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Stiffness instability in short-range critical wetting

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Recent theoretical work has shown that an interface separating two fluid phases suffers changes in its (bare) effective stiffness, $\tilde{\Sigma}(l)=\tilde{\Sigma}_\infty+\Delta\tilde{\Sigma}(l)$, when located at a distance l from a planar wall: terms varying as $l^k e^{-j\kappa l}$ appear in $\Delta\tilde{\Sigma}$ (where $0\le k\le j=1,2,\ldots$ and κ is the inverse bulk correlation length in the fluid wetting the wall). This may induce *first-order* wetting transitions when critical wetting had been expected. This general behavior of $\Delta\tilde{\Sigma}(l)$ is confirmed using an integral/adsorption constraint to determine l, in place of the original crossing constraint. The exact linearized functional renormalization-group technique is used to analyze the full wetting-phase diagram as a function of T, of $\omega=k_B T_{cW}\kappa^2/4\pi\tilde{\Sigma}(T_{cW})$, and of q, the amplitude of the $-le^{-2\kappa l}$ term in $\Delta\tilde{\Sigma}$. For dimensions $d>3$, any positive q (as generally expected) yields first-order wetting. The same is true for $d=3$ provided $\omega<\frac{1}{2}$; but when $\omega>\frac{1}{2}$ nonclassical critical behavior is still found for small $q<q_t(\omega)>0$. Detailed expressions are obtained for $\langle l\rangle$, $\xi_\parallel$, etc., in the various critical and first-order regions. Numerical estimates show that previous Ising-model simulations probably encountered weakly first-order wetting transitions which might explain discrepancies with earlier renormalization-group predictions.

I. INTRODUCTION

A challenging issue in the theory of wetting phenomena is the nature of the *critical wetting transition* in a $(d=3)$-dimensional system with short-range interactions: this question has attracted particular attention recently.[1–10] It suffices, in a first analysis, to consider a planar $d'=(d-1)$-dimensional wall at Cartesian coordinate $z=0$ bounding a d-dimensional half-space $(\mathbf{y},z>0)$ filled with a medium at or near bulk coexistence. Far from the wall the stable bulk phase α is present; close to the wall a wetting layer of the metastable or potentially coexisting phase β may arise, being stabilized via *short-range* interactions with the wall. We suppose also that only short-rangle forces characterize the *non*critical bulk phases α and β. Separating the wetting layer from the bulk phase will be a $\beta|\alpha$ *interface* at a distance from the wall $z=l(\mathbf{y})$ that undergoes thermally induced statistical fluctuations.

A *critical wetting transition* occurs when the mean layer thickness $\langle l\rangle(T)$ diverges *continuously* to $+\infty$ as the temperature T approaches T_{cW}, the critical wetting temperature, when phases α and β are just on the point of coexistence.[1] Equivalently, the $\beta|\alpha$ interface continuously delocalizes into the half-space $z>0$.[1] The precise nature of the divergence of $\langle l\rangle$ and the behavior of other thermodynamic and correlation properties are the main features demanding elucidation.

The theoretical difficulty and interest of this problem arise from the fact that for the critical wetting transition, the physically relevant dimensionality $d=3$ is also the *marginal dimensionality* in the renormalization-group (RG) sense.[1–5] Furthermore, the original RG theory[5–7] led to striking nonuniversal predictions that have not, however, been borne out by extensive Monte Carlo simulations:[9,10] see also Refs. 2–4.

Recent work by the authors[2–4] has addressed various aspects of critical wetting theory. In particular, a careful systematic account of an appropriate description of the fluctuations of the $\beta|\alpha$ interface has been presented.[2–4] Here, we concentrate on the nature of the critical wetting transition as it is determined by the character of the interfacial fluctuations. Our basic tool is functional renormalization-group theory. The present paper may be regarded as the logical extension and development of Ref. 4, which will thus be referred to as **I**. The conclusions of **I** will be freely quoted and the notation used there will be retained here whenever possible. However, in as far as the material now covered is reasonably general and since we believe the results may be of broader interest, efforts have been made to keep this paper essentially self-contained.

