

Surface-induced order and disorder: Critical phenomena at first-order phase transitions (invited)

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Recent theoretical work about the influence of a surface on first-order phase transitions is reviewed. Several types of surface-induced disorder (SID) and surface-induced order (SIO) transitions are discussed. These transitions exhibit interface delocalization phenomena, long-range correlations, and critical behavior of local surface quantities. As a consequence, a variety of universal surface exponents can be defined although there are no bulk exponents. These surface exponents are calculated within Landau theory which is valid for space dimension $d > 3$, and within effective interface models for $d = 2$ and $d = 3$. An estimate of finite size effects on SID and SIO is also given. Finally, it is discussed which critical effects at SID and SIO should be most easily accessible to experiments and to computer simulations.

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I. INTRODUCTION

The theoretical work described in this paper deals with the influence of a surface on a first-order phase transition. It turns out that the surface can induce critical phenomena. Thus, *universal* surface exponents can be defined although there are no bulk exponents.¹⁻⁴

The basic physical process behind these critical effects is the following. At the surface, the number of nearest neighbors is smaller than in the bulk. As a consequence, the surface may start to disorder as the first-order transition is approached although the bulk is still in its ordered state [see Fig. 3(a)]. Thus, a layer of the disordered phase intervenes between the surface and the bulk, and the material undergoes a *surface-induced disorder* (SID) transition. SID may occur if the microscopic interaction parameters are comparable or weaker than those in the bulk. On the other hand, if the microscopic surface couplings are sufficiently stronger, the surface may begin to order as the coexistence curve is approached from the other side where the bulk is still disordered [see Fig. 3(b)]. This is a *surface-induced order* (SIO) transition.

Both at SID and at SIO, several critical effects occur: (1) *continuous depinning of the interface* between the two (almost) coexisting phases; (2) *long-range correlations* parallel to the surface; (3) *critical behavior of local surface quantities* such as the surface order parameter.

SID and SIO can occur if a disordered phase coexists with several ordered phases. A disordered phase can always be distinguished among the coexisting phases if a symmetry is spontaneously broken at the transition as e.g., (1) in magnetic materials such as metamagnets⁵ or type I antiferromagnets⁶; (2) in binary alloys⁶; (3) at a Potts-like transition^{6,7}; (4) at the freezing transition of a crystalline solid.⁸

SID and SIO are two examples of interface delocalization or depinning transitions. Similar transitions occur in fluids and binary liquid mixtures in contact with walls. In this context, they are called wetting and drying transitions. Such transitions have been investigated for semi-infinite lattice gas models,^{9,10} by van der Waals theory,¹¹ and for a Landau-Ginzburg (LG) model.^{9,12,13} This LG model is intimately related to one of the LG models used for SID.¹⁴ As a

consequence, the physically different phenomena SID and wetting can be studied within the same theoretical framework e.g., Refs. 15-17. Interface delocalization has also been discussed for the nonequilibrium phenomenon of kinetic disordering,¹⁸ and in a different geometry for ferroelectrics¹⁹ and for the Blume-Emery-Griffiths model.²⁰

This paper reviews the theory for SID and SIO as developed in Refs. 1-4, 16, and in some unpublished work. This theory consists of several steps, and I try to emphasize the systematics of these steps. The interested reader can find more details in the above references and in Refs. 25, 29, 31 to be published soon.

The paper is organized as follows. In Sec. II, continuous Landau-Ginzburg models for a scalar order parameter are motivated and defined. These are the starting points for the theoretical work described in Sec. III-IX which naturally divides into four parts: (1) Landau or mean field theory (Sec. III, IV); (2) a scaling phenomenology (Sec. V) which is obtained as a reformulation of the results of Landau theory; (3) a Ginzburg criterion (Sec. VI) which shows that Landau theory is invalidated by interface fluctuations for space dimension $d \leq 3$; (4) effective models for these interface fluctuations (Sec. VII-IX).

In Sec. X, the effects due to the finite size of a real sample are briefly discussed. These effects are important in order to predict which critical properties at SID and SIO should be most easily accessible to experiments and to computer simulations (Sec. XI).

II. LANDAU-GINZBURG MODELS

The coexistence of several thermodynamic phases at a first-order transition can be described by a Landau-Ginzburg (LG) potential f with several degenerate minima. If a symmetry is spontaneously broken, one of the minima is distinguished from the others since it corresponds to the disordered phase with a vanishing order parameter.

