Two-dimensional layered Ising models: Exact variational formulation and analysis

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Ising models on the plane square lattice with an *arbitrary* variation of the bond strengths, $J^{\parallel}(z)$ and $J^{\perp}(z)$, with one of the two axial coordinates, z, are considered. The total entropy is exactly represented as a functional of contributions $\varepsilon_q(z)$ to the local energy density arising from the Onsager fermions with wave vector q parallel to the layer axis, y. The resulting explicit local expression provides an effective variational principle for the free energy and energy-density profiles. In the scaling limit the problem reduces to a set of independent second-order differential equations for each $\varepsilon_q(z)$. The power of the method is demonstrated by application to an interface between two uniform but distinct regions; this includes the problem of a wall with a surface field, h_1, as a special case. Previous results for the bulk and surface exponents and for the energy-energy correlation function are easily recovered. Near criticality the method yields, in addition, universal, scaled energy-density profiles, $\varepsilon(z;T)$, which exhibit rich crossovers and *nonmonotonic* variation with z.

I. INTRODUCTION

A. Functionals for inhomogeneous systems

Continued advances in sensitive experimental techniques make it increasingly possible to measure profiles of spatially varying local densities of composition, magnetization, strain, etc. Such spatial variations generally occur near localized (quenched) defects such as walls, steps, interfaces between different phases, grain boundaries, etc. The defects can be isolated or may form patterns, either regular as, e.g., domain walls in incommensurate phases or steps at a vicinal surface, or they may be irregular, as in disordered systems. In bulk ($d=3$)-dimensional samples the defects may be compact or may be localized in lower-dimensional manifolds: films, surfaces, chains, etc. Theoretical knowledge of the profiles of the important densities allows computation of extensive thermodynamic quantities characterizing the inhomogeneity in question, such as surface (or line) specific heats and adsorptions, or interfacial tensions, etc. These in turn may be compared with data obtained from other types of experimental measurements, etc.[1]

From a general viewpoint one sees that in all these cases one is dealing with the response of a statistical mechanical system to a *strong* local perturbation. This problem is beyond the scope of the well-developed linear response theories that relate the profiles induced by *weak* external perturbations, such as periodic probing fields used in scattering experiments, to the two-point correlation functions of the unperturbed bulk system. The strong, rapidly varying perturbations provided by defects may thus be viewed as natural probes for nonlinear response and multiparticle correlations, otherwise unavailable to experimental study.

Especially interesting effects are to be expected for systems which, in the absence of the spatial inhomogeneities, would be at or close to bulk *criticality*. In these cases even a very weak perturbation by a *relevant* field[2] leads to a strong nonlinear response in the physical densities. Furthermore, in the case of *non*critical systems the finite microscopic correlation length, ξ, limits the induced perturbations to a thin, bounded shell of thickness ξ surrounding the defect, beyond which linear response theory will be valid;[3] by contrast, in critical or near-critical systems the perturbations decay slowly, via strong interactions with the sea of bulk critical fluctuations, and are essentially unbounded in extent. Indeed long-range effective interactions between defects appear via this mechanism.

We are thus led to an outstanding problem in the theory of critical phenomena, namely, to describe the response of a critical system to arbitrary *position-dependent relevant* fields. For Ising-type systems these are the ordering (or "magnetic") field $h(\mathbf{r})\equiv H(\mathbf{r})/k_BT$ and the variation in the coupling constant $J(\mathbf{r})$ as conveniently embodied in the temperaturelike field $t(\mathbf{r})=K_c-K(\mathbf{r})$ where $K(\mathbf{r})=J(\mathbf{r})/k_BT$ while K_c is the bulk critical value of K. While many interesting and significant examples of critical behavior in the presence of spatial inhomogeneities have been successfully studied in the literature[4-8] we believe that the theory still lacks an effective general formalism for this class of problems.

In this paper[9] we extend our previous discussion (see Ref. 10, hereafter referred to as I) which argued the merits of an approach based on a variational principle. An example of a widely effective variational approach is provided by the classical van der Waals–Landau–Ginzburg or local-mean-field theory.[11] Within the latter the effect of the fields $h(\mathbf{r})$ and $t(\mathbf{r})$ is considered on the basis of a free energy functional, say, $\mathcal{A}[t(\mathbf{r});m(\mathbf{r})]=\int d\mathbf{r}\mathcal{L}[t;m]$ where $m(\mathbf{r})$ is a local order parameter conjugate to the

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ordering field $h(\mathbf{r})$. The desired "grand canonical" free energy[10] $F \equiv \mathcal{F}[t(\mathbf{r}), h(\mathbf{r})]$ is given variationally via

$$F = \min_{m(\mathbf{r})} \left\{ \mathcal{A}[t(\mathbf{r}); m(\mathbf{r})] - \int d\mathbf{r}\, h(\mathbf{r}) m(\mathbf{r}) \right\} . \quad (1.1)$$

The profiles of the order parameter and of the local energy density[12] $\varepsilon(r)$ follow from

$$m(\mathbf{r}) = -\delta\mathcal{F}/\delta h(\mathbf{r}) , \quad \varepsilon(\mathbf{r}) = -\delta\mathcal{F}/\delta t(\mathbf{r}) . \quad (1.2)$$

Note that the energy density is expected to be particularly important in *symmetric* situations: for example, when h vanishes identically and t is not sufficiently negative to generate spontaneous symmetry breaking, so that m vanishes everywhere in the system. Consider superfluid helium close to but above the λ transition.[1(b),1(d)]

For the "canonical" or $(t;m)$ free-energy density, $\mathcal{L}$, the mean-field approximation gives a local expansion in powers of the order parameter and its gradients, namely,

$$\mathcal{L}(t; m, \nabla m, \ldots) = \frac{1}{2} t m^2 + \frac{1}{4!} u m^4 + \cdots + \frac{1}{2} c (\nabla m)^2 + \cdots . \quad (1.3)$$

This approach has provided invaluable insights into many important problems:[5,11] Thus it accounts for the leading scaling behavior of Ising-type systems in dimensions $d > 4$ and works well for certain other systems, like low-T_c superconductors in $d = 3$. However, the approximation (1.3) fails badly in realistic two- and three-dimensional systems near critical points having *non*classical exponents α, $\eta \neq 0$, $\nu \neq \frac{1}{2}$, etc.[2,12] Consequently there is a strong need for more adequate functionals: these should be based, if possible, on exact solutions or at least on improved approximations that encompass nonclassical exponents; if feasible the functionals should also be *local*.

Recently,[10] we have proposed that such a program might be realized by seeking "microcanonical" or entropylike functionals $\mathcal{S}[\varepsilon(\mathbf{r}), m(r)]$, in which *all* the *relevant* critical densities, i.e., those with scaling dimensions ω satisfying $\omega_m = \beta/\nu$, $\omega_\varepsilon = (1-\alpha)/\nu, \ldots < d$, should appear.[13] For Ising-like criticality only m *and* ε are required, so that, provided $\mathcal{S}(\varepsilon, m)$ is explicitly known, the basic grand canonical potential $\mathcal{F}$ is given by

$$\mathcal{F}[t, h] = \min_{\varepsilon(\mathbf{r}), m(\mathbf{r})} \left\{ \mathcal{S}[\varepsilon, m] - \int d\mathbf{r} (t\varepsilon + hm) \right\} . \quad (1.4)$$

It is clear that the inclusion of $\varepsilon(\mathbf{r})$ in the argument of the variational functional $\mathcal{S}$ in addition to the local order parameter, $m(\mathbf{r})$, normally used in the phenomenological theories, is *necessary* to render $\mathcal{S}$ local. Thus in a symmetric problem, like a neutral wall[1,5] at T slightly above T_c, the order-parameter density $m(\mathbf{r})$ vanishes identically throughout the system, while $\varepsilon(\mathbf{r})$ clearly varies and, in fact, provides singular contributions to the thermodynamic quantities.[1(b),1(d)] Second, the coupling of the energy to the square of magnetization together with the long-range correlations of energy near criticality imply effective power-law interactions $\propto z^{-\omega_\varepsilon}$, $\omega_\varepsilon = d - \lambda_t$, between local distributions of magnetization (mediated by the perturbations of the energy field). The situation is qualitatively similar to classical electrodynamics: while the Lagrangian invoking *both* the matter field and the massless electromagnetic field is local, eliminating the latter leaves one with nonlocal (Coulomb and retarded) interactions.

B. Layered Ising models

To investigate this idea further we define a class of *layered Ising models* which naturally generalize the standard d-dimensional Ising model and carry it one step towards a fully spatially inhomogeneous system: see Fig. 1. The various coupling constants depend on just one spatial coordinate, z, remaining uniform in the other $(d-1)$-directions. Formally the models are defined on a d-dimensional rectangular lattice, which for our purposes is conveniently viewed as a sequence of $(d-1)$-dimensional hypercubic sublattices or *layers* stacked along the z axis and parallel to the y hyperplane: see Fig. 1. The lattice spacings are taken as $a_\parallel$ and $a_\perp$ in and perpendicular to the layers, respectively. We let an integer index j label successive layers while the integer $(d-1)$-component vector $\mathbf{i}$ labels the sites within each layer. A standard Ising spin variable $s_{\mathbf{i},j} = \pm 1$ is assigned to each site of the lattice. Then the fully classical, reduced Hamiltonian of the model is

$$\mathcal{H}/k_B T = -\sum_j \left\{ K_j^\perp \sum_{\mathbf{i}} s_{\mathbf{i},j} s_{\mathbf{i},j+1} + K_j^\parallel \sum_{\langle \mathbf{i},\mathbf{i}' \rangle} s_{\mathbf{i},j} s_{\mathbf{i}',j} + h_j \sum_{\mathbf{i}} s_{\mathbf{i},j} \right\} , \quad (1.5)$$

where $\langle \mathbf{i},\mathbf{i}' \rangle$ denotes nearest-neighbor pairs of lattice sites in a layer.

The model is thus completely specified by the sequences (i) of the nearest-neighbor couplings within each layer or hyperplane, $\{K_j^\parallel = J_j^\parallel / k_B T\}$, (ii) of the layer-to-layer couplings $\{K_j^\perp = J_j^\perp / k_B T\}$, and (iii) of the magnetic fields $\{h_j = H_j / k_B T\}$, while the spacings $a_\perp$, $a_\parallel$ set the overall length scales. Note that due to the intrinsic an-

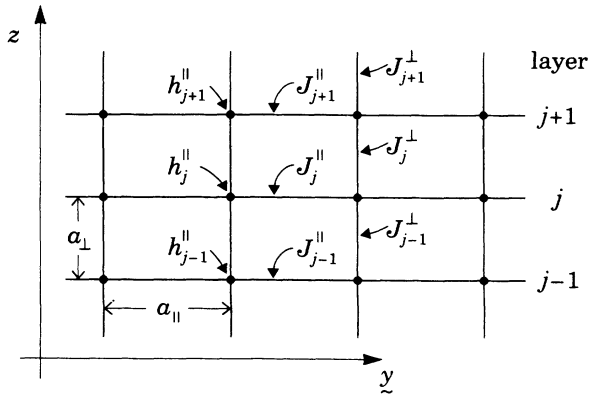

FIG. 1. A general layered Ising model with ferromagnetic couplings $J_j^\parallel (\equiv k_B T K_j^\parallel)$ and $J_j^\perp (\equiv k_B T K_j^\perp)$ parallel and perpendicular to layers labeled $j = 1, 2, 3, \ldots$, and with reduced magnetic fields h_j acting on the layer spins $s_{\mathbf{i},j}$.

isotropy of the model, in which all quantities vary in just *one* of the d directions, there is no reason to set the $K_j^{\perp}$ equal or even close to the $K_j^{\parallel}$. The impact of this anisotropy on the nature of the critical state of the model constitutes one of the problems of the theory.

The fundamental grand canonical thermodynamic potential of the model (compare with I) is

$$A_{\parallel}\mathcal{F}[K_j^{\parallel},K_j^{\perp},h_j] = -k_BT\ln\left[\sum_{s_{i,j}=\pm1}\exp\{-\mathcal{H}[s_{i,j}]/k_BT\}\right], \quad (1.6)$$

where, in the thermodynamic limit, we naturally expect the potential to be proportional to the area $A_{\parallel}$ of the layers. The basic densities per unit area in the layers then follow according to

$$\varepsilon_j^{\parallel} = -\frac{\partial\mathcal{F}}{\partial K_j^{\parallel}}, \quad \varepsilon_j^{\perp} = -\frac{\partial\mathcal{F}}{\partial K_j^{\perp}}, \quad m_j = -\frac{\partial\mathcal{F}}{\partial h_j}. \quad (1.7)$$

Again there is no *a priori* reason for not distinguishing the energies $\varepsilon_j^{\parallel}$ and $\varepsilon_j^{\perp}$ of the bonds parallel and perpendicular to the layers, respectively. Note that the index j for the perpendicular quantities, $K_j^{\perp}$ and $\varepsilon_j^{\perp}$, relates to the bonds connecting the *pair* of jth and $(j+1)$th layers: this somewhat asymmetric notation, accepted here for brevity, differs from that used in I.

The motivation for studying these layered models, apart from some technical advantages discussed below, is that they represent a number of experimentally interesting systems. A particular example shown in Fig. 2 includes (a) two boundary surfaces or "walls" with magnetic fields h_1, h_1' acting on them, (b) an interface between two regions with different values of coupling constants,

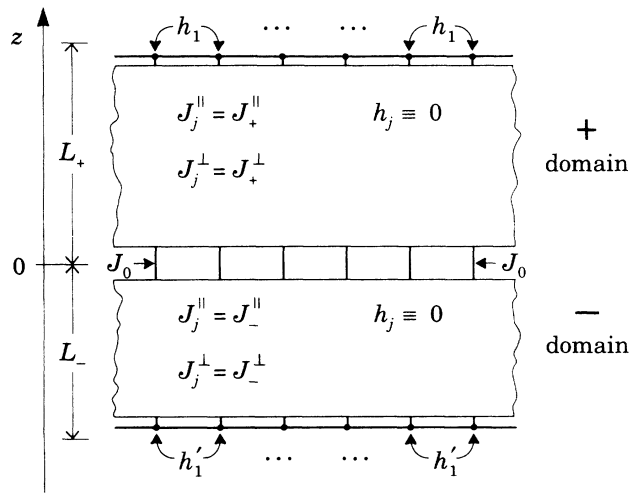

FIG. 2. A particular two-dimensional layered Ising model solvable by the methods expounded here which exhibits two boundary "walls" with (reduced) surface fields h_1 and h_1', and two uniform but, in general, differing finite domains of thicknesses L_+ and L_- with reduced couplings $K_j^{\parallel}=K_+^{\parallel}=J_+^{\parallel}/k_BT$, etc., for $j\geq 1$, and similarly for $j\leq -1$, with layers $j=+1$ and $j=-1$ coupled by interfacial or defect bonds of strength $J_0(\equiv k_BTK_0)$.

say, J_+ and J_- connected via a transition region with a coupling J_0, as well (c) as the effects of interaction between those planar structures, including the finite-thickness effects in the d-dimensional "film." We also anticipate that the rapidly advancing technologies for the preparation of *multi*layered structures[14] will soon allow detailed experiments on phase transitions in periodic, as well as random and quasiperiodic sequences of alternating layers with sharp and diffuse interfaces between them, etc.

The one-dimensional dependence of the parameters of the model allows us to reformulate the problem in the layer-to-layer transfer-matrix representation. Using the standard methods[15] we obtain

$$A_{\parallel}F/k_BT = -\ln\left[\mathrm{Tr}\left\{\prod_j \hat{T}_j\right\}\right], \quad (1.8)$$

where

$$\hat{T}_j = (2\sinh 2K_j^{\perp})^{N_{\parallel}/2}\exp\left[K_j^{\perp *}\sum_{\mathbf{i}}\hat{\sigma}_1(\mathbf{i})\right] \times\exp\left[K_i^{\parallel}\sum_{\langle \mathbf{i},\mathbf{i}'\rangle}\hat{\sigma}_3(\mathbf{i})\hat{\sigma}_3(\mathbf{i}')+h_i\sum_{\mathbf{i}}\hat{\sigma}_3(\mathbf{i})\right], \quad (1.9)$$

where the $\hat{\sigma}_p(\mathbf{i})$ $(p=1,2,3)$ are the usual Pauli matrices acting in the two-state phase space of the (now quantal) spin at each layer site $\mathbf{i}$. Note that

$$K_j^{\perp *} = -\tfrac{1}{2}\ln\tanh K_j^{\perp} \quad (1.10)$$

represents the standard definition of the dual coupling constant while $N_{\parallel}$ is the number of sites in each layer. This transfer-matrix representation forms the basis for our detailed consideration of the planar, $(d=2)$ model in zero bulk field.

Our analysis will achieve a variational formulation applicable to the full lattice problem in which the $K_j^{\parallel}$ and $K_j^{\perp}$ vary in any way whatsoever. However, since a primary interest concerns the critical phenomena we will focus more especially on the problem of finding the singular parts of the thermodynamic functions and energy profiles. Technically this will be done below in the spirit of field-theoretic renormalization,[6,16] by taking the limit of vanishing lattice spacing: $a_{\perp}, a_{\parallel}\to 0$. This is normally a singular limit and finite answers are obtained if and only if the relevant fields t and h are properly redefined according to the scalings $t \Longrightarrow a^{\omega_\varepsilon}t$, $h \Longrightarrow a^{\omega_m}h$, with the unique choice of the scaling dimensions ω_ε, ω_m. Implementation of this procedure in our lattice model is significantly simplified when the values of the parameters $K_j^{\perp}$, $K_j^{\parallel}$, h_j are everywhere sufficiently close to their critical values so as to ensure relatively large values of the various correlation lengths (in the different regions). Then all interesting physical quantities will vary slowly on the scale of the lattice spacings.

This scaling limit necessarily involves (although the converse is false) that $K_j^{\perp}$, $K_j^{\parallel}$, and h_j, regarded as functions of the coordinate $z=ja_{\perp}$, are slowly varying. Then, in the $a_{\perp}\to 0$ limit one can use

$$\hat{T}\equiv\exp[-a_{\perp}\hat{\mathcal{H}}(z)]\approx 1-a_{\perp}\hat{\mathcal{H}}(z), \quad (1.11)$$

which serves to define the *quantum* Hamiltonian $\hat{\mathcal{H}}$ of the equivalent $(d-1)$-dimensional zero-temperature quantum spin-$\frac{1}{2}$ system with coupling constants and fields depending on the imaginary "time" z. Establishing a local variational principle then reduces this quantum-mechanical problem to a classical mechanical one: instead of solving the Schrödinger equation for the N-spin wave function, one has to solve a system of differential equations for a set of local densities. Note that in the $(1+1)$-dimensional case considered below, one can equally run a transfer matrix along the y axis, thus establishing equivalence to a one-dimensional quantum spin chain with coupling parameters depending on the "spatial" coordinate z but fixed in the "time" y: compare with the discussion in Ref. 17.

