Effective interface Hamiltonians for short-range critical wetting

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The derivation of effective interface Hamiltonians on the basis of an underlying noncritical bulk order-parameter theory is critically examined for use in studying critical wetting transitions in $(d=3)$-dimensional systems with short-range forces. A crossing constraint on the interfacial profile is used to define the fluctuating interface location $l(\mathbf{y})$ and exact general expressions are obtained for the effective wall-interface potential $W[l(\mathbf{y})]$ and for the wall-modified interfacial stiffness $\tilde{\Sigma}[l(\mathbf{y})]$ in terms of a constrained planar order-parameter profile. Previous discussions in the literature are shown to be inadequate. Explicit formulas for W and $\tilde{\Sigma}$ are obtained when the bulk thermodynamic potential for the wetting-layer phase is purely parabolic. Novel terms varying as $le^{-j\kappa l}$ $(j=2,3,\ldots)$ appear in the decay of $\tilde{\Sigma}(l)$ to the free-interface limit $\tilde{\Sigma}_\infty$; here, $1/\kappa\equiv\xi_\beta$ is the true correlation length of the bulk wetting-layer phase. General nonparabolic bulk potentials are analyzed perturbatively, leading to terms in $W(l)$ decaying as $w_{jk}l^k e^{-j\kappa l}$ for $0\le k\le j=1,2,\ldots$. An alternative, generalized adsorption definition for $l(\mathbf{y})$ can be solved exactly for a φ^4 bulk potential and yields closely similar results for $W(l)$. On approach to critical wetting at $T=T_{cW}$ the important coefficients w_{jk} for $k\ge 1$ vanish rapidly with $|T-T_{cW}|$; hence previous renormalization-group (RG) treatments of critical wetting remain essentially unchanged. However, these treatments neglect the variation of $\tilde{\Sigma}(l)$ with l which, under RG flow, is seen here to destabilize wetting criticality; further analyses reported elsewhere, show that first-order transitions then arise in many cases.

I. INTRODUCTION AND SUMMARY

In the theory of wetting transitions an extensively studied but still quite controversial topic is the nature of the *critical wetting transition*[1,2] in a $(d=3)$-dimensional system with short-range interactions *in* the bulk system and *between* the wall and the bulk. Renormalization-group (RG) theory[3–9] predicts striking *nonuniversality* for $d=3$, which is the marginal dimensionality[1–3] for this transition. Specifically, all the critical properties should depend strongly on the dimensionless parameter[1–8]

$$\omega=k_B T_{cW}/4\pi\tilde{\Sigma}(T_{cW})\xi_\beta^2(T_{cW}) , \tag{1.1}$$

where $\tilde{\Sigma}(T)$ is the *stiffness* of the free $\beta|\alpha$ interface between the bulk wetting phase β and the bulk phase α. At bulk $\alpha-\beta$ coexistence the $\beta|\alpha$ interface delocalizes from the rigid wall when $T\to T_{cW}-$; for $T>T_{cW}$ the interface is free at a macroscopic distance from the wall. The (finite) *bulk correlation length of the wetting phase* β is denoted ξ_β and enters the theory[1–8] as the basic length scale. It will follow from our analysis and the RG theory[2–6] that ξ_β is to be taken as the *true correlation length* which determines the exponential decay of correlations and, hence, of the tail of the interfacial profile in the direction normal to the wall and interface.

When ω is negligibly small, local mean-field or classical square-gradient theory[10] should apply. When ω increases from 0 the exponents gain nonclassical values. For instance, the exponent $\nu_\parallel$ of the diverging *interfacial correlation length* $\xi_\parallel$ (parallel to the interface) increases first as $1/(1-\omega)$ for $\omega<\frac{1}{2}$ (regime I), then as $1/(\sqrt{2}-\sqrt{\omega})^2$, which diverges when $\omega\to 2-$, for $\frac{1}{2}<\omega<2$ (regime II). Finally, $\nu_\parallel=\infty$ for all $\omega>2$ (regime III).[1,2,4,6]

Experimental tests of this theory are not yet available for fluids, where it should most directly apply, because of the ubiquitous influence of long-range van der Waals or dispersion forces.[1,2] (For that case see Dietrich and Napiórkowski.[11]) However, extensive Monte Carlo simulations of critical wetting have been performed[12–14] for a semi-infinite, $(d=3)$-dimensional simple cubic Ising model above its roughening temperature T_R. Initial estimates of $\omega(T)$ for the observed critical wetting temperatures (which depend on the surface field h_1, etc.) indicated $\omega\gtrsim 1.0$.[12] Thus regime II behavior was expected. More recent estimates[13,14] (using numerical data for the true bulk correlation length in place of the second-moment correlation length ξ_1) indicate $\omega(T)\gtrsim 0.60$ for $T>T_R$, again pointing to regime II and hence $\nu_\parallel>2$. Surprisingly, however, the Monte Carlo data were found to be consistent merely with classical mean-field theory[10] which predicts $\nu_\parallel=1$ (as for $\omega=0$)!

This discrepancy has, of course, attracted further attention.[13–18] In particular, a new Monte Carlo simulation[15] of the solid-on-solid limit of the simple cubic Ising model and a reanalysis[16] of the original data of Refs. 12(a)–12(c) have been interpreted as indicating nonclassical critical wetting behavior corresponding to $\omega\simeq 0.25$ in the simulated Ising model. Evidently the discrepancy between the RG predictions and the simulations remains significant and disturbing. Various explanations have been advanced;[1,2,15–18] however, few seem to be viable and the issue remains unsettled.

Accordingly, it is appropriate to undertake a careful examination of the foundations of the RG theory,[1–9] which is based on an effective interfacial Hamiltonian,

$\mathcal{H}_I[l(\mathbf{y})]$, where $l(\mathbf{y})$ is the fluctuating, normal distance of the $\beta|\alpha$ interface from the point $\mathbf{y}$ on the $d'=(d-1)$-dimensional planar wall which we suppose is located at $z=0$. A crucial ingredient of this theory is an effective, wall-interface potential $W(l;T,\ldots)$, which depends not only on the interface location l, but also in a vital way on the temperature T and other bulk and surface thermodynamic fields. In a typical critical situation treated by RG theory, most details of the underlying microscopic interaction potentials feature only as *irrelevant* parameters and thus do *not* affect the critical exponents, critical amplitude ratios, etc. However, as mentioned, $d=3$ is the marginal dimensionality for short-range critical wetting and it thence transpires[1–7] that the *detailed* forms of decay of the effective potential $W(l)$, in terms of the bulk correlation-decay factor $\exp(-l/\xi_\beta)$, play a determining role in the values and variation of the critical exponents, etc. For this reason it is important to ascertain the appropriate behavior of $W(l;T,\ldots)$ and of any other significant ingredients of the fundamental interface Hamiltonian $\mathcal{H}_I[l(\mathbf{y})]$. That is the issue we address in this article.[19]

Now in real systems undergoing wetting transitions (which may be reasonably mimicked by a semi-infinite lattice system above the interface roughening temperature, such as the Ising models simulated[12–14]) the $\beta|\alpha$ interface appears only as a result of the interplay of local density variables, say $s(\mathbf{r})$, distributed throughout the bulk d-dimensional space. The fluctuations of these variables are clearly described by some more fundamental microscopic Hamiltonian, say $\mathcal{H}_{\text{mic}}[s(r)]$, where, in an Ising-like system, $s(r)$ may be regarded simply as the spin at position $\mathbf{r}=(\mathbf{y},z\geq 0)$. Since wetting transitions arise (by definition) only in systems that are *not* at bulk criticality, one may with fairly good justification[1,2] hope to describe the bulk phases satisfactorily at an intermediate, order-parameter level with $s(\mathbf{r})\Longrightarrow m(\mathbf{r})$ and $\mathcal{H}_{\text{mic}}[s(\mathbf{r})]$ replaced by a Landau-Ginzburg-Wilson effective Hamiltonian of the form[1,2,10]

$$\mathcal{H}[m(\mathbf{r})]=\int\{[\tfrac{1}{2}K\dot{m}^2+\Phi(m)]dz+\Phi_1(m_1)\}d^{d'}y\ , \quad (1.2)$$

where $\dot{m}\equiv\nabla m(\mathbf{r})$ while $\Phi[m(\mathbf{r})]$ is the noncritical bulk free-energy density. The effect of the wall with short-range, wall-bulk interactions is accounted for by $\Phi_1(m_1)$, where $m_1(\mathbf{y})\equiv m(\mathbf{y},z=0)$ is the surface order parameter. For a bulk system near α-β coexistence, one may normally take

$$\Phi(m;T,h)=\Phi_0(m;T)-hm\ , \quad (1.3)$$

where $\Phi_0(m)$ has the standard double-well functional shape with two equal minima at $m=m_{\alpha 0}<0$ and $m_{\beta 0}>0$, while the bulk thermodynamic field h measures the deviation of the chemical potential from precise coexistence (or, equivalently, represents the external ordering field). We adopt a sign convention such that $h\leq 0-$ stabilizes the α phase at $z=+\infty$. For the effective surface potential it is adequate to take the truncated expansion[1,2,9,20,21]

$$\Phi_1(m_1)=-h_1m_1-\tfrac{1}{2}gm_1^2\ , \quad (1.4)$$

where h_1 is the surface field, with $h_1>0$ favoring the β phase, while g is the surface enhancement parameter. For the sake of the current discussion we may assume that g is *negative,* which corresponds to the typical situation.

Evidently, the appropriate interfacial Hamiltonian $\mathcal{H}_I[l]$ is not obvious *a priori* but, rather, must be derived[1,2] by consideration of the bulk description embodied in (1.2)–(1.4) with the given form of $\Phi_0(m;T)$ and of $\Phi_1(m_1)$. Now the widely accepted conclusion[3–6,18] of such an analysis is

$$\Delta\mathcal{H}_I[l(\mathbf{y})]=\int d\mathbf{y}\{\tfrac{1}{2}\tilde{\Sigma}[\nabla l(\mathbf{y})]^2+W[l(\mathbf{y})]\}\ , \quad (1.5)$$

where $\Delta\mathcal{H}_I$ represents the incremental free energy over a flat, isolated $(l\to\infty)$ interface. As before, $\tilde{\Sigma}$ is the stiffness of an isolated, free interface at $T=T_{cW}$, while the *bare effective wall-interface interaction* is expected to assume the form

$$W(l;T,h)=\bar{h}l+w_1e^{-\kappa_1 l}+w_2e^{-\kappa_2 l}+\cdots\ , \quad (1.6)$$

in which the reduced ordering field is $\bar{h}\sim -\bar{h}(\to 0+)$; the exponential decrements are given by

$$\kappa_n=n\kappa\equiv n/\xi_\beta,\quad n=1,2,3,\ldots, \quad (1.7)$$

that is, they are *integral* multiples of $\kappa=1/\xi_\beta$, the inverse correlation length of the wetting layer which, as mentioned, also controls the exponential decay of the interfacial profile and of the correlations into the bulk β phase. The l-independent coefficients $w_1(T,\ldots)$, $w_2(T,\ldots),\ldots$ are smooth functions of the controlling thermodynamic fields T, h, h_1, and g. In particular, for $h=0$ and h_1 and g fixed one has $w_1\sim(T-T_{cW}^0)$ where T_{cW}^0 is the mean-field critical wetting temperature and we may assume that $w_2,\ldots>0$ near the transition.

Nevertheless, as reported previously,[2,19] it appears that the conclusions embodied in (1.5)–(1.7) are rather poorly founded. Indeed, we find, as explained below,[19] that they are *not,* in general, accurate. Rather we show that (1.6) should be replaced by

$$\begin{aligned}W(l;T,h,h_1,g)=\bar{h}l&+(w_{10}+w_{11}\kappa l)e^{-\kappa l}\\&+[w_{20}+w_{21}\kappa l+w_{22}(\kappa l)^2]e^{-2\kappa l}\\&+\cdots\ ,\end{aligned} \quad (1.8)$$

with, however, rather special dependences of the polynomial coefficients $w_{10}(T,\ldots),\ldots,w_{22}(T,\ldots),\ldots$ on the thermodynamic parameters near the mean-field critical wetting transition.

We also show explicitly, as is natural to anticipate,[5(b)] that for $l<\infty$ the coefficient of $(\nabla l)^2$ in (1.5) picks up terms depending, albeit relatively weakly, on l, h, h_1, and g. In other words, the *interfacial stiffness* becomes the *function* $\tilde{\Sigma}(l;T,h,h_1,g)$ which approaches the stiffness $\tilde{\Sigma}=\tilde{\Sigma}_\infty(T)$ of an isolated, free interface only when $l\to\infty$. An explicit expansion of $\tilde{\Sigma}(l;T,\ldots)$ for large l parallels (1.8).[19(b)] The consequences of these modifications to the form of $W(l;T,\ldots)$ and of $\tilde{\Sigma}(l;T,\ldots)$ for critical wetting and other wetting transitions are discussed in the body of this article; the effects of the l dependence of $\tilde{\Sigma}$ can be dramatic.[19(b)]

Our derivation of the effective interfacial Hamiltonian $\mathcal{H}_I[l(\mathbf{y})]$ is based on the introduction of the "collective coordinate" $l(\mathbf{y})$ via a suitable *constraint* on the microstates accessible to the full bulk system. Such a procedure is, of course, not at all new in condensed matter physics. Nevertheless the literature[22,23] is fairly sparse as regards explicit and precise calculations of the sort that are needed here. In particular, the significance of $\tilde{\Sigma}(l)$ and its analogs seems mostly unappreciated.[5(b)] The discussion and concrete analysis we present should, therefore, have value beyond the particular topic of critical wetting theory.

In outline the paper is set out as follows: In Sec. II the precise definition of the effective potential is developed in terms of an explicit *level crossing criterion* for specifying the interface conformation $l(\mathbf{y})$. For fixed $l(\mathbf{y})$, this may be embodied in a constraint on the interfacial profile $m(\mathbf{r})$. Explicit expressions are thence obtained for the potential $W(l)$ and for the effective interfacial stiffness $\tilde{\Sigma}(l)$ in terms of the profile $m_{\Pi}(z;l)$ of a *planar* interface constrained to lie at $l(\mathbf{y})=l_\pi$ fixed: see Eqs. (2.13) and (2.26). A critique of previous derivations[3,5,20] of the effective potential, all leading to the simple exponential form (1.6), is presented in Sec. III and various inadequacies are noted. However, the computation of $m_{\Pi}(z;l)$ to sufficient precision proves to be difficult in general. Accordingly, in Sec. IV, a particular, somewhat artificial expression for the underlying potential $\Phi_0(m,T)$ [in (1.3)] is adopted, namely an asymmetric double-parabolic form.[24] The problem then becomes tractable and can be analyzed completely. At this level, indeed, the purely exponential form (1.6) is captured with explicit general expressions for the coefficients $\bar{h}, w_1, w_2, \ldots$: see (4.20)–(4.22); but for $\tilde{\Sigma}(l)$ the sequence of new terms varying as $le^{j\kappa l}$ for $j=2, 3, \ldots$ already appears: see (4.29)–(4.33).

To proceed further a perturbative approach[19(a)] is introduced in Sec. V: the potential well describing the β phase (which wets the wall) is, in zeroth approximation, represented by a truncated parabola in m; the neglected cubic, quartic, etc. terms can then be handled systematically to yield the asymptotic behavior of $W(l)$ and $\tilde{\Sigma}(l)$. This yields the modified form (1.8), with $w_{21}\neq 0$ and $w_{11}=w_{22}=\cdots=0$ (for $h=0$) and a related form for $\tilde{\Sigma}(l)$ with corresponding coefficients s_{jk} for all $k\leq j=0,1,\ldots$.[19]

An alternative *integral criterion*[19(a)] for defining generalized "adsorption thicknesses" $\bar{l}(\mathbf{y})$, parametrized by a power $p>1$, is discussed in Sec. VI: see also Eq. (2.11). The corresponding constraint equations for the profile can be solved in closed form for $p=2$, 3, and 4 with the aid of a Lagrange multiplier; the case $p=2$ is studied in detail via an exact expression for the profile for general T, h, h_1, g, and $\bar{l}$. The resulting wall potential has, when expressed in terms of $\bar{l}$, a pure exponential form like (1.6). However, if the thickness is reexpressed in terms of the corresponding crossing positions l, all terms in the modified form (1.8) are generated, thus confirming the conclusions of Sec. V. [The stiffness $\tilde{\Sigma}(l)$ can also be analyzed within the formulation.[19]]

Finally, in Sec. VII, the effects of the new form of the interfacial Hamiltonian on the nature of the critical wetting transition are analyzed using (for $d=3$) the linearized functional renormalization-group method.[6] If the stiffness variation is *neglected* one finds that the terms in $W(l)$ of the form $w_{jk}l^k e^{-j\kappa l}$ with $k\geq 1$ can in general lead to significant effects in the critical behavior, at least in regimes I and II where $\omega<2$.[19(a)] However, the new coefficients $w_{jk}(T,h)$ for $k\geq 1$ turn out, as a result of the calculations in Secs. IV–VI, to vanish sufficiently rapidly as $T\to T_{cW}^0$ that, except for small terms in the correction factors to the leading critical behavior, *no changes* to the original RG predictions[4,6] result![19(a)] This situation is dramatically changed, however, when the leading variation of $\tilde{\Sigma}(l)$ is allowed for. As explained briefly in Sec. VII C, the wetting transition in zero field may then become *first order*. However, the somewhat involved analysis needed to elucidate this is postponed for subsequent presentation.

II. DEFINITION OF THE EFFECTIVE HAMILTONIAN

As indicated in the Introduction, we define the interface Hamiltonian $\mathcal{H}_I[l(\mathbf{y})]$ via the introduction of a constraint which specifies restrictions on the accessible microstates of the underlying bulk Hamiltonian $\mathcal{H}[m(\mathbf{y},z)]$ that are compatible with the given interfacial configuration $z=l(\mathbf{y})$. If $\mathrm{Tr}_{l(\mathbf{y})}^{m(\mathbf{r})}$ denotes the appropriate trace (or functional integral) over the bulk variables $m(\mathbf{r})$ as *constrained* by the conformation of $l(\mathbf{y})$, then $\mathcal{H}_I$ is naturally defined[2] via

$$\exp(-\beta\mathcal{H}_I[l(\mathbf{y})])=\mathrm{Tr}_{l(\mathbf{y})}^{m(\mathbf{r})}\{\exp(-\beta\mathcal{H}[m(\mathbf{r})])\}\ , \qquad (2.1)$$

with $\beta=1/k_BT$. Taking the complementary trace $\mathrm{Tr}^{l(\mathbf{y})}$ over the interface configurations then reproduces the exact partition function $Z(T,h,h_1,g)\equiv Z\{\mathcal{H}[m(\mathbf{r})]\}$. This step, once $\mathcal{H}_I[l]$ is obtained, is to be the subject of renormalization-group analysis, etc.[1–9]

A. Constrained profile

Unfortunately, a direct implementation of (2.1) represents an intractable problem, typically as difficult as computing Z directly. In the spirit of previous workers, we therefore argue that the only dangerous, divergent fluctuations at a wetting transition (critical *or* complete) arise from the capillary waves on the delocalizing interface. If the interfacial configuration is frozen one has only the fluctuations associated with the bulk phases α and β in the presence of a wall. These phases are both *noncritical*, their fluctuations being controlled by finite correlation lengths ξ_α and ξ_β; in terms of these, the effects of any local perturbations must decay at least as fast as e^{-r/ξ_α} or e^{-r/ξ_β}, respectively; furthermore, in general, the effects cannot decay any *more* rapidly (except for power-law factors, $1/r^{(d-1)/2}$, etc.). We thus postulate that a saddle-point or mean-field treatment of the constrained trace in (2.1) will be adequate to describe the asymptotics of a wetting transition in which $l\to\infty$. It is clear from this discussion that ξ_α and ξ_β refer to the *true* correlation lengths as against, say, the second-moment correlation lengths $\xi_{1\alpha}$ and $\xi_{1\beta}$.[25]

Consequently, if the *interfacial profile* which minimizes $\mathcal{H}[m(\mathbf{r})]$ subject to the constraint represented by the interface configuration $l(\mathbf{y})$ is

$$m(\mathbf{r})=m_{\Xi}[r;l(\cdot)]\ , \tag{2.2}$$

we accept the approximation

$$\mathcal{H}_I[l(\cdot)]=\mathcal{H}[m_{\Xi}(\mathbf{r};l(\cdot))]=\min_{m(\mathbf{r})}{}^{l(\cdot)}\mathcal{H}[m(\mathbf{r})]\ . \tag{2.3}$$

Relaxation of the constraint or, equivalently, minimizing $\mathcal{H}_I[l(\mathbf{y})]$, yields the overall *optimal* (mean-field) *profile* $\check{m}(z;T,h,h_1,g)$ which, by translational symmetry parallel to the wall, will describe a planar interface, with no $\mathbf{y}$ dependence, at the *optimal location* $l=\check{l}(T,h,h_1,g)$. One must thus have

$$\check{m}(z)=m_{\Xi}(0,z;l=\check{l})\ , \tag{2.4}$$

with

$$\mathcal{H}_I[l=\check{l}]=\mathcal{H}[\check{m}(z)]=\mathcal{H}_{\min}\ . \tag{2.5}$$

Various possibilities arise in choosing a constraint to represent the interface.[22,23] We focus initially on the natural *crossing criterion*[19,21] specified by

$$m[\mathbf{y},z=l(\mathbf{y})]=m^{\times}\quad \text{for all } \mathbf{y}\ , \tag{2.6}$$

in which $m^{\times}$ is a fixed reference level lying between the values $m_{\alpha\infty}$ and $m_{\beta\infty}$ that characterize the bulk α and β phases: see Fig. 1. For convenience we will suppose

$$m_{\alpha\infty}(T,h)<0<m_{\beta\infty}(T,h)\ . \tag{2.7}$$

Then, without loss of generality [since a uniform shift in $m(\mathbf{r})$ is always allowed], one may take $m^{\times}=0$: see Fig. 1.