In general, f depends on several densities ψ_α , $\alpha = 1, 2, \dots$ which include the order parameter fields and, perhaps, some nonordering densities. Consider, for instance, a metamagnet, i.e., an Ising model with competing interactions on a simple cubic lattice in a magnetic field.⁵ There are

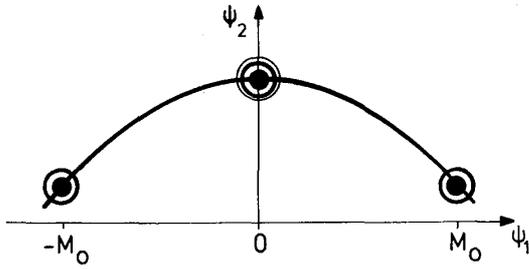


FIG. 1. Landau-Ginzburg potential $f(\psi_1, \psi_2)$ for a metamagnet on a simple cubic lattice. The minima of f are indicated by encircled dots, and the full curve indicates the trough which connects these minima.

two distinct sublattices with sublattice magnetizations m_1, m_2 . The order parameter is $\psi_1 = 1/2(m_1 - m_2)$ whereas the magnetization $\psi_2 = 1/2(m_1 + m_2)$ is a nonordering density. In the vicinity of the first-order transition, the LG potential $f(\psi_1, \psi_2)$ has three minima as shown in Fig. 1. The minima are indicated by encircled dots, and the full lines indicate the troughs of f which connect these minima. At the transition, all three minima have the same depth, and two ordered phases ($\psi_1 = \pm M_0$) coexist with the disordered phase ($\psi_1 = 0$). A more complicated example is obtained if such an Ising model is placed on a fcc lattice. This model describes type I antiferromagnets and binary alloys such as Cu_3Au .⁶

In a semi-infinite geometry, the expectation values $\bar{\psi}_\alpha \equiv \langle \psi_\alpha \rangle$ depend on the distance z from the surface. Within Landau theory, the $\bar{\psi}_\alpha$ are obtained from

$$d^2 \bar{\psi}_\alpha / dz^2 = \partial f / \partial \bar{\psi}_\alpha; \quad \alpha = 1, 2, \dots \quad (1)$$

with appropriate boundary conditions at $z = 0$ and $z = \infty$. Equation (1) is a classical equation of motion of a particle with coordinates $\bar{\psi}_\alpha$, $\alpha = 1, 2, \dots$ which moves in the potential $-f$. SID occurs if the particle starts for $z = 0$ in the vicinity of the minimum of f with vanishing order parameter (see Fig. 1), and arrives for $z \rightarrow \infty$ at one of the minima corresponding to an ordered phase. SIO occurs if the particle moves from one of the ordered phases to the disordered one.

If one wants to investigate the complete phase diagram of the physical system under consideration, one has to solve the multidimensional Eq. (1) for both the order parameter fields and the nonordering densities. In general, this has to be done numerically even for the simple two-dimensional case shown in Fig. 1. On the other hand, if one wants to study the universal aspects of SID and SIO, the multidimensional problem may be reduced to a one-dimensional one since all "particle motions" which give rise to critical effects approach asymptotically one "critical trajectory" which connects the two minima of f .²¹ This "critical trajectory" is typically quite close to the trough between the two minima. Thus, one may consider effective LG models for a scalar order parameter field ϕ which is the coordinate along this "critical trajectory".

For a semi-infinite geometry, these effective LG models have the generic form¹⁻⁴

$$F\{\phi\} = \int d^{d-1} \rho \int_0^\infty dz \{ 1/2(\nabla\phi)^2 + f(\phi) + \delta(z)f_1(\phi) \}, \quad (2)$$

z is the coordinate perpendicular to the surface at $z = 0$. The $(d - 1)$ coordinates parallel to it are denoted by $\vec{\rho}$. The bulk potential $f(\phi)$ is taken to be²²

$$f(\phi) = 1/2(\xi_d^*)^{-2} \phi^2 (1 + t - 2\phi^p + \phi^{2p}). \quad (3)$$

The disordered phase with $\phi = M_d = 0$ and the ordered phase with $\phi = M_0 > 0$ coexist for $t = 0$. ϕ has been rescaled in such a way that $M_0^* = 1$ where * means "at coexistence ($t = 0$)". Thus, t measures the distance from bulk coexistence. The correlation lengths of the disordered and the ordered phase are $\xi_d = \xi_d^*(1 + t)^{-1/2}$ and $\xi_0 = \{d^2 f(M_0) / dM_0^2\}^{-1/2}$, respectively. Equation (3) implies $\xi_d^* = \xi_0^* / p$.

For $p = 1$, Eq. (3) describes systems such as the q -state Potts model with a cubic term $\propto \phi^3$. In the case of a Potts model, t is the temperature deviation from the transition temperature T^* .^{1,2} Furthermore, this model with $p = 1$ is equivalent to the LG model studied in the context of wetting.^{9,12,13} If wetting is described in the magnetic language via the equivalence between the lattice gas and the Ising model, the variable t corresponds to the bulk magnetic field of the Ising model for temperatures below the critical temperature T_c .¹⁴ For $p = 2$, Eq. (3) is applicable to systems such as a metamagnet where odd powers of ϕ are not possible due to an underlying symmetry. In the following, p is taken to be an arbitrary positive integer.