A general word of caution is in order here: many physically interesting systems involve local perturbations with at least one microscopic dimension: see the surfaces and the interface or grain boundary illustrated in Fig. 2. It is then known, in particular from studies of the critical behavior at surfaces, that such abrupt perturbations usually require *additional* renormalization of the local quantities which lead to a new scaling dimensions describing local critical behavior, which have no direct connection to bulk critical exponents or properties. One may hope that the effect of such "discontinuous" perturbations will be equivalent to imposing appropriate boundary conditions on a continuum formulation.[5,6,11] However, since there is no *a priori* obviously correct recipe for formulating such boundary conditions, one really needs to have control of the problem formulated on the lattice scale, in order to properly generate the scaling limit *with* boundary conditions.

C. Inhomogeneous linear Ising chains: Recapitulation

The program outlined in Sec. I A above has already been fully realized for the simplest member of the family of layered Ising models, namely, a one-dimensional nearest-neighbor ferromagnetic Ising chain. Completely local expressions for the functional $\mathcal{S}[\varepsilon,m]$ have been obtained both in the lattice representation[18] and, in I, in the scaling limit. As the parallel dimension is absent in the $d=1$ case, the microscopic model is specified by the set of fields h_j and couplings $K_j^{\perp}\equiv K_j$ between the jth and the $(j+1)$th spins. The corresponding order parameter and energy densities may be defined as

$$m_j=\langle s_j\rangle \quad \text{and} \quad \varepsilon_j=(1-\langle s_j s_{j+1}\rangle)\ . \tag{1.12}$$

It proves convenient to add a constant to the definition of the (reduced) energy density introduced in (1.7) in order to make $\varepsilon_j=0$ for a fully ordered bond. [This is equivalent to defining the interaction part of the Hamiltonian with $(s_{ij}s_{i'j'}-1)$ replacing $s_{ij}s_{i'j'}$ in (1.5): the former definition was, in fact, accepted in I.]

The exact lattice result obtained by Percus[18] takes its most elegant form when expressed in terms of the singlet and pair-spin probabilities $\mathcal{P}_j(s_j)$ and $\mathcal{P}_{j,j+1}(s_j,s_{j+1})$: specifically one can write

$$\mathcal{S}=\sum_{s_j=\pm1}\sum_j[\mathcal{P}_{j,j+1}(s_j,s_{j+1})\ln\mathcal{P}_{j,j+1}(s_j,s_{j+1}) -\mathcal{P}_j(s_j)\ln\mathcal{P}_j(s_j)]\ , \tag{1.13}$$

where

$$\mathcal{P}_j(\pm1)=\tfrac{1}{2}(1\pm m_j)\ , \tag{1.14}$$

$$\mathcal{P}_{j,j+1}(\pm1,\pm1)=\tfrac{1}{2}-\tfrac{1}{4}\varepsilon_j\pm\tfrac{1}{4}(m_j+m_{j+1})\ , \tag{1.15}$$

$$\mathcal{P}_{j,j+1}(\pm1,\mp1)=\tfrac{1}{4}\varepsilon_j\mp\tfrac{1}{4}(m_{j+1}-m_j)\ . \tag{1.16}$$

Note that with our conventions the microcanonical potential $\mathcal{S}$ is equal to $-S/k_B$, where S is the conventional total entropy of the system; in addition the definition of ε accepted here differs from that of I by a factor of 2.

The continuum functional representation for linear Ising systems was obtained in I by working with the Schrödinger equation for the equivalent two-state quantum system. The result can be written

$$\mathcal{S}_{d=1}[\varepsilon,m]=\tfrac{1}{2}\int dz\ \varepsilon(z)\left\{-1+\ln\tfrac{1}{2}\varepsilon(z)-\tfrac{1}{2}\ln[1-m^2(z)]+\mathcal{C}\left[\frac{\dot{m}(z)}{\varepsilon(z)}\right]\right\}\ , \tag{1.17}$$

where the gradient, $\dot{m}(z)\equiv(\partial m/\partial z)$, enters through

$$\mathcal{C}(v)=\tfrac{1}{2}\ln(1-v^2)+v\tanh^{-1}v\ . \tag{1.18}$$

Here we have chosen units of length so as to preserve the definitions (1.12).

As commented above, both representations have their advantages: the lattice result (1.13) allows for treatment of arbitrarily strong and rapidly varying perturbations; but with respect to the criticality at $h_c=0$, and $T_c=0$ (or $K_c=+\infty$) the scaling result (1.17) represents the whole $(d=1)$-dimensional smoothly inhomogeneous Ising universality class, rather than just nearest-neighbor chains. Other advantages of the form (1.17) include (i) its manifest conformal covariance: see I and below; (ii) that, consequently, it yields all results automatically in scaling form; and (iii) that the evident classical Lagrangian form allows application of standard theorems of mechanics.[19] While the continuum result (1.17) was, in fact, obtained independently of (1.13), the general renormalization procedure yielding (1.17) as the appropriate scaling procedure for the lattice formulation (1.13) will be discussed in Sec. III below.

D. Outline

In this paper we derive an exact local variational principle for a two-dimensional layered Ising model in zero bulk magnetic field. The latter limitation comes as no

surprise, of course, since the corresponding homogeneous problem has not been solved. Our variational principle is then applied to a number of simple cases to obtain some novel results. More complicated applications are left for future work.

In detail the layout of the paper is as follows. Section II starts by summarizing some basic results obtained by Shankar and Murthy[20] (SM) in their studies of a random layered Ising model in $d=1+1$ dimensions. With some generalizations (and corrections) we thence find that the basic, zero-field thermodynamic potential $\mathcal{F}_{d=2}[K_j^{\parallel},K_j^{\perp},h_j\equiv 0]$ of the general two-dimensional layered Ising model decouples exactly into a sum of separate potentials for a set of virtual one-dimensional Ising chains labeled by a wave number q conjugate to the layer coordinate y. The couplings K_{qj} and fields h_{qj} of the linear chains are explicitly and locally related to the couplings $K_j^{\parallel}$, $K_j^{\perp}$ of the original planar model. This result is then combined with the exact lattice expressions for the chains, (1.13)–(1.16), to yield an explicit variational principle for the planar model in its full lattice form. The critical manifold can be expressed in general form.[4,21,22]

Obtaining the universal scaling limit of the lattice variational principle is the subject of Sec. III. We present first the result obtained just by combining the decoupling of the potential $\mathcal{F}_{d=2}$ into those for linear chains, with the continuum forms (1.4) and (1.17) of the variational principle for the individual chains. We then verify that the same result can be obtained directly by proper scaling and renormalization of the full lattice form of Sec. II when $a_{\perp}, a_{\parallel}\to 0$. An especially appealing simple continuum scaling form is obtained after noticing that the conformal covariance of the one-dimensional result can be used to absorb the anisotropy of the planar model into a rescaling of the spatial coordinates. The anisotropy thus appears to be a marginal perturbation just as in the homogeneous case.[23] At this stage one sees that the variational fields, now called $\varepsilon_q(z)$, are essentially transverse Fourier coefficients of the overall local energy density $\varepsilon(z)$ of the layered planar system. Indeed an integral over q yields $\varepsilon(z)$ directly.

Some general properties of the continuum scaling functional are discussed in Sec. IV. The methods of Lagrangian mechanics lead to nonlinear "equations of motion" for each energy-density component $\varepsilon_q(z)$ and provide an "energy" integral of motion, namely, a combination of the local energy-density components and their gradients, $\dot{\varepsilon}_q(z)=(\partial\varepsilon_q/\partial z)$, conserved whenever the temperature field $t(z)$, in other words the sequence $\{K_j^{\parallel}, K_j^{\perp}\}$, is constant. The existence of this first integral allows us to explicitly integrate the equations of motion for the important case $t(z)$ piecewise constant. A simple application of this result reproduces the thermodynamic and correlation scaling properties of the standard planar Ising model.

In the subsequent three sections the formalism is applied to the problem of a single planar structure or "defect," either bounding a homogeneous half-plane so forming a wall (Sec. VI) or separating two unlike inhomogeneous half-planes and so representing an interface or grain boundary (Sec. VII). The latter problem, which to our knowledge has not been addressed in the literature previously, seems important as a natural basis for the theory of more elaborate *multilayered* structures. The *boundary conditions* at wall/interface needed to supplement the continuum formulation, which is applicable within the individual uniform half-planes, are obtained in Sec. V. The derivation proceeds via analysis of the exact lattice representation. At the end of Sec. V we point out, however, that the final result appears to follow correctly from fairly simple *macro*scopic arguments. This is, of course, most encouraging in view of the further applications to more complicated discontinuities in $t(z)$, for which explicit expressions might not be readily available. In studying the general solution of the wall and interface problems later, we pay special attention to the energy profiles, $\varepsilon(z)$, which, as mentioned, follow naturally from the variational solutions. We show that the variation of $\varepsilon(z)$ with distance from the boundary resembles renormalization-group flow trajectories for various surface phase transitions. Indeed, the profiles $\varepsilon(z)$ exhibit rich crossovers and, in particular, nonmonotonic variation with z in accord with the flow diagrams for the corresponding surface-criticality regimes.

The paper concludes in Sec. VIII with a discussion of the results obtained and a review of perspectives for the future development of the idea of microcanonical functionals for critical systems.

II. EXACT VARIATIONAL FORMULATION

A. Decoupling of chains

In this subsection we employ the transfer-matrix representation (1.8), (1.9) which maps the zero-field $(d=2)$-dimensional layered Ising model in question onto a $(d=1)$-dimensional quantal spin chain in *discrete* time j, whose evolution operator is

$$\hat{T}_j=(2\sinh 2K_j^{\perp})^{N_{\parallel}/2}\exp\left[K_j^{\perp *}\sum_i \hat{\sigma}_1(i)\right]\times\exp\left[K_j^{\parallel}\sum_i \hat{\sigma}_3(i)\hat{\sigma}_3(i+1)\right]. \tag{2.1}$$

Note that in $d=1+1$ dimensions i is just an integer successively labeling the columns of the rectangular lattice, while j counts the layers (or rows).

We will now closely follow Shankar and Murthy[20] (SM) to show that this quantal spin chain decouples into a sequence of two-state systems evolving independently of one another, even though the parameters $K_j^{\perp}$, $K_j^{\parallel}$ depend on the "time" j. We will then map each of the quantal two-state systems onto a classical Ising chain with position-dependent ferromagnetic couplings K_j and magnetic fields h_j. This finally allows us to use the results of Percus[18] described in Sec. I C.

The derivation starts by making a transformation from the spin variables in (1.9) to two sets of Majorana fermions, $\psi_1(i)$ and $\psi_2(i)$, further decomposed into Fourier coefficients with wave numbers q $(0\le q\le\pi)$, conjugate to the y coordinate: see SM Eqs. (2.3) and (2.6). Then one observes that the coefficients defining the transformation do *not* depend on the values of the varying coupling constants $K_j^{\perp}$ and $K_j^{\parallel}$. The transformation can thus be per-

formed globally with *each* matrix $\hat{T}_j$ achieving a block-diagonal form.

Each block describes transitions within the four-state space corresponding to the pair of fermions with the given wave number q. SM then notice that both the fully occupied state with $n_{1q}=n_{2q}=1$ and the completely empty state with $n_{2q}=n_{2q}=0$ are eigenstates of the transfer matrix $\hat{T}_j$ with eigenvalues unity [apart from the simple prefactor $(2\sinh 2K_j^{\perp})^{1/2}$ which we will account for separately], again independent of the values of the constants $K_j^{\perp}$ and $K_j^{\parallel}$. One is left with a set of independently evolving two-state spaces, the only allowed transitions being the transformation of a type-1 fermion into a type-2 fermion with the same wave number, and the inverse. Any 2×2 matrix can be expressed as a linear combination of Pauli matrices and so by properly choosing the axes of the latter we can write

$$a_{\parallel}\mathcal{F}_{d=2}[K_i^{\perp},K_i^{\parallel}]=-\frac{1}{2}\sum_j \ln(2\sinh 2K_j^{\perp}) - \int_0^{\pi}\frac{dq}{2\pi}\ln\left[2+\mathrm{Tr}\left\{\prod_{j=1}^{N_{\perp}}\hat{T}_j(q)\right\}\right], \tag{2.2}$$

where $\hat{T}_j$ is essentially given by SM Eq. (2.14) as

$$\hat{T}_j(q)=\exp[2K_j^{\perp *}(\hat{\tau}_3\cos q+\hat{\tau}_1\sin q)]\exp(-2K_j^{\parallel}\hat{\tau}_3) . \tag{2.3}$$

Here $N_{\perp}$ is the number of layers in the model, i.e., the length L_z in units of $a_{\perp}$.

Note that we have completely ignored the difficulties related to the boundary conditions in the y or layer direction.[15] This is surely harmless as regards the thermodynamic limit of $\mathcal{F}_{d=2}$ taken with $N_{\parallel}\to\infty$, which is our only present concern; we leave questions related to the finite size of the layers for future work. We will also argue below that we may take $N_{\perp}\to\infty$ and still obtain the leading scaling contributions to the effects of finite size in the z direction: the trick is simply to keep the corresponding correlation length $\xi_{\perp}$ also growing so that $N_{\perp}a_{\perp}/\xi_{\perp}$ stays finite: see Sec. III. This latter limit allows us to neglect the additive term 2 in the argument of the second logarithm in (2.2).

In the homogeneous case the 2×2 blocks $\hat{T}_j(q)$ are conveniently diagonalized by application of the Bogoliubov-Valatin transformation.[15] It is easily seen, however, that the coefficients of the latter *do* depend on the couplings $K_j^{\perp}$ and $K_j^{\parallel}$. Therefore the rotations diagonalizing $\hat{T}_j(q)$ for different j generally do not commute and thus do not help in calculating the trace $\mathrm{Tr}\{\prod_j \hat{T}_j\}$.

The situation is thus quite similar to that considered in I in relation to the inhomogeneous classical Ising chain problem. Indeed, for each q the transfer-matrix product $\prod_j \hat{T}_j(q)$ turns out to be equivalent to that of a classical chain, the two states of the quantum subsystem being associated with the two states of a classical Ising spin.

To see this note first that, up to a constant factor, the product of the transfer matrices in (1.8) reduces for $d=1$ to

$$\cdots\exp(K_j^{*}\hat{\sigma}_1)\exp(h_j\hat{\sigma}_3)\exp(K_{j+1}^{*}\hat{\sigma}_1)\exp(h_{j+1}\hat{\sigma}_3)\cdots . \tag{2.4}$$

We will be able to recast $\prod_j \hat{T}_j(q)$ into the same form if one can manage to represent the first factor in (2.3) in the symmetric form

$$\exp[2K_j^{\perp *}(\hat{\tau}_3\cos q+\hat{\tau}_1\sin q)]=e^{B_j\hat{\tau}_3/2}e^{A_j\hat{\tau}_1}e^{B_j\hat{\tau}_3/2} . \tag{2.5}$$

After projecting both sides onto the four basic matrices 1, $\hat{\tau}_1,\hat{\tau}_2,\hat{\tau}_3$ it is an exercise in the algebra of the Pauli matrices to see that this relation is satisfied by the unique choice

$$A_j(q)=\sinh^{-1}[\sinh(2K_j^{\perp *})\sin q] , \tag{2.6}$$

$$B_j(q)=\tanh^{-1}[\tanh(2K_j^{\perp *})\cos q] . \tag{2.7}$$

At first sight the solution of the system of *four* scalar equations implied by (2.5) by a choice of just *two* parameters may seem miraculous. In fact it is not. Rather, the symmetric form of the right-hand side of (2.5) ensures that both sides represent a rotation around an axis in the (1,3) plane (the $\hat{\tau}_2$ component being identically zero). Thus the orientation of the axis and the amplitude of the rotation are the only two degrees of freedom to be fixed by A and B.

On combining (2.6) and (2.7) with (2.5), (2.3), and (2.4), we see that for each q the layers of the two-dimensional model are mapped onto the sites of a linear Ising chain subject to local reduced magnetic fields

$$H_{qj}=\tfrac{1}{2}B_{j-1}(q)+\tfrac{1}{2}B_j(q)-2K_j^{\parallel} =K_{j-1}^{\perp *}+K_j^{\perp *}-2K_j^{\parallel}+O(q^2) , \tag{2.8}$$

while the layer-to-layer bonds are mapped onto the bonds of the chain: the corresponding bond strengths[24] $\tau_{qj}\equiv K_{qj}=J_{qj}/k_BT$ can be conveniently defined via the fugacities

$$\zeta_{qj}=e^{-2\tau_{qj}}=\tanh K_{qj}^{*}=\tanh A_j(q) =\sinh(2K_j^{\perp *})\sin q/[1+\sinh^2(2K_j^{\perp *})\sin^2 q] =\sinh(2K_j^{\perp *})\sin q+O(q^3) . \tag{2.9}$$

The low-q behavior exhibited here and in (2.8) is of direct relevance to the continuum scaling limit discussed below in Sec. III.

B. Full lattice functional

The results of the previous subsection are summarized by the identity

$$a_{\parallel}\mathcal{F}_{d=2}[K_j^{\perp},K_j^{\parallel}]=\int_0^{\pi}\frac{dq}{2\pi}\mathcal{F}_{d=1}[K_{qj},H_{qj}]+\sum_j C_j , \tag{2.10}$$

$$C_j=-\tfrac{1}{2}k_BT\ln[2\sinh(2K_j^{\perp})\cosh^2(2K_j^{\perp *}\sin^2 q)] . \tag{2.11}$$

Here the couplings K_{qj} and the magnetic fields H_{qj} of the fictitious or virtual linear chains are given by (2.8) and

(2.9). The last sum in (2.10) accounts for various background pieces usually dropped off in the process of transformation. It is nonsingular on the critical manifold of the planar model and its precise form depends, in fact, on the background terms assumed in the planar Hamiltonian (1.5). Here we follow the conventions of SM and I and define $\mathcal{H}_{d=1}$ in a way[10,20] that makes the energy density positive definite. We will see, however, that in the limit $K_j^{\perp}\to 0$, corresponding physically to decoupling the planar model into two noninteracting half-planes, the background part provides a singular contribution $C_j \approx -\frac{1}{2}\ln K_j^{\perp}$. Accounting for these terms turns out to be essential for maintaining analyticity of the total free energy $\mathcal{F}_{d=2}$ in this limit. (See Sec. VI below.)

We now combine (2.10) with (1.4) and the lattice expression (1.13) to obtain the exact local variational functional, namely,

$$
\begin{aligned}
a_{\parallel}\mathcal{F}_{d=2}[K_j^{\perp},K_j^{\parallel};h_j\equiv 0]-\sum_j C_j
&= \min_{M_q,\mathcal{E}_{qj}} k_B T\left\{\int_0^{\pi}\frac{dq}{2\pi}\sum_j\left[-L(1+M_{qj})-L(1-M_{qj})+L(1-\tfrac{1}{2}\mathcal{E}_{qj}+\tfrac{1}{2}(M_{q,j}+M_{q,j+1}))\right.\right.\\
&\quad +L(1-\tfrac{1}{2}\mathcal{E}_{q,j}-\tfrac{1}{2}(M_{q,j}+M_{q,j+1}))+L(\tfrac{1}{2}\mathcal{E}_{q,j}+\tfrac{1}{2}(M_{q,j}-M_{q,j+1}))\\
&\quad \left.\left.+L(\tfrac{1}{2}\mathcal{E}_{q,j}+\tfrac{1}{2}(M_{q,j+1}-M_{q,j}))-H_{qj}M_{qj}+\tau_{qj}\mathcal{E}_{qj}\right]\right\}. \qquad (2.12)
\end{aligned}
$$

where $L(x)=\frac{1}{2}x\ln x$ and we have chosen M_q and $\mathcal{E}_q$ to denote the magnetization and the energy density of the virtual spin chains, just as H_q and τ_q denote the corresponding magnetic and thermal fields. Note that we use the linear-chain bond strengths $\tau_{qj}=K_{qj}\sim -t_{qj}$ as the thermal field here because for $d=1$ we have $K_c=\infty$.

