The interface between the domains with positive and negative magnetization (indicated symbolically by the thick arrows) starts out at the left wedge ($x=-L/\sqrt{2}$, $z=+L/\sqrt{2}$) and ends at the right wedge ($x=z=L/\sqrt{2}$). Above the temperature of the filling transition, the interface fluctuates weakly around its mean position $z=L/\sqrt{2}$, i.e., $\ell(x)\equiv z-|x| =L/\sqrt{2}-|x|$. Below this transition temperature, the interface is either bound to the surfaces where negative surface fields act (as assumed in the sketch) or, equivalently, to the surfaces where positive surface fields act. Only in the immediate proximity of the bottom of the wedge ($x=0,z=0$) [or at the top ($x=0$, $z=L\sqrt{2}$), respectively] does a minority domain (with roughly triangular cross section) exist, characterized by the maximum distance $\ell_0=\ell(x=0)$ (or $L\sqrt{2}-\ell_0$, respectively) of the interface from the surfaces. The distance of a point at the interface near the wedge from the two boundaries forming the wedge is indicated, namely, $\ell/\sqrt{2}$ and $c=\sqrt{2}(|x|+\ell/2)$, respectively. (b) Fluctuations of ℓ_0 along the wedge are characterized by two correlation lengths. ξ_y describes the fluctuations of the interface bound to a wedge, while ξ_y^{1D} refers to the length of domains, where the interface is bound to the upper or lower wedge.

$$\mathcal{H}=-J\sum_{\langle i,j\rangle_{\rm bulk}} S_iS_j-J_s\sum_{\langle i,j\rangle\in W_1\cup W_2} S_iS_j-H_s\sum_{i\in W_1} S_i +H_s\sum_{i\in W_2} S_i\,, \tag{5}$$

where $J\equiv 1$ denotes the exchange constant of the Ising model in the bulk and the spin variables S_i can take values ± 1. In addition, the exchange constant J_s in the surface planes may differ from the exchange in the bulk. In this way, a ''double wedge'' is created, where two planes (W_2) with negative surface fields meet at the line $x=0$, $z=0$ (the y axis of our coordinate system), while the two other planes (W_1) with positive surface fields meet in the opposite line $x=0$, $z=L\sqrt{2}$. Of course, the actual orientation of the lattice planes of the Ising lattice is rotated relative to the y-axis by the angle $\pi/4$, such that the surfaces become simple lattice planes of the simple cubic lattice again, but this is not important for the phenomenological considerations that we will present below. Apart from the different choice of boundary conditions, the model is identical to that used for a study of critical wetting [21–23] and interface localization [27–30]. At this point, we recall again that the Ising model can be reinterpreted as a lattice model for the liquid-gas transition via the lattice gas interpretation. A zero bulk field $H=0$ then corresponds to the pressure of the liquid-gas coexistence in the bulk. However, for this application to fluids it would be more realistic to assume long-range van der Waals–type surface forces rather than strictly local surface forces. We shall comment on this problem below. We are mostly interested in the location $\ell(x)$ of the interface above the wall, disregarding the dependence on the y coordinate (the y axis runs perpendicular to the xz plane shown in Figs. 1 and 2, of course), which needs to be considered in the discussion of interface fluctuations. We define $\ell(x)$ simply as

$$\ell(x)=z-|x|, \tag{6}$$

z being the position of the contour separating the two domains of positive and negative magnetization (in this description, we treat the interface in the sharp kink approximation, neglecting a possible ''intrinsic profile '' of the interface [11–13]).

B. Phenomenological mean-field theory

Following the treatment of Rejmer, Dietrich, and Napiorkowski [5], we first formulate the problem in terms of an effective interface Hamiltonian $\mathcal{H}[\ell]$, which we write as

$$\mathcal{H}[\ell(x)]=L_y\int_{-L/\sqrt{2}}^{+L/\sqrt{2}}dx\left\{\sigma\left(\sqrt{1+\left[\frac{d\ell(x)}{dx}+\mathrm{sgn}(x)\right]^2}-\sqrt{2}\right)+\sqrt{2}V_{\rm tot}(\ell,x)\right\}. \tag{7}$$

Here σ is the interface free energy per unit area and $V_{\rm tot}(\ell,x)$ is the total interface potential experienced at the interface position $[x,y,z=|x|+\ell(x,y)]$ due to the interaction with all four boundaries on which the surface fields act. The standard approximation $\sqrt{1+(d\ell/dx)^2}\approx 1+(1/2)(d\ell/dx)^2$, which also is used in the theoretical treatments of the wedge filling transition [6,7], assumes that the angle α in Fig. 1 is very small. This leads to the capillary wave Hamiltonian [12–14] in its usual form, but this cannot be used here since $\alpha=\arctan 1=\pi/4$ is of order unity and the expansion of the square root is unwarranted. We also have chosen the convention to measure the interface energy relative to that in the state above the filling transition temperature, where $\ell(x)=L/\sqrt{2}-|x|$. The extra factor $\sqrt{2}$ in the last contribution accounts for the ratio between $L_y dx$ and the surface area.

For an interface that interacts with a flat wall with short-range forces and is located at (constant) height h above this straight wall, the standard assumption for the potential is [11–14,29,31]

$$V(h)=a\exp(-\kappa h)+b\exp(-2\kappa h), \tag{8}$$

where a, b, and κ are phenomenological constants. The coefficient a changes sign at the second-order wetting transition temperature T_w such that $a<0$ for $T<T_w$; κ is of the same order as the bulk inverse correlation length ξ_b^{-1}, but probably not identical [28,29]. For $a<0$ the film thickness $h^\star$ is finite. Using $(dV/dh)_{|h^\star}=0$ one obtains $\exp(-\kappa h^\star)=-a/(2b)$ and $V(h^\star)=-a^2/(4b)$. Using the Young equation [12,13], we can relate the minimum of the interface potential to the contact angle Θ via $V(h^\star)=\sigma(\cos\Theta-1)$.

In the present geometry (Fig. 2), however, the treatment needs to be extended to include interactions with all four walls. Simple geometric considerations show (Fig. 2) that the normal distances of a point $[x,y,z=|x|+\ell(x)]$ at the interface from the four walls are $\ell/\sqrt{2}$, $c=\sqrt{2}|x|+\ell/\sqrt{2}$, $L-\ell/\sqrt{2}$, $L-c=L-\ell/\sqrt{2}-\sqrt{2}|x|$, and hence in our case Eq. (8) needs to be replaced by

$$V_{\rm tot}(\ell,x)=4a\exp(-\kappa L/2)\cosh\left(\frac{\kappa x}{\sqrt{2}}\right)\cosh\left(\frac{\kappa}{\sqrt{2}}\left[\frac{L}{\sqrt{2}}-\ell(x)-|x|\right]\right)+4b\exp(-\kappa L)\cosh(\sqrt{2}\kappa x)\times\cosh\left(\sqrt{2}\kappa\left[\frac{L}{\sqrt{2}}-\ell(x)-|x|\right]\right). \tag{9}$$

Note that our result for $V_{\rm tot}(\ell,x)$ does not reduce to the result of Rejmer, Dietrich, and Napiórkowski [5] even in the limit $L\to\infty$, because Rejmer, Dietrich, and Napiórkowski [5] take into account the interaction with the nearest boundary only, and neglect the interaction with the more distant boundary. Their approximation should become accurate for widely open edges (i.e., $\alpha\ll 1$), which is not the case here, where $\alpha=\pi/4$. As a consequence, the potential $V_{\rm tot}(\ell,x)$ depends on x not only implicitly [via the x dependence of $\ell(x)$], but also explicitly. This fact complicates the treatment even on the level of the mean-field theory considerably.

Now mean-field theory for this problem is equivalent to the minimization of the Hamiltonian $\mathcal{H}[\ell]$ with the appropriate boundary conditions, $\ell(x=-L/\sqrt{2})=\ell(x=L/\sqrt{2})=0$. The resulting Euler-Lagrange equation following from Eq. (7),

$$\sigma\frac{d^2\ell(x)/dx^2}{\left(1+\left[\dfrac{d\ell(x)}{dx}+\mathrm{sgn}(x)\right]^2\right)^{3/2}}=\sqrt{2}\,\frac{\partial}{\partial\ell}V_{\rm tot}(\ell,x), \tag{10}$$

generalizes the result of Rejmer, Dietrich, and Napiórkowski [5]. Since it was possible to solve the Euler-Lagrange equation of Ref. [5] only in special limits, there is little hope that the explicit analytic solution of Eq. (10) could be found, and in fact we have been unable to do so. If we approximate $V_{\rm tot}(\ell,x)$ by $V_{\rm eff}[\ell]\approx a\exp(-\kappa\ell/\sqrt{2})+b\exp(-\sqrt{2}\kappa\ell(x))$ we can write $\partial V_{\rm tot}(\ell,x)/\partial\ell\approx dV_{\rm eff}/d\ell$, and thus recover Eq. (3.3) of Ref. [5]. Using this approximation and multiplying both sides of Eq. (10) with $d\ell/dx$, we can integrate:

$$-\left.\frac{2+(d\ell/dx)}{\sqrt{1+[(d\ell/dx)+1]^2}}\right|_{\ell(0^+)}^{\ell(x)}=\sqrt{2}[V_{\rm eff}(\ell(x))-V_{\rm eff}(\ell(0))]. \tag{11}$$

Far away from the corner the distance between the interface and the surface will be equal to the value of a planar surface, i.e., $|d\ell/dx|=0$ and $V_{\rm eff}(\ell(x))=V(h^\star)=\sigma(\cos\Theta-1)$. Here, we disregard the immediate neighborhood of $x=\pm L/\sqrt{2}$ and assume that the effects on the profile $\ell(x)$ near $x=0$ from this region are negligible.