The surface term $f_1(\phi)$ in Eq. (2) will be assumed to be

$$f_1(\phi) = -h_1 \phi + (1/2) a_1 \phi^2 - \frac{1}{p+2} b_1 \phi^{p+2} + c_1 \phi^{2p+2}. \quad (4)$$

This expression can be obtained from mean-field approximations for appropriate lattice models. In the continuum limit,^{9,11} one finds that h_1 is the difference between the symmetry breaking fields in the surface and in the bulk, and a_1 is related to the ratio of the coupling constants in the surface to those in the bulk. If the continuum limit is performed in a specific way, one obtains $b_1 = c_1 = 0$. However, finite values for b_1 and c_1 affect the phase diagram and can lead to higher-order multicritical behavior.^{2,14}

Two physically important limitations of the model (2)-(4) should be mentioned: (1) it deals with short range interactions only. Thus, long-range forces such as dipole-dipole forces in magnets, or elastic forces in binary alloys are not taken into account²³; (2) the effects due to the discreteness of the underlying lattice are not included. The lattice becomes important if the transition temperature T^* is below the roughening temperature T_R of the interface between the two coexisting phases.¹⁰ Thus, the above model should be valid for systems with $T^* > T_R$.

III. DIFFERENT TYPES OF SURFACE CRITICALITY

The type of transition which occurs in the semi-infinite system as bulk coexistence is approached depends crucially on the values for the Landau coefficients in (4). For simplicity, I will mainly discuss the case $b_1 = c_1 = 0$. The correspond-

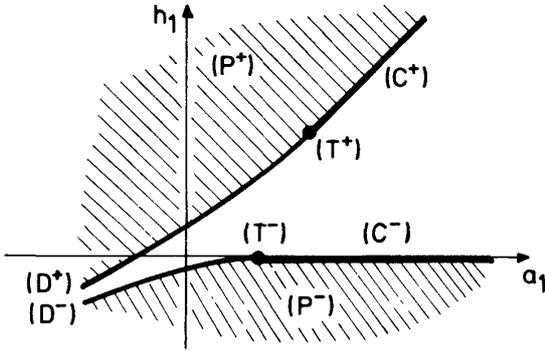


FIG. 2. Phase boundaries inside the coexistence surface ($t = 0$) SID and SIO transitions are indicated by a superscript $-$ and $+$ since they occur as the coexistence surface is approached from $t < 0$ and $t > 0$, respectively.²⁴

ing phase diagram for $t = 0$ is displayed in Fig. 2. A superscript $-$ ($+$) indicates a SID (SIO) transition corresponding to $t \rightarrow 0^-$ (0^+).²⁴ The transition (P^-) occurs for (a_1, h_1) values which belong to the lower shaded area in Fig. 2. This area is bounded by two curves: by the line of discontinuous transitions (D^-), and by the line of critical transitions (C^-). These two lines meet at the tricritical transition (T^-) with $(a_1, h_1) = (1/\xi_0^*, 0)$.

The critical phenomena at these transitions are most easily understood if one considers the order parameter profiles $M(z) = \langle \phi \rangle$. The profiles for SID are displayed in Fig. 3(a).³ At (P^-), the interface at $z = \hat{l}$ moves continuously to infinity with

$$\hat{l} = \xi_0^* \ln(1/|t|). \quad (5)$$

At (C^-) and (T^-), the local order parameter $M_1 \equiv M(z=0)$ in the surface goes continuously to zero as the interface becomes delocalized:

$$\hat{l} = \xi_0^* \ln(1/M_1), \quad (6a)$$

$$M_1 \propto |t|^{\beta_1}, \quad (6b)$$

with the surface exponent $\beta_1 = 1/2$ at (C^-) and $\beta_1 = 1/(p+2)$ at (T^-) with p from Eq. (3).¹⁻⁴ Finally, at (D^-) the SID transition is discontinuous since the interface jumps

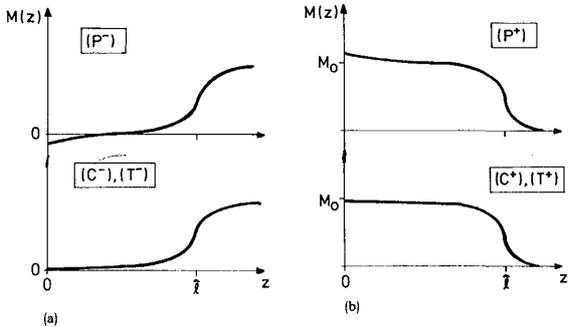


FIG. 3. Order parameter profiles $M(z)$: (a) at the SID transitions (P^-), (C^-), and (T^-); (b) at the SIO transitions (P^+), (C^+), and (T^+).^{3,24} The interface position is denoted by $z = \hat{l}$ in each case.

from a finite \hat{l} to $\hat{l} = \infty$. For $b_1, c_1 \neq 0$ in Eq. (4), one finds a line of tricritical transitions (T^-) which ends in a higher multicritical point (Q^-)²⁴ at $(h_1, a_1, b_1) = (0, 1/\xi_0^*, 1/\xi_0^*)$. At (Q^-), Eq. (6) still holds but with $\beta_1 = 1/(2p+2)$.²