For completeness we write down the variational equations following from (2.12) by differentiating the right-hand side with respect to M_{qj} and $\mathcal{E}_{qj}$, respectively. They are

$$
\begin{aligned}
&-\tanh^{-1}(M_{q,j})+\frac{1}{2}\tanh^{-1}\left[\frac{M_{q,j-1}+M_{q,j}}{2-\mathcal{E}_{q,j-1}}\right]+\frac{1}{2}\tanh^{-1}\left[\frac{M_{q,j}+M_{q,j+1}}{2-\mathcal{E}_{q,j}}\right]\\
&\qquad -\tanh^{-1}\left[\frac{M_{q,j}-M_{q,j-1}}{\mathcal{E}_{q,j-1}}\right]-\tanh^{-1}\left[\frac{M_{q,j+1}-M_{q,j}}{\mathcal{E}_{q,j}}\right]=H_{q,j}\ , \qquad (2.13)
\end{aligned}
$$

$$
\frac{\mathcal{E}_{q,j}^2-(M_{q,j+1}-M_{q,j})^2}{(2-\mathcal{E}_{q,j})^2-(M_{q,j}+M_{q,j+1})^2}=\exp(-4\tau_{q,j})=\xi_{q,j}^2\ . \qquad (2.14)
$$

The expressions (2.12)–(2.14) provide a full variational formulation for the layered planar Ising model. They are obviously local in real space since the variables $M_{q,j},\mathcal{E}_{q,j}$ are coupled only to those at nearest-neighbor sites. The price one has to pay for locality in this representation is the necessity to deal with a whole continuum of variational densities for each layer, parametrized by the wave vector q. However, the densities with different q's are completely decoupled, so one merely has to solve an independent set of equations, namely (2.13) and (2.14) for each q. This task becomes much easier if the *difference* equations (2.13) and (2.14) may be approximated by *differential* equations. Such an approximation is developed in the next section.

C. Critical manifold of the layered model

Before turning to the scaling limit we locate the critical manifold of the planar model. This is easier to achieve in the discrete representation. Following SM we notice that the only way $\mathcal{F}_{d=2}$ can become singular is via a singularity in the integrand in (2.10), i.e., via criticality in one of the $d=1$ chains. But a linear spin chain can become critical only when $K_{q,j}\equiv\infty$ (corresponding to fictitious temperature $T_{d=1}=0$). This induces a singularity at an end point of integration: $q=0$ and/or $q=\pi$. In the limit $K_j\to\infty$, the density of one-dimensional domain walls (or pairs of neighboring antiparallel spins) in a linear chain freezes out and the configurational space of the system reduces to just two states: all spins up and all spins down. The corresponding energies are clearly $E_{\uparrow}=-\sum_j H_{qj}=-E_{\downarrow}$. A singularity may occur only when the gap $E_{\uparrow}-E_{\downarrow}$ closes, i.e., in zero *total* one-dimensional magnetic field $\sum_j H_{qj}$. As our original planar model is ferromagnetic: $K^{\perp},K^{\parallel}>0$, the values of the fictitious fields $H_{q,j}$ at $q=\pi$ are by (2.7) and (2.8) negative definite: $H_{\pi,j}<0$. The singularity can thus arise only if one satisfies the formal condition

$$
\sum_j H_{0,j}=2\sum_j[K_j^{\perp *}-K_j^{\parallel}]=0\ . \qquad (2.15)
$$

In the homogeneous case this condition immediately reproduces the well-known condition of self-duality:[4,5] $K^{\perp *}=K^{\parallel}$. As a phase transition can occur only in the limit of an infinite $q=0$ chain, $N_{\perp}\to\infty$, the condition (2.15) makes sense only if the infinite sum involved there is suitably convergent; more precisely one should prob-

ably ask for convergence of its value per layer, i.e.,

$$\lim_{N_\perp\to\infty}\sum_{j=1}^{N_\perp}[K_j^{\perp *}-K_j^{\parallel}]/N_\perp=0\ . \tag{2.16}$$

Convergence in this latter case is certainly achieved for an infinite periodic system with $K_j^\perp=K_{j+p}^\perp$ and $K_j^\parallel=K_{j+p}^\parallel$ for some integer $p>0$, where the condition of criticality

$$\sum_{j=1}^{p}K_j^{\perp *}=\sum_{j=1}^{p}K_j^{\parallel}\ , \tag{2.17}$$

has been obtained by different methods some 25 years ago by Ferdinand and one of us[21] (see also Kardar and Berker[22]). The more dubious, albeit natural, extrapolation to the homogeneous random layered model solved exactly by McCoy and Wu,[4] namely,

$$\langle\langle K_j^{\perp *}\rangle\rangle=\langle\langle K_j^{\parallel}\rangle\rangle\ , \tag{2.18}$$

where $\langle\langle\ \cdots\ \rangle\rangle$ denotes an average over the distribution of the random coupling variables, seems to work as well (see SM). A ferromagnetic phase transition *does* take place at the temperature defined implicitly by (2.18). However, the existence in the random model of arbitrarily large domains of the fields H_{0j} of one sign provides additional, Griffiths-type singularities. The danger of overlooking infinitely large clusters of a single orientation of the fields $H_{0,j}$ in interpreting the criterion (2.15) is most clearly seen in the simplest case of the models consisting of two unlike half-planes studied below. There, obviously, each half-plane is self-sufficient in producing a singularity at its own value of the critical temperature. Criterion (2.15) is hardly appropriate in that case. Instead one ought to consider the sum $\sum_j H_{0,j}$ taken over each of the infinite clusters.

At any rate, the derivation of (2.15) makes it natural to anticipate that the critical properties of the system will most probably come from the $q\to 0$ part of the integral in (2.12). The corresponding low-q asymptotics is developed in the next section.

III. CONTINUUM AND SCALING LIMITS

A. Expectations

Generalizing slightly the concept of scaling and universality at critical points,[2,12,13,16] we anticipate that the universal singular part of the free energy $\mathcal{F}_{d=2}$ of *any* two-dimensional system belonging to the Ising universality class with the strength of the couplings $t(z)$ depending on only one of the two spatial coordinates z, will be correctly given by the scaling limit of the functional (2.12). In this limit one deals with coarse-grained fields $\varepsilon(z)$, $t(z)$, etc., and thus loses information about the microscopic features of the phenomena; in exchange one gains universality and, as we will see below, also a mathematical form which is much more convenient for analytical treatment.

One way of obtaining the scaling form of the variational principle for the layered $d=2$ Ising model, is to proceed directly from the transfer-matrix representation (2.3) to the scaling form obtained in I for the variational principle for each $d=1$ chain, namely (1.13). That scaling form was derived under the condition that the relevant fields, H_{qj} and $\zeta_{qj}=\exp(-2\tau_{qj})$ (in our present notation), are much less than unity for every j. This essentially means that the local correlation length $\xi_{d=1}=(H_q^2+\zeta_q^2)^{-1/2}$ is everywhere much larger than the lattice spacing $a_\perp$. Of course, once the result is obtained under these restrictions we expect it to describe correctly the *scaling part* of the free energy for a much wider class of systems in which the fields have rapidly varying components and may even violate the $H_{qj},\zeta_{qj}\ll 1$ constraint.

Recalling the correspondences (2.8) and (2.9) between the $d=1$ and $d=2$ variables, we immediately notice that the condition $\zeta_{qj}\ll 1$ is automatically satisfied in the $q\to 0$ limit. The latter is naturally required to achieve scaling: the lattice dispersion appearing in the nonlinear forms $\cos q$, $\sin q$ is clearly nonuniversal and breaks scale invariance. The interpretation in the two-dimensional system of the other constraint appearing in the chain formalism, namely, $H_{qj}\ll 1$, follows from the results of the previous subsection. In the limit $q\to 0$, one sees from (2.15) that $H_{qj}\approx H_{0j}$, and $H_{qj}\ll 1$ become the natural conditions for local proximity to the critical locus, $H_0=0$, in the uniform or homogeneous model. Indeed, as we will see in the next section, the inverse bulk correlation length of the homogeneous model is given by $\xi_b^{-1}(K^\perp,K^\parallel)=H_0(K^\perp,K^\parallel)$. The condition $H_{qj}\approx H_{0j}\ll 1$ is thus again the requirement $\xi_b(K_j^\perp,K_j^\parallel)\gg a_\perp$, for every j.

To summarize, for every layered planar Ising model satisfying (i) $K_j^{\perp *}-K_j^\parallel\ll 1$ and (ii) the natural condition that $K_j^\perp$, $K_j^\parallel$ vary slowly relative to the lattice spacing $a_\perp$, the low-q part of the variational principle (2.12) is correctly given by the scaling form

$$\mathcal{F}_{d=2}^{<}[K^\perp,K^\parallel]=\min_{M_q(z),\mathcal{E}_q(z)}\int_0^\Lambda\frac{dq}{2\pi}\mathcal{S}_{d=1}[\mathcal{E}_q(z),M_q(z)]+\int dz[\tau_q(z)\mathcal{E}_q(z)-H_q(z)M_q(z)]\ , \tag{3.1}$$

where $\mathcal{S}_{d=1}[\mathcal{E},M]$ is given by the local form (1.13) while $\tau_q(z)$ and $H_q(z)$ depend on the local values of the slowly varying couplings $K^\perp(z)$ and $K^\parallel(z)$ via the previous functional forms (2.8) and (2.9). The superscript $<$ to the symbol $\mathcal{F}$ on the left-hand side of (3.1) signifies that only the contributions of long-wavelength modes, with wave numbers q less than the cutoff $\Lambda\ll\pi/a_\perp$, have been accounted for. We expect that, apart from a fixed number of nonuniversal metric factors, the result will not be sensitive to the precise value of Λ, and thus the superscript will not be retained below.

While the above derivation of the form (3.1) from (1.13) is certainly the easiest in view of the work that has already been done in I, we present a more systematic derivation in the next subsection by formally taking the limit of the lattice spacings $a_\perp$, $a_\parallel$ approaching zero in (2.12). This is just the procedure implemented in the field-theoretic version of the renormalization group.[16,6] If the exact lattice functional (2.12) approaches a non-

trivial form in this limit, as we explicitly show that it does, then it is automatically scale invariant and so, therefore, are all the results obtained when it is used as the variational principle.

B. Renormalization and rescaling

We start by introducing a dimensional wave vector

$$q' = q/a_{\parallel} \tag{3.2}$$

and taking the limit $a_{\parallel} \to 0$. (However, the prime on q is omitted in what follows.) We obtain [see (2.8) and (2.9)]

$$H_{qj} \approx H_{0j} = K_{j-1}^{\perp *} + K_j^{\perp *} - 2K_j^{\parallel} , \tag{3.3}$$

which is independent of q, while

$$\zeta_{qj} = e^{-2\tau_{qj}} = qa_{\parallel}/\sinh(2K_j^{\perp}) . \tag{3.4}$$

Note that formally $\zeta_{qj} \to 0$ in the $a_{\parallel} \to 0$ limit, so freezing the system in the $T_{d=1} = 0$ state, unless this limit is complemented by the $a_{\perp} \to 0$ limit taken simultaneously. Before proceeding with the latter we note that the integral $\int_0^{\pi} dq/2\pi$, giving the free energy per unit *site* in the y direction, transforms into $\int_0^{\Lambda} dq/2\pi$ giving the free energy per unit *length* in the y direction (measured in units of $a_{\parallel}$). The upper cutoff $\Lambda \lesssim \pi/a_{\parallel}$ will be set equal to infinity whenever possible. The (trivial) dependence of the results on Λ in the remaining cases can be eliminated by introducing additive counterterms[16,6] in (2.12); but we will not trouble to do that here.

We now turn to the $a_{\perp} \to 0$ limit. It is convenient to transform the sum over the rows j ("sites" in the $d=1$ representation) in (2.12) into a sum over the row-to-row bonds $k = (j, j+1)$ (or nearest-neighbor bonds of the linear chains). One immediately notices that $\mathcal{E}_{qj}$ is indeed a bond variable related to the $(j, j+1)$ bond, so that $\mathcal{E}_{qk} \equiv \mathcal{E}_{qj}$, and likewise $\tau_{qk} \equiv \tau_{qj}$ while the M variables have to be rearranged according to

$$M_{q,k} = (M_{q,j} + M_{q,j+1})/2 , \quad \Delta M_{q,k} = M_{q,j+1} - M_{q,j} ,$$

and each of the row terms $L(1 \pm M_{q,j})$ has to be split between the two neighboring bonds. As a result the sum over j on the right-hand side of (2.12) transforms into

$$\sum_k [L(1 - \mathcal{E}_{qk} + M_{qk}) + L(1 - \mathcal{E}_{qk} - M_{qk}) + L(\mathcal{E}_{qk} + \tfrac{1}{2}\Delta M_{qk}) + L(\mathcal{E}_{qk} - \tfrac{1}{2}\Delta M_{qk}) - \tfrac{1}{2}L(1 + M_{qk} + \tfrac{1}{2}\Delta M_{qk}) - \tfrac{1}{2}L(1 + M_{qk} - \tfrac{1}{2}\Delta M_{qk}) - \tfrac{1}{2}L(1 - M_{qk} + \tfrac{1}{2}\Delta M_{qk}) - \tfrac{1}{2}L(1 - M_{qk} - \tfrac{1}{2}\Delta M_{qk}) + \tau_{qk}\mathcal{E}_{qk} - \tfrac{1}{2}(H_{q,j} + H_{q,j+1})M_{qk}] , \tag{3.5}$$

where we recall that $L(x) = \frac{1}{2}x \ln(x)$. The next step is to introduce the continuous coordinate $z = ka_{\perp}$, so that the sum over k approaches an integral $\int dz/a_{\perp}$ with corrections vanishing as $a_{\perp} \to 0$. In the same limit we can write $M_{qk} = M_q(z = ka_{\perp}) + O(a_{\perp}^2)$, $\Delta M_{qk} = a_{\perp}\dot{M}_q(z = ka_{\perp}) + O(a_{\perp}^2)$, etc., where $M_q(z)$ and $\mathcal{E}_q(z)$ are supposed continuous and differentiable functions of z.

The last step, as discussed before, is multiplicative renormalization: we have to multiply the densities $\mathcal{E}_q$, M_q and the conjugate fields τ_q, H_q by suitable powers of $a_{\perp}$ so that the functional (3.5) has a nontrivial $a_{\perp} \to 0$ limit. It is easily seen that a proper limit is obtained if we put

$$\mathcal{E}'_q(z) = \mathcal{E}_{qk}/a_{\perp} \quad (z = ka_{\perp}) , \tag{3.6}$$

$$H'_q(z) = H_{qk}/a_{\perp} , \tag{3.7}$$

$$\zeta'_q(z) \equiv \exp[-2\tau'_q(z)] = \zeta_{qk}/a_{\perp} , \tag{3.8}$$

leaving $M_q(z)$ dimensionless. The result, which is of course identical to (3.1), can be expressed, on dropping the primes, as

$$\mathcal{F}_{d=2}[K^{\perp}, K^{\parallel}] = \min_{M_q(z), \mathcal{E}_q(z)} \int_0^{\Lambda} \frac{dq}{2\pi} \int dz \{\tfrac{1}{2}\mathcal{E}_q(z)[-1 - \tfrac{1}{2}\ln(1 - M_q^2(z)) + \tfrac{1}{2}\ln(1 - \dot{M}_q^2/\mathcal{E}_q^2) + (\dot{M}_q/\mathcal{E}_q)\tanh^{-1}(\dot{M}_q/\mathcal{E}_q) + \ln(\mathcal{E}_q/2q)] + \mathcal{E}_q(z)\tau_{\Delta}(z) - M_q(z)H_0(z)\} , \tag{3.9}$$

where now

$$H_0(z) = 2[K^{\perp *}(z = ka_{\perp}) - K^{\parallel}(z = ka_{\perp})]/a_{\perp}$$

and we have broken the temperature field $\tau_q(z)$, defined via (3.8) and (3.4), into its dominant part $\frac{1}{2}\ln(1/q)$, which has been absorbed into the term $\ln(\mathcal{E}_q/2q)$, and a residual, position-dependent part

$$\tau_{\Delta}(z) = \tfrac{1}{2}\ln[\sinh(2K^{\perp}(z))a_{\perp}/a_{\parallel}] . \tag{3.10}$$

Note that the choice of the scaling dimensions ω determinating the powers of $a_{\perp}$ multiplying different variables in (3.6)–(3.8) is not *a priori* obvious. More precisely, one knows that (compare with Ref. 12) $\omega_M + \lambda_H = \omega_{\mathcal{E}} + \lambda_{\tau} = d' = 1$, since one has to absorb the factor $a_{\perp}^{-1}$ resulting after the transformation $\sum_k \Rightarrow \int dz/a_{\perp}$ into the prod-

ucts $\mathcal{E}_q\tau_q$ and M_qH_q. However, the way this factor must be split between the density and its conjugate field requires, essentially, calculating the scaling dimensions for the problem. The dimensions $\omega_M=0$, $\omega_{\mathcal{E}}=1$, which are of course well known for the $d=1$ Ising model,[10] can be illustrated by an appealing physical picture of a near-critical chain as consisting of large domains of the two different spin orientations. If l_+ and l_- are the characteristic sizes of the two types of domains near the point z, then $M(z)\simeq(l_+-l_-)/(l_++l_-)$ is dimensionless, while the energy is proportional to the density of the domain walls, $\mathcal{E}(z)\simeq 4/(l_++l_-)$, and thus has the dimensions of inverse length. The dimensions of the fields, $\lambda_H=1$ and $\lambda_\tau=0$ then follow automatically. Note that the rescaling (3.8) defines an *additive* renormalization, i.e., a nonuniversal shift of the temperature field τ_q, which is logarithmically dependent on $a_\perp$. Its appearance can be justified by recalling the symmetry between the fields H and ζ in the scaling limit of the $d=1$ Ising chain: see I. Otherwise this shift in τ appears to be necessary to achieve the proper $a_\perp, a_\parallel\to 0$ limit of $\mathcal{S}$ under the natural condition that the ratio $a_\perp/a_\parallel$ stays finite: see also (3.10).

Apart from the formal procedure of taking $a_\perp, a_\parallel\to 0$, the transformation from (2.12) to (3.9) also requires neglecting terms $O(a_\perp\mathcal{E}_q)$ and $O(a_\perp\dot{M}_q)$ relative to $1-|M_q|$. Using the domain picture of the linear chain criticality one can show that both inequalities

$$a_\perp\mathcal{E}_q \ll 1-|M_q| \ , \tag{3.11}$$

$$a_\perp|\dot{M}_q| \ll 1-|M_q| \ , \tag{3.12}$$

are equivalent to the natural condition that both characteristic domain sizes l_+ and l_- are much larger than the lattice spacing $a_\perp$. To see this, use again $\mathcal{E}\simeq 4/(l_++l_-)$, $1\pm M\simeq 2l_\pm/(l_++l_-)$, and note that M cannot change significantly over scales less than l_++l_-, which bounds $|\dot{M}|$ from above.