We follow Rejmer, Dietrich, and Napiórkowski [5] and require that the solution is symmetric, $|x|+\ell(x)=|-x|+\ell(-x)$, and hence $d\ell/dx=-1$ for $x=0^+$. At the filling transition $\ell(0)\sim L/\sqrt{2}$ and, hence, $V_{\rm eff}(\ell(0))$ is of the order $\exp(-\kappa L/\sqrt{2})$. We expect the effective potential $V_{\rm eff}$ only to estimate the order of magnitude; clearly, in the situation where the interface runs along the diagonal of the wedge, interactions with all surfaces need to be considered. Then, the right-hand side of Eq. (11) takes the following form:

$$\sqrt{2}\left[-\frac{a^2}{4b}+\mathcal{O}(\exp(-\kappa L/\sqrt{2}))\right]=\sqrt{2}[\sigma(\cos\Theta-1)+\mathcal{O}(\exp(-\kappa L/\sqrt{2}))] \tag{12}$$

at the filling transition. The left-hand side of Eq. (11) equals $-\sqrt{2}+1=-\sqrt{2}(1-\cos\alpha)$, where we have used $\cos\alpha=1/\sqrt{2}$ for our double-wedge geometry. Therefore $\cos\Theta=\cos\alpha+\mathcal{O}(\exp(-\kappa L/\sqrt{2}))$ at the filling transition.

Note that this condition differs substantially from the analogous result for the interface localization-delocalization transition between competing flat walls a distance L apart, which rather reads [29,31]

$$a+4b\exp(-\kappa L/2)=0. \tag{13}$$

While Eq. (13) shows that the transition temperature of the interface localization transition for $L\rightarrow\infty$ converges towards the wetting transition temperature, the filling transition temperature for $L\rightarrow\infty$ differs substantially from the wetting transition temperature, in fact, it occurs when the contact angle Θ on the planar substrate approaches the opening angle α. Similar to the interface localization-delocalization transition in a film, however, mean-field theory suggests that the transition temperature in the double-wedge geometry differs from the transition temperature for $L\rightarrow\infty$ by terms of order $\exp(-\kappa L/\sqrt{2})$.

C. Fluctuations of the interface in the "disordered phase" within mean-field theory

In this section we consider the region of temperatures above the filling transition temperature, where the interface in our double-wedge geometry is not bound to either the lower wedge or the upper wedge, but runs more or less straight from the left corner of the square cross section to the right corner (at $z=L/\sqrt{2}$) in Fig. 2. Since we know that this trivially is the solution for the average position of the interface, it is a straightforward matter to expand the effective free energy quadratically around this solution. In the analogous case of the interface localization-delocalization transition between parallel walls, this approach has yielded mean-field prediction for the "susceptibility" of the interface localization transition [29], and it clearly is of interest to try such an approach in the present problem too.

Defining $f=|x|+\ell(x,y)$ we rewrite Eq. (7) as

$$\mathcal{H}[f]=\int_{-L/\sqrt{2}}^{+L/\sqrt{2}}dx\int_0^{L_y}dy\left\{\sigma\left(\sqrt{1+\left(\frac{\partial f}{\partial x}\right)^2+\left(\frac{\partial f}{\partial y}\right)^2}-\sqrt{2}\right)+\sqrt{2}V_{\text{tot}}(\ell(x,y),x)\right\}. \tag{14}$$

Since for the considered conditions $|\partial f/\partial x|\ll 1$, $|\partial f/\partial y|\ll 1$, also $\delta f=f-L/\sqrt{2}$ is small, one can expand Eq. (14) as follows (constant terms being omitted):

$$\mathcal{H}[f]\approx\int_{-L/\sqrt{2}}^{+L/\sqrt{2}}dx\int_0^{L_y}dy\left\{\frac{\sigma}{2}\left[\left(\frac{\partial\delta f}{\partial x}\right)^2+\left(\frac{\partial\delta f}{\partial y}\right)^2\right]+2a\sqrt{2}\exp(-\kappa L/2)\cosh(\kappa x/\sqrt{2})[1+\kappa^2(\delta f)^2/4]+2b\sqrt{2}\exp(-\kappa L)\cosh(\kappa x\sqrt{2})[1+\kappa^2(\delta f)^2]\right\}. \tag{15}$$

One readily sees from Eq. (15), however, that the coefficient of $(\delta f)^2$ is not uniformly positive in the interval $-L/\sqrt{2}\leqslant x\leqslant +L/\sqrt{2}$, as would be required for this expansion to be applicable. Rather, one finds that the coefficient of $(\delta f)^2$ is only positive close to the left and right corners while further inside the double wedge there occurs a critical value $\pm x_c(a)$, where this coefficient changes sign. This value x_c is found from the solution of the equation

$$a=-4b\exp(-\kappa L/2)\cosh(\kappa x_c\sqrt{2})/\cosh(\kappa x_c/\sqrt{2}). \tag{16}$$

Thus we expect that fluctuations of the interface are stable (when $a<0$, i.e., below the wetting transition temperature of the flat surface) only in the regions $\pm(L/\sqrt{2}\leqslant x\leqslant x_c)$, while interfacial fluctuations are unstable in the regime $-x_c\leqslant x\leqslant +x_c$. When the interface localization-delocalization transition is approached, $x_c\rightarrow L/\sqrt{2}$, the interface gets unstable in its "unbound" position everywhere. Therefore the transition to the states where the interface is bound to one of the wedges must occur.

D. Beyond mean-field theory

Using Eq. (14) we obtain the free energy from $F=-k_BT\ln Z$, where $Z=\int\mathcal{D}f\exp(-\mathcal{H})$ with a factor $1/k_BT$ absorbed in the definition of $\mathcal{H}[f]$. This would be a rather formidable problem. In fact, fluctuations have only been considered [6,7] for the simpler case of a single infinite wedge (Fig. 1) with $\alpha\ll 1$. Analyzing this simplified model in the mean-field approximation for a critical filling transition with short-range forces, one finds that the exponents [see Eq. (1)], for the short ranged boundary potential Eq. (8) are [7]

$$\beta_s=0,\quad \nu_\perp=1/4,\quad \nu_y=1/2. \tag{17}$$

Here $\beta_s=0$ means that the midpoint interface position ℓ_0 in Fig. 1 grows only logarithmically in $t=1-T/T_f$ as the filling transition temperature T_f is approached from below, i.e., $\langle\ell_0\rangle\propto|\ln t|$. On the other hand, the result that $\xi_\perp\propto t^{-1/4}$ as $t\rightarrow 0$ shows that mean-field theory for this problem is inadequate, since the "contact condition" [32] $\xi_\perp/\langle\ell_0\rangle\ll 1$ is violated. Thus, fluctuations *beyond mean field* need to be considered. Rather than treating the full Hamiltonian—which should be able to describe both wetting (where $\alpha=0$) and filling (when $\alpha>0$)—Parry *et al.* [6,7] argue that it suffices to consider a simpler Hamiltonian where only fluctuations in y direction are included. Then, $\ell(x,y)\equiv l_0(y)-\alpha|x|$ for $\alpha\ll 1$,

$$\mathcal{H}_{\text{fill}}(\ell_0)=\int dy\left\{\frac{\sigma\ell_0}{\alpha}\left(\frac{d\ell_0}{dy}\right)^2+V_{\text{fill}}(l_0)\right\}, \tag{18}$$

with [for large l_0 the subleading term proportional to $\exp(-2\kappa l_0)$ can be omitted]

$$V_{\text{fill}}(l_0)=\frac{\sigma(\Theta^2-\alpha^2)l_0}{\alpha}+a_F\exp(-\kappa l_0). \tag{19}$$

Θ is the contact angle at the filling transition and a_F is related to the parameter a of Eq. (8). Note that both a and a_F are negative in the regime of interest. Of course, the condition $\partial V_{\text{fill}}/\partial\ell_0=0$ would yield

$$\kappa\langle l_0\rangle=-\ln[\sigma(\Theta^2-\alpha^2)/(|a_F|\kappa\alpha)], \tag{20}$$

and since $\Theta-\alpha\propto t$ [remember, $\Theta(T=T_f)=\alpha$], the above result $\langle l_0\rangle\propto|\ln t|$ follows. For the Hamiltonian Eq. (18), however, a treatment of fluctuations yields the exponents quoted in Eq. (2) [6,7] rather than the mean-field results, Eq. (17). This treatment also yields a scaling prediction for the response of $\langle \ell_0 \rangle$ to a bulk magnetic field, involving a gap exponent $\Delta = 5/4$ [6,7]:

$$\langle l_0 \rangle = t^{-1/4} \tilde{\ell}(H t^{-\Delta}), \tag{21}$$

where $\tilde{\ell}$ is a scaling function which behaves as $\tilde{\ell}(\zeta \to \infty) \propto \zeta^{-1/4\Delta}$, which yields Eq. (3).