Similar phenomena occur when the system undergoes one of the SIO transitions (see Fig. 2). The tricritical transition (T^+) occurs at $(a_1, h_1) = (1/\xi_0^*, 1/\xi_0^*)$ with ξ_0^* defined after Eq. (3). The order parameter profiles at SIO are shown in Fig. 3(b). At (P^+), the interface position diverges as³

$$\hat{l} = \xi_0^* \ln(1/|t|). \quad (7)$$

At (C^+) and (T^+), one finds

$$\hat{l} = \xi_0^* \ln(1/\Delta M_1), \quad (8)$$

$$\Delta M_1 \equiv M_0 - M_1 \propto t^{\beta_1},$$

with $\beta_1 = 1/2$ at (C^+) and $\beta_1 = 1/3$ at (T^+) for all p values in Eq. (3).

So far, the phase boundaries within the coexistence surface $t = 0$ have been discussed. There are additional phase boundaries for $t \neq 0$ which are attached to the coexistence surface along the discontinuous transitions (D^\pm). These extended phase diagrams are discussed in Refs. 2 and 3.

IV. GAUSSIAN FLUCTUATIONS WITH A SOFT MODE

The Gaussian fluctuations are obtained if the expression

$$\phi(\vec{\rho}, z) = M(z) + \eta(\vec{\rho}, z) \quad (9)$$

with the order parameter profile $M(z)$ from Landau theory is inserted into Eq. (2), and the resulting functional is expanded up to second order in η . As a consequence, one has to study a Schrödinger-type equation as discussed in Ref. 16. It turns out that the ground state energy E_0 goes to zero at the depinning transitions, i.e., the ground state $g_0(z)$ is a soft mode.

Upper and lower bounds for E_0 yield

$$E_0 \propto |t| \quad (10)$$

for all depinning transitions, and

$$E_0 \propto h_1^{1+1/\delta_{1,1}} \quad (11)$$

with $1/\delta_{1,1} = 1, 1/(p+1)$, and $1/(2p+1)$ at (C^-), (T^-), and (Q^-)^{25,16} For $t = 0$ and $p = 1$, the eigenvalue problem is exactly solvable.¹³

The correlation function $\langle \eta(\vec{\rho}, z_1) \eta(\vec{0}, z_2) \rangle$ has the singular part

$$\mathbf{G}(\vec{\rho}, z_1, z_2) = \rho^{-(d-3)} \Omega(\rho/\xi_{||}) g_0(z_1) g_0(z_2), \quad (12a)$$

with the correlation length

$$\xi_{||} = E_0^{-1/2}. \quad (12b)$$

$g_0(z)$ is the soft mode with energy E_0 . Equations (10) and (12b) imply $\xi_{||} \propto |t|^{-\nu_{||}}$ with $\nu_{||} = 1/2$.²

Thus, there are long-range correlations parallel to the surface. Note, however, that t enters in Eq. (12) not only through $\xi_{||}$ but also via $g_0(z)$ since

$$g_0(z=0) \propto |t|^{\psi_1}, \quad (13)$$

with $\psi_1 = 1$ at (P^\pm) and $\psi_1 = \beta_1$ otherwise.²⁵ As a consequence, the amplitude of $\mathbf{G}(\vec{\rho}, z_1, z_2)$ is decreased by a factor $|t|^{2\psi_1}$ near the surface.

V. SCALING PHENOMENOLOGY

Within Landau theory, additional power laws for many other surface quantities have been derived, and a large number of surface exponents has been defined.^{2,3} In the case of a second-order bulk transition, all power laws describing the critical surface behavior can be derived from a scaling form for the surface free energy f_s .^{26,27} This is also possible for the physical systems studied here although the bulk transition is first order.^{2,12,14}

Consider, for instance, the critical SID transition (C^-) (see Fig. 2). There are two relevant scaling fields, namely t and h_1 . The surface-free energy has the singular part²

$$f_s = |t|^{2-\alpha_s} \Omega(|t|^{-\Delta_1} h_1). \quad (14a)$$

In Landau theory, one obtains

$$f_s = |t|^{2-\alpha_s} \{ \Omega_1(|t|^{-\Delta_1} h_1) + \ln(|t|^{2-\alpha_s} |t|^{-\Delta_1} \Omega_2[|t|^{-\Delta_1} h_1]) \}, \quad (14b)$$

with $\alpha_s = 1$ and $\Delta_1 = 1/2$.^{2,3} All surface exponents can be expressed in terms of α_s and Δ_1 via scaling laws,² e.g.,

$$\beta_1 = 2 - \alpha_s - \Delta_1. \quad (15)$$

For the transitions (P^\pm), t is the only relevant scaling field. At the multicritical transitions (T^\pm) and (Q^-), there are three and four such fields, respectively.^{2,14}

Scaling relations such as Eq. (15) which do not depend on the space dimension d should hold beyond Landau theory. This can be verified for the two-dimensional interface models discussed in Sec. VIII. On the other hand, one expects that the singular part (14) of f_s is related to the correlation length $\xi_{||}$ [see Eq. (12)] by $f_s \propto \xi_{||}^{-(d-1)}$.¹⁵ This implies the hyperscaling relation $2 - \alpha_s = (d-1)\nu_{||}$ (Ref. 2) which is fulfilled in $d = 2$ since $\alpha_s = 4/3$ and $\nu_{||} = 2/3$ in this case. If the Landau exponents $\alpha_s = 1$ and $\nu_{||} = 1/2$ are inserted into this relation one obtains $d = 3$. Thus, one expects that $d_c = 3$ is the upper-critical dimension for SID and SIO. This is supported by a simple criterion below.