C. The incorporation of anisotropy

In this subsection we will use the conformal covariance of the one-dimensional form (1.13) (see I) to incorporate the residual position-dependent temperature field $\tau_\Delta(z)$ in (3.9) into a position-dependent rescaling of the coordinate z. The easiest way to present the transformation is by noticing that the microscopic length $a_\perp$ involved in the rescalings of the previous subsection need *not* be taken equal to the actual lattice spacing. We employ this freedom by using, instead, a z-dependent length

$$a(z)=a_\parallel/\sinh[2K^\perp(z)] \ , \tag{3.13}$$

chosen so that $\tau_\Delta(z)$ vanishes everywhere. The price one has to pay is the nontrivial dependence

$$z'(z)=\int_0^z a(\bar{z})d\bar{z}/a_\perp \ , \tag{3.14}$$

of the basic coordinate z' of the new model on the natural coordinate $z=ka_\perp$ of the original model. Correspondingly, the rescaling (3.7) then changes the field to

$$H_0(z')=H_0(z)a_\perp/a(z)\equiv 2[K^{\perp *}(z)-K^\parallel(z)]/a(z) \ , \tag{3.15}$$

where z' is related to z by (3.14). The similar rescaling of $\mathcal{E}_q$ may be omitted from (3.9), since $\mathcal{E}_q$ is just a variational field that disappears after the minimization has been performed. Since the transformations (3.14) and (3.15) are analytic whenever $K^\perp(z)$ is smooth and positive, the critical properties of all models related via (3.14) and (3.15) are equivalent to one another. It will be sufficient therefore to consider the simplest representative of each class, namely that with $\tau_\Delta\equiv 0$.

We note further that at the critical point of the isotropic homogeneous model $a_\perp=a_\parallel$ one has[4,15]

$$\sinh 2K^\perp=\sinh 2K^\parallel=\sinh 2K_c=1 \ , \tag{3.16}$$

where $K_c=\frac{1}{2}\ln(1+\sqrt{2})$. Therefore the residual field $\tau_\Delta=\frac{1}{2}\ln[\sinh(2K^\perp)a_\perp/a_\parallel]$ is negligibly weak for any layered model constructed by *microscopically* weak perturbations from isotropic criticality, i.e., with $|K_j^{\perp,\parallel}-K_c|\ll K_c$. The transformation (3.14)–(3.15) can thus be thought of as reducing the problem to that of the isotropic limit. Henceforth we will work in the vicinity of isotropic criticality unless stated otherwise. We should stress again, perhaps, that the condition $|K_j^{\perp,\parallel}-K_c|\ll 1$ is just a convenient limit eliminating irrelevant lattice effects. It does *not* imply the weakness of the perturbation from the point of view of scaling theory: owing to the scale invariance of the critical state any perturbation by the relevant field $t\propto K-K_c$ is "strong."

Note also that the "total magnetic field" $\int H_0(z)dz$ entering the condition of criticality (2.15) is invariant under the transformation (3.14)–(3.15) and so, therefore, is the critical manifold of the planar layered Ising model given by (2.15). This manifold is extended by the group of conformal transformations (3.14)–(3.15) with arbitrary $a(z)>0$, into universality classes, which are natural generalizations of the critical manifold $K^{\perp *}=K^\parallel$ of the uniform model.

D. Scaling form of the functional

Having eliminated the position dependence of the temperature field $\tau_q(z)$ in (3.1) and (3.9) we can readily perform the minimization with respect to $\varepsilon_q(z)$ which yields

$$\tfrac{1}{2}\varepsilon_q(z)=E_q(\varepsilon_q,\dot{\varepsilon}_q)\equiv[\tfrac{1}{4}\dot{\varepsilon}_q^2+q^2(1-\varepsilon_q^2)]^{1/2} \ , \tag{3.17}$$

where $M_q(z)$ has been renamed $\varepsilon_q(z)$ and remains dimensionless. Substituting this into (3.9) we obtain

$$\mathcal{F}_{d=2}[K^\perp(z),K^\parallel(z)] = \min_{\varepsilon_q(z)} k_BT\int_0^\Lambda\frac{dq}{2\pi}\int dz[\mathcal{L}_q(\varepsilon_q,\dot{\varepsilon}_q)-t(z)\varepsilon_q] \ ,$$

$$\mathcal{L}_q(\varepsilon_q,\dot{\varepsilon}_q)=-E_q(\varepsilon_q,\dot{\varepsilon}_q)+\tfrac{1}{2}\dot{\varepsilon}_q\tanh^{-1}\left[\frac{\dot{\varepsilon}_q}{2E_q}\right] \ , \tag{3.18}$$

where $t(z)$ is just a new name for the basic thermal field

$$t(z)\equiv H_0(z)=2[K^{\perp *}_{k=z/a_\perp}-K^\parallel_{k=z/a_\perp}]/a_\perp \ , \tag{3.19}$$

which carries dimensions of inverse length. The "Lagrangian density" $\mathcal{L}_q$ is measured per unit length parallel to the layers. The expressions (3.17)–(3.19) together with (3.13)–(3.15) to specify $t(z')\equiv H_0(z')$, constitute the main result of this paper.

The reason for renaming $H_0 \Longrightarrow t$, $M_q \Longrightarrow \varepsilon_q$ is clear. The results of Sec. II C show that H_0 provides a natural measure of deviation from the critical manifold in the $[K^{\perp}(z),K^{\parallel}(z)]$ functional space. In the vicinity of *isotropic criticality*, $K^{\perp}=K^{\parallel}=K_c$, $a_{\perp}=a_{\parallel}=a$, of the uniform model, the relevant direction taking the system away from criticality is along the diagonal $K^{\perp}=K^{\parallel}$, while anisotropy represents a marginal perturbation:[23] see Fig. 3. Since $\partial K^{\perp *}/\partial K^{\perp}=-1$ at $K^{\perp}=K_c$, our $t\equiv H_0=2[K^{\perp *}-K^{\parallel}]/a$ differs from the conventional $\tilde{t}=(T-T_c)/T_c$ for the case of a small overall change in the temperature T of the system, by only a constant nonuniversal factor, i.e., $t\approx 4K_c\tilde{t}/a$. Correspondingly, the energy density of the system defined as $\varepsilon(z)=-\partial\mathcal{F}/\partial t(z)$ is seen from (1.2) to be, up to a nonuniversal factor, given by

$$\varepsilon(z)=k_BT\int_0^{\Lambda}\frac{dq}{2\pi}\varepsilon_q(z)/a\ , \tag{3.20}$$

thus identifying each ε_q as the contribution to the energy density from the Majorana or Onsager fermions with wave vector q.

More precisely, we can define separate energy densities for the two types of bonds [see (1.7)]: $\varepsilon^{\perp,\parallel}(z)=-\partial\mathcal{F}/\partial K^{\perp,\parallel}(z)$. Along the relevant direction, $K^{\perp}=K^{\parallel}$, the two densities are equal, $\varepsilon^{\perp}=\varepsilon^{\parallel}=2\varepsilon(z)$, so that the total singular part of the energy density $\varepsilon^{\perp}+\varepsilon^{\parallel}$ differs from $\varepsilon(z)$ by a factor of 4. This factor will, however, differ for general anisotropic systems where its calculation must involve analysis of the transformation (3.13)–(3.15).

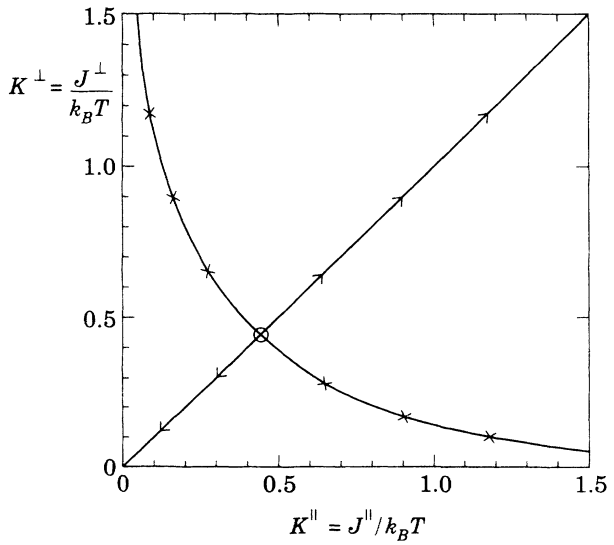

FIG. 3. Critical manifold of the homogeneous rectangular Ising model. The arrows near the isotropic critical point, $K_c^{\parallel}=K_c^{\perp}=J/k_BT_c=\frac{1}{2}\ln(1+\sqrt{2})$, indicate the relevant directions along the isotropic axis $K^{\parallel}=K_{\perp}$. The crosses on the critical locus indicate the marginal character of the anisotropy (measured by $K^{\parallel}-K^{\perp}$ near isotropy).

IV. BASIC PROPERTIES OF THE CONTINUUM FUNCTIONAL

A. Equations of motion and thermodynamics

In this section we explore the basic properties of the functional (3.18) pointing out its formal equivalence to the classical action[19] of a system of classical particles, whose one-dimensional "coordinates" ε_q evolve in "time" z. The particles do not interact with one another, but are subject to an external field $t(z)$. Note that the mean-field approximation to the free energy functional, quadratic in the spatial derivative of the order parameter density, is equivalent to the Newtonian limit of classical mechanics: the Lagrangian is $\mathcal{L}(m,\dot{m})=-U(m)+T(\dot{m})$, while the "kinetic energy" is $T(\dot{m})\propto\dot{m}^2$. This analogy has been extensively explored previously.[11] Here we see that the nonclassical statistical mechanics of the planar layered Ising model leads to a non-Newtonian form of the Lagrangians $\mathcal{L}_q$ in (3.18). We can still apply, however, the general theorems and ideas of Lagrangian mechanics.

The canonical momenta p_q conjugate to the coordinates ε_q are given by

$$\begin{aligned}p_q&=\partial\mathcal{L}_q/\partial\dot{\varepsilon}_q=\tfrac{1}{2}\tanh^{-1}[\dot{\varepsilon}_q/2E_q(\varepsilon_q,\dot{\varepsilon}_q)]\\&=\tfrac{1}{2}\sinh^{-1}[\dot{\varepsilon}_q/2q(1-\varepsilon_q^2)^{1/2}]\ .\end{aligned} \tag{4.1}$$

The classical energy in the absence of the field t, namely,

$$\begin{aligned}E_q(\varepsilon_q,\dot{\varepsilon}_q)&=p_q(\varepsilon_q,\dot{\varepsilon}_q)\dot{\varepsilon}_q-\mathcal{L}_q(\varepsilon_q,\dot{\varepsilon}_q)\\&=[\tfrac{1}{4}\dot{\varepsilon}_q^2+q^2(1-\varepsilon_q^2)]^{1/2}\ ,\end{aligned} \tag{4.2}$$

appears then equal to E_q as defined in (3.17). We note in passing that the canonical Hamiltonian of each of the q particles has the rather elegant form

$$\mathcal{H}_q(\varepsilon_q,p_q)=q(1-\varepsilon_q^2)^{1/2}\cosh(2p_q)\ , \tag{4.3}$$

but we will not use this here.

The variational equations of motion given by the standard Euler-Lagrange formula[19]

$$-\frac{d}{dz}\frac{\partial\mathcal{L}_q}{\partial\dot{\varepsilon}_q}+\frac{\partial\mathcal{L}_q}{\partial\varepsilon_q}=t(z)\ , \tag{4.4}$$

are found to be

$$\tfrac{1}{4}\ddot{\varepsilon}_q-q^2\varepsilon_q=-E_q(\varepsilon_q,\dot{\varepsilon}_q)t(z)\ . \tag{4.5}$$

However, instead of directly taking the derivatives entailed in (4.4), these equations of motion can be more easily obtained from the equations

$$\frac{d}{dz}E_q=-\dot{\varepsilon}_qt(z)\ , \tag{4.6}$$

describing the dissipative balance of energy in the mechanical analogy: the product "velocity" times "force" on the right-hand side expresses the dissipation of the energy E_q.

The set of equations (4.5) constitute the main result of this subsection. If a solution, say $\varepsilon_{q0}(z)$, is available for every q then the energy-density profiles $\varepsilon(z)$ are obtained via a single integration over the wave numbers q: see (3.20). The basic thermodynamic potential $\mathcal{F}[t]$ is given by substituting $\varepsilon_{q0}(z)$ into the right-hand side of (3.18). The latter can be simplified by integrating the second term in (3.19) by parts and using the equations of motion (4.5) satisfied by $\varepsilon_{q0}(z)$. After a few cancellations the result takes the simpler form

$$\mathcal{F}[t(z)]=-\int_0^{\Lambda}\frac{dq}{2\pi}\int dz\frac{E_q(\varepsilon_{q0},\dot{\varepsilon}_{q0})}{1-\varepsilon_{q0}^2(z)}\ , \tag{4.7}$$

provided the spatial derivatives $\partial\varepsilon_{q0}/\partial z$ vanish at the boundaries of the system, as they will do in the case of an infinite system with a localized perturbation $t(z)$. Otherwise, for a system confined between two boundaries, $L_-<z<L_+$, one must add the extra boundary contribution

$$\mathcal{F}_s=\tfrac{1}{2}\varepsilon_{q0}(L_+)\tanh^{-1}[\tfrac{1}{2}\dot{\varepsilon}_{q0}(L_+)/E_q] -\tfrac{1}{2}\varepsilon_{q0}(L_-)\tanh^{-1}[\tfrac{1}{2}\dot{\varepsilon}_{q0}(L_-)/E_q]\ . \tag{4.8}$$

Note that as the conditions used in deriving the scaling form of the functional (3.18) are almost certainly violated at sharp boundaries, there are in general further boundary contributions to $\mathcal{F}$ beyond the $\mathcal{F}_s$ given here. These will be considered in Sec. V.

One should perhaps also stress that the simplified expression (4.7) for the free energy $\mathcal{F}$ using the components ε_{q0} of the energy density by no means replaces the original form (3.18): it is useful *only* provided one has already solved the variational equations (4.5) following from the variation of the latter.

B. Uniform systems

The equations of motion (4.5) can be explicitly solved in the important case of a locally homogeneous system, $t(z)=$const. In this case (4.6) immediately gives an integral of motion

$$[q^2(1-\varepsilon_q^2)+\tfrac{1}{4}\dot{\varepsilon}_q^2]^{1/2}+t\varepsilon_q=I_q\ , \tag{4.9}$$

for each q. Note that one always has to choose the positive branch of the square root here since [see (3.17)] $E_q=\frac{1}{2}\mathcal{E}_q$ is equal to the density of domain walls in the corresponding one-dimensional chain and thus must be positive. Remembering that, we may transfer $t\varepsilon_q$ to the right-hand side and square both sides arriving at a quadratic form in ε_q and $\dot{\varepsilon}_q$. After a shift to the variables

$$x_q=\varepsilon_q-I_q t/(t^2+q^2)\ , \tag{4.10}$$

this reduces to

$$[\dot{x}_q/2\tilde{\kappa}(q)]^2-x_q^2=[I_q^2/\tilde{\kappa}^2(q)-1]q^2/\tilde{\kappa}^2(q)\equiv A_q\ , \tag{4.11}$$

where we have introduced the inverse length scales

$$\tilde{\kappa}(q)=\sqrt{t^2+q^2}\ . \tag{4.12}$$

Equations (4.11) describe hyperbolas in the $(x_q,\dot{x}_q)$ phase plane corresponding to the unstable evolution of a Newtonian particle of mass $\frac{1}{2}\tilde{\kappa}^{-2}$ with coordinate x_q in the potential $U(x_q)=-x_q^2$. The complete set of solutions is given by

$$x_q(z)=\pm A_q^{1/2}\sinh[2\tilde{\kappa}(q)(z-z_0)]\ ,\quad \text{if } |I_q|>\tilde{\kappa}(q)\ ,$$

$$=\pm|A_q|^{1/2}\cosh[2\tilde{\kappa}(q)(z-z_0)]\ ,\quad \text{if } |I_q|<\tilde{\kappa}(q)\ , \tag{4.13}$$

$$=C_q\exp[\pm 2\tilde{\kappa}(q)z]\ ,\quad \text{if } |I_q|=\tilde{\kappa}(q)\ . \tag{4.14}$$

Evidently the second integration entails an arbitrary choice z_0 of the origin of z. In the case of the separatrix solutions $e^{\pm 2\tilde{\kappa}z}$, one arbitrary constant C_q accounts for both the choice of origin and for the overall amplitude and sign.

When shifting the variables back from x_q to $\varepsilon_q=x_q+I_q t/(t^2+q^2)$ one must notice that since (4.11) involves only I_q^2, each solution corresponds to two values of I_q differing in sign. The shift splits each function (4.13)–(4.14) into two, so the set of solutions is overcomplete. This degeneracy goes back, of course, to the two choices of the sign of the square root in (4.9): indeed, it is removed by invoking the inequality

$$I_q-t\varepsilon_q>0\ , \tag{4.15}$$

as discussed above. The picture is simplified further by recalling that the variables ε_q are equal to the magnetizations M_q of the virtual linear chains and thus are restricted by

$$|\varepsilon_q|<1\ . \tag{4.16}$$

The $(\varepsilon_q,\dot{\varepsilon}_q)$ phase plane in this domain, Fig. 4, is divided into four different regions by the straight separatrix lines, $|\dot{\varepsilon}_q|/2\tilde{\kappa}=|\varepsilon_q-t/\tilde{\kappa}(q)|$, corresponding to $I_q=1$ and the solutions

$$\varepsilon_q=C_q\exp[\pm 2\tilde{\kappa}(q)z]+t/\tilde{\kappa}(q)\ . \tag{4.17}$$

In the domains I and III, where $|\dot{\varepsilon}_q|/2\tilde{\kappa}(q)>|\varepsilon_q-t/\tilde{\kappa}(q)|$, the constant I_q exceeds unity

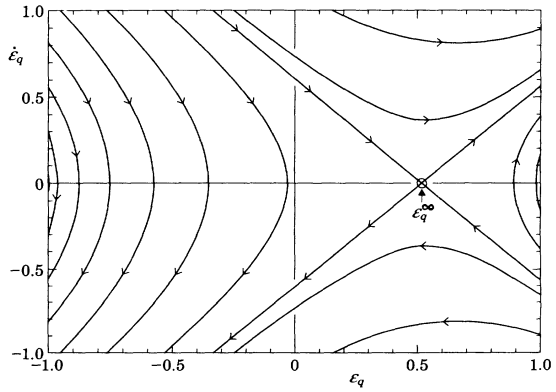

FIG. 4. Flows in the phase plane $(\varepsilon_q,\dot{\varepsilon}_q)$ generated by Eq. (4.5) for constant $t=0.3$ and $q=0.5$. There is only one fixed point at ε_q^{∞}: the separatrices flowing to and from this are described by Eqs. (4.17) and (4.28).

and is conveniently parametrized by an imaginary angle ψ_q via $I_q=\tilde{\kappa}(q)\cosh\psi_q$. The complete set of solutions in these domains is then given by

$$\varepsilon_q=(\sinh\psi_q)[q/\tilde{\kappa}(q)]\sinh[2\tilde{\kappa}(q)(z-z_0)] +(\cosh\psi_q)t/\tilde{\kappa}(q)\ , \tag{4.18}$$

with ψ_q spanning the whole real axis. (Note that $\psi_q\gtrless 0$ corresponds to the domains I and III, respectively; see Fig. 4). In the domains II and IV one has $|\dot{\varepsilon}_q|/2\tilde{\kappa}(q)<|\varepsilon_q-t/\tilde{\kappa}(q)|$ and a convenient representation is then $I_q=\tilde{\kappa}(q)\cos\theta_q$ so that the complete set of solutions is

$$\varepsilon_q=(\sin\theta_q)[q/\tilde{\kappa}(q)]\cosh[2\tilde{\kappa}(q)(z-z_0)] +(\cos\theta_q)t/\tilde{\kappa}(q)\ , \tag{4.19}$$

with θ_q spanning the interval

$$-\tfrac{1}{2}\pi-\tan^{-1}(t/q)<\theta_q<\tfrac{1}{2}\pi-\tan^{-1}(t/q)$$

(while $\theta_q\gtrless 0$ corresponds to domains II and IV, respectively).