For the sake of completeness, we mention that Eq. (2) is valid not only for systems with strictly short-range surface forces but also for surface forces that decay with a power law $V(h) \propto h^{-p}$, provided $p \geq 4$. In contrast, for $p < 4$ Eq. (17) is replaced by

$$\beta_s = 1/p, \quad \nu_\perp = 1/4, \quad \nu_y = 1/2 + 1/p, \tag{22}$$

and one can show that mean-field theory is self-consistent when $t \to 0$ [7].

E. Phenomenological finite size scaling considerations

Finally we note another important distinction between the interface localization transition and the wedge filling transition: while the interface localization transition can occur for any finite distance L between the two planar boundaries, also when fluctuations are taken into account, the wedge filling transition exists only in the limit $L \to \infty$. It is rounded off for any finite L because then the system is quasi-one-dimensional and cannot maintain true long-range order in the y direction. Thus, there is a characteristic domain size ξ_y^{1D} [cf. Fig. 2(b)] over which the magnetization of the double wedge for $T < T_f$ is positive (as assumed in the cross section Fig. 2, since the area of the positive domain is larger), while then an interface occurs where the interfaces move up from the line $z = \langle l_0 \rangle$ (between $x = -\langle \ell_0 \rangle$ and $x = +\langle l_0 \rangle$) to the line $z = L\sqrt{2} - \langle \ell_0 \rangle$ (also between $x = -\langle \ell_0 \rangle$ and $x = +\langle l_0 \rangle$). Here we have assumed that the cross section of the interface between positive and negative domains in the double wedge is essentially a horizontal straight line at height $z = l_0$ in Fig. 2. Thus the area of such an interface across the wedge (needed to change the sign of the magnetization) is $L^2 - 2\langle \ell_0 \rangle^2$, and hence the free energy cost (in units of temperature, having absorbed a factor $1/k_B T$ in our Hamiltonian) is $(L^2 - 2\langle \ell_0 \rangle^2)\sigma$. As a consequence, we estimate that the typical domain size in y direction should be

$$\xi_y^{1D} \propto \exp\{\sigma(L^2 - 2\langle \ell_0 \rangle^2)\} \equiv \exp\{(4\pi\omega)^{-1}[(L/\xi_b)^2 - 2(\langle \ell_0 \rangle/\xi_b)^2]\}, \tag{23}$$

where in the last step we have used the capillary parameter [12–14] $\omega = (4\pi\xi_b^2\sigma)^{-1}$, $\omega \approx 0.86$ [33] for the Ising model. Thus for $L_y \gg \xi_y^{1D}$ one should observe that the magnetization of the double wedge is always zero, due to the formation of many domains of typical size ξ_y^{1D}. However, if L is sufficiently large and L_y not too large, one should observe typically single domain states of the type as sketched in Fig. 2 (or their mirror image along the mirror plane $z = L/\sqrt{2}$) only.

We now discuss the fluctuations of the total magnetization $m = (L^2 L_y)^{-1} \Sigma_i S_i$ in the limit where L is sufficiently large that we can approach the filling transition rather closely and still have $L_y \ll \xi_y^{1D}$ for a large value of L_y such that $L_y \gg \xi_y$. We then expect that the magnetization fluctuations scale as

$$L^2 L_y(\langle m^2 \rangle - \langle m \rangle^2) \propto m_b^2 \xi_\perp \xi_x \xi_y \propto t^{-(\nu_\perp + \nu_x + \nu_y)} = t^{-5/4}. \tag{24}$$

Equation (24) is based on the speculative suggestion that magnetization fluctuations here are predominantly caused by random fluctuations of the interface; if the interface passes a volume element, the magnetization in the volume element changes from $+m_b$, the value of the spontaneous magnetization in the bulk, to $-m_b$, and vice versa. This magnetization fluctuation is correlated in a correlation volume, which is $\xi_\perp \xi_x \xi_y$ for the filling transition. This reasoning assumes that the amplitude of the interface fluctuations is comparable to the lateral dimension L itself. We shall confirm this assumption by Monte Carlo simulations (cf. Fig. 12) and also justify it by relating the interface localization-delocalization transition in a double wedge to the predictions of Parry *et al.* [6,7] via some plausible phenomenological arguments [26].

Of course, we always can write a fluctuation relation for the susceptibility:

$$k_B T \chi = k_B T \frac{\partial m}{\partial H} = L^2 L_y(\langle m^2 \rangle - \langle m \rangle^2), \tag{25}$$

where in a finite system actually it is appropriate to replace $\langle m \rangle^2$ by $\langle |m| \rangle^2$ in the phase where one expects symmetry breaking [34,35]. Hence Eqs. (24) and (25) imply that $\chi \propto t^{-5/4}$, i.e., we speculatively predict that $\gamma = 5/4$ for the filling transition.

Now we discuss finite size scaling for this problem more generally, but assuming $\xi_x \propto \xi_\perp$, so that two nontrivial correlation lengths $\xi_\perp \propto t^{-\nu_\perp}$, $\xi_y \propto t^{-\nu_y}$ remain [cf. Eq. (2)]. Then the most general scaling assumption for the susceptibility would be [36]

$$\chi = t^{-\gamma} \tilde{\chi}(L_y/\xi_y, L/\xi_\perp) = t^{-\gamma} \tilde{\chi}(L_y t^{\nu_y}, L t^{\nu_\perp}), \tag{26}$$

$\tilde{\chi}$ being a suitable scaling function [in the last step of Eq. (26) we actually have suppressed amplitude prefactors in the arguments of this scaling function]. Alternatively, we may write

$$\chi = t^{-\gamma} \tilde{\tilde{\chi}}(L_y/L^{\nu_y/\nu_\perp}, L^{1/\nu_\perp} t), \tag{27}$$

where $\tilde{\tilde{\chi}}$ is another scaling function, and now only one argument depends on temperature, the other argument $L_y/L^{\nu_y/\nu_\perp}$ [$= L_y/L^3$, if Eq. (2) holds] is a generalized aspect ratio [36]. Similar relations can be written for the fourth-order cumulant of the magnetization [36,37]:

$$U_{L,L_y} \equiv 1-\langle m^4\rangle/(3\langle m^2\rangle^2)=\tilde{U}(L_y/\xi_y, L/\xi_\perp)$$
$$=\tilde{\tilde{U}}(L_y/L^{\nu_y/\nu_\perp}, L_y^{1/\nu_y}t), \tag{28}$$

where $\tilde{U}$, $\tilde{\tilde{U}}$ are suitable scaling functions.

It turns out that a similar scaling as for the cumulant applies for the magnetization of the Ising model in the double-wedge geometry:

$$\langle m\rangle = m_b\tilde{m}(L_y/\xi_y, L/\xi_\perp)=m_b\tilde{\tilde{m}}(L_y/L^{\nu_y/\nu_\perp}, Lt^{\nu_\perp}), \tag{29}$$

where $\tilde{m}$ and $\tilde{\tilde{m}}$ are suitable scaling functions and m_b is the spontaneous magnetization of the bulk three-dimensional Ising model. Normally, at a second-order transition one would have a power law $\langle m\rangle \propto t^\beta$ and a corresponding prefactor in Eq. (29), but here this exponent $\beta=0$. This also implies that the "gap exponent" $\Delta=\gamma+\beta=\gamma$, and Eq. (24) is consistent with Eq. (21). We may motivate the result Eq. (29) by noting that for finite "aspect ratio" $L_y/L^{\nu_y/\nu_\perp}$, we expect from geometry (Figs. 1 and 2) the following relation for the magnetization:

$$\langle m\rangle = m_b\left(1-2\frac{\langle \ell_0\rangle^2}{L^2}\right)=m_b[1-\text{const}(t^{1/4}L)^{-2}], \tag{30}$$

which is compatible with Eq. (29), since $\nu_\perp=1/4$ [Eq. (2)]. For $t \ll 0$ we expect then a double Gaussian form for $P_L(m)$ if $L_y/L^{\nu_y/\nu_\perp}$ is kept finite and m is near $\pm\langle m\rangle$:

$$P_L(m)\propto \exp\left[\frac{(m-\langle m\rangle)^2L^2L_y}{2k_BT\chi}\right]+\exp\left[-\frac{(m+\langle m\rangle)^2L^2L_y}{2k_BT\chi}\right]. \tag{31}$$