VI. A SIMPLE GINZBURG CRITERION

An estimate of the effect of fluctuations can be obtained when the contribution Δf_s of the Gaussian fluctuations to the surface free energy f_s is compared to the Landau approximation for this quantity. The singular part of the Gaussian contribution is¹⁶

$$\Delta f_s = (1/2) \int^A \frac{d^{d-1}k}{(2\pi)^{d-1}} \ln(k^2 + E_0), \quad (16)$$

A is an ultraviolet momentum cutoff, and E_0 is the energy of the soft mode (see Sec. IV). Equation (16) leads to

$$\Delta f_s \propto \begin{cases} E_0 \ln(1/E_0), & d = 3 \\ E_0^{(d-1)/2}, & d \neq 3. \end{cases} \quad (17)$$

It follows from Eq. (9) that $\Delta f_s \propto |t|^{(d-1)/2}$ for $d \neq 3$, and $\Delta f_s \propto |t| \ln(1/|t|)$ for $d = 3$. This should be compared with the Landau result $f_s \propto |t| \ln(1/|t|)$. Thus, Δf_s is less singular than f_s for $d > 3$, and more singular for $d < 3$. In $d = 3$, both terms are equally important. If Eq. (11) is inserted into Eq. (17), one obtains

$$\Delta f_s \propto \begin{cases} h_1^\gamma \ln(h_1), & d = 3 \\ h_1^{\gamma(d-1)/2}, & d \neq 3. \end{cases} \quad (18)$$

with $\gamma = 1 + 1/\delta_{1,1}$. The Landau result is $f_s \propto h_1^\gamma$. Again, Δf_s is less singular for $d > 3$, and more singular for $d < 3$. In this case, Δf_s dominates over f_s even for $d = 3$ due to the additional factor $\ln(h_1)$ in Eq. (18).

Thus, Landau theory should be valid for $d > 3$.¹⁶ $d_c = 3$ is rather special since the scaling dimension of t may be correctly described by Landau theory in $d = 3$ whereas the scaling dimension of h_1 is certainly changed by fluctuations. For the LG model (3) with $t = 0$ and $p = 1$, a different line of arguments for $d_c = 3$ has been given in Ref. 13.

VII. EFFECTIVE INTERFACE MODELS

The fluctuations which invalidate Landau theory for $d < 3$ are due to the soft mode $g_0(z)$ of Sec. IV. At the depinning transitions, $g_0(z) \simeq dM(z)/dz$. Thus, if one projects the fluctuation variable $\eta(\vec{\rho}, z)$ in Eq. (9) on this soft mode, one obtains

$$\phi(\vec{\rho}, z) \simeq M(z) - \zeta(\vec{\rho}) \frac{dM}{dz} \simeq M[z - \zeta(\vec{\rho})] \quad (19)$$

where $\zeta(\vec{\rho})$ is a collective coordinate.¹⁶ This indicates that the dominant fluctuations are those of the local interface position $l(\vec{\rho}) = \hat{l} + \zeta(\vec{\rho})$ where \hat{l} is the interface position as obtained from Landau theory (see Fig. 3). If Eq. (19) is inserted into Eq. (2), one obtains an effective field theory $F\{\zeta\}$. After some simplifications, one arrives at an effective model

$$F\{\zeta\} = \int d^{d-1}\rho \{ (1/2)\sigma(\nabla l)^2 + V(l) \}, \quad (20a)$$

for the local interface position $l(\vec{\rho})$. σ is the surface tension of the fluctuating interface. For the critical transition (C^-)

$$V(l) = 1/2(a_1 - 1/\xi_d^*)e^{-2y} - h_1 e^{-y} + A|t|y \quad (20b)$$

with $y = l/\xi_d^*$ and $A > 0$. At (T^-) and (Q^-), $V(l)$ contains the additional terms

$$c_1 e^{-(2p+2)y} + \frac{1}{p+2} (1/\xi_d^* - b_1) e^{-(p+2)y}.$$

Similar expressions can be derived for SIO. It is convenient to absorb a factor $\sigma^{1/2}$ in the field variable $l(\vec{\rho})$. As a consequence, the interface model depends only on

$$\tau \equiv 1/(\xi_d^* \sigma^{1/2}). \quad (21)$$

For $t = 0$ and $p = 1$, Eq. (20) has been obtained in Ref. 13 by a different approach.