Equations (4.17)–(4.19) represent the complete general solution to the equations of motion (4.5) for constant $t(z)$. In order to use (4.7) for free energy calculations we present corresponding expressions for the energy, namely,

$$E_q/q=q/\tilde{\kappa}(q)-C_q(t/q)\exp[\pm 2\tilde{\kappa}(q)z]\ , \tag{4.20}$$

$$=(\cosh\psi_q)q/\tilde{\kappa}(q)-(\sinh\psi_q)[t/\tilde{\kappa}(q)]\sinh[2\tilde{\kappa}(q)(z-z_0)]\ , \tag{4.21}$$

$$=(\cos\theta_q)q/\tilde{\kappa}(q)-(\sin\theta_q)[t/\tilde{\kappa}(q)]\cosh[2\tilde{\kappa}(q)(z-z_0)]\ , \tag{4.22}$$

which correspond, in turn, to (4.17)–(4.19). One should keep in mind that although the functional (3.18) and, correspondingly, the flow generated by (4.5) display no singularities on the lines $|\varepsilon_q|=1$ where the inequality (4.16) breaks down, the conditions under which the transition to the scaling limit (3.1) and (3.18) has been achieved entail, in fact, the stronger inequality (3.11). In the present notation that reads

$$[q^2(1-\varepsilon_q^2)+\tfrac{1}{4}\dot{\varepsilon}_q^2]^{1/2}\ll(1-|\varepsilon_q|)a_\perp^{-1}\ . \tag{4.23}$$

This inequality reduces to (4.16), however, in the formal limit $a_\perp\to 0$, corresponding physically to $q,\ t\ll a^{-1}$.

At $C_q=0$, $\psi_q=0$ and $\theta_q=0$ all three solution sets (4.17)–(4.19) yield the unique fixed point of the flow, namely

$$\varepsilon_q=\varepsilon_q^\infty\equiv t/\sqrt{t^2+q^2}\ , \tag{4.24}$$

which corresponds to Onsager's solution of the homogeneous Ising model. Indeed, integrating ε_q^∞ over q, following (3.20), yields

$$\varepsilon^\infty(T)=\int_0^\Lambda\varepsilon_q^\infty\,dq/2\pi=(2\pi)^{-1}t\ln(2\Lambda/|t|)\ , \tag{4.25}$$

for $|t|\ll\Lambda$, reproducing the famous logarithmic singularity of the energy, namely,

$$\varepsilon_{\rm sing}^\infty(T)=A_\pm t^{1-\alpha},\quad \alpha=0(\log)\ , \tag{4.26}$$

so that the specific heat $C\propto\partial\varepsilon/\partial t$ diverges as $\ln t$.

To compare the values of the critical amplitudes $A_\pm$ with those known for the *isotropic* model one must recall that our definition of t differs from the conventional $\tilde{t}=(T-T_c)/T_c$ by a constant factor: $t=4K_c\tilde{t}/a+O(\tilde{t}^2)$, with $K_c=\frac{1}{2}\ln(1+\sqrt{2})$; that also alters the definition of the energy density $\tilde{\varepsilon}=\partial\mathcal{F}/\partial\tilde{t}$. Taking this factor into account we obtain $\tilde{\varepsilon}=\tilde{A}_\pm(\pm\tilde{t})^{1-\alpha}$ with

$$\tilde{A}_+=\tilde{A}_-=\frac{8}{\pi}K_c^2=\frac{2}{\pi}[\ln(1+\sqrt{2})]^2\ , \tag{4.27}$$

in agreement with Onsager's solution.[4]

In a semi-infinite domain, $z>z_0$, the profiles $\varepsilon_q(z)$ should approach equilibrium values: $\varepsilon_q\to\varepsilon_q^\infty$ as $z\to+\infty$. This $z=+\infty$ boundary condition is satisfied only by the separatrix solutions (4.17): these yield

$$\varepsilon_q(z;T)=\varepsilon_q^\infty(T)+(\varepsilon_q^0-\varepsilon_q^\infty)\exp[-2\tilde{\kappa}(q)(z-z_0)]\ , \tag{4.28}$$

which describes the relaxation of the energy-density components from their surface values to the bulk ones. While the detailed behavior of the energy profile $\varepsilon(z)=\int_q\varepsilon_q(z)$ depends on the q dependence of the surface value ε_q^0 and will be considered below, the exponential decay at large distances from the wall is always governed by the low-q limit of the exponential factor so that

$$\ln|\varepsilon_q-\varepsilon_q^\infty|=-2\tilde{\kappa}(0)z+O(\ln z) =-2|t|z+O(\ln z)\ . \tag{4.29}$$

On general grounds (see Ref. 3 and Sec. IV C below) one expects the rate of exponential decay of the energy perturbations to be identical to that of the energy-energy correlation functions. Therefore, we identify $2|t|$ with the inverse correlation length of the energy, which in turn[25] is expected to be $2\xi_b^{-1}$, where ξ_b is the conventional bulk correlation length defined via decay of the spin-spin correlations. We therefore conclude that

$$\xi_b\approx|t|^{-1}\ , \tag{4.30}$$

confirming the standard hyperscaling relation[12] for the exponent $\nu=(2-\alpha)/2=1$. The critical amplitudes in the law $\xi_b\approx\xi_\pm^0|t|^{-\nu}$, are equal to unity, $\xi_+^0=\xi_-^0=1$, under our definition of t, and also check against the standard results after the rescaling $t\approx 4K_c(T-T_c)/aT_c$.

We close this section by noting that substitution of the separatrix solution (4.17) or (4.20) into (4.7) and (4.8) yields an extra contribution to the free energy per unit

length in the y direction, namely,

$$\mathcal{F}_q^s=\frac{1}{4}\left[(1-\varepsilon_q^0)\ln\frac{1-\varepsilon_q^0}{1-\varepsilon_q^\infty}+(1+\varepsilon_q^0)\ln\frac{1+\varepsilon_q^0}{1+\varepsilon_q^\infty}\right], \tag{4.31}$$

in addition to the q component of the free energy *density*, f_q^b, of a homogeneous system which is

$$f_q^b(T)=-\sqrt{t^2+q^2}\ . \tag{4.32}$$

The latter expression agrees, of course, with that obtained from (4.24) via $f(T)=-\int_0^t \varepsilon(t')dt'$, where we adopt the convention that the free-energy density and the energy density of the uniform critical state, $t\equiv 0$, are equal to zero.

C. Energy-energy correlations in the uniform case

If we knew the full microcanonical functional $\mathcal{S}[\varepsilon(\mathbf{r})]$, the energy-energy correlation functions would simply follow from the functional derivatives[10,16] of $\mathcal{S}$. Unfortunately our result (3.18) is a functional of $\varepsilon_q(z)$ rather than $\varepsilon(\mathbf{r})$. Still there is an easy way of calculating the *pair* energy-energy correlation function

$$G_{\varepsilon\varepsilon}(\mathbf{r})=\langle\varepsilon(\mathbf{r}_1)\varepsilon(\mathbf{r}_1+\mathbf{r})\rangle \tag{4.33}$$

in our formalism if we may assume that in the scaling limit of the isotropic model $G_{\varepsilon\varepsilon}(\mathbf{r})$ does not depend[21,25] on the direction of $\mathbf{r}$. In that case the Fourier transform $\hat{G}_{\varepsilon\varepsilon}(\mathbf{k})$ also depends only on the absolute value of $\mathbf{k}$. Therefore knowing $\hat{G}_{\varepsilon\varepsilon}(\mathbf{k})$ for $\mathbf{k}$ along one particular direction is sufficient. We can calculate $\hat{G}_{\varepsilon\varepsilon}(\mathbf{k})$ for $\mathbf{k}$ parallel to the z axis within our formalism by computing the linear response of the energy profile $\varepsilon(z)$ to a probe temperature field $\delta t=\hat{t}_k e^{ikz}$ superimposed on the uniform field $t(z)=t$.

Linearizing (4.5) around the uniform solution $\varepsilon_q^\infty=t/\sqrt{t^2+q^2}$, one obtains

$$\tfrac{1}{4}\delta\ddot{\varepsilon}_q-(t^2+q^2)\delta\varepsilon_q=-q^2(q^2+t^2)^{-1/2}\delta t(z)\ . \tag{4.34}$$

Substituting $\delta t=\hat{t}_k e^{ikz}$ yields

$$\delta\varepsilon_q(z)=\frac{q^2/\sqrt{q^2+t^2}}{\frac{1}{4}k^2+t^2+q^2}\hat{t}_k e^{ikz}\ , \tag{4.35}$$

so the response of the energy density is

$$\delta\varepsilon(z)=\int\delta\varepsilon_q(z)\frac{dq}{2\pi}$$
$$=\int_0^\Lambda\frac{q^2/\sqrt{q^2+t^2}}{\frac{1}{4}k^2+t^2+q^2}\frac{dq}{2\pi}\hat{t}_k e^{ikz}=\hat{G}_{\varepsilon\varepsilon}(k)\delta t\ , \tag{4.36}$$

which leads to

$$\hat{G}_{\varepsilon\varepsilon}(\mathbf{k})=\frac{1}{2\pi}\left\{\ln(2\Lambda/t)-\frac{\sinh^{-1}(k/2t)}{\tanh[\sinh^{-1}(k/2t)]}\right\}. \tag{4.37}$$

The correlations in real space can be determined by inversion via

$$G_{\varepsilon\varepsilon}(\mathbf{r})=\int_0^\Lambda\frac{k\,dk}{2\pi}\hat{G}_{\varepsilon\varepsilon}(k)J_0(kr)\ . \tag{4.38}$$

where $J_0(x)$ is the standard Bessel function.

In accordance with general principles[2,12,16] the limit $\hat{G}_{\varepsilon\varepsilon}(k=0)=\ln(2\Lambda/et)/2\pi$ is equal to the specific heat $C=\partial\varepsilon^\infty/\partial t$ with ε^∞ given by (4.25). For $t\ll k\ll\Lambda$ the form (4.37) reduces to $\hat{G}_{\varepsilon\varepsilon}(k)\approx\ln(2\Lambda/k)/2\pi$. The corresponding real-space dependence is obtained from (4.38) using a smooth cutoff[2] leading to

$$G_{\varepsilon\varepsilon}(r)\approx\frac{1}{2\pi}r^{-2\omega_\varepsilon}=\frac{1}{2\pi}r^{-2}\ . \tag{4.39}$$

This describes the critical part of the correlation function valid for $a\ll r\ll t^{-1}$. The long-distance part at $t\neq 0$ is determined by the behavior of $\hat{G}_{\varepsilon\varepsilon}(\mathbf{k})$ for $k\lesssim t$. While $\hat{G}_{\varepsilon\varepsilon}(k)$ is a smooth function of k at $k=0$, it lacks a simple pole in the complex k plane which would yield the Ornstein-Zernike form $r^{-1/2}e^{-\kappa_\varepsilon r}$ in real space.[12] Instead, $G_{\varepsilon\varepsilon}(k)$ has a branch point at $k=2it$, leading to[12,25]

$$G_{\varepsilon\varepsilon}(r)\approx\frac{1}{8\pi}r^{-2}e^{-\kappa_\varepsilon r}=\frac{1}{8\pi}r^{-2}e^{-2tr}\ . \tag{4.40}$$

V. BOUNDARY CONDITIONS AT SHARP INHOMOGENEITIES

A. Formulation and the scaling ansatz

We now derive the boundary conditions supplementing the scaling form (3.18) at locations where the two inequalities

$$\xi_b\approx|t|^{-1}\gg a\ , \tag{5.1}$$

$$|d\ln|t|/dz|\ll a^{-1}\ , \tag{5.2}$$

used in taking the scaling limit in Sec. III are violated. In this paper we restrict ourselves to the case of a sharp boundary between two distinct regions which includes the important limit of a free surface.

The simplest realization of a boundary is a stepwise variation of the basic field t, namely,

$$t(z)=t_-\Theta(-z)+t_+\Theta(+z)\ , \tag{5.3}$$

where Θ is the Heaviside step function: see Fig. 5. If both t_+ and t_- satisfy (5.1), i.e., the scaling limit is valid on both sides of the boundary, then the discontinuity can be realized as a limit of a sequence of continuous functions. Using any of those sequences in (4.5) leads to the natural conditions

$$\varepsilon_q(0-)=\varepsilon_q(0+)\ , \tag{5.4}$$

$$\dot{\varepsilon}_q(0-)=\dot{\varepsilon}_q(0+)\ , \tag{5.5}$$

of continuity of the basic densities ε_q and their first spatial derivatives at the jump. This is, of course, the standard situation for second-order differential equations, as, for example, in Schrödinger's equation.[26]

However, a closer look into possible microscopic realizations of a boundary in terms of the underlying layered Ising model shows that the simple jump (5.3) does *not*

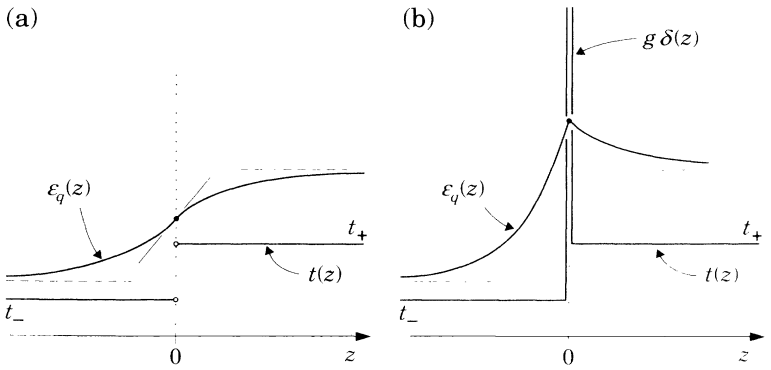

FIG. 5. Sketch of the local thermal field, $t(z)$, and the corresponding profiles of the energy-density components, $\varepsilon_q(z)$, in two continuum models of a boundary at $z=0$ between two domains as in Fig. 2: (a) is appropriate if the couplings, $K^{\perp}$ and $K^{\parallel}$, in both domains lie near the same point on the critical locus in Fig. 3 and so have comparable local anisotropies; (b) contains an extra δ-function contribution of strength g [see Eq. (5.7)] needed to allow for disparate anisotropies on the two sides of the boundary: this induces a discontinuity in $\dot{\varepsilon}_q(z)\equiv\partial\varepsilon_q/\partial z$.

provide a description of the general situation in which the two adjacent regions are near *different* points of the critical locus $K^{\parallel}=K^{\perp *}$; see Fig. 3. In this case the jumps in the absolute values of the coupling constants $K^{\perp}$, $K^{\parallel}$ are large, even if both $|t_+|$, $|t_-|$ are small: unless the variation of $K_j^{\perp}$ and $K_j^{\parallel}$ is correlated in a very special way that keeps H_{0j} small everywhere, the latter will take large, noncritical values in the interfacial zone, so violating (5.1) and (5.2).

The simplest model displaying this feature is sketched in Fig. 2. We will refer to it as model A. It is composed of two uniform Ising half-planes, rows $j=1,2,\ldots,+\infty$ or $z>0$ and $j=-1,-2,\ldots,-\infty$ or $z<0$, characterized by the parameters $K_{\pm}^{\perp}$, $K_{\pm}^{\parallel}$, $a_{\perp\pm}$, $a_{\parallel\pm}$, and $t_{\pm}=2(K_{\pm}^{\perp *}-K_{\pm}^{\parallel})/a_{\perp\pm}$ with subscripts $\pm$ corresponding to $j\gtrless 0$. The two half-planes are coupled via vertical bonds of strength $K_0=J_0/k_BT$ and length b. It is clear now from (2.8) that the

$$H_{q=0,\pm 1}=K_0^*+K_{\pm 1}^{\perp *}-2K_{\pm 1}^{\parallel}=a_{\perp\pm}t_{\pm}+K_0^*-K_{\pm}^{\perp *}$$

are not small, unless the two half-planes are indeed similar so that $K_+^{\perp}\simeq K_-^{\perp}$ and the boundary is then "coherent", i.e., $K_0\simeq K_{\pm}^{\perp}$.

The natural temptation now is to try to account for the anomalously large values of the field $H_{q=0}$ in the boundary region by adding a δ-function feature to the model (5.3) to obtain

$$t(z)=t_-\Theta(-z)+t_+\Theta(+z)+g\delta(0)\ . \tag{5.6}$$

See Fig. 5. As we have seen in Secs. II C and III B, the zeroth moment of the field, $\sum_j H_{q=0,j}\approx\int t(z)dz$, plays a special role in the theory. We conjecture further, therefore, that the strength g of the δ function is fixed by the requirement that the zeroth moment is correctly given by (5.6). For the particular model described above this means

$$g=2K_0^*-K_+^{\perp *}-K_-^{\perp *}+O(t_+b,t_-b)\ . \tag{5.7}$$

This result represents an intuitively appealing limit of the microscopic model when both $a_{\perp+}$, $a_{\perp-}$ and the interface width b approach zero. However, we cannot be sure it is correct until the boundary conditions obtained in the frame of the macroscopic representation (5.6) are compared with the long-wavelength limit of those appearing in the analysis of the exact lattice functional (2.12). This will be done below.