With this crossing criterion and the explicit form (1.2) for $\mathcal{H}[m]$, minimization yields the bulk equation

$$K\nabla_{\perp}^2 m+K\frac{\partial^2 m}{\partial z^2}=\frac{\partial\Phi}{\partial m}\equiv\Phi'(m)\ , \tag{2.8}$$

in which $\nabla_{\perp}^2$ denotes the d'-dimensional Laplacian operator in $\mathbf{y}$. This equation must be satisfied by the constrained profile $m_{\Xi}[\mathbf{r};l(\cdot)]$ both in the wetting-layer or β region $\{0\le z<l(\mathbf{y})\}$ and in the bulk or α region $\{z\ge l(\mathbf{y})\}$. In the wetting layer the *wall condition*

$$K\frac{\partial m}{\partial z}(z=0)=\frac{\partial\Phi_1}{\partial m}\equiv\Phi_1'(m_1)\qquad \text{with } m_1\equiv m(z=0) \tag{2.9}$$

must be imposed. Finally, the constrained profile must obey the asymptotic *bulk condition*

$$m(z\to\infty)\to m_{\alpha\infty}(T,h)\ , \tag{2.10}$$

as well, of course, as the constraint (2.6) on the boundary separating the α and β regions. The optimal profile $\check{m}(z)$ satisfies just (2.8)–(2.10) for all z.

It follows from (2.8) that when the potential $\Phi(m)$ is continuous, as is physically desirable, the optimal profile $\check{m}(z)$ is everywhere smooth [even if $\Phi'(m)$ has discontinuities]. On the other hand, the *constrained* profile $m_{\Xi}[\mathbf{r};l(\cdot)]$ will in general have a *kink*, i.e., a discontinuity in gradient, whenever $\mathbf{r}$ crosses the interface location $z=l(\mathbf{y})$: see Fig. 1. (It may be remarked that Fig. 5 in Ref. 22 is misleading in this respect since no kinks are

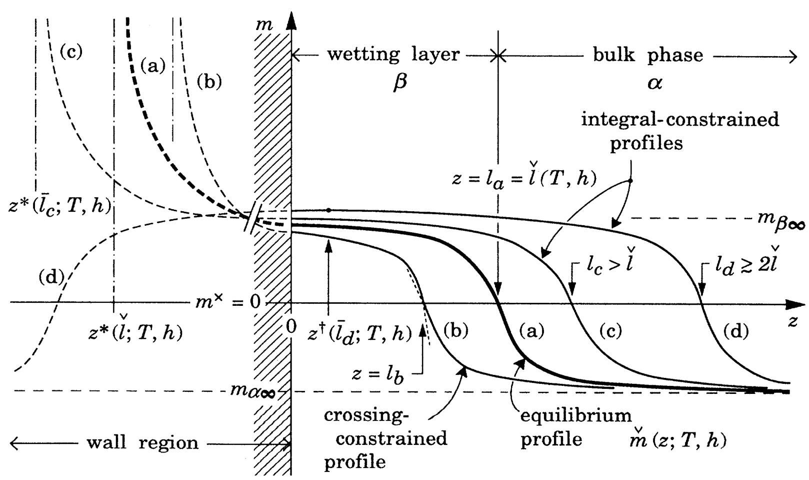

FIG. 1. Schematic order-parameter profiles near a critical wetting transition derived via mean-field theory. Solid curves: (a) denotes the optimal or equilibrium profile $\check{m}(z;T,\ldots)$, which is everywhere smooth and crosses the reference level $m^{\times}=0$ at the equilibrium interface position $z=\check{l}(T,h,h_1,g)$; (b)–(d) represent constrained profiles $m_{\Xi}(z;T,\ldots)$ with crossings at $l_b,l_c,l_d\neq\check{l}$. All the constrained profiles satisfy the wall boundary condition at $z=0$ and approach the bulk phase limit $m=m_{\alpha\infty}(T,h)$ as $z\to\infty$. More specifically, (b) is constrained by the *crossing criterion* and has a kink (slope discontinuity) at $z=l_b$. Two profiles derived under the *integral criterion* are represented by (c) and (d); they are everywhere smooth (with no kinks). Dashed curves represent the analytic extensions of (a)–(d) from $z\ge 0$ to $z\le 0$. Profiles with $\check{l}-l$ small or positive typically diverge to $+\infty$ at $z=z^*\simeq-\check{l}$; profiles with $l-\check{l}\gg\xi_\beta$ have a symmetry about a maximum at $z^{\dagger}$. The wall value m_1 increases monotonically with l, but the slope $\dot{m}_1$ changes sign.

shown in the constrained profiles although they must be present.) A sharp kink could be avoided by utilizing some smooth but strongly localized constraint potential, say $\Psi[m,\mathbf{r};l(\cdot)]\simeq\Psi_0\delta(m-m^{\times})\delta[z-l(\mathbf{y})]$, to specify the interface.[22] Clearly, however, the subsequent analysis would be more complicated. Furthermore, if, as would be reasonable, $\Psi(\mathbf{r})$ were localized about $z=l(\mathbf{y})$ to within distances of ξ_α, ξ_β, or smaller, the behavior for $l\gg\xi_\alpha,\xi_\beta$, which is of principal interest, should be negligibly disturbed.

On the other hand, in Sec. VI below we will explore an *integral criterion* in which the interface location, which we now denote by $z=\bar{l}(\mathbf{y})$, is specified by

$$\bar{l}(\mathbf{y})=\int_0^\infty dz[m(\mathbf{y},z)-m_{\alpha\infty}]^p/(m_{\beta\infty}-m_{\alpha\infty})^p , \qquad (2.11)$$

with $p>0$. In the case $p=1$, the interface thickness $\bar{l}$ corresponds to the adsorption (of phase β on the wall). The corresponding constraint can be imposed (for $p>1$) with the aid of a Lagrange multiplier and leads to a *smooth* constrained profile $\bar{m}_{\Xi}[\mathbf{r};\bar{l}(\cdot)]$: see Fig. 1. (The difficulties associated with the choice $p=1$ are explained in Sec. VI.)

B. Wall-interface potential and stiffness

On the basis of the crossing criterion it is natural to consider, first, planar interfaces for which $l(\mathbf{y})=l_\pi$ is constant; as remarked, the optimal interface is planar. Let us denote the corresponding constrained profile by

$$m_{\Pi}(z;l_\pi)\equiv m_{\Xi}(\mathbf{r};l(\cdot)=l_\pi) . \qquad (2.12)$$

It satisfies (2.6), (2.8) with vanishing $\nabla_{\perp}^2 m$ term, and (2.9), and (2.10). The corresponding value of $\mathcal{H}_I$ follows from (2.3) and, by comparison with the presumed form (1.5), we thence obtain the effective *wall potential* explicitly as

$$W(l;T,h,h_1,g)=\int_0^\infty\left[\frac{1}{2}K\left[\frac{\partial m_{\Pi}}{\partial z}\right]^2+\Delta\Phi(m_{\Pi}(z;l))\right]dz +\Phi_1(m_{\Pi}(0;l))-W_\infty(T,h,h_1,g) , \qquad (2.13)$$

where

$$\Delta\Phi(m;T,h)=\Phi(m;T,h)-\Phi_{\min}(T,h) , \qquad (2.14)$$

in which $\Phi_{\min}(T,h)$ for $h\le 0$ denotes the free-energy density of the bulk α phase. The last term on the right-hand side of (2.13) represents the l-independent terms; for $h=0$ it may be determined simply from the requirement $W(l;h=0)\rightarrow 0$ as $l\rightarrow\infty$. However, one must more generally have $W_\infty=\Sigma_{\alpha|\beta}(T)+\Sigma_{\omega|\beta}(T,h,h_1,g)$ where $\Sigma_{\alpha|\beta}$ is the tension of an isolated $\alpha|\beta$ interface while $\Sigma_{\omega|\beta}$ represents the wall free energy against the β phase. Of course, both $\Sigma_{\alpha|\beta}$ and $\Sigma_{\omega|\beta}$ will be represented only at the mean-field level corresponding to $\mathcal{H}[m]$.[10]

To check the form (1.5) for $\mathcal{H}_I$ as regards the $(\nabla l)^2$ dependence, and to evaluate the coefficient $\tilde{\Sigma}$ clearly require interface configurations $l(\mathbf{y})$ that vary with $\mathbf{y}$. We adopt a perturbative approach and set

$$l(\mathbf{y})=l_\pi+\delta l(\mathbf{y}) , \qquad (2.15)$$

so that $\nabla l(\mathbf{y})=\nabla\delta l(\mathbf{y})$, and write

$$m_{\Xi}(\mathbf{r};l(\cdot))=m_{\Pi}(z;l_\pi)+\delta m(\mathbf{r};l(\cdot)) . \qquad (2.16)$$

Then by (2.8)–(2.10) the correction $\delta m(\mathbf{r})$ satisfies the bulk equation

$$K\nabla^2\delta m=\Phi''(m_{\Pi}(z))\delta m+O(\delta m^2) , \qquad (2.17)$$

with wall and asymptotic conditions

$$K(\partial\delta m/\partial z)_{z=0}=\Phi_1''(m_{\Pi}(0))\delta m_1(\mathbf{y})+O(\delta m_1^2) , \qquad (2.18)$$

$$\delta m(\mathbf{y},z;l(\cdot))\rightarrow 0 \quad \text{as } z\rightarrow\infty , \qquad (2.19)$$

for all $\mathbf{y}$, where $\Phi''=(d^2\Phi/dm^2)$, $\Phi_1''=(d^2\Phi_1/dm_1^2)$, and $\delta m_1\equiv\delta m(\mathbf{y},z=0)$. The interfacial constraint (2.6) now becomes

$$m_{\Pi}[l_\pi+\delta l(\mathbf{y});l_\pi]+\delta m[\mathbf{y},z=l_\pi+\delta l(\mathbf{y});l(\cdot)]=m^{\times} \qquad (2.20)$$

(for all $\mathbf{y}$), which may be expanded in powers of δl to yield

$$\delta m(\mathbf{y},l_\pi;l(\cdot))=-\frac{\partial m_{\Pi}}{\partial z}(l_\pi;l_\pi)\delta l(\mathbf{y})[1+O(\delta l)] , \qquad (2.21)$$

where we have supposed that $(\partial/\partial z)\delta m(\mathbf{r})$ is of order δm near $l=l_\pi$.

To solve (2.17) subject to (2.18), (2.19), and (2.21) to leading (linear) order consider the function

$$n(z;l)=\frac{\partial}{\partial l}m_{\Pi}(z;l) . \qquad (2.22)$$

By differentiating (2.8)–(2.10) with $m=m_{\Pi}(z;l)$, with respect to l we see that $n(z)$ satisfies the full linear homogeneous partial differential equation (2.17) [neglecting the $O(\delta m^2)$ terms] and the homogeneous boundary conditions (2.18) [again neglecting $O(\delta m^2)$] and (2.19). Finally (2.6) implies

$$m_{\Pi}(l;l)=0 , \qquad (2.23)$$

which on differentiation yields the inhomogeneous boundary condition

$$n(l;l)=-\frac{\partial m_{\Pi}}{\partial z}(z=l,l) \qquad (2.24)$$

at $z=l$. But, except for a supplementary factor $\delta l(\mathbf{y})[1+O(\delta l)]$ on the right-hand side of (2.24) in comparison with (2.21), these equations and boundary conditions are identical to those specifying $\delta m(\mathbf{r};l(\cdot))$ in leading order. We thus conclude that the perturbed constrained profile is given by

$$\delta m(\mathbf{r};l(\cdot))=n(z;l_\pi)\delta l(\mathbf{y})[1+O(\delta l)] . \qquad (2.25)$$

Now we can restrict attention to variations δl satisfying $\int\delta l(\mathbf{y})d\mathbf{y}=0$, substitute again in (2.3), and compare with (1.5) to obtain

$$\tilde{\Sigma}(l;T,h,h_1,g)=K\int_0^\infty\left[\frac{\partial m_{\Pi}}{\partial l}(z;l)\right]^2 dz . \qquad (2.26)$$

It is to be anticipated that the right-hand side has a definite, positive limit $\tilde{\Sigma}_{\infty}(T)$, independent of h_1 and g, when $l \rightarrow \infty$ with $h=0$. This limit represents the interfacial stiffness of a free $\alpha|\beta$ interface which, since the Hamiltonian $\mathcal{H}[m(\mathbf{r})]$ describes a system with no spatial anisotropy, will satisfy $\tilde{\Sigma}_{\infty}=\Sigma_{\alpha|\beta}$ (where, as before, the tension is expressed only at the mean-field level). Note that higher-order terms in $\mathcal{H}_I[l]$ proportional to $(\nabla l)^4, (\nabla^2 l)^2$, etc., also arise and can be computed.[26]

The expressions (2.13) for $W(l)$ and (2.26) for $\tilde{\Sigma}(l)$ are the principal results of this section; the latter is exact for all square gradient theories and seems to be quite new. The results rest on the solution $m_{\Pi}(z;l)$, of the variational equation (2.8) for a planar, $\mathbf{y}$-independent profile $l(\mathbf{y})=$const, subject to the boundary conditions (2.9), (2.10), and (2.6) which may be embodied in (2.23).

Although our approach is fairly straightforward, and seems to have been adopted more or less implicitly or explicitly by previous workers, it turns out to be tricky to implement precisely for a general form of potential $\Phi_0(m)$ [in (1.3)], even if one seeks, as we do, only the behavior of $W(l)$ and $\tilde{\Sigma}(l)$ for large l. Restricting the calculations to the standard phenomenological form

$$\Phi_0(m)=\tfrac{1}{2}rm^2+\frac{1}{4!}um^4 \tag{2.27}$$

leads to implicit expressions involving elliptic integrals; however, these prove difficult to analyze asymptotically. Furthermore, as we explain briefly in Sec. III, previous treatments in the literature prove, on examination, to be rather unsatisfactory. In particular, the crucial profile $m_{\Pi}(z;l)$ has not been evaluated adequately. Readers uninterested in our critique may proceed directly to Sec. IV. There we approach the problem by choice of a special, simplified form of $\Phi_0(m)$ for which a fully explicit solution can be developed. Subsequently, we treat the general situation as a perturbation around the special case finding, in fact, new features not present in the family of simplified models.

III. CRITIQUE OF PREVIOUS DERIVATIONS

As mentioned above, this section is *not* needed for the technical development of our analysis. However, insofar as there are essentially three distinct previous discussions in the literature[3,5,20] which treat the derivation of $W(l)$ from $\mathcal{H}[m(\mathbf{r})]$ and obtain the simple exponential form (1.6), it seems appropriate to review the methods used briefly and to explain why they are not satisfactory. This will also bring out some of the physical subtleties involved.

An elementary observation is worth making. If one has correctly derived the effective potential $W(l)$, then solving the equation

$$(\partial W/\partial l)|_{l=\check{l}}=0 \tag{3.1}$$

must yield the exact optimal location $\check{l}(T,h,h_1,g)$ of the equilibrium planar interface that follows from the original bulk Hamiltonian $\mathcal{H}[m(\mathbf{r})]$: see (1.5) and (2.3)–(2.5). This, in turn, yields the full wetting phase diagram.[10] Conversely, if some calculation yields a form for the potential, say,

$$W(l)=\bar{h}l+(w_{10}+w_{11}\kappa l)e^{-\kappa l}+(w_{20}+w_{21}\kappa l)e^{-2\kappa l}, \tag{3.2}$$

which on minimization generates the exact expression for $\check{l}$, it does *not* follow that the result found for $W(l)$, as embodied in $w_{10}(T,h,h_1,g)$, etc., is correct. Indeed, the fact that quite disparate potentials can have identical minima is clear on general grounds; but, to be more specific, one may check directly that the family of potentials given by

$$\begin{aligned} &w_{10}=\lambda(1+\theta)w_1, \quad w_{11}=\lambda\theta w_1, \quad w_{20}=\lambda(1+\tfrac{1}{2}\theta)w_2, \\ &w_{21}=\lambda\theta w_2, \quad \lambda\equiv 1/[1+\theta\kappa\check{l}_0(T,\ldots)], \end{aligned} \tag{3.3}$$

with θ sufficiently small, have the same minima at $l=\check{l}_0(T,\ldots)$ as the pure exponential form given by $\theta=0$. Other more explicit examples, which do not entail an implicitly defined function like $\check{l}_0(T,\ldots)$, are also not hard to find.

Now both Refs. 3 (hereafter referred to as BHL) and 5 (hereafter referred to as LKZ) consider the standard m^4 form (2.28) for the bulk potential $\Phi_0(m)$ and use a surface potential $\Phi_1(m_1)$ as given by (1.4) although expressed in different notations). Beyond that, BHL restrict attention to the case $h=0$ and it is not clear how to extend their approach to $h\neq 0$. Indeed, in none of the works cited is the method to be used set out in an unambiguous manner. BHL notes that the optimal equilibrium profile has the form

$$\check{m}(z;T,\ldots)=-m_0\tanh\{\tfrac{1}{2}\kappa[z-\check{l}(T,\ldots)]\}, \tag{3.4}$$

with $m_0(T)\equiv m_{\beta\infty}(T,h=0)>0$ while $\check{l}(T,\ldots)$ may, in fact, be determined from the wall boundary condition (2.9). Of course, this identification of the interface location amounts to a zero-crossing criterion (although this is not explicitly enunciated). In effect, the next step is to assert that the constrained profile m_{Ξ} is approximated to sufficient accuracy by the ansatz

$$m_{\Xi}[\mathbf{r};l(\cdot)]\simeq\check{m}[z-\Delta l(\mathbf{y})], \tag{3.5}$$

where $\Delta l=l(\mathbf{y})-\check{l}(T,\ldots)$. This ansatz certainly looks plausible. In the BHL analysis it leads to the pure exponential form (1.6) for $W(l)$ which arises, essentially, solely from the mismatch of $\check{m}(z-\Delta l)$ at the wall via $\Phi_1(m_1)$.