A. Background and preliminaries

As mentioned, our understanding of short-range critical wetting in $d=3$ dimensions has appeared deficient because of a long-standing disagreement between the predictions of renormalization-group treatments[1,5–8] and of careful and seemingly reliable Monte Carlo simulations.[1,2,9–11] Specifically, the RG theories[5–8] have employed the rather standard basic *interfacial Hamiltonian*

$$\mathcal{H}_I[l(\mathbf{y})]=\int d^{d'}y\{\tfrac{1}{2}\tilde{\Sigma}[\nabla l(\mathbf{y})]^2+W[l(\mathbf{y})]\}\ , \qquad (1.1)$$

with a *bare wall-interface potential* of the form

$$W(l;T,h,\ldots)=\bar{h}l+w_1e^{-\kappa l}+w_2e^{-2\kappa l}+\cdots \qquad (1.2)$$

to describe the fluctuations of the wall-interface separation $l(\mathbf{y})$ in systems with short-range interactions. In this formulation: (i) the coefficient $\tilde{\Sigma}=\tilde{\Sigma}(T,\ldots)$ is the *stiffness* of an isolated, free $\beta|\alpha$ interface; (ii) the exponential decays in the potential $W(l)$ are controlled by the scale $\xi_\beta \equiv 1/\kappa$, the (bounded) *true correlation length*[12] in the wetting layer β; (iii) the reduced ordering field $\bar{h} \sim -h\,(\to 0+)$ measures the bulk free-energy difference between the α and β phases; and (iv) the coefficients in the effective potential $W(l)$ behave as $w_1(T,h,\dots) \sim (T-T_{cW}^0)\to 0-$, $w_2(T,h,\dots)>0$, etc., near the mean-field critical wetting transition at $T=T_{cW}^0$.

Assuming that $l(\mathbf{y})$ undergoes only negligible capillary fluctuations, this Hamiltonian leads to a phase diagram and transition behavior fully consistent with the appropriate mean-field, order-parameter-based theory.[1,2,13] When such fluctuations are treated by the RG theory,[1,5–8] however, one finds strong nonuniversality for critical wetting at the marginal dimensionality[5] $d=3$. Three distinct regimes of behavior emerge, depending sensitively on the fundamental interfacial fluctuation or capillary parameter[5,7,8]

$$\omega = k_B T_{cW}/4\pi\tilde{\Sigma}(T_{cW})\xi_\beta^2(T_{cW}) \ . \tag{1.3}$$

Thus the exponent $\nu_\parallel$ of the diverging *interfacial correlation length* $\xi_\parallel$ (parallel to the wall and, thus, along the interface) is predicted to vary as

$$\nu_\parallel = \begin{cases} 1/(1-\omega) & \text{for } \omega < \frac{1}{2} \quad \text{(Regime I)} \\ 1/(\sqrt{2}-\sqrt{\omega})^2 & \text{for } \frac{1}{2} < \omega < 2 \ \text{(Regime II)} \\ \infty & \text{for } \omega > 2 \quad \text{(Regime III)} \ . \end{cases} \tag{1.4}$$

Beyond that, the transition temperature T_{cW} remains unshifted from T_{cW}^0, the mean-field value, when $\omega \le 2$, but drops below T_{cW}^0 in the strong fluctuation Regime III (when $\omega > 2$).[3–6]

Unhappily, the principal tests of the theory, namely, Monte Carlo simulations[9,10] of semi-infinite, $(d=3)$-dimensional Ising models above the roughening temperature T_R have failed[1–3,11] to confirm these predictions. On the one hand, careful estimates[11] indicate $\omega(T) \gtrsim 0.7$ for the temperatures simulated, pointing to Regime II, where $\nu_\parallel(T) \gtrsim 2.5$ is predicted. On the other hand, the Monte Carlo data are found to be consistent with $\omega(T) \lesssim 0.25$ (i.e., $\nu_\parallel \lesssim 1.3$) and even with the classical order-parameter-based mean-field theory,[13] which predicts $\nu_\parallel = 1$ (corresponding to $\omega = 0$)!