Variation of the basic functional (3.18) with $t(z)$ given by (5.6) is readily achieved by separating each integral over z in (3.18) into three pieces:

$$\int_{-\infty}^{\infty}dz[\mathcal{L}_q-t\varepsilon_q]=\int_{-\infty}^{0}dz[\mathcal{L}_q-t_-\varepsilon_q]+\int_0^{\infty}[\mathcal{L}_q-t_+\varepsilon_q]-g\varepsilon_q(0)\ . \tag{5.8}$$

Variation of the first and second pieces gives the usual bulk equations of motion (4.4) with $t=t_-$ or t_+ plus the boundary contributions

$$\pm\left[\frac{\partial\mathcal{L}}{\partial\dot{\varepsilon}_q}\right]_{z\to\mp 0}\delta\varepsilon_q(0)=\pm p_q(0\mp)\delta\varepsilon_q(0)\ ,$$

which appear after the integration of $\int(\partial\mathcal{L}/\partial\dot{\varepsilon}_q)\delta\dot{\varepsilon}_q dz$ by parts.[19] Here the p_q are the canonical momenta given in (4.1). Combining these contributions with $-g\delta\varepsilon_q(0)$ from the third term in (5.8) results in the following picture: see Fig. 5. Each component $\varepsilon_q(z)$ is continuous through $z=0$, so that (5.4) still holds, but the slope $\dot{\varepsilon}_q(z)$ is discontinuous with a jump in the canonical momentum $p_q(z)$ equal to the strength of the δ function, that is

$$p_q(0+)-p_q(0-)=\tfrac{1}{2}\ln\left\{\frac{\dot{\varepsilon}_q(0+)+\{\dot{\varepsilon}_q^2(0+)+4q^2[1-\varepsilon_q^2(0)]\}^{1/2}}{\dot{\varepsilon}_q(0-)+\{\dot{\varepsilon}_q^2(0-)+4q^2[1-\varepsilon_q^2(0)]\}^{1/2}}\right\}=-g\ . \tag{5.9}$$

Note that the constancy of $t(z)$ for $z\neq 0$ has not been used; the derivation still holds if t_+ and t_- in (5.6) are allowed to vary continuously with z in their respective half-planes. In summary, Eqs. (5.4) and (5.9) specify the necessary conditions at a boundary modeled by a jump in $t(z)$ plus a δ-function contribution.

These boundary conditions are obviously invariant under the transformation $z\Rightarrow z/\lambda$, $q\Rightarrow q\lambda$, $\varepsilon_q\Rightarrow\varepsilon_q$; thus they leave the formulation *scale invariant.* Note that in the general case of different anisotropy on the two sides

of the boundary, the coordinate transformations (3.14) required on the two sides also differ. While the original units of length can be restored at this point, leading to nonuniversal factors multiplying $\dot{\varepsilon}_q(0-)$ and $\dot{\varepsilon}_q(0+)$ in (5.9), it is more convenient to postpone this step until the explicit solution has been obtained. Note also that the definition (5.7) of the strength of the δ function, g, based on the zeroth moment of the temperature field, is invariant under transformation with (3.14).

For the case in which $t_+(z)$ and $t_-(z)$ are both constant in (5.6), which should represent the scaling limit of the lattice model A in Fig. 2 when the thicknesses L_+ and L_- of the + and − domains are infinite, we can go further and solve explicitly for the energy-density components $\varepsilon_q(z)$ and their contributions $\mathcal{F}_q$ to the free energy. Each component takes the form (4.28) on both sides of the boundary so that

$$\varepsilon_q(z)=\varepsilon_q^{\pm}+(\varepsilon_q^0-\varepsilon_q^{\pm})\exp[\mp 2\tilde{\kappa}_{\pm}(q)z]\ ,\quad z\gtrless 0\ , \tag{5.10}$$

where $\varepsilon_q^{\pm}$ and $\tilde{\kappa}_{\pm}(q)$ denote ε_q^{∞} and $\tilde{\kappa}(q)$ of (4.24) and (4.13) on the respective sides, $z\gtrless 0$, of the boundary. Thence follows

$$\dot{\varepsilon}_q(0\pm)=\mp 2\tilde{\kappa}_{\pm}(q)(\varepsilon_q^0-\varepsilon_q^{\pm})\ , \tag{5.11}$$

which when substituted into (5.9) yields the only remaining unknown as

$$\begin{aligned}\varepsilon_q^0&=\tanh[g+\tfrac{1}{2}\tanh^{-1}(\varepsilon_q^+)+\tfrac{1}{2}\tanh^{-1}(\varepsilon_q^-)]\ ,\\&=\tanh[g+\tfrac{1}{2}\sinh^{-1}(t_+/q)+\tfrac{1}{2}\sinh^{-1}(t_-/q)]\ .\end{aligned} \tag{5.12}$$

The same result can, in fact, be obtained by minimizing the total free energy of the interface, namely,

$$\mathcal{F}_q^A(\varepsilon_q^0)=\mathcal{F}_q^s(\varepsilon_q^0,\varepsilon_q^+)+\mathcal{F}_q^s(\varepsilon_q^0,\varepsilon_q^-)-g\varepsilon_q^0\ , \tag{5.13}$$

where $\mathcal{F}_q^s(\varepsilon_q^0,\varepsilon_q^{\infty}=\varepsilon_q^{\pm})$ denotes the contributions of the two exponential pieces in (5.10), as given by (4.31). The advantage of this approach to the problem of the boundary is that the minimization automatically yields the qth component of the excess free energy of the interface as

$$\begin{aligned}\mathcal{F}_q^A&=\frac{1}{4}\ln\frac{[1-(\varepsilon_q^0)^2]^2}{[1-(\varepsilon_q^+)^2][1-(\varepsilon_q^-)^2]}\\&=-\tfrac{1}{2}\ln[Q^2(g,t_+,t_-;q)q^2/\tilde{\kappa}_+(q)\tilde{\kappa}_-(q)]\\Q&\equiv\cosh\left[g+\frac{1}{2}\sinh^{-1}\left[\frac{t_+}{q}\right]+\frac{1}{2}\sinh^{-1}\left[\frac{t_-}{q}\right]\right]\ .\end{aligned} \tag{5.14}$$

The results (5.10), (5.12), and (5.14) represent the complete solution of the problem within the phenomenological approach for the thermal field (5.6). In the following sections we analyze two physically interesting limits of the lattice model A using the full lattice representation (2.12)–(2.14), to confirm that our procedure is correct, i.e., that the solution just obtained precisely reproduces the scaling limit of the lattice model.

B. Analysis of the boundary in the lattice representation

The reason we expect the boundary conditions following from the model potential (5.6) to correctly represent the scaling limit of the problem can be understood quite simply on the basis of the lattice representation (2.12) and the underlying mapping onto the linear Ising chains. The point is that for any given variation of the bond strengths $K_j^{\perp}$, $K_j^{\parallel}$ across the boundary, the $d=1$ fields, H_{qj}, stay finite while the $d=1$ bond strengths, $\tau_{qj}\approx-\frac{1}{2}\ln q$, diverge when $q\to 0$. Therefore, whenever the deviations from the scaling-limit conditions (5.1) and (5.2) are confined to a boundary layer of finite thickness, say b, there is always a finite wave number q_b, such that for $q\ll q_b$ the variation of $\varepsilon_q=M_{qj}$ across the boundary layer is negligible. Furthermore, it is easily seen that when the probability of encountering a $d=1$ domain wall (i.e., a pair of antiparallel neighboring linear-chain spins) within this boundary layer is negligible, the leading contribution to the free energy from this region is just

$$\sum_j H_{qj}M_{qj}\approx\varepsilon_q^0\sum_j H_{qj}\approx g\varepsilon_q^0\ ;$$

here the sum is taken over the boundary region in which the values of the field H_{qj} might get large, and the definition in the previous subsection of the strength g of the δ function in (5.6) has been used. Note that despite the absence of domain walls within the boundary layer, ε_q^0 does not have to equal ± 1: the linear-chain spins of the boundary layer can still coherently fluctuate within domains of size $l\gg b$. Thus, although the continuum representation (3.18) cannot describe the variation of ε_q across the boundary layer, there is no need to do this. All that matters in the long-wavelength limit, $q\ll q_b$, is the value ε_q^0 and its interaction with the local excess, g, of the temperature field, as given by (5.7). Outside the boundary region, ε_q^0 will match smoothly on to the extremal solutions of (3.18): see Fig. 5.

C. Free surface limit

The only case in which this reasoning may be invalid is when the definition of the model entails singular limits in which certain bonds vanish or become infinitely strong. However, this does arise in the physically interesting situation (which we will call model B) of a half-plane Ising model with surface spins subject to a surface magnetic field h_1 (in the original, real planar meaning). This model may be obtained from model A (Fig. 2) by taking the limit[4] $J_-^{\perp}, J_-^{\parallel}\to+\infty$, and, again, $L_+\to\infty$. That freezes the spins of the $z<0$ half-plane in one of the uniform states $s=\pm 1$. Correspondingly, the frozen spins induce a field $h_{j=1}\equiv h_1=\pm K_0$ which acts on the spins of the surface layer $j=+1$. As the basic free energy $\mathcal{F}(h_1,t_+)$ must be an even function of h_1 (in the absence of any bulk field), the lack of information about the sign of the surface field merely adds a term $k_B\ln 2$. That is obviously negligible in the thermodynamic limit. This device reduces the original problem with nonzero field to a layered problem in zero field tractable by available methods. Note that besides taking the limit $K_-^{\perp}, K_-^{\parallel}\to+\infty$, necessary to freeze

the spins of the ($z<0$) half-plane, we wish to allow $K_0 \to 0$ in order to obtain the important free surface limit, $h_1 = 0$. In all these cases one cannot reasonably expect that M_{qj} changes by only a small amount between $j=-1$ and $j=+1$: thus it is appropriate to resort to the lattice formulation.

Substituting the values of the bond strengths $K^{\perp}, K^{\parallel}$ into (2.8) and (2.9) we determine the fields H_{qj}, $\zeta_{qj} = \exp(-2\tau_{qj})$ entering the functional (2.12). For $q \ll a^{-1}$ we obtain

$$H_{q,-1} = K_{-}^{\perp *} + K_0^{*} - 2K_{-}^{\parallel} = -\infty \ , \tag{5.15}$$

$$\zeta_{q,0} \equiv e^{-2\tau_{q,0}} = \zeta_{q(-1,1)} = q/[\sinh^2(2K_0) + q^2]^{1/2} \ , \tag{5.16}$$

$$H_{q,1} = K_0^{*} + K_{+}^{\perp *} - 2K_{+}^{\parallel} = H_{q+} + (K_0^{*} - K_{+}^{\perp *}) \ , \tag{5.17}$$

$$\begin{aligned} H_{q,j} &= H_{q+} \equiv 2(K_{+}^{\perp *} - K_{+}^{\parallel}) \ , \\ \zeta_{qj} &= \zeta_{q+} \equiv q/\sinh(2K_{+}^{\perp}) \ , \quad j \geq 2 \ . \end{aligned} \tag{5.18}$$

[Recall that for notational convenience the $j=0$ row is dropped in our definition of model A: see Fig. 2; instead we use 0 to label the quantities related to the $(-1,+1)$ bonds.] Being interested in the critical behavior of the ($z>0$) half-plane, we suppose $H_{q+}, \zeta_{q+} \ll 1$. Note also that for $K_0 \ll 1$ one has

$$K_0^{*} \approx -\tfrac{1}{2} \ln K_0 \gg +1 \ . \tag{5.19}$$

We proceed to analyze (2.12)–(2.14). In the language of the $d=1$ analogy, the infinite negative fields $H_{q,j}$ for $j \leq -1$ freeze the $j=-1$ linear-chain spin so that $M_q = -1$: compare with (5.15). Note that the linear-chain spin-density maps onto the real, planar energy density, so the result $M_{qj} = -1$ for $j \leq -1$ indicates the absence of domain walls in the $z<0$ half-plane, rather than the actual freezing of the planar spins in the "down" state. Minimization with respect to ε_{q0} leads to the expected result: the linear-chain bond of strength $\tau_{q,0} = -\tfrac{1}{2} \ln \zeta_{q,0}$, connecting the $d=1$ spin at $j=1$ to the one frozen in the down state, adds an effective magnetic field $M_{q,-1}\tau_{q,0} = -\tau_{q,0}$ to $H_{q,+1}$. The problem is thus reduced to that of the uniform ($j \geq +1$) half-chain, the effects of the anomalous fields and bonds for $j<+1$ being accounted for by an extra $d=1$ magnetic field, namely,

$$\begin{aligned} g_1(q;T) &= H_{q,1} - \tau_{1,0} - H_{q+} \\ &= K_0^{*} - K_{+}^{\perp *} + \tfrac{1}{2} \ln q - \tfrac{1}{4}[\sinh^2 2K_0 + q^2] \ , \end{aligned} \tag{5.20}$$

acting on the first spin of the chain. Analysis of the further variational equations (2.13) and (2.14) down the chain confirms that the reasoning of the previous subsection is applicable at this stage: the correct scaling description is provided by the continuum functional (3.18) defined on the half-space $z>0$ with an extra δ-function piece

$$\begin{aligned} \mathcal{L}_s^{B} = [&-g_1 \varepsilon_q + \tfrac{1}{4}(1+\varepsilon_q)\ln(1+\varepsilon_q) \\ &+ \tfrac{1}{4}(1-\varepsilon_q)\ln(1-\varepsilon_q)]\delta(z) \ , \end{aligned} \tag{5.21}$$

added to the Lagrangian $\mathcal{L}_b$. While the first term in the brackets accounts for the interaction with the local excess of the field, g_1, the second and the third terms represent one half of the first and the second terms, respectively, in the brackets in the first, $j=1$, member of the sum in (2.12). These two pieces represent the $O(1)$ correction to the approximation of the sum in (2.12) by the integral in (3.18), as the $a_{\perp} \to 0$ limit is taken.[27] This kind of term does not appear in (5.6) since the sum, being converted into an integral in model A, is taken from $j=-\infty$ to $j=+\infty$ rather than from $j=+1$ to $j=+\infty$ as in the present case.

The derivation of the boundary conditions proceeds now exactly as in Sec. V A, the difference being the absence of the first piece on the right-hand side of (5.8) and the more complicated form of the surface term. Correspondingly, (5.9) becomes

$$\begin{aligned} p_q(0+) &= \tfrac{1}{2} \sinh^{-1}\{\dot{\varepsilon}_q(0+)/2q[1-(\varepsilon_q^0)^2]\} \\ &= -g_1 + \tfrac{1}{2} \ln[1-(\varepsilon_q^0)^2] \ , \end{aligned} \tag{5.22}$$

which, just as before, applies equally when t_+ is a continuous function of $z>0$. If, however, t_+ is constant, as in model B, we can go further and, substituting (4.28) into (5.22), actually solve to obtain

$$\begin{aligned} \varepsilon_q^0 &= \tanh[g_1 + \tfrac{1}{2} \tanh^{-1}(\varepsilon_q^{\infty})] \\ &= \tanh[g_1 + \tfrac{1}{2} \sinh^{-1}(t/q)] \ , \end{aligned} \tag{5.23}$$

where $\varepsilon_q^{\infty} = \varepsilon_q^{+} = t_+/(t^2+q^2)^{1/2}$. Again we can obtain the same result, together with the excess surface free energy, by minimizing

$$\begin{aligned} \mathcal{F}_q^{B} &= \min_{\varepsilon_q^0}[\mathcal{F}_q^{s}(\varepsilon_q^0, \varepsilon_q^{\infty}) - g_1\varepsilon_q^0 + \tfrac{1}{4}(1+\varepsilon_q^0)\ln(1+\varepsilon_q^0) \\ &\qquad + \tfrac{1}{4}(1-\varepsilon_q^0)\ln(1-\varepsilon_q^0)] \\ &= \tfrac{1}{2} \ln\{[1-(\varepsilon_q^0)^2][1-(\varepsilon_q^{\infty})^2]^{-1/2}\} \\ &= -\tfrac{1}{2} \ln\{\cosh^2[g_1 + \tfrac{1}{2} \sinh^{-1}(t/q)]q/\tilde{\kappa}(q)\} \ , \end{aligned} \tag{5.24}$$

where we have omitted the subscripts on $\tilde{\kappa}(q) \equiv \tilde{\kappa}_+(q)$ and $t \equiv t_+$: compare with (5.13) and (5.14).

Note the striking similarity of (5.23) and (5.24) to (5.12) and (5.14). Indeed, we will see in Sec. VII that most of the features of model B can be obtained directly in the appropriate $t_- \to -\infty$, $K_0 \to 0$ limit of the *scaling* equations (5.12) and (5.14) which describe model A.

VI. WALL FREE ENERGIES AND PROFILES

In this and the following section we analyze some of the applications of the formalism and methods presented above. We start with the classical problem of a semi-infinite system subject to a surface magnetic field[4,5] h_1, named model B in the previous subsection. First we recover in a very simple and straightforward manner the previously known results regarding the surface magnetization m_1 and the surface specific heat C_s, specifically, the surface exponents Δ_1 and β_1, and the exact scaling forms for $m_1(t,h_1)$ and $C_s(t)$. Then the energy-density profiles $\varepsilon(z;t,h_1)$, which follow naturally from the formulation, are analyzed. It is found that the decay of the sur-

face perturbation, $\Delta\varepsilon(z)$, with distance from the wall, which has not been studied previously, closely reflects the renormalization-group flow of the surface thermodynamic quantities.

A. General solution: Surface scaling

Formally the surface free energy $\mathcal{F}_s^B$ and the energy profile $\varepsilon(z)$ follow directly from (5.23), (5.24), and (4.28) by performing the integration over q: see (3.18) and (3.20). However, the scaling of those quantities is not immediately apparent owing to the complicated q dependence of $g_1(q;T)$ which is given by (5.20). [Note by contrast that the dimensionless constant g in (5.12) and (5.14) does *not* depend on q, so the scaling in model A *is* easily seen.] Now, from (5.21) we see that the scaling dimension of g_1 must be zero. But, by (5.20), the only way g_1 can be kept dimensionless in the $a_\parallel \to 0$ limit after introducing a dimensional wave vector via $q' = q/a_\parallel$ [see (3.2)], is by assigning a finite value to a new scaling field: recall (5.19). We thus introduce

$$h_1 = (2a_\parallel)^{-1/2} K_0 \exp(-K_+^{\perp *}) \approx (2a_\parallel)^{-1/2} K_0 \exp(-K_+^{\parallel}) , \tag{6.1}$$

where we have used $K_+^{\parallel} - K_+^{\perp *} = O(ta_\perp) \ll 1$. Then the scaling limit, $a_\parallel \to 0$, of (5.20) can be taken and yields

$$g_1 \approx \tfrac{1}{2} \ln(q/h_1^2) = \ln(q^{\omega_1}/|h_1|) , \tag{6.2}$$

which defines the scaling dimension $\omega_1 = \frac{1}{2}$ of the surface field h_1. The formal approach of taking the $a_\parallel \to 0$ limit we have followed here in order to determine ω_1 has, in fact, a simple meaning which is clear from (5.20) and (5.23): when $t \to 0$ we expect the important contributions to come from the integration over $q = O(t)$, so that we have $\sinh^{-1}(t/q) = O(1)$ in (5.23). The important dependence on h_1 comes from those values that also yield $g_1(q;h_1) = O(1)$. The latter, as we have seen, is possible if and only if $h_1 = O(q^{1/2}) = O(t^{1/2}) = O(t^{\Delta_1})$, where by the last equality we have introduced the surface gap exponent

$$\Delta_1 = \omega_1/\omega_t = \tfrac{1}{2} , \tag{6.3}$$

in agreement with the established results.[5]

Now we can substitute (6.2) into (5.23) and (5.24) to obtain universal expressions for the scaling parts of the energy profile and the surface energy, respectively.