The interface model (20) can be easily analyzed within Landau theory where $\langle l \rangle \equiv \hat{l}$ is determined from $\partial V/\partial l|_{\hat{l}} = 0$. It turns out that all critical properties at all SID transitions discussed in Sec. III and IV are recovered.

Note, however, that the interface position $l(\vec{\rho})$ in a semi-infinite geometry is restricted to $l > 0$. Thus, a hard wall at $l = 0$ should be added to the potential $V(l)$ in Eq. (20). In $d = 2$, such a wall does not affect the critical properties at the depinning transitions.¹⁵ In $d = 3$, the effects of a hard wall on the critical singularities are presently not known.

VIII. INTERFACE MODELS IN $d = 2$

In $d = 2$, no phase boundaries away from bulk coexistence are possible. As a consequence, the phase boundaries (D^\pm) and (T^\pm) inside the coexistence surface (see Fig. 2)

must also disappear in $d = 2$.¹⁴ Thus, a two-dimensional system can only undergo the depinning transitions (P^\pm) and (C^\pm).

The field theory (20) with $d = 2$ can be replaced by a one-dimensional eigenvalue problem via transfer matrix methods.²⁸ One has to consider a Schrödinger-type equation with the potential $V(x)$ given by Eq. (20). One finds that the coexistence surface is still given by $t = 0$ whereas the phase boundaries (C^\pm) inside this surface are shifted by the fluctuations.¹⁶ At (C^\pm), the scaling form Eq. (14a) for f_s is obtained with $\alpha_s = 4/3$ and $\Delta_1 = 1/3$. For $|t| \rightarrow 0$, $\hat{l} \propto |t|^{-1/3}$, $\xi_{\parallel} \propto |t|^{-2/3}$, and $M_1 \propto |t|^{1/3}$. In addition, the interface width $\xi_1 \equiv \langle l^2 \rangle - \langle l \rangle^2$ diverges as $\xi_1 \propto |t|^{-\nu}$ with $\nu_1 = 1/3$. Thus, the relation $\nu_1 = (3 - d)\nu_{\parallel}/2$ holds in $d = 2$.² In $d = 3$, the first-order cumulant approximation (see Sec. IX) yields $\xi_1 \propto |\ln(|t|)|^{1/2}$, and thus, $\nu_1 = 0$. For $d > 3$, $\nu_1 = 0$ from Landau theory.

IX. INTERFACE MODELS IN $d = 3$

For $d = 3$, the field theory (20) may be tackled by a cumulant expansion.²⁹ So far, only the first nontrivial term of this expansion has been investigated.¹⁵⁻¹⁷ This first term can be obtained either by a normal-ordering procedure,^{15,17} or by a variational method.¹⁶ In this first-order cumulant approximation, the scaling dimension of t in $d = 3$ is the same as in Landau theory: $\hat{l} \propto \ln(1/|t|)$ and $\xi_{\parallel} \propto |t|^{-1/2}$, i.e., $\alpha_s = 1$ and $\nu_{\parallel} = 1/2$ are recovered.¹⁶ On the other hand, the scaling dimension of h_1 is changed in a complicated way.¹⁵⁻¹⁷ Note that this difference was to be expected from the simple Ginzburg criterion of Sec. VI.

For $t = 0$, the properties of the critical and the multicritical transitions are found to depend on the variable τ given by Eq. (21) which is dimensionless in $d = 3$. Consider, for instance, the critical transition (C^-). For $t = 0$ and $\tau < \tau_c \equiv 2\sqrt{\pi}$, the interface becomes delocalized as $\hat{l} \propto \ln(1/h_1)$, and $f_s \propto h_1^{x(\tau)}$ where the exponent x depends on τ in a nonuniversal manner. For $t = 0$ and $\tau = \tau_c$, an additional phase boundary not present in Landau theory is found. Along this phase boundary, $\hat{l} \propto 1/(\tau_c - \tau)$, and f_s has an essential singularity. For $t = 0$ and $\tau > \tau_c$, the interface is delocalized even for a finite surface field h_1 .¹⁶

In a field-theoretic description, the interface width ξ_1 diverges at all depinning transitions. This should be valid if the transition temperature is above the roughening temperature. The first-order cumulant approximation yields $\xi_1 \propto [\ln(\xi_{\parallel})]^{1/2} \propto (\hat{l})^{1/2}$.

What happens if one goes beyond the first-order term in the cumulant expansion? It turns out that normal ordering is not sufficient to renormalize the effective interface models. Consider, for instance, an interaction term $\propto e^{-q\tau l}$ in $d = 3$. After normal ordering, the n th order term of the cumulant expansion is still ultraviolet divergent for $\tau^2 > 8\pi/(q^2 n)$.²⁹ Whether a field theory such as Eq. (20) is renormalizable at all in $d = 3$ beyond the first-order term has to be seen in the future.

One may estimate the validity of the first-order cumulant approximation by applying it to the field theory (20) in $d = 2$ since exact results are available in this case (Sec. VIII).