We note that the argument of the exponentials can be rewritten as

$$\left(\frac{m}{\langle m\rangle}\pm 1\right)^2\frac{\langle m\rangle^2L^2L_y}{2k_BT\chi}=L^2L_yL^{-\gamma/\nu_\perp}\tilde{f}(L_y/L^{\nu_y/\nu_\perp}, L^{1/\nu_\perp}t)$$
$$=L^{2+\nu_y/\nu_\perp-\gamma/\nu_\perp}\tilde{\tilde{f}}(L_y/L^{\nu_y/\nu_\perp}, L^{1/\nu_\perp}t), \tag{32}$$

where $\tilde{f}$, $\tilde{\tilde{f}}$ are suitable scaling functions that result from inserting the scaling expressions for $\langle m\rangle$ [cf. Eq. (29)] and χ [cf. Eq. (27)]. Now, Eqs. (31) and (32) are compatible with a scaling description of $P_L(m)$ at the filling transition itself (where $t=0$) only if the power law prefactor of L in Eq. (32) vanishes. (If a positive power of L remained, a two-delta function distribution would also appear at $T=T_f$. Such a description in terms of a two-delta function distribution at T_f would be expected if the interface localization-delocalization transition in the double-wedge geometry was a standard first-order transition.) This requires that a (generalized) hyperscaling relation holds:

$$2\nu_\perp+\nu_y=\gamma, \tag{33}$$

which is nothing but a special case of the generalization of hyperscaling to uniaxially anisotropic criticality [36],

$$(d-1)\nu_\perp+\nu_y=\gamma+2\beta \tag{34}$$

noting that we deal with $d=3$, $\beta=0$ here. The exponents suggested above [$\nu_\perp=\frac{1}{4}$, $\nu_y=\frac{3}{4}$, cf. Eq. (2)] and $\gamma=\frac{5}{4}$ [see Eq. (24)] are indeed fully consistent with Eq. (33).

Now a convenient way to estimate exponents such as $1/\nu_\perp$, $1/\nu_y$ is to take temperature derivatives at these common intersection points of the cumulants or magnetizations, from which we predict slopes that scale as $L_y^{4/3}$ (keeping the generalized aspect ratio L_y/L^3 fixed).

We emphasize that unlike Eqs. (2) and (21) which are based on a calculation [6,7] using the approximate effective Hamiltonian Eq. (18), Eqs. (23)–(34) are highly speculative. Thus, a Monte Carlo test of these conjectures, as well as of Eq. (2), is clearly warranted. While the filling transition for a single infinite wedge (Fig. 1) corresponds to a singularity of the surface excess free energy only, Eqs. (26)–(34) imply a special type of "bulk" transition in the limit $L\to\infty$, $L_y\to\infty$, $L_y/L^{\nu_y/\nu_\perp}=\text{const}$.

III. MONTE CARLO RESULTS

A. Direct analysis of the wedge filling

First of all we emphasize that for our simulations it is more convenient to vary H_s at fixed T (rather than varying T at fixed H_s), as in our studies of wetting transitions [21–23]. Thus, we reinterpret the distance t from the filling transition as $t=(H_{sc}-H_s)/H_{sc}$, where $H_s=H_{sc}(T)$ is the inverse function of $T=T_f(H_s)$. Of course, it should not matter in which way the line of filling transitions is approached in the (T,H_s) plane as long as it is not tangential to the line. This choice is preferable because the bulk properties of the Ising model (spontaneous magnetization m_b and susceptibility and correlation length ξ_b in the bulk, as well as the interface free energy σ) then stay strictly constant and none of these properties can depend upon H_s.

As a first estimate of the wedge-filling transition we use the macroscopic criterion that the filling occurs when the contact angle Θ on a planar substrate equals the wedge angle $\alpha=\pi/4$. The contact angle Θ is given by the Young equation:

$$\cos\Theta=\frac{\sigma_{s+}(H_s)-\sigma_{s-}(H_s)}{\sigma}=\frac{\Delta\sigma(H_s)}{\sigma}, \tag{35}$$

where σ denotes the interface tension between the coexisting phases in the bulk, σ_{s+} and σ_{s-} are the surface free energies of the bulk phase with positive and negative magnetization, respectively. By virtue of the symmetry of the Ising model the difference of the surface free energies $\Delta\sigma$ at surface field H_s can be written as $\Delta\sigma(H_s)=\sigma_{s+}(+H_s)-\sigma_{s+}(-H_s)$. The latter quantity can be obtained readily via thermodynamic integration [38]:

$$\frac{\Delta\sigma(H_s)}{J}=\int_{-H_s}^{+H_s}dH_s'\langle M_{s+}\rangle, \tag{36}$$

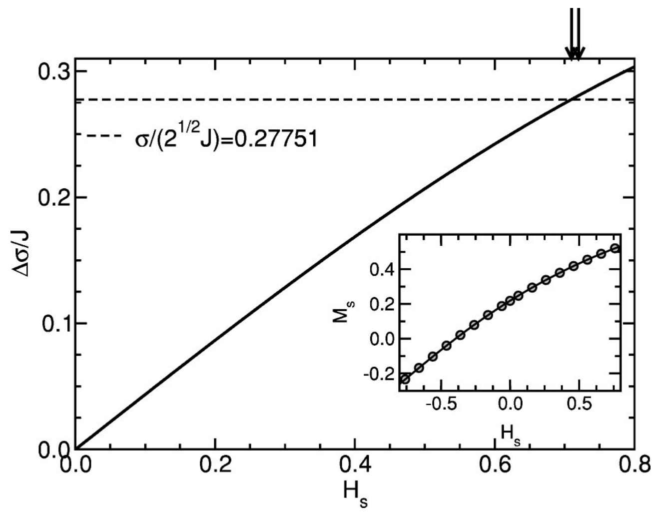

FIG. 3. Surface free energy difference $\Delta\sigma$ as a function of the surface magnetic field H_s at $J/k_BT=0.25$. Data are obtained from a film with symmetric surfaces and $L=L_z=80$. Arrows on the top mark $H_{sc}=0.71$ and 0.72, respectively. The inset shows the surface magnetization as a function of the surface field.

where $M_{s+}=(\Sigma_{i\in \text{surface}}S_i)/L^2$ denotes the surface magnetization of a planar surface when the bulk has a positive spontaneous magnetization. The Monte Carlo results for the dependence of M_s on the surface magnetic field H_s at $J/k_BT=0.25$ are presented in the inset of Fig. 3. For these simulations we have used a thin film with two symmetric walls and periodic boundary conditions in the lateral directions. The main panel compares the difference in surface free energy $\Delta\sigma(H_s)/J$ with the value $\sigma/(J\sqrt{2})=0.277\,51$, where we have used the accurate values of the interface tension of the Ising model [39]. The intersection point yields the estimate $H_{sc}\approx 0.71$ for the wedge filling transition. This estimate is compatible with the value $H_{sc}=0.72$ obtained from a more detailed finite size scaling analysis (cf. below). The deviations are presumably due to inaccuracies of the surface magnetization M_{s+} at large negative values of the surface field H_s. Under these conditions the system is metastable with respect to capillary condensation to a state with a negative magnetization in the middle of the film. (Note that the wetting transition is of second order for the planar substrate and unlike the situation at a first-order wetting transition metastable states cannot be observed close to the wetting transition.) Therefore, we can monitor the surface magnetization only for a finite time and systematically overestimate the surface magnetization. This, in turn, leads to an overestimation of $\Delta\sigma$ and a concomitant underestimation of H_{sc}.

Figure 4 shows typical results for the magnetization distribution in the wedge, in the form of contour diagrams for four choices of H_s near the filling transition H_{sc} (which is not known *a priori*, however). These contour diagrams show that the magnetization decays very smoothly from $+m_{\text{sp}}$ (≈ 0.75 at the considered temperature) in the bulk to negative values in the lower left corner of the cross sections. This variation is very gradual, and also at those cases ($H_s=0.68$ and 0.695) where one can see that in large parts of the system the interfaces are bound to the left and lower boundaries and run parallel to them, the thickness of the interfacial profiles is much broader than expected from the "intrinsic" interfacial width (which should be $2\xi_b$, with a bulk correlation length of the order of only about a lattice spacing at the considered temperature). These observations already indicate that strong interface fluctuations are indeed present, and become much more pronounced in the diagonal direction, when the interface has become unbound from the left lower wedge, e.g., at $H_s=0.720$ (note the large spacing between adjacent contours near $m=0$).