B. Surface magnetization and specific heat

This subsection will analyze the derivatives of

$$\mathcal{F}_s^B(t,h_1) = \int_0^\Lambda \frac{dq}{2\pi} \mathcal{F}_q^B(t,g_1) , \tag{6.4}$$

where $\mathcal{F}_q^B(t,g_1)$ is given by (5.24) while g_1 now takes the simple form (6.2). A closer look reveals, however, that the result becomes singular in the important limit $h_1 \sim K_0 \to 0$. The reason is simply that we have so far neglected some trivial, t-independent contributions to the free energy arising from K_0, which nonetheless are singular when $K_0 \to 0$ (upon which the lattice decouples into two independent halves). These contributions are the following: (i) The $C_0 \approx -\frac{1}{2}\ln K_0$ term in (2.10) and (2.12); see (2.11). This represents the free energy per J_0 bond (see Fig. 2) and it contributes doubly, $2C_0 \approx -\ln K_0$, to each q component of the free energy. (Recall that $\int_0^\pi dq/2\pi = \frac{1}{2}$.) (ii) The energy $-K_0^* M_{q,-1} = K_0^* \approx -\frac{1}{2}\ln K_0$ of interaction between the K_0-dependent part of the $(d=1)$ field $H_{q,-1}$ in (5.15) and the "frozen" layer of spins at $j=-1$ with $M_{q,-1} = -1$. (iii) The energy $\tau_{q,0} \approx \frac{1}{2}\ln K_0/q + \text{const}$ representing the $M_{q,+1}$-independent part of the term $\tau_{q0}\mathcal{E}_{q0} = \tau_{q0}(1+M_{q,+1})$ in (2.12). The equality $\mathcal{E}_{q0} = 1 + M_{q,+1}$ is an obvious consequence of the spin at $j=-1$ being frozen in the $s=-1$ state. Summing all these pieces and adding the result to (5.24) we obtain

$$\mathcal{F}_q^B(t,h_1) = -\ln[(1+\varepsilon_q^\infty)^{1/2} + (1-\varepsilon_q^\infty)^{1/2} h_1^2/q] + \text{const} , \tag{6.5}$$

where, as previously, $\varepsilon_q^\infty = t/\tilde{\kappa}(q)$ while the constant stands for the parts of the free energy independent of t and h_1.

We can now calculate the magnetization of the first surface layer. Up to the metrical factor in (6.2), it is given by

$$m_1 = -\partial\mathcal{F}/\partial h_1 = -\int_0^\Lambda \frac{dq}{2\pi} \frac{\partial \mathcal{F}_q^B}{\partial h_1} = \frac{h_1}{\pi} \int_0^\Lambda \frac{dq/q}{(h_1^2/q) + \exp[\sinh^{-1}(t/q)]} = h_1 \mathcal{M}_1^\pm(|h_1|/|t|^{\Delta_1}) = h_1 \mathcal{M}_1^\pm(|h_1|/|t|^{1/2}) . \tag{6.6}$$

Here $\pm$ corresponds to $t \gtrless 0$, and the scaling functions $\mathcal{M}_1^+$, $\mathcal{M}_1^-$ are conveniently calculated by introducing a new integration variable w according to $q = |t|\sinh w$. Note the corresponding change of the cutoff $\Lambda \Longrightarrow w_\Lambda \approx \ln(2\Lambda/|t|)$. Then we find

$$\mathcal{M}_1^\pm(y_1) = \frac{1}{\pi} \int_0^{w_\Lambda} \frac{\cosh w \, dw}{\cosh w \pm 1 + y_1^2} , \tag{6.7}$$

$$\mathcal{M}_1^+(y_1) = \frac{1}{\pi} \left[\ln(2\Lambda/t) - \frac{(1+y_1^2)\sinh^{-1}(y_1/\sqrt{2})}{(1+y_1^2/2)^{1/2} y_1/\sqrt{2}} \right] , \tag{6.8}$$

$$\mathcal{M}_1^-(y_1)=\frac{1}{\pi}\left[\ln(2\Lambda/|t|)+\frac{(1-y_1^2)\cos^{-1}(y_1/\sqrt{2})}{(1-y_1^2/2)^{1/2}y_1/\sqrt{2}}\right], \quad y_1\le\sqrt{2},$$
$$=\frac{1}{\pi}\left[\ln(2\Lambda/|t|)-\frac{(y_1^2-1)\cosh^{-1}(y_1/\sqrt{2})}{(y_1^2/2-1)^{1/2}y_1/\sqrt{2}}\right], \quad y_1\ge\sqrt{2}. \tag{6.9}$$

It is not hard to check that $\mathcal{M}_1^-(y_1)$ is analytic through $y_1=\sqrt{2}$ despite first appearances. Various asymptotic limits can be readily elucidated. In the disordered phase, $t>0$, as $y_1\to 0$, one has

$$m_1=\frac{1}{\pi}\ln(2\Lambda/te)h_1+O(h_1^2), \tag{6.10}$$

and the system is characterized by a finite surface susceptibility $\chi_{11}=\partial m_1/\partial h_1\sim t^{-\gamma_{11}}$, which actually diverges logarithmically when $t\to 0+$ ($\gamma_{11}=0$). On the low-temperature side, when $y_1\to 0$ one finds

$$\mathcal{M}_1^-\approx\frac{1}{\pi}[\ln(2\Lambda/|t|)+\tfrac{1}{2}\pi y_1^{-1}], \tag{6.11}$$

so that the surface magnetization varies as

$$m_1=\mathrm{sgn}(h_1)\left[\frac{-t}{2}\right]^{1/2}+\frac{1}{\pi}h_1\ln\left[\frac{2\Lambda}{|t|e}\right]+O(h_1^2). \tag{6.12}$$

In other words, the system is characterized by a *spontaneous surface magnetization* $m_1^0=m_1(h_1=0+)\sim|t|^{\beta_1}$, with

$$\beta_1=\tfrac{1}{2}, \tag{6.13}$$

while χ_{11} still diverges logarithmically when $t\to 0-$. For large surface fields, $y_1\gg 1$, one finds

$$m_1\approx\frac{1}{\pi}h_1\ln(\Lambda/h_1^2). \tag{6.14}$$

Consequently at the critical temperature, $t=0$, the surface susceptibility χ_{11} varies as $\ln h_1$.

The surface specific heat, $C_s=-\partial^2\mathcal{F}_s(t,h_1)/\partial t^2$, can be obtained similarly. For $h_1=0$ the result is especially simple, namely,

$$C_s(t_1,h_1=0)=-\frac{1}{4\pi}t^{-1}-\frac{1}{2}\delta(t). \tag{6.15}$$

Recall that the *surface* specific heat need not be positive. Although the "latent heat," contributed by the δ-function term looks unusual in the context of a continuous transition, it does not violate scaling: indeed, both terms in (6.15) scale as $t^{-\alpha_s}$ with $\alpha_s=1$. All the surface exponents thus obtained can, of course, be derived via the usual hyperscaling relations[12] from the scaling dimensions $\omega_t=\nu^{-1}=1$, $\omega_1=\nu^{-1}\Delta_1=\frac{1}{2}$ of the bulk temperature and the surface magnetic fields, respectively, and the dimensionality $d'=1$ of a boundary surface of the planar model. Thus one has $\alpha_s=2-d'\nu=1$, $\beta_1=(d'-\omega_1)\nu-2-\alpha_s=\Delta_1=\frac{1}{2}$, $\gamma_{11}=2-\alpha_s-2\Delta_1=0$, etc.

Both the exponents and the amplitudes of the critical power laws in (6.10)–(6.14) agree fully with those obtained in the pioneering study of Binder and Hohenberg,[5] who presented an asymptotic analysis of the exact solution of the semi-infinite lattice model obtained by McCoy and Wu.[4] We believe that our method provides a much simpler way to obtain these results, the basic advantage being that the scaling limit is taken on the level of the variational functional rather than being derived from the fully detailed expressions. In fact, we operate with a field theory representing the scaling limit of the model, which is much simpler than the original lattice representation. Note also that the expression quoted for the scaling function for $m_1(t_1,h_1)$ in Ref. 5 is quite incorrect for $0<h_1<\infty$, even though it reproduces correctly the two limits $h_1=0$ and $h_1=\infty$. Our expressions (6.8) and (6.9) agree precisely with the exact lattice-based calculations of Au-Yang and Fisher.[28]

C. Scaled energy profiles

Consider now the energy profiles $\varepsilon(z)$, or rather $\Delta\varepsilon(z)=\varepsilon(z)-\varepsilon^\infty$, for different values of t and h_1; these profiles have not been studied previously. Substituting ε_q^0 from (5.23), and g_1 from (6.2), into $\varepsilon_q(z)$ as given by (4.28), and integrating over q yields

$$\Delta\varepsilon(z)=\int_0^\Lambda\frac{dq}{2\pi}\{\tanh[\tfrac{1}{2}\ln(q/h_1^2)+\tfrac{1}{2}\sinh^{-1}(t/q)] -\tanh[\sinh^{-1}(t/q)]\}\exp[-2\tilde{\kappa}(q)z], \tag{6.16}$$

where the q-dependent inverse correlation length $\tilde{\kappa}(t,q)=(t^2+q^2)^{1/2}$ was introduced in (4.13). The exponential factor $e^{-2\tilde{\kappa}z}$ ensures convergence of the integral at large q for any $z>0$. Thus the limit $\Lambda\to\infty$ may be taken straightforwardly. The result obviously satisfies the scaling law

$$\Delta\varepsilon(z)=t^{\omega_\varepsilon/\nu}Y_\pm(zt^\nu, h_1/|t|^{\Delta_1}) =tY_\pm(zt, h_1/|t|^{1/2}), \tag{6.17}$$

where Y_+ and Y_- correspond again to $t\gtrless 0$, respectively, and are given explicitly by

$$Y_\pm(x,y_1)=\int_0^\infty\frac{du}{2\pi}\exp[-2x(1+u^2)^{1/2}]V_\pm(u;y_1), \tag{6.18}$$

$$V_\pm(u;y_1)=\tanh\tfrac{1}{2}[\ln(u/y_1^2)\pm\sinh^{-1}(1/u)] \mp(1+u^2)^{1/2}. \tag{6.19}$$

The function $Y_+(x,y_1)$ describing the spatial variation of the energy density in the scaling regime above T_c is shown in Fig. 6 for various fixed values of $y_1=h_1/t^{1/2}$. The qualitative behavior of the profiles can be seen from

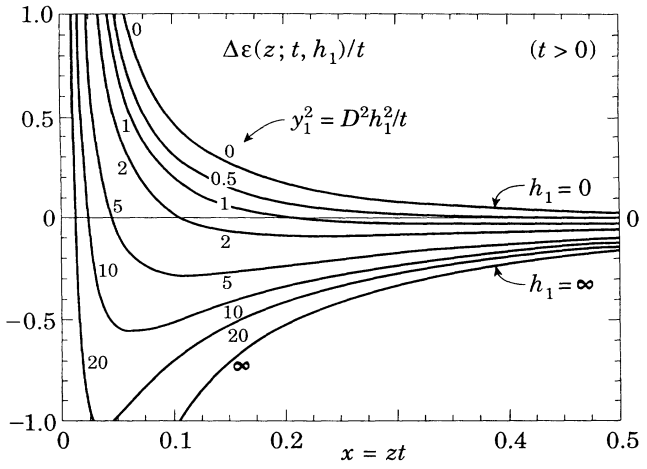

FIG. 6. Net energy-density profiles in the scaling regime at fixed $T > T_c$ near a wall which is subject to a surface field h_1. Note that all profiles are nonmonotonic and display minima except when $h_1 = 0$, which characterizes the *ordinary* surface phase transition, or when $h_1 \to \pm\infty$, corresponding to the *normal* (equivalently, *extraordinary*) surface transition.

various asymptotic results for $Y_\pm$ available in analytical form. Generally, the profile crosses over from the universal power-law decay at criticality with $h_1 = 0$, namely,

$$\Delta\varepsilon_O(z) = 1/4\pi z \ , \tag{6.20}$$

valid also for $z \ll |t|^{-1}, h_1^{-2}$, to the noncritical exponential decay laws

$$\Delta\varepsilon_+ \propto -z^{-1/2}e^{-2tz} \ , \qquad \text{for } t>0 \ , \tag{6.21}$$

$$\Delta\varepsilon_- \propto (2|t| - h_1^2)z^{-3/2}e^{-2|t|z} \ , \quad \text{for } t<0 \ , \tag{6.22}$$

and to the alternative universal critical-point decay law

$$\Delta\varepsilon_{EO}(z) = -1/4\pi z \ , \tag{6.23}$$

when $h_1 \neq 0$. Compare the nontrivial power-law prefactors in (6.21) and (6.22) with the energy-energy correlation function (4.37). The crossover *at* $t=0$ between $\Delta\varepsilon_O(z)$ and $\Delta\varepsilon_{EO}(z)$ is described by

$$\Delta\varepsilon_c(z) = \frac{1}{z}W_c(w = h_1^2 z) = \frac{1}{2\pi z}\int_0^\infty \frac{u-w}{u+w}e^{-2u}du \ . \tag{6.24}$$

This behavior should also be observed on the intermediate scales $z \ll t^{-1}$ for large values of the surface field, $y_1 \gg 1$. Furthermore, the scaling functions $Y_\pm$ in (6.17) can be expressed explicitly for $h_1 = 0$ and h_1 large in terms of the standard Bessel functions, $\mathbf{K}_\nu(z)$, as

$$2\pi Y_\pm(x,0) = \mathbf{K}_1(2x) \mp \mathbf{K}_0(2x) \ , \tag{6.25}$$

$$2\pi Y_\pm(x,\infty) = -\mathbf{K}_1(2x) \mp \mathbf{K}_0(2x) \ . \tag{6.26}$$

In fact, $Y_+(x,0)$ and $Y_+(x,\infty)$ bound the profiles in Fig. 6.

The most remarkable feature of these profiles is their nonmonotonicity. From (6.20)–(6.23) we see that above T_c the profile $\Delta\varepsilon(z)$ must exhibit a minimum for any $h_1 > 0$, as also below T_c when $h_1^2 > 2|t|$: see Fig. 6. To understand this effect, note that owing to the exponential factors $\exp[-2(q^2+t^2)^{1/2}z]$ in (4.28) and (6.17), the dependence of $\Delta\varepsilon(z)$ near a given value of z is determined by the behavior of the prefactor $(\varepsilon_q^0 - \varepsilon_q^\infty)$ for $q \lesssim z^{-1}$ when $zt \ll 1$, but for $q \lesssim (z/t)^{-1/2}$ when $zt \gtrsim 1$. Therefore increasing z in the argument of $\Delta\varepsilon$ is similar to a Wilson momentum-shell renormalization-group operation[2] in that the short-wavelength fluctuations are progressively eliminated. We thus expect the profiles $\Delta\varepsilon(z)$ to exhibit all the crossovers characteristic of surface criticality.[5,6] At short wavelengths the weak fields h_1 and t are unimportant, so the behavior is dominated by the strong disordering effect of the bonds broken at the surface which *increase* the energy density: the correlations transmitting this effect into the bulk are those characteristic of the critical state. [Compare with (4.36).] Thus $\Delta\varepsilon(z)$ is positive and decreases according to the power law (6.20) corresponding to the *ordinary* surface critical behavior[5,6] which occurs in the absence of a local symmetry-breaking field.

However, when $t \gtrsim -h_1^2$ the surface magnetization m_1 exceeds the bulk magnetization, implying that at *large* scales the surface is *more* ordered than the bulk. Indeed, h_1 is a relevant perturbation, its effect increases as $q \to 0$, as is clear from (6.17). Hence, for $t > -\frac{1}{2}h_1^2$ and $q \lesssim h_1^2$, the surface energy-density component ε_q^0 becomes smaller than ε_q^∞. The large-scale fluctuations are then suppressed by the surface field, which is reflected in negative, i.e., lower values of $\Delta\varepsilon(z)$ at large z. When $t=0$ the final destination of the renormalization-group flow is what might best be called the *normal* surface fixed point (since the lack of field symmetry when $h_1 \neq 0$ is generic). This, however, is known to be asymptotically equivalent to the *extraordinary* surface fixed point in which $h_1 = 0$ but the surface spontaneously orders above the bulk T_c owing to enhanced surface couplings.[5,6] This is reflected in the profile (6.23).

Of course, a nonzero bulk thermal field, t, is also a relevant perturbation. The typical effects of t can be seen from the explicit forms (6.25) and (6.26) describing the crossover from the power laws at small z to exponential decay for $z \gtrsim 1/\tilde{\kappa}(q=0) \equiv \xi_b(t)$.

Note that nonmonotonic profiles of $\varepsilon(z)$ are also predicted to occur close to the *special* point in $d = 4-\epsilon$ dimensions by means of operator-product-expansion techniques.[6] (The special point is equivalent to the condition of weak surface field in our $d=2$ case.) These nonmonotonicities were felt, however, to be limited to the critical region, $|t| \ll h_1^2$, since the massive, i.e., noncritical, behavior cannot be obtained directly from the critical operator algebra. Interpolation between our $d=2$ results and those for $d = 4-\epsilon$, however, indicates strongly that nonmonotonicity should also be a generic feature in $d=3$ dimensions.

VII. DOMAIN BOUNDARIES OR INTERFACES

Our interest in the critical behavior at the fixed interface or boundary between distinct domains (see Fig. 2) is twofold. Besides the importance *per se*, especially in

view of the planned studies of criticality in multilayers,[29] we would also like to check the extent to which the surface model (model B) considered in the previous section correctly reproduces the phenomena occurring when one of the two half-planes goes critical, say as $t_+ \to 0$, while the other remains noncritical, $t_- \approx$ const. Most of the work on surface critical behavior[4-8] has been based on the assumption [see hypothesis Ω of Refs. 1(b) and 1(c)] that the response of the "spectator" phase[1(b)] to the fluctuations in the near-critical phase can be neglected, the only significant feature being the presence or absence of local symmetry breaking at the interface. More specifically, we expect for $|t_+| \ll |t_-|$ the difference between the interfacial model (A) and the surface model (B) to be insignificant beyond a surface layer of thickness $z \lesssim \xi_{b-}(T) \approx |t_-|^{-1}$. The effect of symmetry breaking in the spectator phase when $t_- < 0$ should be equivalent to a surface field $h_1 \neq 0$. Correspondingly, an interfacial boundary with a disordered phase, $t_- \gg |t_+| > 0$, should be correctly modeled by symmetric boundary conditions with $h_1 = 0$. We expect matters to be more complicated and interesting, however, when the spectator phase is close to criticality, $|t_-| \ll |t_+|$, so that the fluctuations in the $z > 0$ region are correlated near the surface over distances much longer than in the bulk owing to the *proximity* of the critical phase. Finally, when $t_- = t_+$ we obtain the limiting case of a *defect line* of altered bonds in the planar model, which has independent interest (see, e.g., Ref. 8).