Motivated by this disagreement and by the failure of various possible explanations,[1–4] a careful examination of the foundations of the RG theory[5–8] has been undertaken.[2–4] The central issue is the validity of the interfacial Hamiltonian (1.1) and (1.2). We argue (in **I**) that short-range *noncritical* systems undergoing wetting transitions such as the Ising model simulated[8,9] may be described sufficiently well by a Landau-Ginzburg-Wilson (LGW) order-parameter Hamiltonian of the form[1–4,13]

$$\mathcal{H}[m(\mathbf{r})] = \int d^{d'}y\Big(\big\{\tfrac{1}{2}K[\nabla m(\mathbf{r})]^2 + \Phi(m)\big\}dz + \Phi_1(m_1)\Big) \ , \tag{1.5}$$

where $\Phi[m(\mathbf{r});T,h,\dots]$ is the noncritical bulk free-energy density while $\Phi_1(m_1;T,\dots)$ represents the direct short-range wall-bulk interaction in terms of the surface order parameter $m_1(\mathbf{y}) \equiv m(\mathbf{y},z=0)$.[1,2] Consequently, the appropriate interfacial Hamiltonian $\mathcal{H}_I[l]$ may be derived[1–4] systematically from the underlying bulk description (1.5), with given forms of $\Phi(m)$ and $\Phi_1(m_1)$ by introducing $l(\mathbf{y})$ as a *locally defined* collective coordinate: most directly one may adopt a profile *crossing definition*[2,4] to specify the precise location of the fluctuating interface. Then $\mathcal{H}_I[l(\mathbf{y})]$ can be defined by constraining the profile via, say, $m(\mathbf{y},l(\mathbf{y}))=0$, and taking a trace over the remaining degrees of freedom.

While the full implementation of this program is nontrivial, the analysis of **I** (see also the Appendix to this paper) demonstrates convincingly, we believe, that the conclusions embodied in (1.1) and (1.2) are *not* accurate. Specifically, the expression (1.2) for the wall-interface potential should be replaced by

$$W(l;T,h,\dots) = \bar{h}l + (w_{10} + w_{11}\kappa l)e^{-\kappa l} + [w_{20} + w_{21}\kappa l + w_{22}(\kappa l)^2]e^{-2\kappa l} + \cdots \ , \tag{1.6}$$

and, *in addition,* the fixed interfacial stiffness $\tilde{\Sigma}$ in (1.1) must be replaced by an l-dependent *function* of the form

$$\tilde{\Sigma}(l;T,h,\dots) = \tilde{\Sigma}_\infty + (s_{10} + s_{11}\kappa l)e^{-\kappa l} + [s_{20} + s_{21}\kappa l + s_{22}(\kappa l)^2]e^{-2\kappa l} + \cdots \ . \tag{1.7}$$

Thus the stiffness should have a piece $\Delta\tilde{\Sigma} \equiv \tilde{\Sigma}(l) - \tilde{\Sigma}_\infty$ decaying just like $W(l)$ for large l (when $h=0$).

Explicit calculations in **I** and in the Appendix here yield two sets of mutually consistent coefficients w_{jk} and s_{jk} near the mean-field critical wetting transition as controlled by $h \to 0$ and

$$\tau \sim (T - T_{cW}^0) \to 0 \ . \tag{1.8}$$

From the original *crossing-criterion* formulation[2,4] [(5.75) and (5.76) of **I** and associated text], one finds for the potential

$$(\mathbf{A}):\ \bar{h} \sim -h \ , \quad w_{10} \approx a_{10}\tau \ , \quad w_{20} \approx a_{20} \ , \quad w_{jj} = 0 \ (j \ge 1) \ , \quad w_{21} \approx a_{21}\tau^2 \ , \dots \ , \tag{1.9}$$

and for the stiffness

$$(\mathbf{A}):\ \tilde{\Sigma}_\infty = \Sigma_{\alpha|\beta} \ , \quad s_{10} \approx b_{10}\tau \ , \quad s_{21} \approx -b_{21} \ , \quad s_{22} \approx b_{22}\tau^2 \ , \quad s_{20} \approx b_{20} \ , \dots \ , \tag{1.10}$$