In order to obtain an estimate where the filling transition occurs we plot ℓ_0^{-4} versus H_s in Fig. 5: if $\ell_0\propto(H_{sc}-H_s)^{-1/4}$ holds, a plot of ℓ_0^{-4} versus H_s should yield a straight line whose extrapolation intersects the abscissa at the transition field, $H_{sc}\approx 0.706$. The data are more or less compatible with such an analysis, but there is a systematic deviation for $H_s\leqslant 0.6$, presumably because the data are too far away from the filling transition and for $H_s\geqslant 0.7$ due to finite size effects. The inset of Fig. 5 shows that ℓ_0 increases with increasing H_s only very gradually and $\ell_0=L/\sqrt{2}$ (corresponding to a flat interface connecting the wedges where the competing boundaries meet) is not at all reached over the entire range of surface fields, up to $H_s=1.6$. Also the point where the curve ℓ_0 versus H_s has its steepest slope ($H_s\approx 0.73\pm 0.01$) exceeds the value found from the extrapolation somewhat. Thus, this "naive" way to study the filling transition by Monte Carlo simulation is hardly suitable to test the theory.

The situation is much clearer when we investigate the variation with the conjugate field [cf. Fig. 6(a)]. We see that for fields $H/J\geqslant 0.01$ the interface distance from the wedge is too small ($\ell_0\leqslant 4$ lattice spacings), so this region of fields clearly is unsuitable to test the theoretical predictions. For the case where we are deep in the phase where the interface is unbound from the wedges, we can confirm the behavior $\ell_0(H)\propto H^{-1}$ predicted for complete filling [cf. Eq. (4)] at least for $10^{-3}\leqslant H/J\leqslant 10^{-2}$. For smaller fields finite size effects are visible. Fig. 6(b) shows also evidence for Eq. (3); testing this relation is more subtle, since H_{sc} is not known exactly.

B. Finite size scaling analysis of the localization-delocalization transition in the double wedge

Since it is obvious that the parameter L_y plays a crucial role in the analysis of the simulation data, we proceed next to the variation of properties with L_y at fixed L. As we have asserted in the preceding section, we expect that there cannot be a transition when we let $L_y\rightarrow\infty$ at fixed L, because the problem becomes quasi-one-dimensional. Nevertheless, plotting the fourth-order cumulant versus H_s for $L=40$ and various choices for L_y, we find (Fig. 7) rather well characterized intersection points (and this is confirmed by an intersection point of the absolute value of the magnetization) at $H_{sc}\approx 0.72$. Does this render our conclusion about the absence of a transition for $L_y\rightarrow\infty$ obsolete? This is clearly not the case, rather, the correct interpretation presumably is that ξ_y^{1D} [Eq. (23)] for $L=40$ is already very large, and orders of magni-

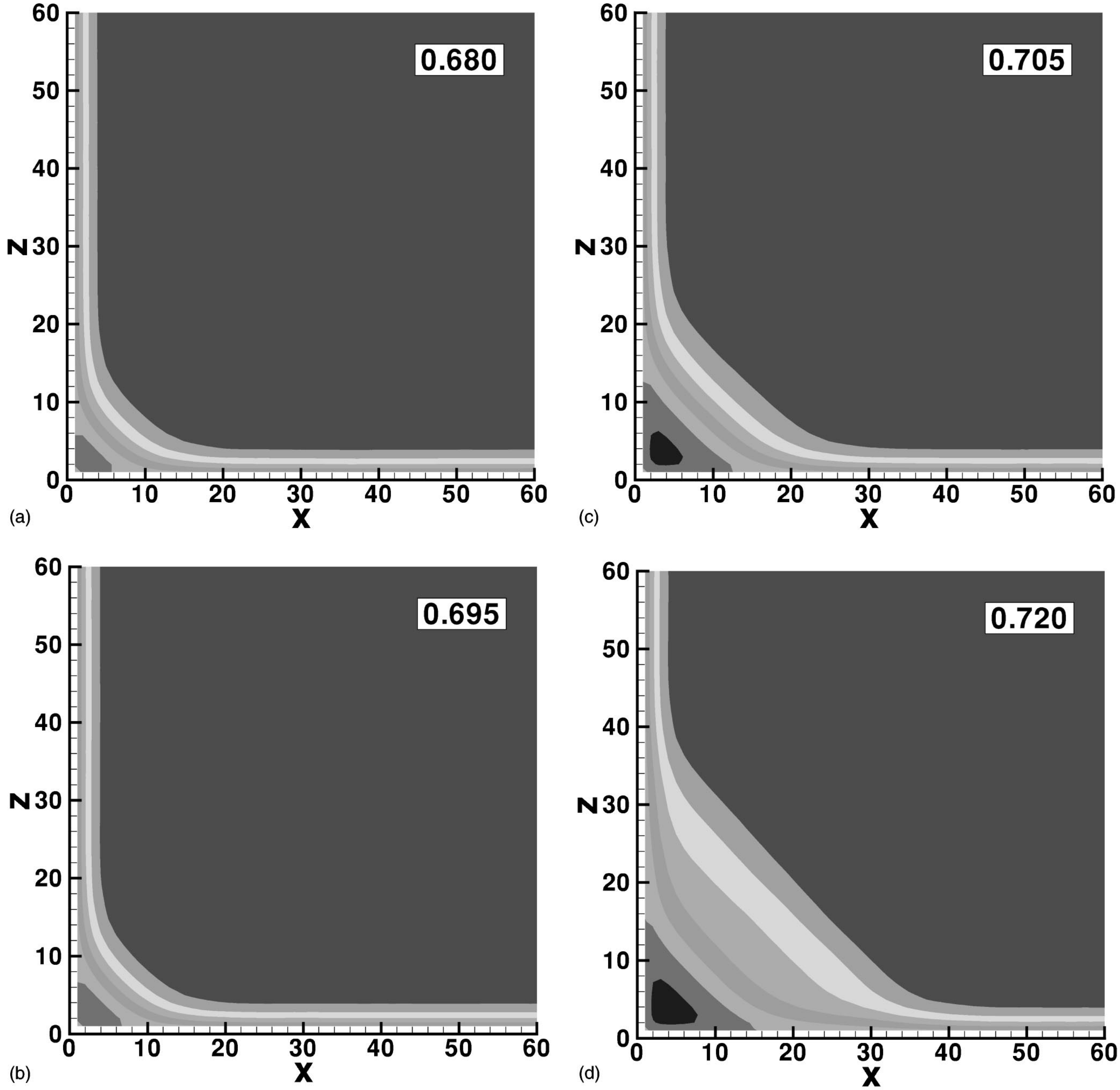

FIG. 4. Contour diagrams of the magnetization distribution in the xy plane (i.e., averaged over the y direction) of $L\times L\times L_y$ Ising lattices with $L=60$, $L_y=120$, $J_s=0.5$, $J/k_BT=0.25$, and four choices of H_s: $H_s=0.68$ (a), 0.695 (b), 0.705 (c), and 0.720 (d). Contours are shown from $m=-0.6$ to $+0.6$ in steps of 0.2. Note that the surface field is negative at the left vertical boundary and at the lower boundary of the cross sections.

tude larger values of L_y would be needed to see the system form domains of opposite magnetization along the y direction. This latter interpretation is corroborated by the finding (Fig. 8) that no longer any intersections occur when we make the cross section much smaller ($L^2=144$ rather than $L^2=1600$). In order to verify Eq. (23) more thoroughly, we have performed measurements of the correlation length of the magnetization in a plane, ξ_y^{1D} along the y direction (Fig. 9). It is seen that in the region $H_s>H_{sc}$ (where the interface runs in diagonal direction across the wedge, and the correlations along the y axis are dominated by interface fluctuations) one finds that $\ln \xi_y^{1D}\propto \mathrm{const.}\,L$, while for $H_s<H_{sc}$ (where the interface is bound in a wedge, and only after a length ξ_y^{1D} jumps over to the opposite wedge) one indeed finds that $\ln \xi_y^{1D}/L\propto L$, i.e., $\ln \xi_y^{1D}\propto L^2$, as predicted [Eq. (23)]. Of course, there is still need to understand these data in more detail; one can already see that too small wedges (such as $L=4$, 6, and 8) are not very helpful to elucidate the behavior, presumably, one must have $L\gg 2\xi_b$ before any of the phenomenological considerations of Sec. II start to make sense. This is plausible, since the constant $(4\pi\omega)^{-1}$ is of the order of 1/10 in Eq. (23).