A. General Expressions

We will focus on the incremental energy-density profiles $\Delta\varepsilon(z)$ for $z \geq 0$ defined with respect to $\varepsilon_+^\infty(T) = \varepsilon(z \to +\infty)$: see (4.25). In view of the results of the previous section we expect these profiles to be representative of the general crossovers in critical behavior. On substituting (5.12) into (4.28) and integrating on q we obtain

$$\Delta\varepsilon(z) = \int_0^\Lambda \frac{dq}{2\pi} \{\tanh[g + \tfrac{1}{2}\sinh^{-1}(t/q) + \tfrac{1}{2}\sinh^{-1}(t_s/q)] - \tanh[\sinh^{-1}(t/q)]\} \exp[-2\tilde{\kappa}(q)z]$$
$$\approx t Y(tz,\ t_s/t,\ g)\ , \tag{7.1}$$

where, we have put $t_+ \equiv t$, $t_- \equiv t_s$, the subscript s denoting the spectator phase. Recall also that the field g, defined in (5.7), measures the strength of the K_0 bonds coupling the $+$ and $-$ domains relative to the couplings within the two domains. In the second part of (7.1) scaling is obtained by taking the $\Lambda \to \infty$ limit as usual: the scaling function is

$$Y(x,\tau_s,g) = \int_0^\infty \frac{du}{2\pi} \{\tanh[g + \tfrac{1}{2}\sinh^{-1}(1/u) + \tfrac{1}{2}\sinh^{-1}(\tau_s/u)] - \tanh[\sinh^{-1}(1/u)]\} \exp[-2x(1+u^2)^{1/2}]\ . \tag{7.2}$$

However, this limit is not applicable if $z \lesssim \Lambda^{-1}$, or if $x \lesssim t/\Lambda \ll 1$. In writing these equations we have also limited ourselves to $t > 0$, which is no real restriction because of the symmetry relation

$$\Delta\varepsilon(z,t,t_s,g) = -\Delta\varepsilon(z,-t,-t_s,-g)\ . \tag{7.3}$$

B. Reduction to ordinary and normal surface behavior

From (7.1) and (7.2) we immediately see that when $t \to 0$ with $t_s =$ const, the scaling field τ_s approaches either $+\infty$ or $-\infty$ depending on the relative sign of t_s and t; the only exception arises when $t_s = 0$, which corresponds to the unstable *special* multicritical point value $\tau_s = 0$ which is discussed in the next subsection. Setting $\tau_s = \pm\infty$ in (7.2) leads to

$$Y(x,+\infty,g) = \frac{1}{2\pi}[\mathbf{K}_1(2x) - \mathbf{K}_0(2x)]\ , \tag{7.4}$$

$$Y(x,-\infty,g) = -\frac{1}{2\pi}[\mathbf{K}_1(2x) + \mathbf{K}_0(2x)]\ , \tag{7.5}$$

in one-to-one correspondence to $Y_+(x,0)$ and $Y_+(x,+\infty)$ in (6.25) and (6.26). We may thus identify, precisely as anticipated, $t_s > 0$ and $t_s < 0$ with the ordinary ($h_s = 0$) and the normal (equivalent to the extraordinary) ($h_s \neq 0$) regimes discussed in Sec. VI. Note that the scaling variable g, now representing the modification of the surface bonds, is irrelevant in this limit ($t \to 0$, t_s, g fixed): thus the symmetry relation (7.3) gives

$$Y_-(x,0) = -Y_+(x,+\infty)\ ,$$
$$Y_-(x,+\infty) = -Y_+(x,0)\ , \tag{7.6}$$

just as follows from (6.25) and (6.26).

The expressions (7.4) and (7.5) for $Y(x,\pm\infty,g)$ describe the profiles when $x = O(1)$, i.e., for $z \gtrsim t^{-1} \gg t_s^{-1}$, which in the language of the surface-field model B corresponds to the limits $y_1^2 = h_1^2/t = +\infty$ or 0, for $t_s < 0$ and $t_s > 0$, respectively. To obtain the intermediate scaling regime involving finite y_1 we may follow the idea behind model B and try to compensate the strong ordering effects of a low-temperature spectator phase, with $\tau_s \to \infty$, by weakening the surface bonds, $K_0 \to 0$ (see Fig. 2). In this limit (5.7) and (5.19) give $g \approx -\ln K_0 \gg 1$, while $\sinh^{-1}(\tau_s/u) \approx -\ln(2\tau_s/u)$. Substituting these asymptotic expressions into (7.2) one directly obtains $Y_+(x,y_1)$ as found in (6.18) with, however, y_1^2 replaced by $|\tau_s| e^{-2g}$. Thus model B is recovered with the surface field identified as

$$h_1 \equiv y_1 t^{1/2} = |t_s|^{1/2} e^{-g} \propto |t_s|^{1/2} K_0\ . \tag{7.7}$$

This result is easily understood on recalling (6.12): the magnetic field h_1 acting on the first row of spins of the $z > 0$ half-space is simply given by $m_{-1} K_0$

$\propto(-t_s)^{\beta_1}K_0=(-t_s)^{1/2}K_0$ (see Fig. 2), where the surface magnetization m_{-1} of the spectator phase should not be significantly influenced by the weak coupling to the critical phase.

C. Long-distance behavior

The two different forms of the long-distance behavior, $\Delta\varepsilon_-\propto z^{-3/2}e^{-2|t|z}$ and $\Delta\varepsilon_+\propto z^{-1/2}e^{-2tz}$ found for $t<0$ and $t>0$ in (6.22) and (6.21), respectively, clearly correspond in this representation to t and t_s having the same or different signs. Indeed, for $z\gg t^{-1}, t_s^{-1}$, the integral in (7.1) is dominated by $q\lesssim(t/z)^{1/2}\ll t, t_s$. We can therefore approximate $\sinh^{-1}(t/q)$ by $\mathrm{sgn}\{t\}\ln(2|t|/q)$, and $\sinh^{-1}(t_s/q)$ by $\mathrm{sgn}(t_s)\ln(2|t_s|/q)$ in the argument of (7.1). Depending on the relative signs of t and t_s the two $\frac{1}{2}\ln q$ terms either reinforce or cancel leading to two different forms, namely, for $t>0$, $t_s>0$,

$$\Delta\varepsilon\approx\frac{1}{16\sqrt{\pi}}t^{1/2}(t^{-1}-t_s^{-1}e^{-2g})z^{-3/2}e^{-2tz}\ , \tag{7.8}$$

while for $t>0$, $t_s<0$,

$$\Delta\varepsilon\approx-\frac{1}{4\sqrt{\pi}}t^{1/2}\{1+\tanh[-g+\tfrac{1}{2}\ln(-t_s/t)]\}\times z^{-1/2}e^{-2tz}\ , \tag{7.9}$$

with corrections of relative order $(tz)^{-1}$ in both cases. For $t\ll|t_s|$ these results are equivalent to the $x\gg1$ limits of (7.4) and (7.5), respectively.

D. A boundary with a critical phase

Consider now the special case $t_s=\tau_s=0$ in (7.1) and (7.2). It yields a still different form of long-distance behavior: at small q the preexponential factor in (7.1) and (7.2) now behaves as q, rather than as q^2 when $\mathrm{sgn}\{t\}=\mathrm{sgn}\{t_s\}$, or as q^0 when $\mathrm{sgn}\{t\}=-\mathrm{sgn}\{t_s\}$. The integration over q then yields

$$\Delta\varepsilon(z)\approx-e^{-2g}e^{-2tz}/4\pi z\ . \tag{7.10}$$

This form also holds asymptotically on intermediate scales when $t\gg|t_s|$.

E. Short-distance behavior

At short distances, in the sense $z\ll t,|t_s|$, the integral in (7.1) is dominated by $q\gtrsim z^{-1}\gg t,|t_s|$. For $g\neq0$ the preexponential factor can then be approximated by $\tanh g$, which on integration leads to

$$\Delta\varepsilon(z)\approx(\tanh g)/4\pi z\ . \tag{7.11}$$

This result has also been obtained recently by other methods;[8(b)] indeed, it becomes *exact* for a layer of altered bonds, $g\neq0$, in a critical phase, $t=t_s=0$. Simple power counting shows[8(b)] that such a layer imposes a *marginal* perturbation on the critical phase: in other words, its scaling dimension $\omega=\omega_t-d'$, where $d'=1$ is the dimensionality of the layer, vanishes identically. The marginality is revealed in the continuous dependence of the *amplitude* of the critical power law on the strength of the perturbation, g. By varying g one can smoothly cross over from the universal amplitude $z\Delta\varepsilon(z)=+1/4\pi$ corresponding to *ordinary* surface critical behavior at $g=+\infty$ [see (6.20)] to the universal value $z\Delta\varepsilon=-1/4\pi$ at $g=-\infty$, corresponding to the *normal* (or extraordinary) form (6.23). Note that, physically, $g=+\infty$ means breaking the bonds so creating two new free surfaces, while $g=-\infty$ represents infinitely strong boundary bonds, completely suppressing energy fluctuations in the interfacial plane.

The long-distance part of the energy profile in the defect layer model is just given by (7.8) with $t_s=t$, which yields

$$\Delta\varepsilon\approx(1-e^{-2g})e^{-2tz}/16\sqrt{\pi}z^{3/2}t^{1/2}\ . \tag{7.12}$$

When $g\ll1$ one enters the linear response realm considered in Sec. IV C and one sees that the forms (7.8) and (7.12) may be viewed as deriving from the asymptotic behavior (4.40) of the energy-energy correlation function $G_{\varepsilon\varepsilon}(r)$ by integrating over the transverse coordinate according to

$$\int G_{\varepsilon\varepsilon}(y,z)dy\propto\int(z^2+y^2)^{-1}\exp[-2t(z^2+y^2)^{1/2}]dy\propto e^{-2tz}/z^{3/2}t^{1/2}\ , \tag{7.13}$$

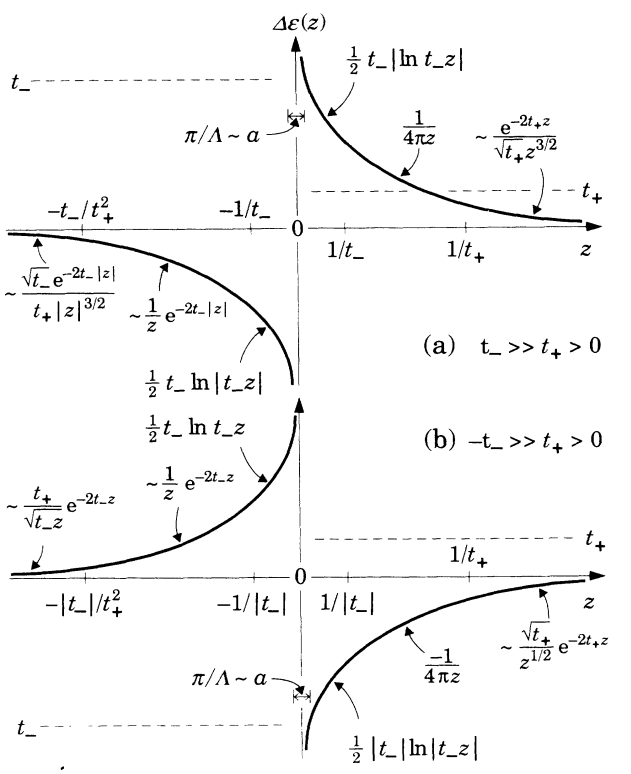

FIG. 7. Schematic depiction of the various asymptotic regimes in the near-critical behavior of the energy profiles, $\Delta\varepsilon(z)$, near a smooth or "matched" (i.e., $g=0$) interface/boundary between two semi-infinite domains with uniform thermal fields (or critical-point deviations) t_+ and t_-. (a) The like case $t_-\gg t_+>0$; (b) the unlike case $-t_-\gg t_+>0$. Note that $\Delta\varepsilon(z)=\varepsilon(z;T)-\varepsilon_\pm^\infty(T)$ where ε_+^∞ and ε_-^∞, the bulk energy densities, differ for $z\gtrless0$: see Eq. (4.25). The total-energy profile, $\varepsilon(z,T)$, varies smoothly through $z=0$: see Fig. 5(a).

for $zt \gg 1$. It is all the more surprising that the long-range part of the energy profile in (7.9) and (7.10) when $\mathrm{sgn}(t_s) \neq \mathrm{sgn}(t)$ differs qualitatively from the predictions of linear response theory.

When $g=0$, which corresponds physically to a smooth or "matched" boundary between the two half-planes (following the discussion in Sec. V), the divergence of $\Delta\varepsilon(z)$ when $z \to 0$ is weaker than (7.11). By using $\sinh^{-1}(t/q) \approx t/q$, and analogously with t_s in place of t, in (7.1) we obtain

$$\Delta\varepsilon(z) \approx \frac{t_s - t}{4\pi} \ln\left[\frac{1}{z t_{\max}}\right], \quad t_{\max} \approx \max[t, |t_s|]\,. \tag{7.14}$$

When $z\Lambda$ approaches unity the upper cutoff Λ in (7.1) can no longer be ignored and $\Delta\varepsilon$ approaches a value of order $(t_s - t)\ln(\Lambda/t_{\max}) \sim (\varepsilon_+^\infty - \varepsilon_-^\infty)$, the difference of the bulk energy densities as given by (4.25). The logarithmic law (7.14) can thus be viewed as a precursor of the smooth behavior across the boundary to be expected for the total, overall profile $\varepsilon(z)$ when $g=0$: see Fig. 5 and recall that $\varepsilon(z;T) = \varepsilon_\pm^\infty(T) + \Delta\varepsilon(z;T)$ where the bulk values $\varepsilon_+^\infty(T)$ and $\varepsilon_-^\infty(T)$, for $z \gtrless 0$, differ whenever $t_+ \neq t_-$. However, the precise form of the profile for $|z| \lesssim \Lambda^{-1}$ is beyond the present scaling-limit considerations.

The results of this section are summarized schematically in Fig. 7 for the case $g=0$. The only qualitative difference appearing when $g \neq 0$ is that the logarithmic law (7.14) goes over to the stronger short-distance divergence (7.11).

VIII. SUMMARY AND PROSPECTS

In summary, we have derived a general variational principle for layered two-dimensional systems belonging to the Ising universality class and have shown that it can be applied effectively to solve physically interesting problems. In place of our original proposal of a functional $\mathcal{S}[m,\varepsilon]$ of just the magnetization and the energy densities, we were forced to include in the argument of the microcanonical functional a whole continuum of variables $\varepsilon_q(z)$ proportional to the densities of the transverse Fourier components of the energy density. Note also that the other Legendre transform, from the magnetic field to the magnetization, has not been performed here: except for surface fields, our analysis has been confined to fixed magnetic field $h=0$. It remains, therefore, to find a way of evaluating the *spontaneous* magnetization below criticality within the present formalism. Luckily, the contributions of different $\varepsilon_q(z)$ decouple: this fact is obviously related to the integrability of planar Ising models. Thus we obtain the set of independent second-order ordinary differential equations (4.5). Reducing the calculational task to solving these equations represents a significant gain relative to the traditional matrix methods, as demonstrated by our analysis here and elsewhere.[29] Even if the equations cannot be solved in a closed form, one may profit from the arsenal of theorems and numerical methods developed for ordinary differential equations; in addition the variational characterization opens the door to the use of trial functions. Another advantage of the present formalism relative to the matrix method is that the scaling limit can be taken at the level of the variational functional itself: see the transition from (2.12) to (3.18). One then automatically obtains all answers in scaling form, describing thereby the whole ($d=2$) Ising universality class. In this respect our method is similar to those based on the conformal symmetry of the critical state;[8(a),30] but, unlike those methods, it is also capable of describing correctly the behavior governed by the noncritical, high- and low-temperature fixed points.

Our study of a linear domain boundary or fixed interface separating two Ising half-planes has revealed a rich variety of crossover phenomena. The crossovers are reflected in the energy profiles which in a sense reproduce the renormalization-group trajectories. A particularly robust feature, which seems likely to extend to $d=3$ dimensions and which should be experimentally detectable, is the nonmonotonicity of the energy profiles near a surface subject to a weak symmetry-breaking field, h_1.

An encouraging technical result of our work is that, while the condition of large local correlation length, $\xi(z) \approx t^{-1}(z) \gg a$, used in justifying the scaling limit (3.18) (see Sec. III A), is likely to fail at a strong, localized defect such as a surface or a boundary, a simple, intuitively appealing extension of the scaling representatation, as in our modeling of a domain boundary using a δ-function contribution to the temperature field $t(z)$, may make it possible to elucidate correctly the essential features of the problem without recourse to the microscopic representation.

From a general viewpoint, one may notice that in both the ($d=1$)- and ($d=2$)-dimensional models with z-dependent inhomogeneities that we have considered so far, the local formulation was achieved by invoking as many independent densities as there are degrees of freedom in the hyperplane perpendicular to the z direction. A formulation very similar to the present one has in fact been obtained also for $d=4-\epsilon$ dimensions.[29] One may thus speculate that this is a general feature of the problem. The integration over a continuum of momenta q allowed us to obtain the nontrivial surface exponent[5] $\Delta_1 = \frac{1}{2}$ determining the scaling $h_1 \propto t^{\Delta_1}$ in the surface-field problem (see Sec. VI). This is an answer to the critique of the earlier local functional formulations presented in Ref. 31. Of course, the existence of a set of transverse modes giving *independent* contributions to the variational functional is probably a special feature of the integrable models considered so far. Whether an interaction between the modes can be included in the framework of an effective local formulation in a more general case, remains to be seen.

In any case, the layered planar Ising model presents a number of interesting problems which may be approached successfully using the present formalism. Apart from the independent interest of these questions, studying the model further may be useful in developing more general insights into the way critical phenomena develop in spatially inhomogeneous systems. Specific prospective further problems include the following:

(i) *Periodic multilayers.* The general solutions of Sec. IV B reduce the problem to algebraic equations which turn out to be solvable in an explicit form.[29] A preliminary analysis reveals a number of interesting, experimentally observable, features.

(ii) *Random multilayers.* It was recently emphasized[17] that while the McCoy-Wu solution[4] of the *random* layered planar Ising model remains almost the only exact calculation available for a nontrivial finite-range random system, our understanding of it is still incomplete. The present formalism reduces the problem to analysis of a nonlinear stochastic differential equation, namely, (4.5) with a randomly varying thermal field $t(z)$ on the right-hand side. This opens the possibility of connecting the problem to other active areas of research. The similarity between the present formalism and that appearing in the perturbative treatment[29] in $d=4-\epsilon$ dimensions, gives some hope of progress for $d=3$, where random multilayers can, in fact, be created by molecular-beam epitaxial growth techniques.[14]

(iii) *Smoothly varying inhomogeneities.* To what extent, say, a smooth periodic modulation, $t(z)=t_0+t_1\cos(Qz)$, can be accurately modeled by a periodic multilayer with sharp interlayer boundaries remains to be seen. This question is relevant both to the general understanding of scaling in spatially inhomogeneous systems and for a number of specific physical problems ranging from the effects of gravity to smooth doping profiles induced by ion implantation, irradiation, etc.[32] While exact analytical solution of the equations of motion (4.5) may be available only rarely, the variational character of our formulation should be particularly useful in such cases.

(iv) *Functional renormalization group for the thermal profiles.* The realization of a functional renormalization-group scheme on the space of profiles $\varepsilon_q(z)$ would be most useful in classifying the various types of critical behavior in layered planar Ising models as well as in suggesting approaches for other dimensionalities and universality classes.

Other possibilities for developing the general variational approach, advanced in Ref. 10 and expounded here, include (a) working with other integrable systems in $d=2$; (b) using conformal invariance principles[30] to study systems with general (rather than layered) inhomogeneities $t=t(\mathbf{r})$; and (c) perturbative approaches[29] for $d>2$.

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