However, this ansatz basically disregards the breaking of translational invariance by the wall when the interface is located *away* from $l=\check{l}$. By relaxing the wall boundary condition, it ignores the *distortion* of the constrained profile induced by the wall-bulk interactions. Thus the true constrained profile must deviate from the simple tanh profile whenever $l\neq\check{l}$. Indeed, as mentioned, the constrained profile $m_{\Xi}(z)$ must have a break in its gradient at $z=l(\mathbf{y})$ that is obviously not represented by the ansatz (3.5). The distortion from the translated optimal profile induces a contribution to $W(l)$ which comes from the whole region of the wetting layer of "bulk" β phase in addition to changing the value of the wall contribution from that computed by BHL. In light of these considerations there are no good grounds for believing that (3.5) is adequate; in fact, our calculations reveal that, in general, it is not.

The defects of the ansatz (3.5) become further apparent when nonzero h is examined. In this case the optimal profile $\check{m}(z;T,h\neq 0,h_1,g)$ which can also be calculated exactly (see Sec. VI) actually diverges to ∞ when extended analytically to negative values of z (see Fig. 1). The ansatz method then generates unphysical terms in $W(l)$ varying like $he^{+\kappa l}$. Indeed, one is led to conclude that $W(l)\rightarrow +\infty$ when $l\rightarrow l_{0c}\simeq 2\check{l}(T,h,\ldots)$. In light of this behavior the ansatz must be considered generally unacceptable in the presence of a wall at a finite distance from the interface.

The arguments of LKZ are not as transparent or explicit. Following Ref. 23(c), a "collective coordinate" $\zeta(\mathbf{y})$ is introduced, essentially as $\zeta(\mathbf{y})=\Delta l(\mathbf{y})$ in (3.4), and an expression for the potential $W(l)$ is stated. [See LKZ, Eq. (12b), where V corresponds to W.] Near the wetting transitions $\Phi_1(m_1)-\Phi_1(m_{\beta\infty})$ is small and an expansion is made. In addition, an expression [LKZ, Eq. (2)] is employed which asymptotically relates $\exp[-\kappa l(T,h,\ldots)]$ to the surface order parameter value $m_1=m(z=0)$. [Although valid to leading order in $e^{-\kappa l}$, it is not evident why this relation should suffice to yield $W(l)$ to order $e^{-2\kappa l}$.] This procedure leads LKZ to the form (1.6) for $W(l)$, including an $e^{-3\kappa l}$ term [see LKZ, Eq. (13)], although the various coefficients $w_1,w_2,\ldots$ seem not to have been completely evaluated. Notwithstanding the differences in the details, we believe that the LKZ analysis is open to the same basic criticisms made of the BHL calculation: specifically, the ansatz (3.5) is inadequate.

Another somewhat more explicit treatment is presented in Ref. 20(a) (hereafter referred to as L) for the simpler case in which $\Phi_0(m)$ is represented by a symmetric pair of parabolas with minima at $m=0$ and m_0. Again a crossing criterion is implicitly adopted. Because the profile is just a sum of exponentials in the two regions defined by $m\geq m_0$ and $m\leq m_0$, the calculations can be performed in detail. (See also Sec. IV below.) However, the constrained profile $m_{\Xi}[\mathbf{r},l(\cdot)]$ is, unfortunately, never explicitly stated. At one point, L appears to set $\check{l}(T,\ldots)$, as specified by the boundary conditions, equal to l, which should be free: see L, Eqs. (15) and (16). This again amounts to improper neglect of the wall boundary condition: see L, Eq. (18). In fact, the procedure followed seems to imply that the constrained profile m_{Ξ}, rather than being always continuous [with a break in slope at $z=l(\mathbf{y})$], exhibits a discontinuity of magnitude

$$\Delta m \propto [e^{-\kappa l}-e^{-\kappa\check{l}(T,\ldots)}] \tag{3.6}$$

when l is close to but no equal to $\check{l}$. This is, of course, quite unacceptable physically.

The conclusion of L is that $W(l)$ again has the simple exponential form (1.6). For the *special case* of the double-parabolic form for $\Phi_0(m)$, this is also our finding in Sec. IV, below. However, the detailed form of the coefficients $w_1,w_2,\ldots$ given by L appears to deviate somewhat from those we find; the differences imply that some mean-field critical amplitudes and fluctuation strengths will differ in magnitude (although qualitative features will agree).

In summary, previous treatments leading to expressions for $W(l)$ have not been clearly formulated and, insofar as they seem to correspond to the systematic procedure outlined in Sec. II above, they have used inadequate approximations or inadmissable substitutions. By way of explanation, it should be noted that the main thrusts of BHL, LKZ, and L were *not* the derivation of $W(l)$ but, rather, other features of the critical wetting transitions. The delicate nature of the analysis needed to derive $W(l)$, which, after all, is required to the rather high order $e^{-2\kappa l}$ or $e^{-3\kappa l}$, was not well appreciated.

IV. CROSSING CRITERION WITH PARABOLIC BULK FREE-ENERGY DENSITIES

In this section we implement explicitly the program set out in Sec. II to calculate the effective wall-interface potential $W(l;T,h,\ldots)$, as given in (2.13), and the perturbed interfacial stiffness $\tilde{\Sigma}(l;T,h,\ldots)$, as given in (2.26). Accordingly, we aim to calculate $m_{\Pi}(z;l;T,h,\ldots)$ the constrained interfacial profile for a planar interface with $l(\mathbf{y})=l_\pi$ fixed independent of $\mathbf{y}$.

A. Model bulk free energy

As a first approach we make the calculations tractable by treating only bulk free-energy-density functions $\Phi_0(m)$ that can be represented as piecewise parabolic. This step, which is motivated by prior uses[20,27] of double-parabola approximations to $\Phi_0(m)$ in place of the usual m^4 form (2.27), enables us to derive explicit, closed expressions for $W(l)$ and $\tilde{\Sigma}(l)$.

Accordingly, consider the *asymmetric double-parabolic* (DP) form, see Fig. 2,

$$\begin{aligned}\Phi_0^{\mathrm{DP}}(m)&=\Phi_\alpha^{\mathrm{DP}}(m)\equiv\tfrac{1}{2}\chi_\alpha^{-1}(m-m_{\alpha0})^2 \quad \text{for } m\leq 0\\ &=\Phi_\beta^{\mathrm{DP}}(m)\equiv\tfrac{1}{2}\chi_\beta^{-1}(m-m_{\beta0})^2 \quad \text{for } m\geq 0\ ,\end{aligned} \tag{4.1}$$

where we impose *continuity* via the matching condition $\Phi_\alpha^{\mathrm{DP}}(0)=\Phi_\beta^{\mathrm{DP}}(0)$ which implies

$$\chi_\alpha/\chi_\beta=m_{\alpha0}^2/m_{\beta0}^2\ . \tag{4.2}$$

Note, furthermore, that Φ_0 depends on T via the temperature dependences of the susceptibilities $\chi_\alpha(T)$ and $\chi_\beta(T)$ of the two bulk phases, and via the coexistence values $m_{\alpha0}(T)$ and $m_{\beta0}(T)$.

Although this model for Φ_0 has a break in slope, i.e., a kink, at $m=0$, it is somewhat more realistic than previously discussed double-parabolic forms in three ways: (i) There is no restriction to situations in which the bulk α and β phases are symmetrically related as implicit, e.g., in the m^4 form. (ii) When $h\neq 0$ the overall thermodynamic potential $\Phi(m)=\Phi_0(m)-hm$ [see (1.3)] has local minima at

$$m_{\alpha\infty}(T,h)=m_{\alpha0}+\chi_\alpha h,\quad m_{\beta\infty}(T,h)=m_{\beta0}+\chi_\beta h\ , \tag{4.3}$$

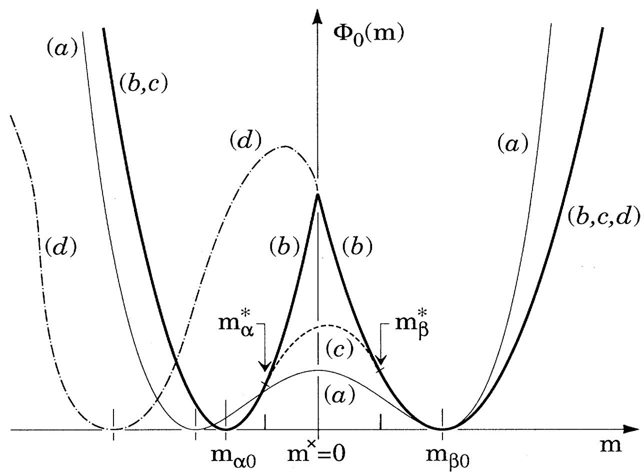

FIG. 2. Bulk free-energy densities $\Phi_0(m)$ at α-β coexistence: (a) standard, classical m^4 form; (b) asymmetric double parabola with crossing criterion specified at $m^\times=0$; (c) asymmetric triple parabola with matching values and slopes at m_α^* and m_β^*; (d) single parabola with arbitrary continuation for $m\leq 0$.

which vary appropriately with h. [Previous forms[20,27] imposed $m_{\alpha\infty}(h)=m_{\alpha 0}=-m_{\beta\infty}(h)$.] (iii) In using the crossing criterion one can naturally fix $m^\times$ at $m=0$ (whereas in the earlier discussions $m^\times$ was shifted with h).

In mean-field theory using (1.2) the inverse correlation lengths are

$$\kappa_\alpha(T)\equiv\xi_\alpha^{-1}=(K\chi_\alpha)^{-1/2}$$

and (4.4)

$$\kappa(T)\equiv\xi_\beta^{-1}=(K\chi_\beta)^{-1/2} .$$

The overall wetting phase diagram for $\Phi_0^{\rm DP}$ can be determined, within mean-field theory, by standard methods.[10,20] As regards critical wetting, quite normal behavior is observed.[10] More specifically, the critical wetting transition at $T=T_{cW}^0$ and $h=0-$ occurs when $\tau=0-$ with

$$\tau\equiv[h_1+gm_{\beta\infty}(T,h)]/[K\kappa(T)-g] , \tag{4.5}$$

provided, as we assume henceforth,

$$\tilde{g}\equiv g/K\kappa=\chi_\beta\kappa g<-1 . \tag{4.6}$$

More generally, however, the parabolic form (4.1) leads to anomalies in regions of the phase diagram that will *not* concern us here. For completeness we mention, nevertheless, that in combination with the truncated expression (1.4) for $\Phi_1(m_1)$, the physical region is limited to $g<\min(K\kappa_\alpha,K\kappa)$ and to T below the bulk α-β critical temperature T_c. In this combination *tricritical* wetting[9] is also unphysical since all the first-order wetting transitions are found to correspond, under the crossing criterion, to jumps in wetting-layer thickness from $l<0$ to $l=\infty$.[28] Some of this pathology can be alleviated by adding cubic and higher order terms to $\Phi_1(m_1)$: see also Ref. 21.

B. Planar profile and effective potential

To obtain the constrained planar profile $m_{\rm II}(z;l)$, we must solve (2.8) subject to (2.9), (2.10), and the crossing condition (2.6) with $m^\times=0$. For the parabolic form (4.1) this reduces to a *piecewise linear* ordinary differential equation. The solution falls naturally into two parts: the first describes the α phase for $z\geq l$ (and $m\leq 0$) and is simply

$$m_{\rm II}=m_\alpha(z;l;T,h)=m_{\alpha\infty}[1-e^{-\kappa_\alpha(z-l)}] ; \tag{4.7}$$

the second piece describes the β phase or wetting-layer part of the profile for $z\leq l$ (and $m\geq 0$) and may be written

$$m_{\rm II}=m_\beta(z;l;T,h)=m_{\beta\infty}+B_+e^{\kappa(z-l)}+B_-e^{-\kappa(z-l)} . \tag{4.8}$$

The amplitudes B_+ and B_-, which depend on l, T, h, h_1, and g, may be determined by imposing the wall condition (2.9) and the crossing condition (2.6). If, for brevity, we write

$$X(l;T)\equiv\exp(-\kappa l) , \tag{4.9}$$

which becomes small in the region of critical and complete wetting ($l\to\infty$), we obtain

$$B_+=-\frac{m_{\beta\infty}+\tau X}{1-\mathcal{G}X^2} , \tag{4.10}$$

and

$$B_-=\frac{\tau+m_{\beta\infty}\mathcal{G}X}{1-\mathcal{G}X^2}X , \tag{4.11}$$

where for convenience we have introduced, in place of (4.6), the bounded, *positive* g-dependent parameter

$$0<\mathcal{G}\equiv-\frac{1+\tilde{g}}{1-\tilde{g}}\equiv-\frac{1+\chi_\beta\kappa g}{1-\chi_\beta\kappa g} . \tag{4.12}$$

One may now substitute our expressions for $m_{\rm II}(z;l)$ in (2.13) and perform the required integrations on z over the intervals $(0,l)$ and (l,∞), the integrands containing only terms varying as $\exp(\pm jkz)$ with $j=0,1,2$. It is important to note that both positive, zero, *and* negative powers of $e^{-\kappa z}$ appear. If the reduced bulk field is defined by

$$\begin{aligned}\bar{h}&\equiv\Phi(m_{\beta\infty})-\Phi(m_{\alpha\infty})\\&=-h\Delta m_\infty(T,h)\\&=-h[m_{\beta 0}-m_{\alpha 0}+\tfrac{1}{2}(\chi_\beta-\chi_\alpha)h] ,\end{aligned} \tag{4.13}$$

and the constrained surface order parameter is

$$m_{1\rm II}(l;T,h,h_1,g)=m_{\beta\infty}+B_+X+B_-X^{-1} , \tag{4.14}$$

the result for the effective potential is

$$\begin{aligned}W(l)=\bar{h}l&+\tfrac{1}{2}K\kappa[B_+^2+X^{-2}B_-^2](1-X^2)\\&-\tfrac{1}{2}h_1m_{1\rm II}-\tfrac{1}{2}gm_{1\rm II}^2+\tfrac{1}{2}K\kappa_\alpha m_{\alpha\infty}^2-W_\infty .\end{aligned} \tag{4.15}$$

The background term $W_\infty(T,h,h_1,g)$ here is fixed by the conditions discussed after (2.14) which amount to $[W(l)-\bar{h}l]\to 0$ as $l\to\infty$. After further algebra one finds

$$W_\infty=\tfrac{1}{2}K\kappa_\alpha m_{\alpha\infty}^2-h_1 m_{\beta\infty}-\tfrac{1}{2}g m_{\beta\infty}^2+\tfrac{1}{2}K\kappa m_{\beta\infty}^2-\tfrac{1}{2}(K\kappa-g)\tau^2=\Sigma_{\alpha|\beta}^{\mathrm{II}}(T,h)+\Sigma_{\omega|\beta}(T,h,h_1,g)\ , \tag{4.16}$$

where the required free interfacial and wall tensions are

$$\Sigma_{\alpha|\beta}^{\mathrm{II}}=\tfrac{1}{2}K\kappa_\alpha(T)m_{\alpha\infty}^2(T,h)+\tfrac{1}{2}K\kappa(T)m_{\beta\infty}^2(T,h)\ , \tag{4.17}$$

$$\Sigma_{\omega|\beta}=\tfrac{1}{2}K\kappa\tau^2-h_1(m_{\beta\infty}+\tau)-\tfrac{1}{2}g(m_{\beta\infty}+\tau)^2\ . \tag{4.18}$$

Note that when $h\to 0$ the tension $\Sigma_{\alpha|\beta}^{\mathrm{II}}(T,h)$ reduces simply to $\Sigma_{\alpha|\beta}(T)$, namely the (mean-field) tension of an isolated or free planar $\alpha|\beta$ interface; when $h\neq 0$, however, this tension corresponds to a similar interface but with an imposed crossing constraint at $m^\times=0$ (and the bulk field energy removed). As regards the wall tension against the wetting phase β, one may note that (4.8)–(4.11) imply

$$m_{1\mathrm{II}}(l\to\infty;T,h,h_1,g)=m_{\beta\infty}+\tau\ . \tag{4.19}$$

Finally, after further reduction, the effective wall-interface potential itself can be written transparently as

$$W(l;T,h,h_1,g)=\bar{h}l+\frac{w_1X+w_2X^2}{1-\mathcal{G}X^2}\ , \tag{4.20}$$

with coefficients given by (4.12), (4.13), and

$$w_1(T,h,h_1,g)=2K\kappa m_{\beta\infty}\tau\ , \tag{4.21}$$

$$w_2(T,h,h_1,g)=K\kappa\mathcal{G}m_{\beta\infty}^2+K\kappa\tau^2\ . \tag{4.22}$$

On recalling $X=e^{-\kappa l}$, it is evident that our closed-form result for $W(l)$ is in full agreement with the generally accepted form (1.6). Furthermore, as expected, $w_1\sim\tau\sim T-T_{cW}^0$ vanishes at mean-field wetting criticality while w_2 remains positive. One may note that w_2 contains explicit positive contributions from the wall, via $\tau(T,h,h_1,g)$, which were not found in previous analyses,[3,5,20] although they vanish near mean-field wetting criticality. When fluctuations are included via renormalization-group theory,[4,6] however, the critical point T_{cW} deviates from T_{cW}^0 when $\omega>2$ and these terms then affect the value of T_{cW}.

The higher-order coefficients $w_3,w_4,\dots$ in (1.6) can be read off from (4.20). One sees that the w_j for $j\geq 3$ all vanish at the wetting tricritical point $w_1=w_2=0$. This is quite anomalous and corresponds to the failures of the parabolic approximations for Φ_0 near tricriticality that were alluded to above.

It is of interest to check the smoothness of the optimal profile $m(z)=m_{\mathrm{II}}(z;l)$ through the crossing level $m^\times=0$ and, more generally, to determine the break in slope of the constrained profile $m_{\mathrm{II}}(z,l)$ at $z=l$ when $l\neq\check{l}$; see Fig. 1. It proves convenient to define

$$\Delta_\pm(l;T,h,h_1,g)=\frac{\partial m_\beta}{\partial z}(l-;l)\pm\frac{\partial m_\alpha}{\partial z}(l+;l) \tag{4.23}$$

so that the magnitude of the break or kink is just $\Delta(l)=\Delta_-(l)$. Calculation yields

$$\Delta_\pm=-\kappa\frac{m_{\beta\infty}+2\tau X+\mathcal{G}m_{\beta\infty}X^2}{1-\mathcal{G}X^2}\pm\kappa_\alpha m_{\alpha\infty}\ . \tag{4.24}$$

Furthermore, one can show that the effective force on the interface can be factorized exactly as

$$-\partial W/\partial l=\tfrac{1}{2}K\Delta_+(l)\Delta_-(l)\ . \tag{4.25}$$

Thus the force vanishes at the minimum of $W(l)$ given by $\Delta_-(\check{l})=0$; hence the kink Δ also vanishes at $l=\check{l}$. An expansion of (4.21) to order X^2 yields

$$\Delta(l)\approx\kappa[2\tau+\mathcal{G}m_{\beta\infty}(X+\check{X})](X-\check{X})\ , \tag{4.26}$$

where $\check{X}\equiv X(\check{l})$; this is generally small in the vicinity of the critical wetting transition.