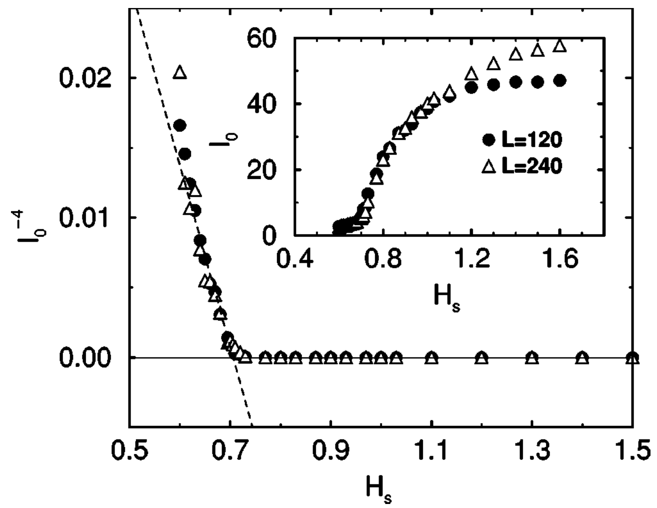

FIG. 5. Plot of the inverse fourth power of the interface distance from the wedge vs surface field strength H_s, showing a possible straight line fit to estimate $H_{sc} \approx 0.706$ from an extrapolation. The system parameters are the same as in Fig. 3, including also a second linear dimension $L = 240$. The inset shows a linear plot of ℓ_0 vs. H_s.

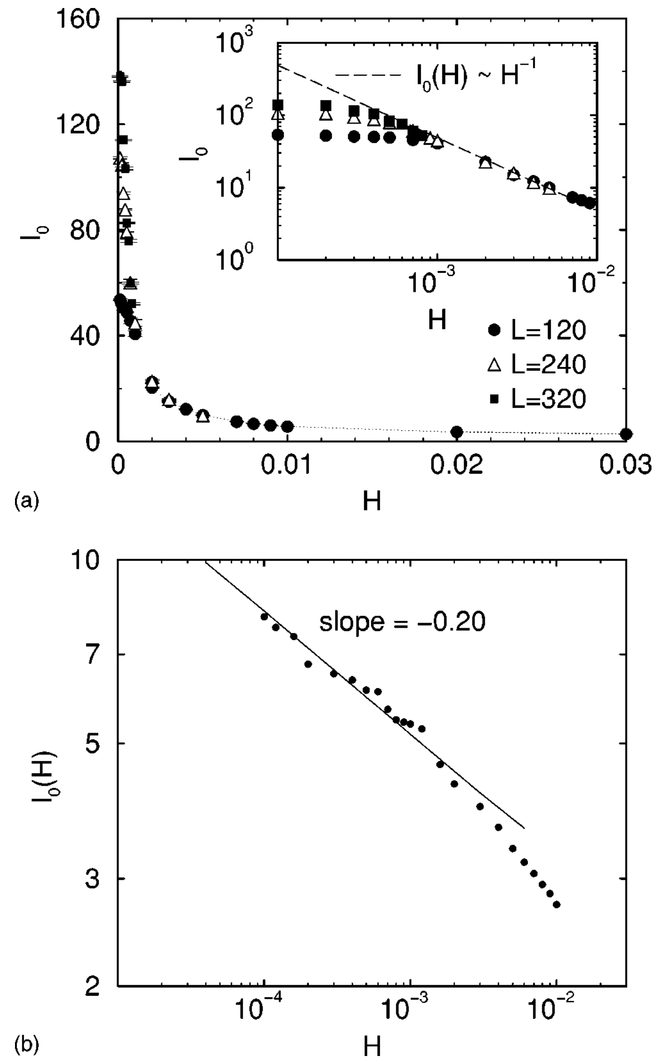

FIG. 6. (a) Interface distance ℓ_0 from the wedge plotted vs bulk field H, for $J_s = 0.5$, $J/k_BT = 0.25$, $H_s = -1.0$, $L_y = 60$, and three choices of L ($L = 120$, 240, and 320, respectively). The inset shows the same data as a log-log plot. (b) Same as (a) but for the critical field $H_{sc} = 0.72$, $L = 60$, $L_y = 80$. The broken straight line on the log-log plot indicates the theoretically predicted slope of $-1/5$.

Since the finite size effects associated with L_y clearly are important, we want to check the finite size scaling ideas of Sec. II, keeping the aspect ratio L_y/L^3 approximately constant. This means doubling L requires increasing L_y by a factor of eight! Figure 10(a) shows that again the cumulant (as well as the absolute value of the magnetization) have a rather well pronounced common intersection point at $H_{sc} \approx 0.72$, the value already found from Fig. 7 (where L_y was varied at fixed L).

Figure 10(b) presents our data for the magnetization fluctuation and the susceptibility χ, respectively. The peak height of $k_BT\chi$ in the finite system clearly scales as $L^2 L_y$, because $\langle m^2 \rangle - \langle |m| \rangle^2$ at the transition is of order unity as $L \to \infty$. The scaling of the peak width $\Gamma \propto L^{-4}$ is exactly what one expects from Eq. (27).

A particular gratifying result is seen in Fig. 11, which demonstrates that the cumulant at fixed aspect ratio L_y/L^3 has the expansion expected from Eq. (28), namely,

$$U_{L,L_y} - \tilde{\tilde{\tilde{U}}}(0, L_y/L^3) \propto t L_y^{4/3} + \cdots, \tag{37}$$

and the theoretical exponent $1/\nu_y = 4/3$ is in good agreement with our simulation data.

Figure 12 studies the probability distribution of the magnetization at our estimated value for the filling transition, $H_{sc} = 0.72$, varying again L_y at fixed aspect ratio L_y/L^3. In order to reduce the influence of the surface spins we regard the distribution of $m - m_s \equiv (M - M_s)/(L-1)^2 L_y$, where M and M_s denote the extensive magnetization of the total system and the surface. The peaks of the distribution do not move inward with increasing size, as they would do if the order parameter exponent β of the magnetization were positive [26], but rather move slightly outward. For $\beta > 0$ the peak positions of $P(m)$ would scale as $L^{-\beta/\nu}$ [26], and this is clearly not the case. Of course, m is bounded between -1 and $+1$, and so these peak positions can ultimately only settle down at constant values. Therefore, this behavior is only compatible with $\beta = 0$, since $\beta < 0$ is physically impossible. Now a first-order transition can formally also be described by $\beta = 0$, but $P(m)$ would then converge for $L \to \infty$ towards the sum of two delta functions, and this is clearly not the case here because $P(m)$ retains a nontrivial shape in the thermodynamic limit. We expect that the shape of $P(m)$ will depend on the generalized aspect ratio L_y/L^3 but we have not studied this problem. In any case, also the existence of correlation lengths and the susceptibility, which all diverge with power laws as $H_s \to H_{sc}$, suggests that this transition should be interpreted as a limiting case of a second-order transition rather than a first-order transition. This behavior corroborates our speculative remarks on the finite size scaling behavior of $P_L(m)$ in Sec. II.

A further test of scaling behavior is provided by Fig. 13,

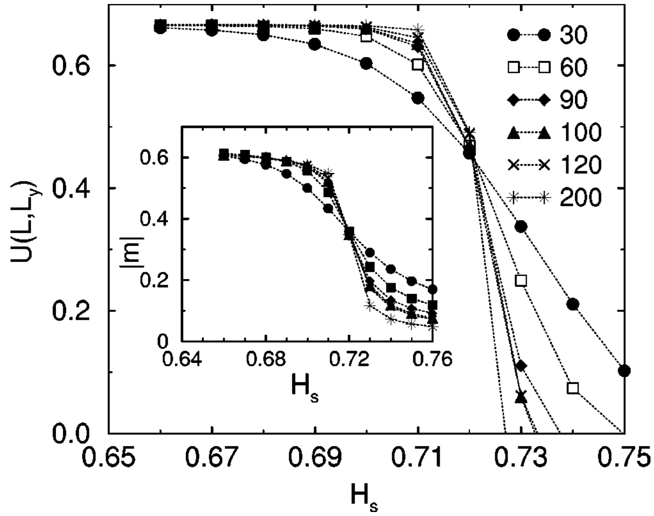

FIG. 7. Fourth-order cumulant U plotted vs H_s for $J_s=0.5$, $J/k_BT=0.25$ $H=0$, $L=40$, and several choices of L_y, as indicated in the figure. The inset shows corresponding data for the absolute value of the magnetization. The intersection of these curves suggests a transition at $H_{sc}=0.72$.

where the magnetization fluctuation is plotted versus $|H_{sc}-H_s|L_y^{1/\nu_y}$. From Eqs. (26) and (27) we predict that for fixed aspect ratio $L_y/L^{\nu_y/\nu_\perp}$ we have a behavior $\langle m^2\rangle-\langle|m|\rangle^2 =t^{-\gamma}/(L^2L_y)\tilde{f}(tL^{1/\nu_\perp}) \quad =(tL^{1/\nu_\perp})^{-\gamma}(L^{\nu_y/\nu_\perp}/L_y)f(tL^{1/\nu_\perp}) =\tilde{f}(tL^{1/\nu_\perp})$. This type of scaling behavior is strongly supported, moreover, for large $\zeta=tL^{1/\nu_\perp}$ the expected behavior $\tilde{f}(\zeta)\propto\zeta^{-\gamma}=\zeta^{-5/4}$ is seen.