with, rather plausibly, $s_{11}=0$, where a_{jk} and b_{jk} are positive (nonvanishing) parameters of order $\Sigma_{\alpha|\beta}$, the free interfacial tension, which depend weakly on details of the order-parameter Hamiltonian $\mathcal{H}[m(\mathbf{r})]$. (We suppose that h and τ are defined to be dimensionless.) Alternatively from an *integral-criterion* formulation[2] [see (6.57)–(6.60) of **I** and (A34)–(A39) below], one obtains

$$(\mathbf{B}):\ \bar{h}_I \approx \bar{h} \ , \quad w_{10}^I \approx a_{10}^I\tau \ , \quad w_{20}^I \approx a_{20}^I \ , \quad w_{jj}^I \approx a_{jj}^I\bar{h}\tau^j \ (j \ge 1) \ , \quad w_{21}^I \approx a_{21}^I\tau^2 + O(h), \dots \ ; \tag{1.11}$$

$$\tilde{\Sigma}_\infty^I = \Sigma_{\alpha|\beta} \ , \quad s_{10}^I \approx b_{10}^I\tau \ , \quad s_{11}^I = 0 \ , \quad s_{21}^I \approx -b_{21}^I \ , \quad s_{22}^I \approx b_{22}^I\tau^2 \ , \quad s_{20}^I \approx b_{20}^I, \dots \ , \tag{1.12}$$

where the superscripts and subscripts I denote the integral criterion, while the a^I_{jk}, b^I_{jk} are also positive parameters of order $\Sigma_{\alpha|\beta}$. Note, as discussed further in I and the Appendix here, that the constraint is imposed via an integral relation but $l(\mathbf{y})$ still denotes the crossing position of the constrained interfacial profile.

Having found these modifications to the original interfacial Hamiltonian, one must ask how the predictions for critical wetting will be affected. If, initially, one assumes that the stiffness variation $\Delta\tilde{\Sigma}(l)$ plays no significant role near criticality,[14] the consequences of the new "anomalous" terms $w_{jk}(\kappa l)^k e^{-j\kappa l}$ ($k \geq 1$) in $W(l)$ can be examined fairly straightforwardly within the framework of the current RG theory.[7] In fact, as shown in I Sec. VII, because the leading coefficients $w_{11} \sim w^I_{11}$, $w_{21} \sim w^I_{21}$, and $w_{22} = w^I_{22}$ are zero or *vanish* with τ, the corrections to $W(l)$ alone do *not* change the critical wetting behavior in any significant qualitative way.

On the other hand, the treatment of the stiffness variation which we undertake below requires an extension of the existing RG flow equation to allow for the renormalization of $\Delta\tilde{\Sigma}(l)$. To our surprise, the subsequent analysis reveals that the stiffness variation $\Delta\tilde{\Sigma}(l)$ generally has a major influence on the critical wetting behavior. Indeed, as we show here,[3] the *nonvanishing* and *negative* coefficients s_{21} and s^I_{21} in (1.9) and (1.11) destabilize the anticipated critical wetting transition in many cases when $d=3$, resulting in fluctuation-induced, weakly *first-order wetting transitions.*[3] We believe that such weak first-order wetting transitions may well characterize the semi-infinite simple cubic Ising models simulated[9] and thus provide a plausible explanation of why these simulations disagree with the original RG predictions.[5,7]

Note that essentially the same conclusions follow using either the set of coefficients **A** [(1.9) and (1.10)] or the set **B** [(1.11) and (1.12)], above. Consequently, in addition to reinforcing confidence in the generality of the new form of the interfacial Hamiltonian (see also the Appendix for a brief discussion), there is no reason to distinguish between the crossing and integral criterion formulations in the text below. Moreover it transpires that the wetting behavior near $T = T^0_{cW}$ at bulk coexistence is determined adequately just by the terms $w_{10}e^{-\kappa l}$, $w_{20}e^{-2\kappa l}$, $w_{21}\kappa l e^{-2\kappa l}$ in $W(l)$, and by $s_{10}e^{-\kappa l}$ and $s_{21}\kappa l e^{-2\kappa l}$ in $\Delta\tilde{\Sigma}(l)$. For the sake of simplicity, therefore, we will keep only a loose check on other more rapidly decaying or vanishing terms.