One finds that it gives the correct phase diagram qualitatively but it overestimates the divergence of \hat{l} , and underestimates the divergence of ξ_{\parallel} .²⁹

X. FINITE SIZE EFFECTS

The theoretical work described in Sec. III-IX has been concerned with a semi-infinite geometry where the thickness \hat{l} of the surface layer diverges. This cannot happen in a real, finite sample. The obvious question is: how far does the surface layer intrude into such a finite sample?

Consider a slab of linear dimension L . The semi-infinite case is recovered for $L = \infty$. The most important effect of L finite is a shift of the bulk coexistence curve from $t = 0$ to $t = t^*(L)$.³⁰ For large $L \gg \xi_d^*$, Landau theory yields^{4,31}

$$t^*(L) \propto -\sigma^*/L, \quad \text{at SID},$$

$$t^*(L) \propto +\sigma^*/L, \quad \text{at SIO}, \quad (22)$$

where σ^* is the surface tension of the interface at coexistence. Equation (22) should hold beyond Landau theory as long as σ^* is finite.^{4,31}

The shift (22) of the coexistence surface implies that the continuous behavior predicted for $L = \infty$ becomes weakly discontinuous for large but finite L . For $t \rightarrow t^*(L)$, the maximal thickness of the surface layer is $\hat{l} \propto L^{1/3}$ for $d = 2$, and $\hat{l} \propto \ln(L)$ for $d = 3$. Thus, the thickness of the surface layer is rather small in $d = 3$ even for a macroscopic sample. The maximal value of the parallel correlation length is $\xi_{\parallel} \propto L^{2/3}$ in $d = 2$, and $\xi_{\parallel} \propto L^{1/2}$ in $d = 3$. At the critical and multicritical transitions, the surface order parameter M_1 makes a small jump $\propto L^{-\beta_1}$ at $t^*(L)$.^{4,31}

XI. OUTLOOK

The theory described above is still far from complete. First of all, the critical singularities in $d = 3$ are still not known precisely (Sec. IX). While the scaling dimension of t may be correctly described by Landau theory, the scaling behavior at coexistence is changed by interface fluctuations in a complicated manner not fully understood. This seems to be the most interesting theoretical problem. Furthermore, one should investigate more realistic Landau-Ginzburg models for magnetic materials and binary alloys which include several densities (see Sec. II) in order to estimate the range of interaction parameters where SID and SIO are expected to occur.

Nevertheless, the above theory already indicates which critical effects at SID and SIO should be most easily accessible to experimental studies and to computer simulations. First, consider $d = 3$. In this case, the diverging thickness \hat{l} of the surface layer cannot be observed easily due to finite size effects (Sec. X). The divergence of the correlation length ξ_{\parallel} is not severely restricted by such effects. However, ξ_{\parallel} is contained in the singular part G of the correlation function (12) which may be difficult to detect at the surface since the amplitude of G goes to zero at the transition [see Eq. (13)]. As a consequence, the most promising quantity to look at in $d = 3$ is the local order parameter M_1 at the surface which may be experimentally investigated by LEED,³² spin polar-

ized LEED,³³ or total reflected x rays.³⁴ Indeed, the continuous behavior of M_1 predicted by Eq. (6b) may have been observed already in a LEED experiment on Cu₃Au,³² and in a Monte Carlo simulation of an Ising model for this alloy.³²

Similar computer studies on two-dimensional lattice models would also be interesting in order to investigate the critical phenomena discussed in Sec. VIII. For example, one could study the q -state Potts model on a simple cubic lattice for large q where SID and SIO have been found within a mean-field approximation.¹ Apparently, SID has also been found in a molecular dynamics study of the melting transition in a two-dimensional Lennard-Jones system.³⁵

Could SID or SIO also be observed experimentally in $d = 2$? Possible candidates are first-order transitions in monolayers of noble gases adsorbed on graphite. The substrate crystallites of such systems have a typical size $L \approx 1000 \text{ \AA}$. Consider, for instance, values for the temperature and the pressure where a two-dimensional solid can coexist with a two-dimensional liquid. As before, t measures the distance from the coexistence curve and $t > 0$ corresponds to the disordered liquid phase. Assume that the microscopic interaction parameters along the one-dimensional boundaries of the substrate crystallites are such that the liquid starts to freeze at these boundaries. In this case, the adsorbate would undergo a SIO transition: strips of the solid phase would appear along the one-dimensional boundaries as $t \rightarrow 0^+$. These strips may be modeled by a random network of rectangles where each rectangle has an approximate size L times \hat{l} . If x rays are scattered from one such rectangle, the scattering intensity around a two-dimensional reciprocal lattice vector is anisotropic: the width of this intensity is $\propto 1/L$ or $1/\hat{l}$ if the momentum transfer is parallel or perpendicular to the long edge of the rectangle which is $\propto L$. An average over the random orientation of the rectangles leads to an isotropic linewidth $\propto 1/\hat{l}$. One may also include the effect of fluctuations of the one-dimensional interface between the solid strips and the liquid in the "middle" of the substrate crystallites. These fluctuations give rise to a diffuse scattering intensity with a linewidth $\propto 1/\xi_1$.^{4,31} Since $\hat{l} \propto \xi_1 \propto t^{-1/3}$ in $d = 2$ (see Sec. VIII), the critical effects of SIO may provide an explanation for the scattering data obtained at the two-dimensional freezing transition of Xenon on graphite.^{36,4}

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¹R. Lipowsky, Z. Phys. **B 45**, 229 (1982); doctoral thesis, University of Munich, 1982 (unpublished).