Up to this point we have employed $J_s=0.5$. In this case the wetting transition on a planar substrate is of second order and the wedge filling transition is also of second order (cf. Fig. 5). In practice there are few experimental realizations of second-order wetting transitions. One important prediction of Parry *et al.* [6,7] is that the wedge filling transition may be second order even if the wetting transition on a planar substrate is of first-order. In the Ising model first order wetting transitions occur for $J_s>J_{\rm tri}$, where the tricritical wetting transition has been estimated to occur for $J_{\rm tri}\approx1.2$ [21,22]. We have studied two cases $J_s=1.3$ and $J_s=1.1$. The larger value corresponds to a first-order wetting transition, while the smaller value is still in the regime of second-order wetting for the planar semi-infinite Ising system. In Fig. 14 we plot ℓ_0 versus the surface field H_s. For $J_s=1.1$ the data give evidence for a critical filling transition. For the stronger enhancement $J_s=1.3$ of the surface interactions we find a clear cut first-order filling transition. The present data indicate that the tricritical filling transition occurs at a similar value of the surface enhancement J_s as the tricritical wetting transition. Our data do not rule out that there might still exist an interval of J_s where the wetting transition is of first order but the wedge filling transition is of second order, but our simulations indicate that this interval is small. For a more concise test of Parry's conjecture the detailed form of the interface potential has to be measured.

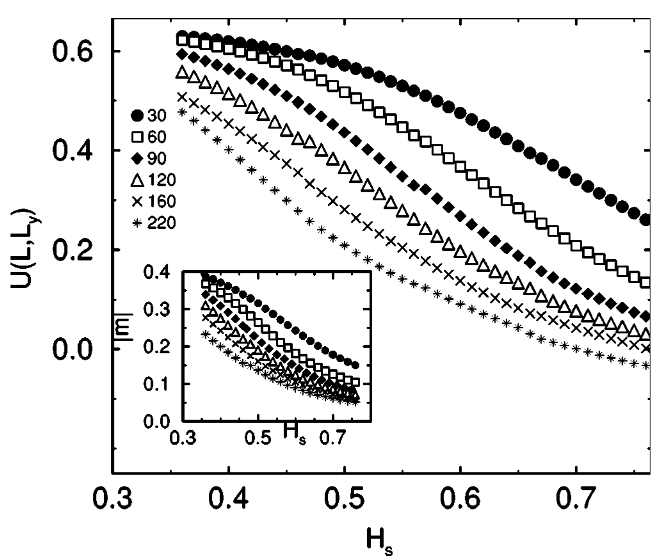

FIG. 8. Same as Fig. 7, but for $L=12$.

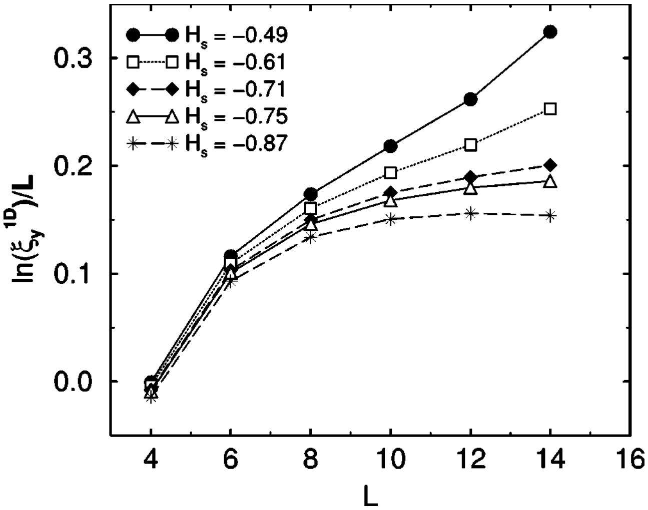

FIG. 9. Logarithm of the correlation length of the magnetization in the z direction, ξ_y^{1D}, divided by L, plotted vs L for a variety of surface fields. For these data a choice of parameters $J_s=0.5$, $J/k_BT=0.25$, and $L_y=1000$ was made.

First-order filling might give rise to a rich prefilling behavior for a finite bulk magnetic field. Prefilling of a wedge has been discussed within mean-field theory by Rejmer, Dietrich, and Napiórkowski [5], and we expect this to modify the phase behavior in a double wedge in a similar way as the prewetting behavior alters the phase diagram of an antisymmetric thin film [40].

IV. OUTLOOK

In this paper, the results of an extensive Monte Carlo study of Ising models in a double-wedge geometry were described, with the aim of testing available theoretical concepts on wedge filling transitions. We have used the same simple cubic lattice model with nearest neighbor ferromagnetic exchange and strictly short-range surface forces, which, was used successfully in previous work to probe critical and first-order wetting (which occurs for strong enough enhancement

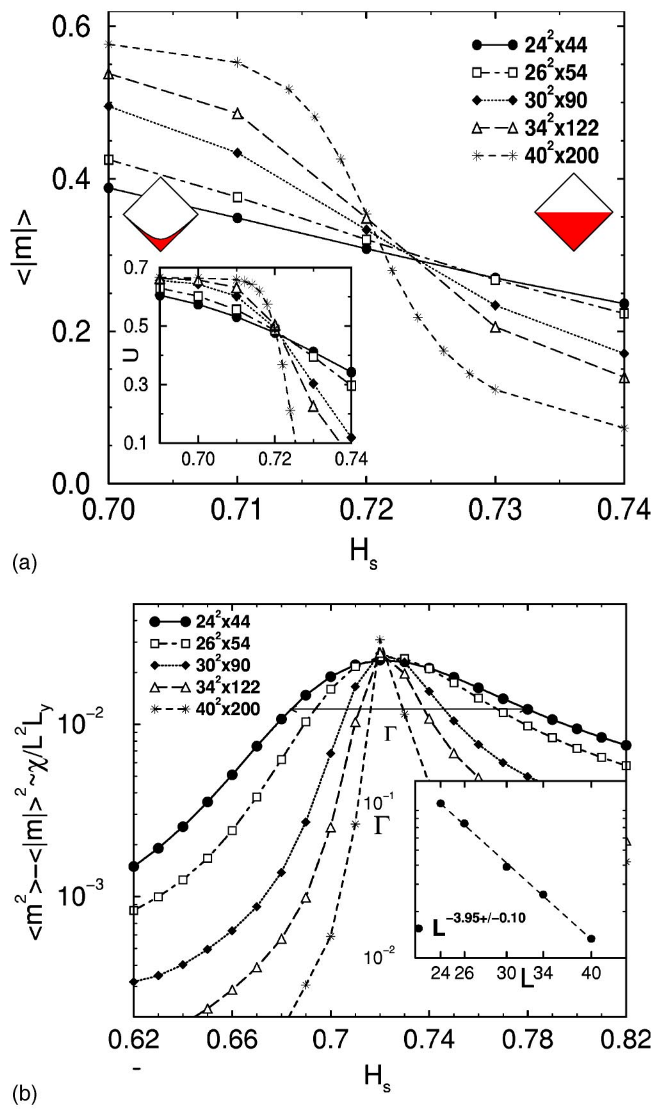

FIG. 10. (a) Magnetization and fourth-order cumulant (inset) plotted vs H_s for $J_s=0.5$, $J/k_BT=0.25$, $H=0$, and several choices of L and L_y, keeping the aspect ratio approximately constant. (b) Magnetization fluctuation $\langle m^2\rangle-\langle|m|\rangle^2$ plotted vs H_s for the same choice of parameters as panel (a). The inset shows a test of the power law for the half-width $\Gamma\propto L^{-1/\nu_\parallel}=L_y^{-4}$.

of the surface coupling J_s relative to the bulk coupling J) and for the study of interface localization transitions in thin films. Since Monte Carlo work necessarily uses lattices which have all linear dimensions finite, one must pay particular attention to finite size effects on phase transitions. We thus carefully analyzed the finite size scaling behavior of the present problem. For systems with a $L\times L\times L_y$ geometry, a very nontrivial and interesting behavior occurs in the limit $L\rightarrow\infty$, $L_y/L^{\nu_y/\nu_\perp}$ finite, where ν_y is the critical exponent of the correlation length of interface fluctuations in the y direction along the wedge, while $\nu_\perp$ is the critical exponent of the correlation length of interface fluctuations, in the direction perpendicular to the interface. The resulting behavior is analyzed in terms of a phenomenological scaling theory, and arguments are presented that the filling transition of a single

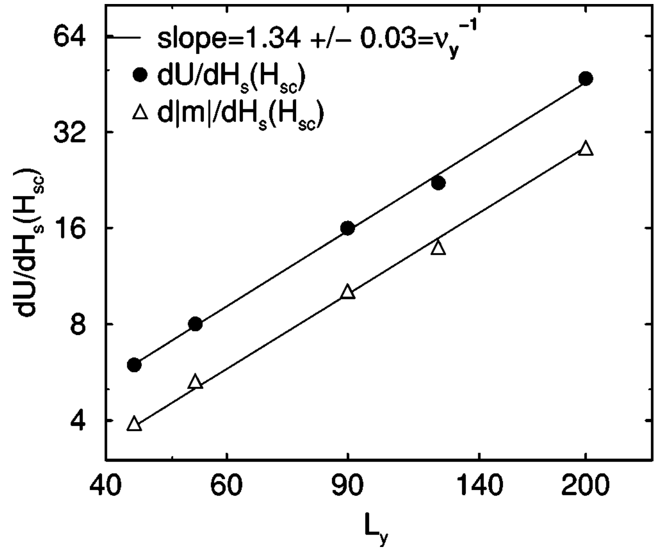

FIG. 11. Log-log plot of the slope of the cumulants and magnetizations at the intersection point vs L_y. The slope of the straight lines is $1/\nu_y=1.34\pm0.03$.