C. Wall-perturbed interfacial stiffness

By using (4.7) and (4.8) in (2.26) we find that the interfacial stiffness in the presence of a wall is given by

$$\tilde{\Sigma}(l)=K\int_0^l dz[A_+e^{\kappa(z-l)}+A_-e^{-\kappa(z-l)}]^2+\tfrac{1}{2}K\kappa_\alpha m_{\alpha\infty}^2\ , \tag{4.27}$$

where

$$A_\pm(l)=(\partial B_\pm/\partial l)\mp\kappa B_\pm\ , \tag{4.28}$$

so that $A_+=O(1)$ and $A_-=O(X^2)$ as $l\to\infty$. Completing the calculation yields the explicit result

$$\tilde{\Sigma}(l)=\tfrac{1}{2}K\kappa_\alpha m_{\alpha\infty}^2+\tfrac{1}{2}K\kappa\tilde{m}^2\times[(1-X^2)(1+\mathcal{G}^2X^2)-4\mathcal{G}\kappa lX^2]\ , \tag{4.29}$$

where one finds

$$\tilde{m}\equiv\frac{A_+}{\kappa}=\frac{m_{\beta\infty}+2\tau X+m_{\beta\infty}\mathcal{G}X^2}{(1-\mathcal{G}X^2)^2}\ . \tag{4.30}$$

For large l this has the expansion

$$\tilde{\Sigma}(l)=\tilde{\Sigma}_\infty(T,h)+s_{10}e^{-\kappa l}+s_{20}e^{-2\kappa l}+\cdots+s_{21}\kappa le^{-2\kappa l}+s_{31}\kappa le^{-3\kappa l}+\cdots\ , \tag{4.31}$$

where the interaction coefficients are

$$s_{10}(T,h,h_1,g)=2K\kappa m_{\beta\infty}\tau\ ,\qquad s_{20}=\tfrac{1}{2}K\kappa m_{\beta\infty}^2(6\mathcal{G}+\mathcal{G}^2-1)+O(\tau^2)\ , \tag{4.32}$$

$$s_{21}(T,h,h_1,g)=-2K\kappa\mathcal{G}m_{\beta\infty}^2\ ,\qquad s_{31}(T,h,h_1,g)=-8K\kappa\mathcal{G}m_{\beta\infty}\tau\ , \tag{4.33}$$

so that $s_{21}=O(1)$ as $\tau\to 0$. As expected, in view of the special isotropy of the underlying model, the stiffness at $l=\infty$ satisfies $\tilde{\Sigma}_\infty(T,h)=\Sigma_{\alpha|\beta}^{\mathrm{II}}(T,h)$; see (4.17).

Now the appearance of terms in $\tilde{\Sigma}(l)$ varying as $le^{-j\kappa l}$ ($j=2,3,\dots$) is rather unexpected since only pure exponentials occur in the formula for $W(l)$. The mechanism by which the factor l arises is, however, quite transparent when the integrand in (4.27) is multiplied out: a term independent of z, namely $2KA_+(l)A_-(l)$, then appears which, on integration, generates the last term in (4.29). A similar mechanism also produces the $\bar{h}l$ term, in $W(l)$, but, in that case, no net factors of $e^{-\kappa l}$ are contributed by the amplitudes $B_\pm(l)$. We will see in Sec. V, however, that this is one mechanism that actually generates terms like $l^k e^{-j\kappa l}$ in $W(l)$ for general $\Phi_0(m)$.

D. Triple-parabola free-energy densities

One of the obvious unphysical features of the double-parabolic models is the sharp cusp in $\Phi_0(m)$ at $m=0$: see Fig. 2. To eliminate this but preserve the ease of analysis, it is natural to consider triple-parabola models $\Phi_0^{\mathrm{TP}}(m)$ in which the central region of $\Phi_0^{\mathrm{DP}}(m)$ is replaced by a third, inverted parabola. The simplest possibility is to take this as

$$\Phi_0=\Phi(0)-\tfrac{1}{2}\Gamma m^2 , \tag{4.34}$$

for $m_{\alpha 0}<m_\alpha^*\le m\le m_\beta^*<m_{\beta 0}$, while restricting (4.1) accordingly to $m\le m_\alpha^*$ and $m\ge m_\beta^*$. By adjusting say, $\Phi(0)$, Γ, m_α^*, and χ_α for fixed $m_{\alpha 0}$, $m_{\beta 0}$, χ_β, and m_β^* one can make $\Phi_0^{\mathrm{TP}}(m)$ continuous and smooth (with no kinks) for all m.

The previous derivations can be repeated in a fairly straightforward manner.[28] The crucial profile $m_{\mathrm{II}}(z;l)$ still has the general character illustrated in Fig. 1 with a kink at $z=l\neq\check{l}$ but continuous slope and curvature elsewhere. However, both parts, $m_\alpha(z;l)$ and $m_\beta(z;l)$ for $m \lessgtr m^\times=0$, are now composed of two pieces: one piece with the original exponential forms in (4.7) and (4.8) and one piece, for $m_\alpha^*\le m\le 0$ or $0\le m\le m_\beta^*$, involving $\sin[\kappa_0(z-l)]$ with $\kappa_0=\sqrt{\Gamma/K}$. The pieces join with matching slope *and* curvature at m_α^* or m_β^*, respectively. The algebra is more complicated than previously and the results are not quite as explicit. Nevertheless, it is easy to see that the trigonometric pieces of $m_{\mathrm{II}}(z;l)$ span an interval in the interfacial region of the profile of width approximately π/κ_0 which, for reasonable choices of the inverted parabolic section, is only of order ξ_α or ξ_β. Thence one reaches, when $l\to\infty$, essentially the same conclusions, (1.5) for $\mathcal{H}_I[l]$, (1.6) for $W(l)$, and (4.30) for $\tilde{\Sigma}(l)$, as previously. Of course, the explicit expressions for $w_1, w_2, \ldots, \Sigma_{\alpha|\beta}^{\mathrm{II}}, s_{10}, s_{21}, \ldots$ will change quantitatively but not qualitatively.

More generally, one learns that it is really only the form of the free-energy density $\Phi_0(m)$ in the *vicinity* of $m=m_{\beta 0}$ that determines the asymptotic form of $\mathcal{H}_I[l]$ as $l\to\infty$. We can exploit that fact, as follows.

E. Single-parabola forms

Consider a "single-parabola" thermodynamic potential $\Phi_0^{\mathrm{SP}}(m)$ which (i) in the β phase, for $m\ge m^\times=0$, takes the simple parabolic form that is given in (4.1), but (ii) for $m\le m^\times$ assumes a *general* form, say $\Phi_\alpha(m)$, restricted only by the requirement that it has a single, second, α-phase minimum at $m=m_{\alpha 0}$: see Fig. 2. We may reasonably assume that there is an *expansion* in powers of $(m-m_{\alpha 0})$ about the α minimum, as in the first member of (4.1), but this will play no essential role.

For such a single-parabola potential the analysis of Sec. IV B above may be followed closely. Consider, first, the profile $m_{\mathrm{II}}(z;l)$ in the α-phase region. In place of the simple exponential expression in (4.7) we will have a more general form, say, $m_\alpha(z-l;T,h)$ which, by using (2.8) in the standard way with the condition (2.10) for $l\to\infty$, is a solution of

$$\partial m_\alpha/\partial z=-\sqrt{2\Delta\Phi_\alpha(m_\alpha)/K} , \tag{4.35}$$

where $\Delta\Phi_\alpha$ is defined as in (2.14). If, as previously, $\check{m}(z)$ is the optimum profile satisfying $\check{m}(\check{l})=m^\times=0$, it is clear that the desired constrained, planar profile in the α phase is simply

$$m_\alpha(z-l)=\check{m}(z-\Delta l) \text{ with } \Delta l=l-\check{l} . \tag{4.36}$$

It may be remarked that these steps essentially justify the ansatz used by previous authors in the α phase (only) and for this special, single-parabola, type of free energy.

Now, as regards $m_{\mathrm{II}}(z,l)$ in the β-phase region $0\le z\le l$, the previous analysis in (4.7)–(4.12) remains unchanged. Indeed, the first new feature arises in the expression (4.15) for $W(l)$: the fourth term here, namely $\frac{1}{2}K\kappa_\alpha m_{\alpha\infty}^2$, represents the contribution, say $\Sigma_\alpha(T,h)$, of the profile for $z\ge l$ to the surface tension of a free $\alpha|\beta$ interface: see (4.17). Evidently this must be recomputed using the new form for $m_\alpha(z-l)$ that solves (4.35). In the usual manner this leads to

$$\Sigma_\alpha(T,h)=\int_{m_{\alpha\infty}}^{0}[2K\Delta\Phi_\alpha(m)]^{1/2}dm , \tag{4.37}$$

where $m_{\alpha\infty}(T,h)$ represents the minimum of $\Phi_\alpha(m)-hm$ which, up to $O(h^2)$, is s till given by (4.3).

The first term $\bar{h}l$ in (4.15) also has a contribution from the α-phase region of integration, but the changes amount only to the redefinition of $m_{\alpha\infty}(T,h)$ already mentioned. Thus, (4.13), which defines $\bar{h}$, remains valid except that in the second line terms of order h^3 will, in general, arise; but these are clearly of no consequence.

To adapt the previous derivation of $W(l)$ it is thus clear that it is necessary only to replace the terms $\frac{1}{2}K\kappa_\alpha m_{\alpha\infty}^2$ in (4.16) and (4.17) by Σ_α. But these changes have no effects on the subsequent expressions (4.18)–(4.22). Thus $W(l)$ behaves *precisely* as previously found. The derivations in (4.23)–(4.26) of the discontinuity in $\dot{m}_{\mathrm{II}}(z;l)$ when $l\neq\check{l}$ also need no modifications.

The analysis of the wall-perturbed stiffness $\tilde{\Sigma}(l)$ in Sec. IV C also stands virtually unchanged beyond the replacement of $\frac{1}{2}K\kappa_\alpha m_{\alpha\infty}^2$ by Σ_α in (4.27). In particular, the results (4.29)–(4.33) remain fully valid.

Recalling that the choice $m^\times=0$ is quite general, since a shift in m can always be made, we conclude that it is *only* the pure parabolic form of $\Phi_0^{\mathrm{SP}}(m)$ around $m_{\beta 0}$ (actually in a neighborhood of magnitude τ) that determines the asymptotic forms of $W(l)$ and $\tilde{\Sigma}(l)$. To go beyond this analysis and treat general free-energy forms it is necessary to allow for cubic and higher-order terms in the expansion of a general $\Phi_0(m)$ about $m=m_{\beta 0}$. That task is undertaken in the next section.

V. PERTURBATIONAL ANALYSIS FOR GENERAL FREE-ENERGY DENSITIES

In this section we consider a general free-energy density $\Phi_0(m;T)$ of double minimum form. As in Sec. IV E, we treat the bulk, α-phase region in $m \le m^{\times} \equiv 0$ exactly; however, the wetting layer or β-phase region will be analyzed perturbatively starting with the single-parabola results of IV E.

A. Wetting-layer formulation

Following the arguments of Sec. IV E, we can straightforwardly reformulate the problem of computing the wall-interface potential $W(l)$ and the perturbed stiffness $\tilde{\Sigma}(l)$ in terms of the wetting-layer properties alone as follows:

$$W(l)=\min_{m(z)} \mathcal{H}_L[m(z)]-\overline{W}_\infty(T,h,h_1,g) , \tag{5.1}$$

where, with $\dot{m}=\partial m/\partial z$, the layer Hamiltonian is simply

$$\mathcal{H}_L[m(z)]=\int_0^l dz[\tfrac{1}{2}K\dot{m}^2+\Delta\Phi(m)]+\Phi_1(m_1) \tag{5.2}$$

with, as before, $m_1\equiv m(z=0;l)$, and $\Delta\Phi$ defined via (1.3) and (2.14); the background $\overline{W}_\infty(T,\ldots)$ is fixed [as in (4.15)] by the condition $[W(l)-\bar{h}l]\to 0$ as $l\to\infty$. In addition, the crossing criterion translates into the condition

$$m(z=l;l)=0 , \tag{5.3}$$

to be imposed on all $m(z)$ used in (5.1). Note that $\mathcal{H}_L$ entails only the β-phase part of the profile [$z \le l$ and $m(z;l)\ge 0$].

The wall-modified interfacial stiffness is, via (2.26) and (4.37), given by

$$\tilde{\Sigma}(l)=K\int_0^l dz(\partial m_{\Pi}/\partial l)^2+\Sigma_\alpha , \tag{5.4}$$

where $m_{\Pi}(z;l)$ is, now, the planar profile (for $z\le l$) minimizing (5.2) subject to (5.3).

To establish a perturbative scheme for calculating m_{Π} we set

$$\varphi(z;l)=m(z;l)-m_{\beta\infty}(T,h) \tag{5.5}$$

and expand $\Phi(m)$ about the β-phase minimum as[29]

$$\Phi(m)=\Phi_{\min}(T,h)+\bar{h}+\tfrac{1}{2}\chi_\beta^{-1}\varphi^2+\sum_{n=3}^{\infty} n^{-1}\varepsilon_n\varphi^n , \tag{5.6}$$

where (4.13) has been used. For the standard m^4 form (2.28) with $r<0$ one finds $m_{\beta 0}=(6|r|/u)^{1/2}$, $\chi_\beta^{-1}=2|r|+O(h)$, and

$$\varepsilon_3=(u|r|/6)^{1/2}+O(h), \quad \varepsilon_4=u/6, \quad \varepsilon_n=0 \quad (n\ge 5) . \tag{5.7}$$

As $u\to 0$ one formally has $\varepsilon_3\sim\sqrt{u}$, $\varepsilon_4\sim u$. More generally we may conveniently suppose

$$\varepsilon_n \propto \varepsilon^{n-2} \quad (n\ge 3) . \tag{5.8}$$

When $\varepsilon=0$ the problem reduces to the single-parabola form solved in Sec. IV E. Then we propose to treat ε (and $\varepsilon_3,\varepsilon_4,\ldots$) as a small parameter and aim to compute the expansion coefficients in the expressions

$$W(l;\varepsilon)=W_0(l)+\sum_{\{k_n\}}{}' V_{k_3k_4\ldots}(l)\prod_{n=3}\varepsilon_n^{k_n} , \tag{5.9}$$

$$\tilde{\Sigma}(l;\varepsilon)=\tilde{\Sigma}_0(l)+\sum_{\{k_n\}}{}' S_{k_3k_4\ldots}(l)\prod_{n=3}\varepsilon_n^{k_n} , \tag{5.10}$$

where the leading terms W_0 and $\tilde{\Sigma}_0$ follow from the previous analysis; here and below the primes on the sums denote the restriction $k_3+k_4+\cdots\ge 1$.

A remark concerning the nature of the free-energy function $\Phi_0(m)$ as the ε_n vary, is worth making. If $\Phi_\alpha\equiv\Phi(m\le 0)$ is held fixed while $\Phi_\beta\equiv\Phi(m\ge 0)$ varies with ε, a discontinuity is, in general, introduced in $\Phi(m;\varepsilon)$ at $m=0$. Now, on the one hand, this could be eliminated (along with discontinuous derivatives) by making appropriate ε-dependent changes in Φ_α which are then easily included in the calculation; on the other hand, a discontinuity in $\Phi(m)$ at $m=0$ may well be tolerated since, as the analysis reveals, it has no effect on the asymptotic behavior of $W(l)$, etc., which is of primary interest. Of course, a discontinuity in $\Phi(m)$ at $m=0$ does induce a break in slope (or kink) at the crossing point even in the optimal profile $\check{m}(z)=m_{\Pi}(z;l=\check{l})$. This is unphysical but, again, harmless as regards the large-l behavior. Thus we will have no reason to discuss this issue again.

B. Perturbation procedure

By (5.1)–(5.3) and (5.6) the planar layer profile $m_{\Pi}-m_{\beta\infty}\equiv\varphi_{\Pi}(z;l)$ (for $z\le l$) satisfies

$$\mathcal{L}\varphi_{\Pi}\equiv K(\partial_z^2-\kappa^2)\varphi_{\Pi}=\sum_{n=3}^{\infty}\varepsilon_n\varphi_{\Pi}^{n-1} , \tag{5.11}$$

where $\partial_z=\partial/\partial z$, together with the boundary conditions

$$\mathcal{B}_1\varphi_{\Pi}\equiv(K\partial_z+g)\varphi_{\Pi}(z=0;l)=-h_1-gm_{\beta\infty} , \tag{5.12}$$

$$\mathcal{B}_2\varphi_{\Pi}\equiv\varphi_{\Pi}(z=l;l)=-m_{\beta\infty} . \tag{5.13}$$

Now if we expand the profile in the form

$$\varphi_{\Pi}(z;l)=\varphi_0(z;l)+\sum_{\{k_n\}}{}'\varphi_{k_3k_4\ldots}(z;l)\prod_{n=3}\varepsilon_n^{k_n} , \tag{5.14}$$

the coefficients $\varphi_{k_3k_4\ldots}$ satisfy the recursion relations

$$\mathcal{L}\varphi_0=0,\quad \mathcal{L}\varphi_{10}=\varphi_0^2,\quad \mathcal{L}\varphi_{01}=\varphi_0^3 , \tag{5.15}$$

$$\mathcal{L}\varphi_{20}=2\varphi_0\varphi_{10},\quad \mathcal{L}\varphi_{11}=2\varphi_0\varphi_{01}+3\varphi_0^2\varphi_{10} ,\quad \mathcal{L}\varphi_{02}=3\varphi_0^2\varphi_{01},\quad \ldots , \tag{5.16}$$

where, for brevity here and below, only the subscripts k_3 and k_4 have been indicated. Likewise the appropriate boundary conditions are

$$\mathcal{B}_1\varphi_0=-h_1-gm_{\beta\infty},\quad \mathcal{B}_1\varphi_{jk}=0 \quad \text{for } j+k\ge 1 , \tag{5.17}$$

$$\mathcal{B}_2\varphi_0=-m_{\beta\infty},\quad \mathcal{B}_2\varphi_{jk}=0 \quad \text{for } j+k\ge 1 . \tag{5.18}$$

The equations for φ_0 are equivalent to those solved for

$m_{\rm II}$ in the β phase in Sec. IV B. As in (4.8)–(4.12) we therefore have

$$\varphi_0(z;l)=B_+e^{\kappa(z-l)}+B_-e^{-\kappa(z-l)}, \qquad (5.19)$$

with $B_+=-m_{\beta\infty}+O(\tau X,X^2)$ and $B_-=O(\tau X,X^2)$. It is then straightforward in principle to solve the system (5.15)–(5.18) recursively. Before undertaking that task, consider the expansion coefficients for $W(l;\varepsilon)$ and $\tilde{\Sigma}(l;\varepsilon)$.

In principle one needs to substitute the expansion (5.14) for $\varphi_{\rm II}$ into (5.2) to obtain $W(l;\varepsilon)$. However, the variational equation

$$\left.\frac{\partial\mathcal{H}[m]}{\partial m}\right|_{m=m_{\beta\infty}+\varphi_{\rm II}}=0 \quad \text{for all } \varepsilon_n \qquad (5.20)$$

yields

$$V_{jk\cdots}(l)=\int_0^l dz\left.\frac{\partial^{j-1+k+\cdots}[\varphi_{\rm II}(z;l)]^3}{3j!k!\cdots\partial^{j-1}\varepsilon_3\partial^k\varepsilon_4\cdots}\right|_{\varepsilon=0} \quad (j\geq 1)$$
$$=\int_0^l dz\left.\frac{\partial^{j+k-1+\cdots}[\varphi_{\rm II}(z;l)]^4}{4j!k!\cdots\partial^{j}\varepsilon_3\partial^{k-1}\varepsilon_4\cdots}\right|_{\varepsilon=0} \quad (k\geq 1), \qquad (5.21)$$

From these relations one can read out the relatively simple results

$$V_{10}=\tfrac{1}{3}\int_0^l dz[\varphi_0(z;l)]^3,$$
$$V_{01}=\tfrac{1}{4}\int_0^l dz[\varphi_0(z;l)]^4, \qquad (5.22)$$

$$V_{20}=\int_0^l dz\,\varphi_0^2\varphi_{10},\quad V_{02}=\int_0^l dz\,\varphi_0^3\varphi_{01}, \qquad (5.23)$$

$$V_{11}=\int_0^l dz\,\varphi_0^2\varphi_{01}=\int_0^l dz\,\varphi_0^3\varphi_{10},\quad \ldots . \qquad (5.24)$$

The last equation here provides the first instance of a useful series of consistency checks on the calculations which reflect the fact that the system $\{\mathcal{L};\mathcal{B}_1,\mathcal{B}_2\}$ is self-adjoint.[30] From (5.4) and (5.10) one similarly finds for the stiffness coefficients

$$S_{10}=2K\int_0^l dz\left[\frac{\partial\varphi_0}{\partial l}\right]\left[\frac{\partial\varphi_{10}}{\partial l}\right],$$
$$S_{01}=2K\int_0^l dz\left[\frac{\partial\varphi_0}{\partial l}\right]\left[\frac{\partial\varphi_{01}}{\partial l}\right], \qquad (5.25)$$

$$S_{20}=K\int_0^l dz\left[\left[\frac{\partial\varphi_{10}}{\partial l}\right]^2+2\left[\frac{\partial\varphi_0}{\partial l}\right]\left[\frac{\partial\varphi_{20}}{\partial l}\right]\right],\quad \ldots . \qquad (5.26)$$

The procedures outlined here enable the formal perturbative expansion for $W(l)$ and $\tilde{\Sigma}(l)$ to be carried through explicitly to any specified order. Note, in particular, that owing to the simplicity of $\mathcal{L}\propto\partial_z^2-\kappa^2$ and to the simple exponential form (5.19) for φ_0, the successive differential equations in (5.15), (5.16), etc. present no technical difficulties. However, in order to understand the asymptotic decay of $W(l)$ and of $\tilde{\Sigma}(l)-\tilde{\Sigma}_\infty$ in the regimes of small τ and of small $X\equiv e^{-\kappa l}$ it proves necessary to analyze the structure of the whole perturbative expansion in some detail. Before embarking on that analysis it is instructive to examine some of the low-order terms explicitly to see what is involved.