B. Outline and summary

The balance of this paper is organized into five sections. In the following section we present a general formulation for treating stiffness variation using the linearized functional RG framework of Fisher and Huse.[7] We derive and solve explicitly a pair of coupled flow equations in functional space for the renormalized interfacial potential $W^{(t)}(l)$ and the renormalized stiffness variation $\tilde{\Sigma}^{(t)}(l)$ in d dimensions. One sees that $\tilde{\Sigma}^{(t)}(l)$ approaches the constant fixed-point value $\tilde{\Sigma}_{\alpha|\beta}$ diffusively but that $W^{(t)}(l)$ picks up contributions both from the bare ($t=0$) wall-interfacial potential *and* from the bare stiffness variation. A direct competition between the (bare) stiffness variation and the (bare) interfacial potential determines the fluctuation-dependent wetting behavior. The standard matching and rescaling procedure[1,4,7] in the critical limit when $t \rightarrow \infty$ is recapitulated for general d.

In Sec. III, the consequences of the derived stiffness variation away from the marginal dimension $d=3$ are discussed. For $d>3$, we establish that the stiffness variation with the expected attractive $le^{-2\kappa l}$ component *always* destabilizes the unperturbed mean-field wetting criticality and results in first-order wetting transitions. However the usual mean-field critical behavior is realized in the limits $d \rightarrow \infty$ and $\omega(d) \rightarrow 0$, where $\omega(d)$ is the natural generalization of the capillary parameter (1.3). In fact both limits may be regarded as locating *tricritical wetting points*[13] since the first-order wetting discontinuities vanish in these limits in a manner explicitly determined.

The discussion for $d<3$ mainly serves as a reminder that the linearized RG treatment is effective only in ($d \geq 3$) dimensions.[7] By recalling other studies,[8,15] it is conjectured that short-range critical wetting remains stable with standard characteristics for $d < d_1(\omega)$, where d_1 is close to 3.

Section IV addresses the marginal dimensionality $d=3$. A detailed phase diagram is constructed near mean-field critical wetting along bulk coexistence in the expanded parameter space (τ,ω,q), where $q \propto -s_{21}$ is regarded as a new thermodynamic variable. A *tricritical wetting locus* is identified in this space; the previously predicted critical wetting transitions are destabilized whenever $q(\omega) > q_{\mathrm{tri}}(\omega)$. Complete phase boundaries, critical singularities, and significant crossover loci are calculated in the three consecutive Regimes I, II, and III.

In Sec. V, the implications of the new predictions for the existing Monte Carlo Ising-model simulations are discussed. On the basis of various unavoidably rather rough numerical estimates we suggest that even though the expected first-order wetting transitions are rather weak, their almost-critical precursors may well have distorted the conclusions of the simulational analyses. Some brief concluding remarks are also offered. In the Appendix, as mentioned, we obtain the behavior of the interfacial stiffness on the basis of the integral criterion.

II. FUNCTIONAL RENORMALIZATION WITH SPATIALLY VARYING STIFFNESS

Our task here is to implement a functional renormalization-group treatment of the extended interface Hamiltonian which we write, following (1.1), (1.2), and (1.7), as

$$\mathcal{H}_I[l(\mathbf{y})] = \mathcal{H}_0[l] + \mathcal{H}_W[l] \ , \tag{2.1}$$

where the free interface Hamiltonian is simply

$$\mathcal{H}_0[l] = \int^{\Lambda} d^{d'}y \, \tfrac{1}{2}\tilde{\Sigma}_\infty(\nabla l)^2 \ . \tag{2.2}$$

The superscript Λ here indicates that in Fourier space the components $\hat{l}(\mathbf{k})$ of $l(\mathbf{y})$ are subject to the wave-number cutoff $|\mathbf{k}| < \Lambda$. The wetting part of the Hamiltonian is similarly given by

$$\mathcal{H}_W[l]=\int^{\Lambda} d^{d'}y[\tfrac{1}{2}\Delta\tilde{\Sigma}(l)(\nabla l)^2+W(l)] , \tag{2.3}$$

where $\Delta\tilde{\Sigma}(l)\equiv\tilde{\Sigma}(l)-\tilde{\Sigma}_\infty\to 0$ as $l\to\infty$. Following Fisher and Huse (FH),[7] and utilizing some of the analysis of Lipowsky and Fisher (LF),[8] we aim to construct momentum-shell renormalization-group recursion relations which are exact to linear order in $\mathcal{H}_W$. This will suffice[7] to discuss critical wetting for $d\geq 3$.