(infinite) wedge is equivalent to the interface localization transition in an (infinitely large) double wedge. For the latter case both second-order and first-order transitions have been studied (as in the case of wetting at planar surfaces, the order of the filling transition depends on J_s: for sufficient enhancement of J_s both first-order wetting and first-order filling transitions occur). If the transition is second order, the critical behavior of the double-wedge Ising model is very unusual. It is characterized by the critical exponents $\beta=0$, $\gamma=\nu_y+2\nu_\perp$. We confirm the exponents predicted by Parry *et al.* [6,7] ($\nu_y=3/4$, $\nu_\perp=1/4$) and also obtain $\gamma=5/4$, thus verifying this scaling law as well. While for critical wetting

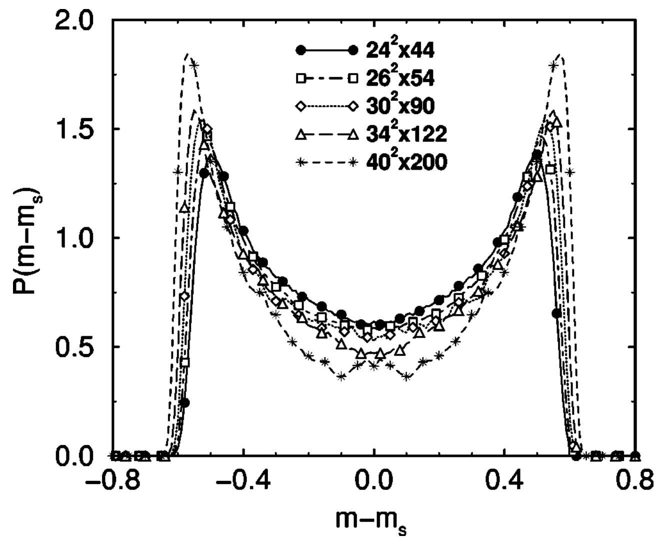

FIG. 12. Probability distribution of the difference between the magnetization M and its surface value M_s normalized per bulk spin, i.e., $m-m_s=(M-M_s)/(L-1)^2L_y$ for $J_s=0.5$, $J/k_BT=0.25$, $H=0$, $H_s=H_{sc}=0.72$, and several choices of L, L_y which approximately correspond to fixed aspect ratio L_y/L^3.

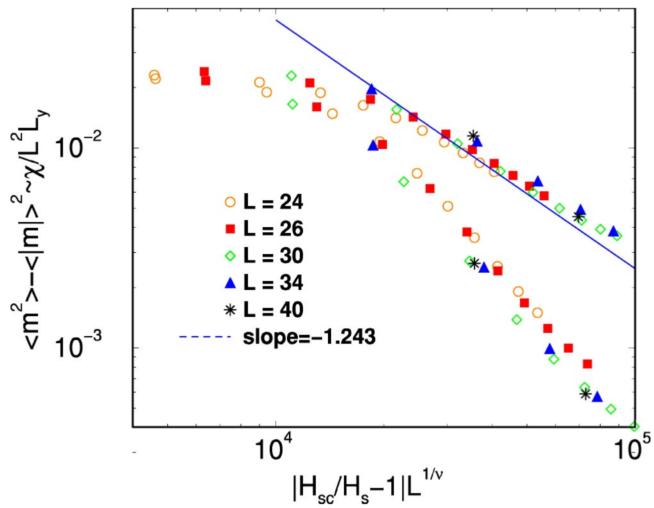

FIG. 13. Scaling plot of the magnetization fluctuation vs $|H_{sc}-H_s|L_y^{1/\nu_y}$. The broken straight line has a slope of -1.243, close to the predicted value $-\gamma=-5/4$.

at planar walls the corresponding simulations were hardly able to detect any significant deviation from mean field results, for the present problem of wedge filling the corresponding non-mean-field theory of Parry *et al.* is straightforwardly verified. We also present evidence that in the limit $L_y\to\infty$ (keeping L finite) no transition occurs, since then the double wedge behaves analogously to a one-dimensional (1D) Ising model, which has a finite correlation length at all nonzero temperatures. In the present problem, this correlation length ξ_y^{1D} describes the distance over which the interface between positively and negatively magnetized domains is bound to the lower wedge or the upper wedge, respectively. The expected scaling $\ln \xi_y^{1D}\propto L^2$ is also verified. This reduction of dimensionality of interface localization-delocalization transitions to the 1D Ising case for the geometry $L\times L\times L_y$ geometry with L finite and $L_y\to\infty$ is the analog of the 2D Ising behavior for the $L\times L_y\times L_y$ geometry with L finite and $L_y\to\infty$.

Nevertheless, these results should be viewed as only a first step: in order to address filling of fluids in real wedges, effects due to long-range forces between the adsorbed molecules and the substrate must be included. Furthermore, the use of an off-lattice model for the fluid would be desirable. While the theory of Parry *et al.* predicts that for a significant range of parameters the same critical filling behavior results, as was found for short-range surfaces, this latter prediction remains to be tested. We also could not verify yet the suggestion that wedge filling may be a second-order transition even if the corresponding wetting transition is a first-order transition: for the cases studied in the present paper, the order of the corresponding filling and wetting transitions was the same. More work on these problems is clearly desirable, as are corresponding experiments. Thus, it is encouraging that an experimental study of "complete filling" already exists [41] and yields results compatible with the theoretical expectations. Further extensions could concern wedges with asymmetry between the left and right surface (for a mean-field treatment of a single asymmetric wedge see Ref. [42]) or the low temperature behavior where wetting is replaced by layering in Ising models at temperatures below the interface roughening temperature [43]. Our phenomenological modeling of the interface in the double wedge ignored the effect of the line tension of the two contact lines of the interface and the wedge (Fig. 1), and the effect of fluctuation in the position of the contact lines [44] along the wedge in the y direction. It would we interesting to look into this problem in future work. Another intriguing problem would be to address the kinetics of wedge filling induced by changes of the external control parameters. We hope to report on such studies in the future.

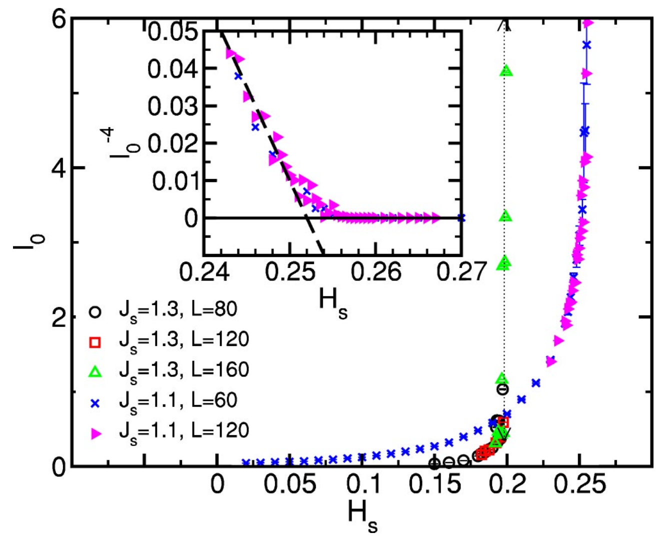

FIG. 14. Interface distance l_0 plotted vs surface field for $J_s=1.3$, $J/k_BT=0.25$, $L_y=60$, and three choices of $L=80$, 120, and 160, as indicated in the figure. The variation of ℓ with H_s for weaker coupling $J_s=1.1$ is also shown (stars and crosses). The inset replots ℓ_0^{-4} vs H for $J_s=1.1$, similar to Fig. 5. The data present evidence that the wedge filling transition is of first order for $J_s=1.3$, while it is of second order for $J_s=1.1$.

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