C. Leading orders in φ^4

It transpires that novel behavior is generated in lowest order (in X and τ) by the φ^4 terms in (5.6); accordingly, consider $\varepsilon_3=\varepsilon_5=\varepsilon_6=\cdots=0$ with $\varepsilon_4>0$ small. To simplify expressions here, we will when convenient also adopt units of distance, energy, and order parameter in which

$$\kappa=1,\quad K=1,\quad m_{\beta\infty}=1 . \qquad (5.27)$$

Substitution of (5.19) in (5.22) and a simple integration yields

$$V_{01}(l)=\tfrac{1}{16}B_+^4(1-X^4)+\tfrac{1}{2}B_+^3B_-(1-X^2)+\tfrac{3}{2}lB_+^2B_-^2$$
$$+\tfrac{1}{2}B_+B_-^3X^{-2}(1-X^2)+\tfrac{1}{16}B_-^4X^{-4}(1-X^4) . \qquad (5.28)$$

On using (4.10)–(4.12) for $B_\pm$ one finds that $V_{01}(l)$ contains the expected positive powers of X plus the novel, "anomalous" term

$$\Delta V_{01}(l)\equiv\tfrac{3}{2}lB_+^2B_-^2=\tfrac{3}{2}\kappa l\tau^2e^{-2\kappa l}+O(\tau le^{-3\kappa l}) \qquad (5.29)$$

(where κ has been temporarily restored). This contribution is, of course, in disagreement with the pure exponential form (1.6) for $W(l)$ suggested by previous arguments and supported by the parabolic models; rather, it is consistent with the more complex form (1.8), namely

$$W(l)=\bar{h}l+W_1(\kappa l)e^{-\kappa l}+W_2(\kappa l)e^{-2\kappa l}+\cdots , \qquad (5.30)$$

with polynomials

$$W_1(x)=w_{10}+w_{11}x,$$
$$W_2(x)=w_{20}+w_{21}x+w_{22}x^2 , \qquad (5.31)$$

etc. More concretely, (5.29) suggests

$$w_{21}\approx\tfrac{3}{2}\tau^2\varepsilon_4,\quad w_{31}\approx O(\tau)\varepsilon_4 \qquad (5.32)$$

to first order in ε_4. Collecting the other terms in (5.28) yields

$$w_{10}=2\tau(1-\tfrac{1}{8}\varepsilon_4+\cdots),$$
$$w_{20}=\mathcal{G}(1-\tfrac{1}{4}\varepsilon_4+\cdots)+O(\tau^2), \qquad (5.33)$$

etc., where the zeroth-order results follow from (4.21) and (4.22). To this order in ε_4, no contributions to w_{11} and w_{jk} for $k\geq 2$ appear.

To go further one needs φ_{01}, the first-order ε_4 correction to $\varphi_{\rm II}\simeq\varphi_0$. To solve (5.15) for φ_{01} we use the special solutions

$$\mathcal{L}^{-1}e^{nz}=e^{nz}/(n^2-1)\quad\text{for } n\neq\pm1$$
$$=\tfrac{1}{2}nze^{nz}\qquad\text{for } n=\pm1 . \qquad (5.34)$$

In combination with the general solutions $C_\pm e^{\pm z}$ this yields

$$\varphi_{01}(z;l)=\tfrac{1}{8}B_+^3e^{3(z-l)}+[\tfrac{3}{2}B_+^2B_-(z-l)+C_+]e^{z-l}$$
$$-(\tfrac{3}{2}B_+B_-^2z-C_-)e^{-z+l}+\tfrac{1}{8}B_-^3e^{-3(z-l)}\,, \tag{5.35}$$

where the boundary conditions (5.17) and (5.18) yield closed expressions for C_+ and C_-, which have been calculated explicitly and have leading behavior

$$C_+=-[\tfrac{3}{2}\tau^2+O(\tau X,\ldots)]lX^2+\tfrac{1}{8}+O(\tau X,\ldots)\,, \tag{5.36}$$

$$C_-=\tfrac{3}{2}\mathcal{G}[\tau+O(X)]lX^3-\tfrac{1}{8}\mathcal{G}X^2+O(\tau^3X,\ldots)\,. \tag{5.37}$$

The novel feature here is, evidently, the appearance of both factors z and l in $\varphi_{\Pi}(z,l)$ related to the "resonance" solutions, $n=\pm1$, in (5.34). Note also that in (5.23) and below the z^k factors multiplying $e^{-j(z-l)}$ terms with j positive, integrate on z from 0 to l to yield a term varying no more strongly than l^k: conversely, z factors multiplying increasing exponentials $e^{+j(z-l)}$ ($j>0$), can be grouped as $(z-l)^ke^{+j(z-l)}$, so that integration yields only l^ke^{-jl}. The corresponding coefficients C_+ and C_- are then found to associate factors X^i ($i\geq1$) with the l^k terms.

Now using (5.25), the expression for φ_{01} leads, via an integration, to the first-order stiffness correction

$$S_{01}(l)=-\tfrac{1}{2}l^2(3B_-^2A_+^2+12B_+B_-A_+A_-+3B_+^2A_-^2)$$
$$+l(2A_-D_++2A_+D_--3B_+B_-A_-)$$
$$+\tfrac{3}{16}B_+^2A_+^2+A_+D_++A_-D_-X^{-2}+\cdots\,, \tag{5.38}$$

where the $A_\pm(l)$ are defined through (4.28), and

$$D_\pm(l)\equiv(\partial C_\pm/\partial l)\mp\kappa C_\pm\quad(\kappa=1)\,, \tag{5.39}$$

so that $D_+=O(\tau^2X^2)l+O(1)$ and $D_-=O(\tau X^3)l+O(X^2)$. The powers of l arise from the resonances, as mentioned, but also from the integration of terms with factors e^{0z}. A direct expansion for large l and, hence, small X yields

$$S_{01}(l)=l^2(-\tfrac{3}{2}\tau^2X^2-15\tau\mathcal{G}X^3+\cdots)$$
$$+l\{[\tfrac{1}{2}\mathcal{G}+O(\tau^2)]X^2+O(\tau)X^3+\cdots\}$$
$$+\tfrac{1}{16}+O(\tau^2)+O(\tau)X+O(1)X^2+\cdots\,. \tag{5.40}$$

Note the presence of l-independent terms which contribute to the stiffness of a free ($l\to\infty$) interface: such terms must clearly be present.

As anticipated, this result suggests that the stiffness $\tilde{\Sigma}(l)$ has the general form

$$\tilde{\Sigma}(l)=\tilde{\Sigma}_\infty+S_1(\kappa l)e^{-\kappa l}+S_2(\kappa l)e^{-2\kappa l}+\cdots\,, \tag{5.41}$$

with polynomials ($j=1,2,\ldots$)

$$S_j(x)=s_{j0}+s_{j1}x+\cdots+s_{jj}x^j\,. \tag{5.42}$$

This structure is obviously similar to that of $W(l)$ in (5.30)–(5.33). Note, however, that the coefficient of lX^2 here does *not* vanish when $\tau\to0$ in *contrast* to the contributions to $W(l)$.

Combining (5.40) with the previous parabolic results (4.31)–(4.33) one reads out

$$\tilde{\Sigma}_\infty\approx\tilde{\Sigma}^0_\infty+\tfrac{1}{16}\varepsilon_4,\quad s_{10}\approx2\tau+O(\tau)\varepsilon_4,\quad\ldots\,, \tag{5.43}$$

$$s_{22}\approx-\tfrac{3}{2}\tau^2\varepsilon_4,\quad s_{32}\approx-15\tau\mathcal{G}\varepsilon_4,\quad\ldots\,, \tag{5.44}$$

$$s_{21}\approx-2\mathcal{G}(1-\tfrac{1}{4}\varepsilon_4),\quad s_{31}\approx-8\mathcal{G}\tau[1+O(1)\varepsilon_4]\,,\quad\ldots\,, \tag{5.45}$$

as well as $s_{11}\approx0$ and $s_{jk}\approx0$ for all $j\geq k\geq3$ to this order in ε_4. Recall that we are using reduced units: see (5.27).

In a parallel way, the expression for φ_{01} yields the second-order ε_4 corrections to the potential via (5.23). After some tedious algebra, one finds

$$V_{02}(l)=l(3B_+^2B_-C_-+3B_+B_-^2C_+-\tfrac{9}{2}B_+^3B_-^3)$$
$$+(\tfrac{1}{48}B_+^6+\tfrac{1}{4}B_+^3C_+-\tfrac{3}{4}B_+^4B_-^2l+\cdots)\,, \tag{5.46}$$

where, as in (5.38), all terms not displayed are of higher order in X and τ. Consequently, one can expand to get

$$V_{02}(l)=l^2\{\tfrac{9}{2}\tau^3X^3+[18\tau^2\mathcal{G}+O(\tau^3)]X^4+\cdots\}$$
$$+l[-\tfrac{3}{4}\tau^2X^2+O(\tau^4X^2,\tau X^3,\ldots)]$$
$$-\tfrac{1}{96}+\tfrac{1}{8}\tau X+\tfrac{5}{32}\mathcal{G}X^2+\cdots\,. \tag{5.47}$$

This accords with the form (5.30) and yields new l^2 terms in $W(l)$ with

$$w_{32}\approx\tfrac{9}{2}\tau^3\varepsilon_4^2,\quad w_{42}\approx18\tau^2\mathcal{G}\varepsilon_4^2,\quad\ldots\,. \tag{5.48}$$

In addition, this calculation shows that the leading variation of those terms that are already nonzero in first order [see (5.32)–(5.33)] are unmodified in character while w_{11}, w_{22}, and all w_{jk} with $j\geq k\geq3$ remain zero in this order. Finally, note the existence in (5.47) of an l-independent term that contributes only to the background to be subtracted off in the final definition of $W(l)$.

D. Some general considerations

Our explicit calculations of the φ^4 corrections in $W(l)$, to second order in ε_4, and in $\tilde{\Sigma}(l)$, to first order, can, clearly, be extended straightforwardly. However, the algebra rapidly becomes unmanageable. Nevertheless, various general features are clear and will be discussed prior to examining the explicit low-order φ^3 corrections. For convenience let

$$P_k(z,l;X)=\sum_{i,j}^{k}p_{ij}(X)l^iz^j \tag{5.49}$$

be a *generic* polynomial in z and l of total degree k ($\geq i+j$); related polynomials of the same degree will be denoted $\bar{P}_k,P_k^\pm$, etc. Then with the operator $\mathcal{L}$ defined by (5.11)–(5.13), one may extend (5.34) to give

$$\mathcal{L}^{-1}P_k(z)e^{nz}=\bar{P}_k(z)e^{nz}\quad\text{for } n\neq\pm1$$
$$=P_{k+1}(z)e^{nz}\quad\text{for } n=\pm1\,. \tag{5.50}$$

Thus, on solving (5.16), one sees that $\varphi_{02}(z;l)$ contains terms $P_0e^{\pm 5z}$, $P_1e^{\pm 3z}$, and $P_2e^{\pm z}$. More generally, in nth order one has

$$\varphi_{0n}(z;l)=\sum_{k=0}^{n}{}^{\pm} P_k^{\pm}(z,l)e^{\pm(2n-2k+1)} , \tag{5.51}$$

where distinct sums over + and − are understood. On the other hand, from (5.21), etc., one obtains the potential contribution in the form

$$V_{0n}(l)=\sum_{\{j\}}^{n-1} a_{\{j\}} \int_0^l dz\, \varphi_{0i}(z;l)\cdots\varphi_{0k}(z;l) , \tag{5.52}$$

the sum being restricted by $i+\cdots+k=n-1$ while the $a_{\{j\}}$ are unimportant combinatorial coefficients. In light of (5.51) this leads to

$$V_{0n}(l)=\int_0^l dz \sum_{k=0}^{n+1}{}^{\pm} P_{m(k,n)}^{\pm}(z,l)e^{\pm 2(n-k+1)z} , \tag{5.53}$$

where $m(k,n)=\min(k,n-1)$. A precisely similar expression is found for the stiffness correction coefficients $S_{0n}(l)$ except that $P_{m(k,n+1)}^{\pm}$ replaces $P_{m(k,n)}^{\pm}$.

Since one has

$$\int_0^l dz\, P_k(z,l)e^{nz}=\tilde{P}_k(l,l) \qquad \text{for } n\neq 0$$
$$=P_{k+1}(l,l) \quad \text{for } n=0 , \tag{5.54}$$

these results clearly reveal the general route by which powers of l appear in the perturbative structure. Indeed one sees that $V_{0n}(l)$ and $S_{0,n-1}(l)$ contain terms with all factors l^j for $0\le j\le n$. Consequently, both $W(l)$ and $\tilde{\Sigma}(l)$ contain terms with prefactors l^k with k arbitrarily large. In these circumstances it is at first unclear why the coefficients $W_n(\kappa l)$ in (5.30) should be finite polynomials as asserted in (5.31). However, if they were not finite polynomials one would have to contemplate the possibility that, for example, the expansion of the first coefficient takes the form

$$W_1(x)=w_{10}+w^*\sum_{k=0}^{\infty}(\lambda\varepsilon_4 x)^k/k!$$
$$=w_{10}+w^*e^{\lambda\varepsilon_4 x} . \tag{5.55}$$

That would change the leading exponential decrement of $W(l)$ from κ to $\kappa(1-\lambda\varepsilon_4)$, a most alarming transformation! The same concerns obviously apply to the stiffness expansion (5.41).

Fortunately, a scenario of this sort is not, in fact, realized. What happens, as can be seen in the calculations reported above and below, is that each factor of l finally appearing in $W(l)$ or $\tilde{\Sigma}(l)$ carries at least one factor of $B_-\sim\tau X$ or of X, thence leading to the polynomial nature of the $W_j(l)$ in (5.31) and of the $S_j(l)$ in (5.42).[19] The reader should examine (5.28), (5.35), (5.38), and (5.46) and note the operation of the boundary-condition mechanism discussed after (5.37). Moreover, as also indicated by the explicit calculations for S_{01} in (5.41) and for V_{02} in (5.47), the higher-order ε_4 corrections do not determine the leading decays of the coefficients $W_1(l)$, $S_1(l)$, $W_2(l)$, and $S_2(l)$ of the crucial $e^{-\kappa l}$ and $e^{-2\kappa l}$ terms.

Before discussing further generalities, we examine the asymmetrical φ^3 perturbations and related issues. By calculating explicitly the leading-order corrections, we will see that the ε_3 terms behave in a closely similar way to the ε_4 terms so that all major conclusions for $W(l)$ and $\tilde{\Sigma}(l)$ remain valid.

E. Leading orders in φ^3

Consider now the case $\varepsilon_4=\varepsilon_5=\cdots=0$ with $\varepsilon_3>0$ small, and follow the program of Sec. V C. On using (5.19) and (5.22) and adopting (5.27), the first-order ε_3 correction is simply

$$V_{10}(l)=\tfrac{1}{9}B_+^3(1-X^3)+\tfrac{1}{9}B_-^3(X^{-3}-1)$$
$$+B_+^2B_-(1-X)+B_+B_-^2(X^{-1}-1) \tag{5.56}$$

which, under expansion, yields

$$V_{10}(l)=-\tfrac{1}{9}+\tfrac{1}{9}\tau^3+[\tfrac{2}{3}\tau+O(\tau^2)]X$$
$$+[\tfrac{2}{3}\mathcal{G}+O(\tau)]X^2+[\tfrac{1}{9}-\mathcal{G}+O(\tau)]X^3+\cdots . \tag{5.57}$$

Evidently this correction preserves the pure-exponential form of the parabolic limit; it results only in background terms and unimportant modifications of the amplitudes of the leading coefficients of $W(l)$. Thus, extending the earlier results (4.20)–(4.22), we find

$$w_1\equiv w_{10}\approx 2\tau(1+\tfrac{1}{3}\varepsilon_3+\cdots) ,$$
$$w_2\equiv w_{20}\approx \mathcal{G}(1+\tfrac{2}{3}\varepsilon_3+\cdots) . \tag{5.58}$$

[In addition, (5.58) leads to $w_3(\varepsilon_3)\approx O(\tau)+(\tfrac{1}{9}-\mathcal{G})\varepsilon_3>0$ when τ and $\mathcal{G}$ are small; this removes the unphysical *tricritical* and higher multicritical wetting behavior[10,19] mentioned after Eqs. (4.6), and (4.22). Indeed, the ε_4 corrections derived from (5.28) and so on, as well as higher-order corrections, fulfill the same function.]

Solving (5.15) now yields the first-order profile correction

$$\varphi_{10}(z;l)=\tfrac{1}{3}B_+^2Z^2+C_{10}^+Z-2B_+B_-$$
$$+C_{10}^-Z^{-1}+\tfrac{1}{3}B_-^2Z^{-2} , \tag{5.59}$$

where $Z\equiv e^{(z-l)}$, while the boundary conditions (5.17) and (5.18) lead to

$$C_{10}^+=-\tfrac{1}{3}-\tfrac{8}{3}\tau[1+O(\tau)]X-3[\mathcal{G}+O(\tau)]X^2+\cdots , \tag{5.60}$$

$$C_{10}^-=-\frac{1}{3}\left[\mathcal{G}-\frac{1}{1-\tilde{g}}\right]\tau^2[1+O(\tau)]X$$
$$+\tfrac{1}{3}[\mathcal{G}+O(\tau)]X^2+\cdots , \tag{5.61}$$

which have no resonance factors of l. Subsequent iteration, however, yields

$$\varphi_{20}(z;l)=\tfrac{1}{12}B_+^3Z^3+\tfrac{2}{3}C_{10}^+B_+Z^2$$
$$+[C_{20}^+-\tfrac{5}{3}B_+^2B_-(z-l)]Z$$
$$-2(C_{10}^+B_-+C_{10}^-B_+)+(\tfrac{5}{3}B_+B_-^2z+C_{20}^-)Z^{-1}$$
$$+\tfrac{2}{3}C_{10}^-B_-Z^{-2}+\tfrac{1}{12}B_-^3Z^{-3} , \tag{5.62}$$

with new amplitudes

$$C_{20}^{+}=\tfrac{5}{3}[\tau^2+O(\tau X,\dots)]lX^2-\tfrac{5}{36}+O(\tau X,\dots)\ , \quad (5.63)$$

$$C_{20}^{-}=-\tfrac{5}{3}[\tau\mathcal{G}+O(X)]lX^3+\tfrac{5}{36}\mathcal{G}X^2+O(\tau^3 X,\dots)\ . \quad (5.64)$$

Evidently $\varphi_{20}(z;l)$ has both z and l factors: note also the operation of the boundary-condition mechanism discussed after (5.37).