²R. Lipowsky, Phys. Rev. Lett. **49**, 1575 (1982); Z. Phys. **B 51**, 165 (1983).

³R. Lipowsky and W. Speth, Phys. Rev. **B 28**, 3983 (1983).

⁴R. Lipowsky and G. Gompper, University of Munich preprint (1983).

⁵E. D. G. Cohen, in *Fundamental Problems in Statistical Mechanics*, edited by E. D. G. Cohen (North-Holland, Amsterdam, 1975), Vol. 3, p. 47.

⁶K. Binder, Phys. Rev. Lett. **45**, 811 (1980); Z. Phys. **B 45**, 61 (1981).

⁷F. Y. Wu, Rev. Mod. Phys. **54**, 235 (1982).

⁸T. V. Ramakrishnan, Phys. Rev. Lett. **48**, 541 (1982).

⁹R. Pandit and M. Wortis, Phys. Rev. **B 25**, 3226 (1982).

¹⁰R. Pandit, M. Schick, and M. Wortis, Phys. Rev. **B 26**, 5112 (1982).

¹¹References can be found in the recent review by D. M. Kroll, KFA-Jülich preprint (1984).

¹²H. Nakanishi and M. E. Fisher, Phys. Rev. Lett. **49**, 1565 (1982).

¹³E. Brezin, B. I. Halperin, and S. Leibler, J. Phys. **44**, 775 (1983).

¹⁴D. M. Kroll and R. Lipowsky, Phys. Rev. **B** (in press).

¹⁵D. M. Kroll and R. Lipowsky, Phys. Rev. **B 26**, 5289 (1982).

¹⁶R. Lipowsky, D. M. Kroll, and R. K. P. Zia, Phys. Rev. **B 27**, 4499 (1983).

¹⁷E. Brezin, B. I. Halperin, and S. Leibler, Phys. Rev. Lett. **50**, 1387 (1983).

¹⁸T. Meister and H. Müller-Krumbhaar, Phys. Rev. Lett. **51**, 1780 (1983).

¹⁹J. Lajzerowicz, Ferroelectrics **35**, 219 (1981).

²⁰W. Selke and J. Yeomans, J. Phys. **A 16**, 2789 (1983).

²¹Such "particle motions" may start for $z = 0$ far away from the two minima. In this case, the "particle" first comes close to one of the minima, changes direction, and finally moves essentially along the "critical trajectory" into the other minimum.

²²In Refs. 2 and 3, the powers of ϕ have been denoted by $x = p + 2$ and $y = 2p + 2$.

²³For $d = 2$, long-range forces are discussed in Ref. 28. For $d = 3$, mean-field theory should be valid for such forces as discussed in R. Lipowsky, University of Munich preprint (1983).

²⁴The transitions (C^-), (T^-), (Q^-), and (P^+) have been denoted by $\{0_2\}$, $\{s\}$, $\{sp\}$, and $\{E^+\}$ in Refs. 14 and 14.

²⁵R. Lipowsky (to be published).

²⁶K. Binder, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1983), Vol. 8.

²⁷H. W. Diehl, J. Appl. Phys. **53**, 7914 (1982).

²⁸D. M. Kroll and R. Lipowsky, Phys. Rev. **B 28**, 5273 (1983).

²⁹R. Lipowsky, D. M. Kroll, and R. K. P. Zia (to be published).

³⁰In the context of wetting, the qualitative features of this shift have been discussed by H. Nakanishi and M. E. Fisher, J. Chem. Phys. **78**, 3279 (1983).

³¹R. Lipowsky and G. Gompper (to be published).

³²V. S. Sundaram, B. Farrell, R. S. Alben, and W. D. Robertson, Phys. Rev. Lett. **31**, 1136 (1973); Surf. Sci. **46**, 653 (1974).

³³S. Alvarado, M. Campagna, and H. Hopster, Phys. Rev. Lett. **48**, 51 (1982).

³⁴S. Dietrich and H. Wagner, Phys. Rev. Lett. **51**, 1469 (1983).

³⁵F. F. Abraham, Rep. Prog. Phys. **45**, 1114 (1982); Fig. 26.

³⁶P. A. Heiney, R. J. Birgeneau, G. S. Brown, P. M. Horn, D. E. Moncton, and P. W. Stephens, Phys. Rev. Lett. **48**, 104 (1982).