Using these corrections to the profile in (5.23) yields

$$\begin{aligned} V_{20}(l)=&-\tfrac{10}{3}B_+^2B_-^2 l+(\tfrac{1}{12}B_+^4+\tfrac{1}{3}B_+^2C_{10}^{+}+2B_+B_-C_{10}^{+}\\ &+B_+^2C_{10}^{-}-\tfrac{2}{3}B_+^3B_-+\cdots)\\ =&-\tfrac{10}{3}[\tau^2+2\tau\mathcal{G}X+O(\tau^3X,X^2)]lX^2\\ &+\tfrac{5}{9}\tau X-\tfrac{1}{36}+O(\tau^4,\tau^2X,\mathcal{G}X^2,\dots)\ . \end{aligned} \quad (5.65)$$

Thus the ε_3 perturbation also generates anomalous terms with factors of B_- and contributes to the general form (5.30) for $W(l)$; specifically, one has

$$w_{21}\approx-\tfrac{10}{3}\tau^2\varepsilon_3^2,\quad w_{31}\approx-\tfrac{20}{3}\tau\mathcal{G}\varepsilon_3^2,\quad \dots, \quad (5.66)$$

while the w_{j0} with $j=1,2,\dots$ are modified only trivially. To this order in ε_3 the coefficients w_{11}, w_{22}, and w_{jk} with $j\geq k\geq 2$ remain zero.

With φ_{10} and φ_{20} one can go further, since from (5.21), etc., one obtains

$$\begin{aligned} V_{30}=&\int_0^l dz(\varphi_0\varphi_{10}^2+\varphi_0^2\varphi_{20})\\ =&C_{20}^{+}(\tfrac{1}{3}B_+^2+2B_+B_-+\cdots)+C_{20}^{-}(B_-^2+\cdots)\\ &+l(\tfrac{5}{3}B_+^3B_-^2-\tfrac{20}{3}B_+B_-^2C_{10}^{+}+\cdots)+\cdots\\ =&-\tfrac{10}{3}[\tau^2+\tfrac{7}{3}\tau X+O(\tau^3,\tau^2X,X^3)]lX^2\\ &+l^0[\cdots]\ . \end{aligned} \quad (5.67)$$

This demonstrates that V_{30} and V_{20} have equivalent anomalous terms, both being proportional to $\tau^2 lX^2$ as $x,\tau\to 0$.

Likewise the ε_3 corrections for the stiffness may be calculated. Using the $A_\pm$ from (4.28) and defining

$$D_{j0}^{\pm}\equiv(\partial C_{j0}^{\pm}/\partial l)\mp\kappa C_{j0}^{\pm}\quad(\text{with } j=1,2, \text{ and } \kappa=1)\ , \quad (5.68)$$

one obtains from (5.25) the result

$$S_{10}(l)=2(A_+D_{10}^{-}+A_-D_{10}^{+})l+(\tfrac{4}{9}B_+A_+^2+A_+D_+-\tfrac{8}{3}B_+A_+A_--4B_-A_+^2+D_-A_-X^{-2}+\cdots) \quad (5.69)$$

$$=-\tfrac{4}{3}[\mathcal{G}+O(\tau,X)]lX^2-\tfrac{1}{18}[1+2\tau X+(8\mathcal{G}-3)X^2+\cdots]\ , \quad (5.70)$$

and, from (5.26), the second-order result

$$\begin{aligned} S_{20}(l)=&\tfrac{5}{6}(4B_+B_-A_+A_-+B_-^2A_+^2+B_+^2A_-^2)l^2\\ &+(A_-D_{20}^{+}+A_+D_{20}^{-})l+(\cdots)\ ,\\ =&[\tfrac{5}{6}\tau^2+\tfrac{5}{3}\tau\mathcal{G}X+O(X^2)]l^2X^2+\cdots\ , \end{aligned} \quad (5.71)$$

where in the last line, only the l^2 terms have been shown explicitly.

By inspection we see that the first-order correction $S_{10}(l)$ does not generate any new terms beyond those already found in the pure parabolic results (4.31)–(4.33). On the other hand, the second-order correction contributes to the fuller form (5.41)–(5.42) with, specifically,

$$s_{22}\approx\tfrac{5}{6}\tau^2\varepsilon_3^2,\quad s_{32}\approx\tfrac{5}{3}\tau\mathcal{G}\varepsilon_3^2,\quad s_{42}\sim\tau^0\varepsilon_3^2\ . \quad (5.72)$$

F. Higher-order perturbations and cross terms

The explicit calculations of the leading order ε_4 and ε_3 corrections reported above do, in fact, serve to determine the leading behavior of $W(l)$ and $\tilde{\Sigma}(l)$ to order $e^{-2\kappa l}$, which is our primary concern. Examining the details of the calculation reveals the operative mechanisms leading to the correction polynomials in l with, furthermore, in many cases factors vanishing with τ. However, it is also clear that the perturbative structure is rather complex; this has prevented us from developing transparent algorithms for describing the general perturbative term. Nevertheless, further analysis, which we summarize now, enables us to surmise, we believe reliably, the most important structural features of the perturbation expansion.

Consider, first, the effect of further perturbations of degree $n\geq 5$ (which do not, of course, arise in the simple φ^4 model). We find that these may be ignored asymptotically provided the ε_3 and ε_4 terms are present. (In saying this we are, of course, regarding modifications of various amplitudes by factors of order unity when $\tau\to 0$ and $l\to\infty$ as uninteresting.) More concretely, it is easy to see that the first-order contributions to $W(l)$ proportional to ε_{2k} for $k\geq 3$ contain only the anomalous term $\sim lB_-^k\sim\tau^k le^{-k\kappa l}$, while the corresponding second-order correction contains terms $l^2(\tau^{2k-1}X^{2k-1}+\cdots)$ $+l(\tau^kX^k+\cdots)$, etc. All these terms are, in fact, weaker (in powers of τ and X) than the corresponding contributions to the w_{jk} arising from the ε_3 and ε_4 perturbations. Hence we restrict further discussion to the φ^3 and φ^4 potential terms.

As seen explicitly above, the leading contributions to the w_{jk} and s_{jk} in low order come from the (pure) ε_4 terms. Following the analysis in Sec. V D above, one sees more generally that the highest powers of l enter in nth order as

$$V_{0n}(l)\approx b_n l^n B_-^{n+1},\quad S_{0n}(l)\approx c_n l^{n+1}B_-^{n+1}\ , \quad (5.73)$$

where b_n and c_n are of order unity. Furthermore, the $V_{0n}(l)$ and $S_{0,n-1}(l)$ corrections generate nonzero coefficients w_{jn} for all $j\geq n+1$ and s_{jn} for all $j\geq n$. Beyond that, however, they have no other significant consequences.

The low-order calculations also revealed that the first-order φ^3 terms gave no anomalous l dependences whereas the second-order ε_3^2 corrections were equivalent to the first-order ε_4 correction: compare (5.32) with (5.66) and (5.44) with (5.72). Further analysis indicates that these correspondences, for the s_{jk} with $j \geq k$ and for w_{jk} with $j \geq k+1$, hold for general $k \geq 0$.

It is clearly also necessary to understand the cross terms such as $V_{11}(l)$, $V_{12}(l)$, etc. A full calculation, using (5.24), yields

$$V_{11}(l)=3B_+B_-(B_+C_{10}^- + B_-C_{10}^+)l+\tfrac{1}{15}B_+^5+\cdots$$
$$=(\tau^2+3\tau\mathcal{G}X+\cdots)lX^2+O(1,\tau X,X^2) . \quad (5.74)$$

Comparison with (5.28) and (5.29) shows that the $\varepsilon_3\varepsilon_4$ term contributes to $W(l)$ nothing beyond the products of the pure first-order ε_4 term; it merely modifies the amplitudes by factors of order unity. More generally, one surmises that the corrections of order $\varepsilon_3^{2m}\varepsilon_4^n$ and $\varepsilon_3^{2m+1}\varepsilon_4^n$ have the same character as the term of order ε_4^{m+n} $(m,n \geq 0)$.

In summary, we conclude that the general polynomial coefficients, resulting from perturbations $\varepsilon_3 \sim \varepsilon$, $\varepsilon_4 \sim \varepsilon^2$, etc. behave as

$$w_{jk}=\varepsilon^{2k}\tau^{|2k+2-j|^+}[a_{jk}+O(\tau,\varepsilon)] , \quad (5.75)$$

$$s_{jk}=\varepsilon^{2|k-1|^+}\tau^{|2k-j|^+}[b_{jk}+O(\tau,\varepsilon)] , \quad (5.76)$$

where $|x|^+ \equiv \max\{x,0\}$; while the coefficients a_{jk} for $j \geq k+1$ and b_{jk} for $j \geq k$ are of order unity except that b_{10} and b_{11} both vanish as revealed by the explicit calculations of Secs. V D and V E. Furthermore, s_{11} appears to carry a factor of at least τ in all orders and it vanishes identically in ε_4, ε_4^2, ε_3, ε_3^2, and $\varepsilon_3\varepsilon_4$. It follows, as already seen in lower orders, that the w_{jk} are nonvanishing at $T=T_{cW}^0$ if, but only if, $k \leq \frac{1}{2}j-1$; likewise the s_{jk} are nonzero at $T=T_{cW}^0$ only when $k \leq \frac{1}{2}j$.

This completes our analysis of the perturbative contributions to the effective interfacial Hamiltonian: see (5.30) and (5.41). In fact, the leading-order results contained in (5.32), (5.33), (5.43)–(5.45), and (5.48) are quite characteristic of the full expansion.

VI. INTEGRAL CRITERION ANALYSIS

Our conclusions based on the *crossing criterion* are clearly satisfactory, especially since the value of $m^\times$ can be chosen fairly freely. Nevertheless, other choices of the definition for the interface location are possible and, if reasonable, should lead to equivalent asymptotic wetting behavior. As was mentioned in Sec. II, the definition (2.11) provides, for general $p>0$, a set of *integral criteria* providing measures of the total adsorption in the wetting layer. In this section we use this definition and discuss some interesting features of the results.

A. Integral criterion formulation

Clearly the integral definitions (2.11) of $\bar{l}$, the wetting-layer thickness, entail global constraints on the fundamental partial trace in (2.1) through which the effective interfacial Hamiltonian $\mathcal{H}_I[\bar{l}]$ is now to be defined. Accordingly, the previous derivations of the corresponding effective interaction $W(\bar{l})$ and of the effective stiffness $\bar{\Sigma}(\bar{l})$ must be revised. However, the general principles remain unchanged so that we again undertake the following program: First, we obtain the *planar profile* $\bar{m}_{\Pi}(z;\bar{l}) \equiv \bar{m}_{\Xi}[\mathbf{r};\bar{l}(\cdot)=l_\pi]$ from the constrained minimization principle. (Note that we use an overbar to label properties computed using the integral criterion.) Then, with $\bar{m}_{\Pi}(z;\bar{l})$ in place of $m_{\Pi}(z;l)$, we evaluate $W(\bar{l})$ and $\bar{\Sigma}(\bar{l})$ using (2.13) and (2.26), respectively. (Note that these expressions are not dependent on the details of the criterion determining l or $\bar{l}$.)

Now, to obtain the planar constrained profile $\bar{m}_{\Pi}(z;\bar{l})$ we will utilize the method of the Lagrange multiplier to impose the constraint. This leads to a new set of equations for the constrained profile. Specifically, the first one of this set may be taken as the constraint itself, namely

$$\bar{l}=\int_0^\infty dz[\bar{m}_{\Pi}-m_{\alpha\infty}]^p/(m_{\beta\infty}-m_{\alpha\infty})^p , \quad (6.1)$$

where $\bar{l}$ is independent of $\mathbf{y}$ and does not, in general, equal the corresponding equilibrium value $\bar{l}_0$.

Next, the planar profile must still obey the *bulk condition*

$$\bar{m}_{\Pi}(z \to +\infty;\bar{l}) \to m_{\alpha\infty} , \quad (6.2)$$

which is, in fact, also required by (6.1). Finally, the profile must satisfy the minimization requirements, corresponding to integrating out the noncritical bulk fluctuations at a mean-field level: see Sec.II. These derive from

$$\delta\left\{\mathcal{H}[\bar{m}_{\Pi}]+\lambda\int_0^\infty[\bar{m}_{\Pi}-m_{\alpha\infty}]^p dz\right\}\Big/\delta\bar{m}_{\Pi}=0 , \quad (6.3)$$

where λ is the anticipated Lagrange multiplier. On using (1.2) for $\mathcal{H}[m]$, this reduces to

$$K\frac{d^2\bar{m}_{\Pi}}{dz^2}=\Phi'(\bar{m}_{\Pi})+p\lambda(\bar{m}_{\Pi}-m_{\alpha\infty})^{p-1} , \quad (6.4)$$

for the bulk region $0<z<\infty$, and

$$K\frac{d\bar{m}_{\Pi}}{dz}(z=0)=\Phi'(\bar{m}_{1\Pi}) , \quad (6.5)$$

at the wall with $\bar{m}_{1\Pi} \equiv \bar{m}_{\Pi}(z=0+,\bar{l})$, following the notations of (2.8) and (2.9).

Evidently, our task is to solve the nonlinear differential equation (6.4) subject to the two boundary conditions (6.2) and (6.5) and with one parameter λ to be determined through (6.1). It turns out that for the natural choice $p=1$ (as well as for $0<p<1$) certain difficulties arise[11,19] as we now show. However, for integral $p=2,3,4$ and the standard m^4 model (2.27), we can obtain explicit results.

B. Insolubility for p unity or less

We observe, first, that the *equilibrium profile* $\check{m}(z)$ depends only on $\mathcal{H}[m]$ but not on the choice of criterion. Consequently, if $\bar{l}_0(T,h)$ is the *equilibrium value of the wetting-layer thickness,* the relation $\bar{m}_{\Pi}(z;\bar{l}=\bar{l}_0)=\check{m}(z)$ holds for all $p>0$: see Fig. 1. This corresponds, again, to consistency at the mean-field level. Naturally, $\overline{m}_{\rm II}(z;\overline{l}_0)$ also corresponds to $\lambda=0$ in (6.4); conversely, for $\overline{l}\neq\overline{l}_0$ one must have $\lambda\neq 0$.

Second, since $m=m_{\alpha\infty}$ is the global minimum of the bulk potential $\Phi(m)$, (6.2) and (6.4) determine the curvature of $\overline{m}_{\rm II}(z)$ when $z\to\infty$ as

$$d^2\overline{m}_{\rm II}/dz^2\to\lambda p(\overline{m}_{\rm II}-m_{\alpha\infty})^{p-1}/K \ . \tag{6.6}$$

But for $p\leq 1$ (and $\lambda\neq 0$) this implies a nonzero curvature as $z\to\infty$ and $m\to m_{\alpha\infty}$. Clearly, however, that contradicts the bulk condition (6.2), which in fact requires decay of all derivatives $d^n\overline{m}_{\rm II}/dz^n$ to zero when $z\to\infty$. We must conclude therefore that no proper solutions exist for the *constrained profile* when $p\leq 1$ and $\lambda\neq 0$.

In other words, the *integral criterion* as we have accepted it perturbs the vicinity of the pure α phase too strongly whenever $p\leq 1$.[11,19] We remark that the result is somewhat surprising in that (2.11) with $p=1$ corresponds to the most natural definition of the wetting layer thickness on the basis of the adsorption. One can devise various *ad hoc* but reasonable *approximate* procedures to define and solve the problem using $0<p\leq 1$, but they are too artificial to be worth recording here.[26(c)]

On the other hand, (6.6) implies no difficulties whenever $p>1$. Indeed, by choosing tractable bulk free-energy densities $\Phi(m)$ in (6.4) and corresponding values of the parameter $p>1$, one can obtain several sets of exact, explicit solutions. We present below only a representative case with $p=2$ and the standard m^4 model specified by (1.3) and (2.27).

C. Exact profiles in the m^4 model

To begin, we recapitulate briefly some of the known mean-field results for the model.[10]

(a) The m^4 potential has an exact α-β symmetry at coexistence $h=0\pm$ with the order-parameter values

$$-m_{\alpha 0}(T)=m_{\beta 0}(T)=M\equiv(6|r|/u)^{1/2} \ . \tag{6.7}$$

When $H<0$, the α phase is stable and the equilibrium value of the order parameter shifts as

$$m_{\alpha\infty}(T,h)=m_{\alpha 0}+\tfrac{1}{2}|r|^{-1}h+O(h^2)<m_{\alpha 0} \ , \tag{6.8}$$

which is the negative solution of the third-order equation

$$\tfrac{1}{6}um(m^2-M^2)=h \ . \tag{6.9}$$

The β phase is then metastable with the order-parameter value $m_{\beta\infty}(T,h)=-m_{\alpha\infty}(T,-h)$, which is the largest, positive solution of (6.9).

(b) Unlike the parabolic potentials considered in Sec. IV, this m^4 potential together with the usual surface interaction $\Phi_1(m_1)$ of (1.4) generates, in mean-field theory, a full, well-behaved wetting/surface-transition phase diagram in the field space (T,h,h_1,g).[10] In particular, the critical wetting transition corresponds to

$$T-T_{cW}^0\sim\tau\sim h_1+gm_{\beta 0}\to 0- \tag{6.10}$$

at $h=0-$ with $g<-K\kappa_0$, where the inverse bulk correlation length is

$$\kappa_0(T)=(2|r|/K)^{1/2}=\kappa_{\alpha 0}=\kappa_{\beta 0} \ . \tag{6.11}$$

Now in order to solve for the constrained planar profile $\overline{m}_{\rm II}$ it is convenient to define the rescaled profile

$$\rho(z;\overline{l})\equiv[\overline{m}_{\rm II}(z;\overline{l})-m_{\alpha\infty}]/(-2m_{\alpha\infty}) \ . \tag{6.12}$$

The first integral of (6.4) using (6.2) yields

$$(d\rho/dz)^2=\kappa^2[(1-\rho)^2+\mu]\rho^2 \ , \tag{6.13}$$

where the parameters are

$$\mu=(3/um_{\alpha\infty}^2)\lambda+\tilde{h} \ , \tag{6.14}$$

$$\tilde{h}\equiv\tfrac{1}{2}[1-(m_{\alpha 0}^2/m_{\alpha\infty}^2)]\sim -h\to 0+ \ , \tag{6.15}$$

$$\kappa(T,h)\equiv(3K/um_{\alpha\infty}^2)^{-1/2}=\kappa_\alpha(T)+O(h) \ . \tag{6.16}$$

Likewise the wall condition (6.5) becomes

$$\left[\frac{1}{\kappa}\frac{d}{dz}+\tilde{g}\right]_{z=0}\rho=\tilde{h}_1\equiv(h_1+gm_{\alpha\infty})/2m_{\alpha\infty}K\kappa \ , \tag{6.17}$$

while near mean-field wetting criticality one has $\tilde{h}_1\approx\tilde{g}\equiv g/K\kappa$.

In order to proceed correctly, particularly as regards the signs of $d\rho/dz$, it is useful to study the problem with the standard graphical methods.[10,20] One verifies that $\rho(z;\overline{l})$ is always a smooth function for $0<z<\infty$; this is a benefit of the global character of the integral criterion. In particular, $\rho(z;\overline{l})$ crosses the reference value $m^\times=0$ or $\rho^\times=\frac{1}{2}$, smoothly at $z=l$ in contrast to the crossing-criterion profiles: see Fig. 1. We expect $l=\overline{l}+O(\xi_\beta)$ near critical wetting.

Now two distinct cases arise: (i) $\mu\equiv\mu(\overline{l})\geq 0$, which corresponds to $\overline{l}<\overline{l}_c$ where, depending on the relative values of the relevant critical wetting fields h and τ, one has $\overline{l}_c(T,h)\simeq 2\overline{l}_0$. [Recall that $\overline{l}_0(T,h)$ is the equilibrium or unconstrained value of $\overline{l}$.] Furthermore, $\mu(\overline{l})$ decreases monotonically as $\overline{l}$ increases. In case (ii) one has $\mu(\overline{l})\leq 0$, corresponding to $\overline{l}_c\leq\overline{l}\leq\infty$. Now, however, as $\overline{l}$ increases above $\overline{l}_c$, $\mu(\overline{l})$ first decreases (below zero) and then finally rises back to zero as $\overline{l}\to\infty$.

The profiles also differ markedly in the two cases: (i) when $\overline{l}\leq\overline{l}_c$ one finds that $\rho(z)$ increases monotonically as z decreases from $+\infty$ and, on analytic continuation through $z=0$, ultimately *diverges* to $+\infty$ inside the wall region when z approaches a singular point $z^*(\overline{l})<0$. On the other hand, (ii) when $\overline{l}>\overline{l}_c$ there is always a *point of symmetry,* on the analytically extended profile at $z=z^\dagger(\overline{l})$ such that $\rho(z)=\rho(2z^\dagger-z)\geq 0$. In addition, there is a unique maximum at $z^\dagger$ with $\rho(z^\dagger)=1+(-\mu)^{1/2}$: see Fig. 1.

Armed with these insights, the appropriate square roots in (6.13) may be taken. The integral to obtain $z=Z(\rho)$ then proves tractable and, furthermore, can be inverted to yield the explicit constrained profile in the form

$$\rho(z;\overline{l})=\frac{1+\mu}{1+F_+e^{\tilde{\kappa}(z-l)}+F_-e^{-\tilde{\kappa}(z-l)}} \ , \tag{6.18}$$

where the asymptotic decay is given by

$$\tilde{\kappa}^2(T,h)=\kappa^2(1+\mu) \ . \tag{6.19}$$

This form of solution can be checked by direct substitution in (6.4) and (6.2) and is a valid solution for all l provided $F_+F_- = -\frac{1}{4}\mu$. By imposing the crossing condition $m^\times=0$ or $\rho(l)=\frac{1}{2}$ to define l one finds more explicitly

$$2F_\pm = 1+2\mu\pm[(1+\mu)(1+4\mu)]^{1/2} , \tag{6.20}$$

and can check that $l=\bar{l}+O(\xi_\beta)$ for large l. The various features listed under (i) and (ii) above can be explicitly checked.

Note also that (6.19) and (6.20) include the exact solution in the unconstrained, $\lambda=0$ case which is given simply by $\mu=\tilde{h}$. Then one has $\tilde{\kappa}=\kappa\sqrt{1+\tilde{h}}$, $F_+=1+\frac{9}{4}\tilde{h}+O(\tilde{h}^2)$, and $F_-=-\frac{1}{4}\tilde{h}+O(\tilde{h}^2)$. When $h\to 0-$ the standard $\tanh[\frac{1}{2}\kappa(z-l)]$ profile of m^4 theory is reproduced. We remark that this explicit solution for the standard theory does not seem to be recorded in the literature for $h\neq 0$. When $T>T^0_{cW}$ the equilibrium profiles, imposed by appropriate wall conditions, have the form

$$\check{m}(z;T,h=0)=M\{1+\coth[\tfrac{1}{2}\kappa(z-z^*)]\} . \tag{6.21}$$

These display the advertised divergence at $z=z^*$: see Fig. 1.

D. Effective wall-interface potential

Although the explicit form (6.18)–(6.20) of the constrained profile is relatively simple, it is still necessary to impose the wall boundary condition (6.17) and the actual constraint (6.1). To that end it is convenient to introduce the wall deviation and reduced gradient via

$$x\equiv\rho_1(\bar{l})-1=(\bar{m}_{1\mathrm{II}}+m_{\alpha\infty})/(-2m_{\alpha\infty}) , \tag{6.22}$$

where, as previously, the subscript 1 means evaluation at $z=0+$, and

$$\dot{\rho}_1\equiv\frac{1}{\kappa\rho_1}\left[\frac{d\rho}{dz}\right]_1=\frac{1}{\kappa}\left[\frac{d\bar{m}_{\mathrm{II}}}{dz}\right]_{z=0}\Big/(\bar{m}_{1\mathrm{II}}-m_{\alpha\infty}) . \tag{6.23}$$

These are related via (6.13) as

$$\dot{\rho}_1^2=x^2+\mu . \tag{6.24}$$

Then, using the appropriate square root in (6.13) one can integrate (6.1) for $p=2$ to find

$$\tilde{\kappa}\bar{l}=-\dot{\rho}_1-\sqrt{1+\mu}-\ln\left[\frac{x-\dot{\rho}_1}{\sqrt{1+\mu}-1}\right] , \tag{6.25}$$

which is valid for all $\bar{l}$ with

$$\tilde{\kappa}(T,h)\equiv\tfrac{1}{4}\kappa[1-(m_{\beta\infty}/m_{\alpha\infty})]^2=\kappa+O(h) . \tag{6.26}$$

Note, however, as discussed in Sec. VI C, that $\dot{\rho}_1$ can change sign. Finally (6.17) may be rearranged to give

$$(1+x)\dot{\rho}_1=-\tilde{\tau}-\tilde{g}x \tag{6.27}$$

with, recalling (4.5) and (4.6),

$$\tilde{\tau}\equiv(h_1-gm_{\alpha\infty})/(-2m_{\alpha\infty}K\kappa)\sim\tau . \tag{6.28}$$

The variable $\tilde{\tau}$ will serve as our primary control parameter.

Now Eqs. (6.24)–(6.28) determine the variation of x, $\dot{\rho}_1$, and μ with the layer thickness $\bar{l}$ and the thermodynamic fields T, h, h_1, and g (via $\tilde{\tau}$, $\tilde{g}$, etc.). We aim initially, therefore, to express the wall potential $W(\bar{l};T,\dots)$ in terms of x, $\dot{\rho}_1$, and μ.

To proceed we write the expression (2.13) for $W(\bar{l};\dots)$ as

$$W(\bar{l})=W_{\alpha\beta}(\bar{l})+W_\omega(\bar{l})-W_\infty(T,\dots) , \tag{6.29}$$

where the direct wall contribution is

$$W_\omega=\Phi_1(\bar{m}_{1\mathrm{II}})=-h_1\bar{m}_{1\mathrm{II}}-\tfrac{1}{2}g\bar{m}^2_{1\mathrm{II}}$$
$$=\Sigma_0(T,h)[\tfrac{1}{2}\tilde{g}-2\tilde{\tau}-4\tilde{\tau}x-2\tilde{g}x^2] , \tag{6.30}$$

in which $\Sigma_0\equiv K\kappa m^2_{\alpha\infty}$ reduces simply to $\frac{3}{2}\Sigma_{\alpha|\beta}(T)$, when $h\to 0$, where $\Sigma_{\alpha|\beta}$ is the mean-field interfacial tension for this model.[10] The background term $W_\infty(T,\dots)$ may, as explained after (2.13), be determined at the end of the calculation from the requirement $W(\bar{l};h=0)\to 0$ as $\bar{l}\to\infty$.

The bulk term $W_{\alpha\beta}(\bar{l})$ is more complicated but after substituting for $(\partial m_{\mathrm{II}}/\partial z)^2$ using (6.13) and performing an integral similar to that yielding (6.25), one can obtain

$$W_{\alpha\beta}(\bar{l})=2\Sigma_0\left\{\tilde{h}\ln\left[\frac{x-\dot{\rho}_1}{\sqrt{1+\mu}-1}\right]+\tfrac{1}{3}(1+\mu-3\tilde{h})\sqrt{1+\mu}-\tfrac{1}{3}\dot{\rho}_1[2x^2+3x-\mu+3\tilde{h}]\right\} , \tag{6.31}$$

which is valid for $\dot{\rho}_1$ positive, negative, or zero. The first step now is to eliminate the logarithmic term here with the aid of (6.25). That yields the expected linear, bulk field term $\bar{h}\,\bar{l}$ in $W(\bar{l})$ with

$$\bar{h}\equiv 2\Sigma_0\tilde{h}\tilde{\kappa}=\frac{(m_{\beta\infty}-m_{\alpha\infty})^2}{2m_{\alpha\infty}}h\sim -h , \tag{6.32}$$

as $h\to 0-$. Note, however, that there are still weak, residual field dependences in μ, $\dot{\rho}_1$, etc. Next one can eliminate $\dot{\rho}_1$ in (6.24) and (6.31) using (6.27) and express the reduced Lagrange multiplier as

$$\mu=\frac{(\tilde{\tau}+\tilde{g}x)^2}{(1+x)^2}-x^2 . \tag{6.33}$$

After some algebra one can then write

$$W(\bar{l})=\bar{h}\,\bar{l}+V[x(\bar{l})]-W_\infty , \tag{6.34}$$

with x now regarded as a function of $\bar{l}$, T, h, h_1, and g, and

$$V(x)=\Sigma_0\{\tfrac{1}{2}\tilde{g}-2\tilde{\tau}+\tfrac{2}{3}[1+\mu(x)]^{3/2}-2\tilde{\tau}x-gx^2-\tfrac{2}{3}(\tilde{\tau}+\tilde{g}x)[\mu(x)-3x-2x^2]/(1+x)\} . \tag{6.35}$$

Note that this may readily be expanded in powers of x for small $\tilde{\tau}$.

On the other hand, one can rearrange (6.25) in the form

$$\bar{X}(\bar{l})\equiv e^{-\bar{\kappa}\bar{l}}=[\sqrt{1+\mu}-1](x-\dot{\rho}_1)^{-1}\exp[\dot{\rho}_1+\sqrt{1+\mu}]$$
$$=\tfrac{1}{2}e[1+O(\tilde{\tau})][\tilde{\tau}+(\tilde{g}-1)x-\tilde{g}^2x^2+O(x^3)] , \quad (6.36)$$

where the expression follows by eliminating $\dot{\rho}_1$ and μ in favor of x as before. The expansion can then be inverted for small $\bar{X}$, that is, for $\bar{l}\to\infty$, to yield

$$x(\bar{l})=\frac{1+O(\tilde{\tau})}{1-\tilde{g}}\left[\tilde{\tau}-\frac{2}{e}\bar{X}-\frac{4\tilde{g}^2}{e^2(1-\tilde{g})}\bar{X}^2+O(\bar{x}^3)\right] , \quad (6.37)$$

which, in turn, may be substituted into the expansion of (6.34) in powers of x.

Finally, one obtains the desired expansion for the wall potential as $\bar{l}\to\infty$ in the form

$$W(\bar{l})=\bar{h}\,\bar{l}+\bar{w}_1e^{-\bar{\kappa}\bar{l}}+\bar{w}_2e^{-2\bar{\kappa}\bar{l}}+\bar{w}_3e^{-3\bar{\kappa}\bar{l}}+\cdots , \quad (6.38)$$

where we recall that $\bar{h}$ is defined in (6.23) while $\bar{\kappa}(T,h)$ is given by (6.26), (6.16), and (6.11). The coefficients are found to be

$$\bar{w}_1=(4/e)(1+\mathcal{G})\Sigma_0\tilde{\tau}+O(\tilde{\tau}^2) , \quad (6.39)$$

$$\bar{w}_2=(4/e^2)\mathcal{G}\Sigma_0+O(\tilde{\tau}) , \quad (6.40)$$

$$\bar{w}_3=[16\tilde{g}^3(\tilde{g}+\tfrac{1}{3})/(1-\tilde{g})^3e^3]\Sigma_0+O(\tilde{\tau}) , \quad (6.41)$$

as $\tilde{\tau}\sim\tau\to0$. Note that $\tilde{\tau}$ is defined in (6.28), the numerical coefficients $\tilde{g}$ and $\mathcal{G}$ are defined in (4.6) and (4.12) and satisfy $-\tilde{g}>1$ and $0<\mathcal{G}<1$, while $\Sigma_0(T,h)=K\kappa m^2_{\alpha\infty}$ reduces to three halves of the bulk tension $\Sigma_{\alpha|\beta}$ when $h\to0$. This completes the derivation of the wall-interface potential.

One also finds that the background piece is given by

$$W_\infty=(\tfrac{2}{3}+\tfrac{1}{2}\tilde{g})\Sigma_0+O(\tilde{\tau}) , \quad (6.42)$$

which approaches $\Sigma_{\alpha|\beta}+\frac{1}{2}gM^2$ when $h,\tilde{\tau}\to0-$. This value is, of course, calculable directly from the mean-field theory.[10]

E. Relation between the integral and crossing constraints

The most striking feature of the result (6.38) is that the thickness $\bar{l}$ enters only in the bulk term $\bar{h}\,\bar{l}$ and as powers of $\bar{X}=e^{-\bar{\kappa}\bar{l}}$; there are no terms like $\bar{l}^k\bar{X}^j$ with polynomial factors as found generally when using the crossing constraint. To understand the relationship between the two apparently contrasting results in more detail we examine the dependence of $\bar{l}$ on the *corresponding* crossing point l that follows from the integrally constrained profile (6.18).

To this end we evaluate $\rho(z;\bar{l})$ and $d\rho/dz$ at $z=0$ using (6.18), (6.22), with (6.23) to get

$$(\mu-x)/(1+x)=F_+\tilde{X}+F_-\tilde{X}^{-1} , \quad (6.43)$$

$$\dot{\rho}_1(1+\mu)^{1/2}/(1+x)=-F_+\tilde{X}+F_-\tilde{X}^{-1} , \quad (6.44)$$

where, by (6.20), we have

$$\tilde{X}\equiv e^{-\bar{\kappa}l}=-2F_-[\mu-x-\dot{\rho}_1\sqrt{1+\mu}]/\mu(1+x) . \quad (6.45)$$

Now note that near criticality τ, x, and thence $\dot{\rho}_1$ and μ are all small. Then with the aid of (6.24) one can expand in the form

$$\tilde{X}=-\frac{x+\dot{\rho}_1}{1+x}[1-\tfrac{9}{4}\mu+\tfrac{1}{2}(2-\dot{\rho}_1)(x-\dot{\rho}_1)+O(\dot{\rho}_1\mu,\mu^2)] . \quad (6.46)$$

On the other hand, from the expression (6.25) for $\bar{l}$ one can obtain

$$x+\dot{\rho}_1=-(2/e)\bar{X}[1-\tfrac{1}{4}\mu-\dot{\rho}_1+\tfrac{1}{2}\dot{\rho}_1^2+O(\dot{\rho}_1^3,\mu^2)] . \quad (6.47)$$

Combining this with (6.46) and using (6.37) for x yields

$$\tilde{X}=(2/e)\bar{X}[1+2\tilde{g}x+O(x^2,\tilde{\tau})]$$
$$=\frac{2}{e}\bar{X}\left[1-\frac{4\tilde{g}}{(1-\tilde{g})e}\bar{X}+O(\bar{X}^2,\tilde{\tau})\right] . \quad (6.48)$$

Finally, using (6.19), one obtains

$$\kappa l=[\bar{\kappa}\bar{l}+1-\ln2+O(\tilde{\tau},\bar{X})]/(1+\mu)^{1/2} . \quad (6.49)$$

Now from (6.33) and (6.37) one finds

$$\mu=\frac{2}{e}\bar{X}\left[\frac{2}{1-\tilde{g}}\tilde{\tau}+\frac{2}{e}\mathcal{G}\bar{X}+O(\bar{X}^2)\right][1+O(\tilde{\tau})] . \quad (6.50)$$

Hence from (6.49) we can conclude, as $h\to0$,

$$l=\bar{l}+(1-\ln2)\xi_\beta+O(\tilde{\tau}\bar{l}\,\bar{X},\ \bar{l}\bar{X}^2) . \quad (6.51)$$

This confirms the basic expectation $\bar{l}-l=O(\xi_\beta)$. In the limit that the profile approaches the standard tanh profile this is, of course, easily seen directly.

We now seek to reexpress the potential $W(\bar{l})$ in terms of l, the crossing thickness. To that end notice that $X\equiv e^{-\kappa l}=\tilde{X}^{1/\sqrt{1+\mu}}$ and from (6.48) thence obtain

$$\bar{X}=\tfrac{1}{2}eX^{\sqrt{1+\mu}}\left[1+\frac{2\tilde{g}}{1-\tilde{g}}X^{\sqrt{1+\mu}}+O(\bar{X}^2)\right] . \quad (6.52)$$

Then by using (6.50) and noting that $X^\mu=\exp(-\mu\kappa l)$ one can expand this for small $\tilde{\tau}$ and X in the form

$$(2/e)\bar{X}=X+\sum_{j=2}^{\infty}\sum_{k=0}^{j-1}c_{jk}(\kappa l)^kX^j , \quad (6.53)$$

where the leading coefficients are found to be

$$c_{21}=\tilde{\tau}/(1-\tilde{g}),\quad c_{20}=2\tilde{g}/(1-\tilde{g})+O(\tilde{\tau}) , \quad (6.54)$$

$$c_{32}=\tfrac{1}{2}\tilde{\tau}^2/(1-\tilde{g}),\quad c_{31}=\tfrac{1}{2}\mathcal{G}+O(\tilde{\tau}),\quad c_{30}=O(1) . \quad (6.55)$$

The appearance of the terms $(\kappa l)^ke^{-j\kappa l}$ is striking in view of the results originally obtained with the crossing criterion! Indeed, we may now substitute (6.53) into the previous results (6.38)–(6.41) for $W(\bar{l})$ to obtain the same potential expressed in terms of l. This yields

$$W^I(l;T,\ldots)\equiv W(\bar{l};T,\ldots)=\bar{h}_I l+\sum_{j=1}^{\infty}\sum_{k=0}^{j} w_{jk}^I(\kappa l)^k X^j , \quad (6.56)$$

where the new potential coefficients are, in leading orders,

$$\bar{h}_I=\kappa\bar{h}/\bar{\kappa}\approx\bar{h}, \quad w_{10}^I=2(1+\mathcal{G})\Sigma_0\tilde{\tau}+O(\tilde{\tau}^2,h) , \quad (6.57)$$

$$w_{11}^I=\bar{h}\tilde{\tau}/\bar{\kappa}(1-\tilde{g})[1+O(\tilde{\tau},h)] ,$$
$$w_{20}^I=\mathcal{G}\Sigma_0+O(\tilde{\tau},h) , \quad (6.58)$$

$$w_{21}^I=-2\mathcal{G}\Sigma_0\tilde{\tau}^2+O(\tilde{\tau}^3,h), \quad w_{31}^I\sim\tilde{\tau}+O(h) , \quad (6.59)$$

$$w_{22}^I=\bar{h}\tilde{\tau}^2/\bar{\kappa}(1-\tilde{g})^2[1+O(\tilde{\tau},h)] ,$$
$$w_{32}^I\sim\tilde{\tau}^3+O(h) , \quad (6.60)$$

$$w_{30}^I=2\tilde{g}^3(\tilde{g}+\tfrac{1}{3})\Sigma_0/(1-\tilde{g})^3 . \quad (6.61)$$

Finally, therefore, we have an extremely close correspondence with the results (5.30)–(5.31) obtained wholly on the basis of the crossing criterion. Note in particular how the coefficients w_{jk}^I for $k\geq 1$ vanish as powers of $\tilde{\tau}\sim\tau$ when $T\to T_{cW}^0$ as do the original coefficients w_{jk}. The compatibility of the two approaches reinforces our general conclusions.

It should be further remarked that the explicit planar profile (6.18) allows us to determine the l-dependent stiffness coefficient as indicated in Sec. VI A. However, the expressions for $\tilde{\Sigma}(l)$ now entail complicated integrals so that more elaborate analysis (to be presented elsewhere[31]) is required to extract the asymptotic decay. Here we merely report that the type of behavior found for the parabolic potentials with perturbations is, in fact, reproduced.[31]

VII. CONSEQUENCES OF NONEXPONENTIAL TERMS

Having established that the effective potential $W(l)$ in general contains terms of the form $w_{jk}(\kappa l)^k e^{-j\kappa l}$ for $j\geq k\geq 0$, as in (1.8), and that the perturbed stiffness $\tilde{\Sigma}(l)$ has similar terms, it is appropriate to ask what effects such deviations from pure exponential form will have on the critical wetting behavior. Recalling that the borderline dimensionality is[3-9] $d=3$, there are three cases to address: (i) $d<3$, (ii) $d>3$, and (iii) $d=3$.

The functional renormalization-group treatment for $d<3$ reveals[8,9] the existence of well-defined fixed-point potentials $W^*(l)$ describing wetting criticality with nonclassical exponents. The fixed-point potentials have single wells and rapidly decaying tails; on the critical manifold in the full Hamiltonian space they are attractive for all similar potentials which decay faster than $1/l^{\tau}$ with $\tau=2(d-1)/(3-d)$.[8,9] The only two relevant perturbations correspond to the deviations $\Delta T=(T-T_{cW})\neq 0$ and $\bar{h}>0$. Consequently, the changes in $W(l)$ we have found can do no more than change the values of T_{cW} and of the nonuniversal metrical factors; universal aspects of the critical behavior will remain unchanged.

The spatial dependence of the stiffness $\tilde{\Sigma}(l)$ that we have uncovered has not been explicitly studied in current renormalization-group treatments.[3-8] However, its presence considerably complicates the analysis and, accordingly, details will be presented elsewhere.[31] Nevertheless, one can be confident, in view of the exact planar Ising model solutions,[32] that no deviations from critical point universality will be induced by this source when $d=2$.

By contrast, for $d>3$ mean-field theory should be valid and the behavior will be sensitive to the details of $W(l)$ even if $\tilde{\Sigma}(l)$ should play no role.[31] Thus considering *complete wetting,* as $\bar{h}\to 0+$ with $T>T_{cW}$, and neglecting $\tilde{\Sigma}(l)$ one finds for $w_{11}>0$ a wetting layer thickness diverging as

$$\langle\kappa l\rangle\approx\ln(\bar{h}/\kappa)^{-1}+\ln[\vartheta w_{11}\ln(\bar{h}/\kappa)^{-1}]+\cdots . \quad (7.1)$$

The singular correction term here is absent for pure exponentials ($w_{11}=0$); the factor $\vartheta\simeq 1$ allows for renormalization by residual fluctuations (which generally shift the bare parameters). In a similar way if $w_{22}>0$ and $w_{11}<0$ and w_{10} both vanish linearly when $\Delta T\to 0-$, *critical wetting* in zero field is described by

$$\kappa\langle l\rangle\approx\ln(c/|\Delta T|)-\ln[\vartheta w_{22}\ln(c/|\Delta T|)]+\cdots , \quad (7.2)$$

where c is a constant and the next correction varies as $w_{10}/w_{11}\ln(c/|\Delta T|)$. Again the leading log-log correction is absent for pure exponentials. All other properties also follow in a straightforward way[1,2] from $W(l)$ [assuming, still, that the effects of $\tilde{\Sigma}(l)$ can be neglected[31]].

At the borderline dimension $d=3$, on which we now focus, one might guess that the changes in critical behavior could be no worse than for $d>3$. However, although essentially correct, that conclusion is *not* obvious in view of the complex wetting transition behavior found at $d=3$ in the renormalization-group treatments;[4-9] recall, in particular, the continuous dependence of the exponents on the parameter ω defined in (1.1). To study this we follow the analysis of D. S. Fisher and Huse[6] still *neglecting* any possible role of $\tilde{\Sigma}(l)$.

A. Renormalization-group analysis for $d=3$

Fisher and Huse[6] (FH) consider the standard interface Hamiltonian (1.5) with $\tilde{\Sigma}$ *independent* of $l(\mathbf{y})$ and a momentum cutoff $|\mathbf{k}|<\Lambda$ imposed. Now FH argue persuasively that to understand asymptotic ($l\to\infty$) wetting criticality a linearized RG treatment suffices. They then implement an exact linearization of the standard momentum shell integration procedure: fluctuations with momenta satisfying $\Lambda/b<|\mathbf{k}|\leq\Lambda$ are integrated out followed by the rescaling

$$\mathbf{y}'=\mathbf{y}/b \text{ and } l(\mathbf{y}')=b^{(d-3)/2}l(\mathbf{y}) . \quad (7.3)$$

In this formula we allow for general d, but will usually set $d=3$ below. Introducing a continuous renormalization flow parameter t (called l by FH, who use z for our l) via $b=e^{\delta t}\to 1$ leads to a linear partial differential equation for the renormalized wall-interface potential $W^{(t)}(l)$.

To obtain the critical behavior of the wetting-layer thickness $\langle l\rangle$, the parallel correlation length $\xi_{\parallel}$, and F_s, the singular part of the free energy (per unit wall area), the RG transformation is carried through up to a matching point $t=t^{\dagger}(T,h,\ldots)$ where at the (presumed unique) *minimum* $l=l^{\dagger}$ of $W^{(t^{\dagger})}(l)$ one has

$$\partial^2 W^{(t^\dagger)}/\partial l^2|_{l=l^\dagger}=\tilde{\Sigma}/\xi_\beta^2 . \tag{7.4}$$

At this point mean-field theory suffices and yields

$$\langle l^{(t^\dagger)}\rangle \simeq l^\dagger,\ \ \xi_\parallel^{(t^\dagger)}\simeq\xi_\beta,\ \ F_s^{(t^\dagger)}\simeq W^{(t^\dagger)}(l^\dagger) . \tag{7.5}$$

Then, via rescaling, the original, unrenormalized properties are given by

$$\begin{aligned}&\langle l\rangle(T,h,\dots)\approx e^{-(d-3)t^\dagger/2}l^\dagger ,\\ &\xi_\parallel(T,h,\dots)\approx e^{t^\dagger}\xi_\beta ,\\ &F_s(T,h,\dots)\approx e^{-(d-1)t^\dagger}W^{(t^\dagger)}(l^\dagger) .\end{aligned} \tag{7.6}$$

Because of the linearization employed one cannot treat an infinitely repulsive wall for $l<0$. Rather, in the spirit of FH, we write for all l

$$W(l)\equiv W^{(0)}(l)=\Theta(-l)W_\omega(l)+\Theta(l)\left[\bar{h}l+\sum_{j\ge k\ge 0}W_{jk}(l)\right] , \tag{7.7}$$

where $\Theta(z)=1,0$ for $z\gtrless 0$, is the usual step function. We then adopt a "soft wall" of strength $0<w_0<\infty$ and take

$$W_\omega(l)=w_0,\ \ W_{jk}(l)=w_{jk}(\kappa l)^k e^{-j\kappa l} . \tag{7.8}$$

Solving the linearized flow equation for $d=3$ yields[6]

$$W^{(t)}(l)=\frac{e^{2t}}{\sqrt{2\pi}\delta(t)}\int_{-\infty}^{\infty}dl'\,W^{(0)}(l')\exp\left[-\frac{(l-l')^2}{2\delta^2(t)}\right] , \tag{7.9}$$

where the width of convolution is given by

$$\delta^2(t)=2\omega\xi_\beta^2 t . \tag{7.10}$$

We may now analyze the renormalized potential asymptotically for large l and t. It transpires[6] that expressions are needed only for $\mu\equiv l/\xi_\beta t$ of order ω. We thence obtain the Gaussian forms

$$W_\omega^{(t)}(l)\approx w_0\frac{\delta(t)}{\sqrt{2\pi}l}e^{2t-l^2/2\delta^2(t)} , \tag{7.11}$$

$$[\bar{h}l]^{(t)}\approx\bar{h}le^{2t}+\frac{\bar{h}\delta^3(t)}{\sqrt{8\pi}l^2}e^{2t-l^2/2\delta^2(t)} \tag{7.12}$$

for $l>0$, and for $0<l<2j\omega\xi_\beta t$

$$W_{jk}^{(t)}(l)\approx\frac{w_{jk}k!}{\sqrt{2\pi}\kappa\delta}\left[j-\frac{\kappa l}{2\omega t}\right]^{-k-1}e^{2t-l^2/2\delta^2(t)} ; \tag{7.13}$$

however, for $l>2j\omega\xi_\beta t$ one still has the exponential decays

$$W_{jk}^{(t)}(l)\approx w_{jk}(\kappa l-j\kappa^2\delta^2)^k e^{(2+j^2\omega)t-j\kappa l} . \tag{7.14}$$

The further corrections to these expressions are of relative order $1/t$ as $l^2/t\sim t\to\infty$ or smaller.

Now FH showed for the $k=0$ case ($w_{jk}=0$ for $k>0$) that the changeover of the renormalized potentials from Gaussian to exponential decays is the crucial feature leading to the three regimes of critical behavior, namely I, $\omega<\frac{1}{2}$; II, $\frac{1}{2}<\omega<2$; III, $\omega>2$. This changeover is evidently independent of the exponent k of the κl factors in $W(l)$. Consequently, the same three regimes arise quite generally. The more detailed changes in critical behavior can be determined from (7.11)–(7.14) following directly the methods of FH. We will, primarily, just summarize the results.

B. Wetting criticality with nonexponential terms

For generality we may first regard the potential coefficients w_{jk} ($j\ge k$) as independent fields and thus ignore the rather special dependences of the "bare" or initial values of the w_{jk} on T, h, h_1, and g uncovered in the preceding sections. (Under renormalization one would not normally expect such dependences to be preserved unless particular symmetries were involved; however, in the present case, since we operate with the linearized functional renormalization group, the bare values have an enhanced significance.) A little reflection shows, however, that a host of different types of wetting transition scenarios might then arise as various different combinations of the w_{jk} compete with one another under renormalization! Our aim here is only to study the *changes* induced in the ordinary critical wetting transition found for pure exponentially decaying effective potentials. This results[6] from a competition between the "attractive" part of the renormalized potential, which we generalize as

$$A^{(t)}(l)\equiv[\bar{h}l]^{(t)}+W_{10}^{(t)}(l)+W_{11}^{(t)}(l) , \tag{7.15}$$

and the remaining "repulsive" part which is thus

$$R^{(t)}(l)\equiv W_\omega^{(t)}(l)+\sum_{j\ge 2}\sum_{k=0}^{j}W_{jk}^{(t)}(l) . \tag{7.16}$$

Now in the FH analysis[6] the attractive part is totally negative for $T<T_{cW}^0$ but approaches zero when $T\to T_{cW}^0-$, while the repulsive part remains everywhere positive throughout the transition region. We will assume that the same situation pertains when the factors polynomial in l are present with, in particular, the $j=2$ terms in (7.16) not all vanishing. One may check that for the specific potential coefficients computed previously this will be the case. It is then easily seen that the higher-order terms with $j\ge 3$ in (7.16) may be neglected.

In the circumstances postulated, the three critical wetting regimes will arise just as previously[6] being determined as follows: regime I, $\omega<\frac{1}{2}$: the global minimum of $W^{(t^\dagger)}(l)$ lies in the exponential tails of both $A^{(t^\dagger)}(l)$ and $R^{(t^\dagger)}(l)$ [see (7.14)]; regime II, $\frac{1}{2}<\omega<2$: the minimum lies, now, in the Gaussian region of $R^{(t^\dagger)}(l)$ [see (7.11)–(7.13)]; regime III, $\omega>2$: the Gaussian parts of both attractive and repulsive potentials determine the global minimum of $W^{(t^\dagger)}(l)$. It transpires, furthermore, that the results can be expressed compactly in terms of the polynomials $W_1(x)=w_{10}+w_{11}x$ and $W_2(x)$, as defined in (5.31).

Suppose then, that the critical wetting point is approached along the phase boundary with $\bar{h}=0$ and one can write

$$W_1(x) \approx \Delta T U_1(x) \quad \text{with } \Delta T = (T - T_{cW}^0)/T_{cW}^0 \to 0- \ . \tag{7.17}$$

In regime I ($\omega < \frac{1}{2}$) the transition remains at $\Delta T = 0$ and one finds the parallel correlation length varies as

$$\xi_\parallel \sim \frac{[W_2(\vartheta \ln|\Delta T|^{-1})]^{\nu_\parallel/2}}{|W_1(\nu_\parallel \ln|\Delta T|^{-1})|^{\nu_\parallel}} , \tag{7.18}$$

where the exponent $\nu_\parallel = 1/(1-\omega)$ takes its previous value[6] while $\vartheta = (1-2\omega)\nu_\parallel$. Similarly one has a wetting-layer thickness diverging as

$$\langle \kappa l \rangle \approx -\frac{1+2\omega}{1-\omega} \ln|W_1(\nu_\parallel \ln|\Delta T|^{-1})| + \frac{2+\omega}{2(1-\omega)} \ln W_2(\vartheta \ln|\Delta T|^{-1}) , \tag{7.19}$$

while the singular part of the surface free energy obeys

$$F_s \sim \frac{|W_1(\nu_\parallel \ln|\Delta T|^{-1})|^{2\nu_\parallel}}{[W_2(\vartheta \ln|\Delta T|^{-1})]^{(1-2\omega)\nu_\parallel}} . \tag{7.20}$$

In regime II ($\frac{1}{2} < \omega < 2$) the critical wetting transition is again at $\Delta T = 0$, but the singularities are described by

$$\xi_\parallel \sim \xi_\beta \left[\frac{(\ln|\Delta T|^{-1})^{-\sqrt{\omega/8}}}{|W_1(\vartheta_1 \ln|\Delta T|^{-1})|} \right]^{\nu_\parallel} , \tag{7.21}$$

with exponent $\nu_\parallel = (2+\omega-\sqrt{8\omega})^{-1}$, as previously[6] and

$$\langle \kappa l \rangle \approx \sqrt{8\omega}\,\nu_\parallel \{ \ln|\Delta T|^{-1} - \tfrac{1}{8}(2+\omega) \ln\ln|\Delta T|^{-1} - \ln[W_1(\vartheta_1 \ln|\Delta T|^{-1})/\Delta T] \} , \tag{7.22}$$

with $\vartheta_1 \equiv (2-\omega)\nu_\parallel$.

Finally, in regime III ($\omega > 2$) the transition temperature is shifted[6] according to $\Delta T_{cW} = T_{cW} - T_{cW}^0 \approx -c(\omega-2) \to 0$ as $\omega \to 2+$. The values of ΔT_{cW} and c depend on all the coefficients w_{jk} and the critical divergences are

$$\xi_\parallel \sim \exp\left[\frac{1}{C\Delta\tau} \left[\ln\frac{1}{C\Delta\tau} + \ln\ln\frac{1}{C\Delta\tau} + \cdots \right] \right] , \tag{7.23}$$

$$\langle \kappa l \rangle \approx \frac{\sqrt{8\omega}}{C\Delta\tau} \left[\ln\frac{1}{C\Delta\tau} + \ln\ln\frac{1}{C\Delta\tau} + \cdots \right] , \tag{7.24}$$

where $\Delta\tau \sim T_{cW} - T \to 0+$ and C depends on w_{jk}, w_0, ω, etc.

The previous results[4,6] correspond simply to $W_1(x) = a_1 \Delta T \le 0$ and $W_2(x) = a_2 > 0$. One can thus see clearly that polynomial factors in $W(l)$ can induce significant differences (which are somewhat more noticeable in regimes I and II). For instance, if both w_{11} and w_{10} vanish linearly with ΔT and $w_{22}(T_{cW}^0) > 0$, one finds from (7.19) and (7.22) that $\langle \kappa l \rangle$ picks up divergent corrections of the form $A(\omega)\ln\ln|\Delta T|$ (although in regime III, one encounters only shifts in the nonuniversal transition locus, in the amplitudes, etc.).

On the other hand, our explicit calculations in Secs. V and VI actually showed that, for short-range critical wetting, w_{11}, w_{21}, and w_{22} either vanish identically or approach zero much more rapidly than linearly with ΔT: see (5.75) and (6.57)–(6.61). When this is recognized, further expansions of (7.18)–(7.24) may be made, revealing that such w_{jk} terms with $k \ge 1$ generate nothing more than unimportant modifications of correction factors to the leading behavior in regimes I and II. In regime III only the nonuniversal transition locus and various amplitudes are effected.[19] In other words, the previous results of Brézin, Halperin, and Leibler and of FH are fully adequate: all the deviations from pure exponential behavior found in $W(l)$ are quite inessential to the asymptotic critical wetting behavior!

Closely similar conclusions hold for the approach to critical wetting by varying the bulk field at $T = T_{cW}$. We find, in fact, two distinctive types of behavior corresponding to $\omega < \frac{1}{2}$ (regime I) and $\omega > \frac{1}{2}$ (regimes II and III) that are adequately determined by the *pure* exponential terms together with $[\bar{h}l]^{(t)}$ and $W_\omega^{(t)}(l)$. Thus, *provided* the stiffness variation is neglected, all the original RG predictions for critical wetting remain valid, in spite of the nonexponential terms in $W(l)$.

Finally, we remark that by extending calculations along the lines of FH,[6] one can obtain[33] closed-form expressions for the scaling functions for $\xi_\parallel(T,h)$, $\langle l(T,h) \rangle$, and $F_s(T,h)$ in regime I as a function of the scaled combination $\Delta T/|h|^{(1-\omega)/2}$. These scaling functions allow, in principle, better analysis and assessment of the Monte Carlo simulations.[12,15,16,18] However, in doing this one seems only to reinforce the earlier conclusions that for the Ising-model simulated one has $\omega_{\text{fit}} \lesssim 0.25$ in contrast to the actual value[13] $\omega \gtrsim 0.6$. Therefore, our analysis to this point does not cast light on the sharp discrepancy between the theory and simulations.

C. Effects of stiffness variation

It is evident that to finish the story the effects of the l-dependent terms $\Delta\tilde{\Sigma}(l)$ in the stiffness coefficient of the full interfacial Hamiltonian must be studied. As mentioned, the necessary analysis is rather elaborate and will be reported separately;[31] the overall conclusions and a few details have been summarized briefly.[19(b)] For completeness the main issues arising are sketched here.

The renormalization-group flows must now be studied in the functional space specified by $\{\Delta\tilde{\Sigma}^{(t)}(l), W^{(t)}(l)\}$. The first essential feature is that the fluctuation contributions controlled by $\Delta\tilde{\Sigma}(l)$ feed through into $W^{(t)}(l)$. Within the linearized RG theory, the result has a surprisingly simple form: it is simply as if, after renormalization to stage t, the bare potentials $W_{jk}(l)$ in (7.7) and (7.8) are replaced by

$$\check{W}_{jk}(l) = [w_{jk} + \tfrac{1}{2}\omega\xi_\beta^2\Lambda^2(1-e^{-2t})s_{jk}](\kappa l)^k e^{-j\kappa l} , \tag{7.25}$$

in which the s_{jk} are the stiffness coefficients [from (4.31)] while Λ is the momentum cutoff.

Next one notices the explicit results found previously, in particular, $w_{10} \sim s_{10} \sim \Delta T$, $w_{20} \sim s_{20} \sim \Delta T^0$, $w_{21} \sim \Delta T^2$, and, most crucially, the fact that $s_{21}(T,h)$ remains of order unity and *negative* as $\Delta T \to 0-$: see (4.33) and (5.45). Consequently the term $s_{21} l e^{-2\kappa l}$ plays a dominating role in $R^{(t)}(l)$, at least for $l > 4\omega\xi_\beta t$: see (7.14). Furthermore, since this contribution is negative it violates the positivity of the renormalized repulsive potential $R^{(t)}(l)$ for large t and l. This has an obvious destabilizing effect. Indeed, it follows that in regime I ($\omega < \frac{1}{2}$) the critical wetting transition must become a *first-order* transition!

In regimes II and III the fluctuations are enhanced; then more detailed analysis is needed.[31] One finds[19(b),31] that there is a nonuniversal *tricritical* value ω_t above which the critical wetting transition remains continuous and with unaltered singular behavior; below ω_t the wetting transition is again of first order.

It also transpires[31] that the first-order transitions induced by the stiffness variation are comparatively weak so that, in simulations of finite systems, they might easily be viewed as critical in nature. In light of this, it seems likely that the discrepancies with the previous Monte Carlo simulations can be attributed to the fact that the transitions simulated in the three-dimensional Ising model are actually weakly first-order. However, further numerical studies (analytically based or via simulations) will be needed to cement that conclusion firmly.

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