A. Linearized functional recursion relations

As explained by FH (see also I Sec. VII), it is appropriate to write

$$l(\mathbf{y})=l^<(\mathbf{y})+l^>(\mathbf{y}) \tag{2.4}$$

and to integrate out the short-wavelength fluctuations

$$l^>(\mathbf{y})=\int_{\Lambda/b}^{\Lambda} e^{i\mathbf{k}\cdot\mathbf{y}}\hat{l}(\mathbf{k})d^{d'}k/(2\pi)^{d'} , \tag{2.5}$$

having wave numbers in the shell $\Lambda/b<|\mathbf{k}|\leq\Lambda$, where $b=e^t$ is the spatial rescaling factor, so that $\mathbf{y}'=\mathbf{y}/b$, while t is the usual renormalization parameter. The corresponding "wave-function rescaling"

$$l'(\mathbf{y}')=l(\mathbf{y})/b^{\zeta(d)} \quad \text{with } \zeta(d)=\tfrac{1}{2}(3-d) \tag{2.6}$$

ensures that the free interface Hamiltonian $\mathcal{H}_0[l]$ is a nontrivial fixed point of the RG transformation.

On taking the partial trace of $\exp(-\beta\mathcal{H}_I[l^<+l^>])$, with $\beta=1/k_BT$, in order to define the renormalized Hamiltonian $\mathcal{H}_I'[l^<]$, we expand in $\mathcal{H}_W$ and retain only the first-order term. We further set $b=e^{\delta t}$ and consider $\delta t\to 0$ so as to derive differential recursion relations. It then proves adequate to expand $\mathcal{H}_I$ to quadratic order in $l^>$. This leads to the symbolic formula

$$\mathcal{H}'[l^<]=\mathcal{H}_0[l^<]+k_BT\ln N_0(b) +\mathcal{R}_b\left\{\mathcal{H}_W[l^<]+\frac{\partial}{\partial l}\mathcal{H}_W[l^<]l^> +\frac{1}{2}\frac{\partial^2}{\partial l^2}\mathcal{H}_W[l^<](l^>)^2+\cdots\right\} , \tag{2.7}$$

where $\mathcal{R}_b=N_0(b)^{-1}\int\mathcal{D}l^>\exp(-\beta\mathcal{H}_0[l^>])$, while the normalization of this linear operator is set by $\mathcal{R}_b\{1\}=1$. After allowance for symmetry, etc., only the two terms

$$\mathcal{R}_b\{(l^>)^2\}\approx A^2\delta t \ , \quad \mathcal{R}_b\{(\nabla l^>)^2\}\approx B^2\delta t \tag{2.8}$$

need to be computed. Higher powers of $l^>$ contribute only $o(\delta t)$. Performing the momentum-space integrals following FH and LF yields

$$A^2=B^2/\Lambda^2=\frac{k_BT}{\tilde{\Sigma}_\infty}\frac{2^{2-d}\Lambda^{d-3}}{\pi^{(d-1)/2}\Gamma[\frac{1}{2}(d-1)]}\equiv 2\xi_\beta^2\omega(d) , \tag{2.9}$$

which also serves to define the generalized capillary parameter $\omega(d)$. Evidently, $\omega(d)$ is dimensionless and $\omega(3)$ is equal to ω as defined in (1.3).

Finally, the rescaling (2.6) is to be implemented and terms must be matched on both sides of (2.7). Apart from a constant "background" contribution which we will neglect, no new terms appear in $\mathcal{H}'_I(l)$. Thus we obtain the coupled differential recursion relations or flow equations

$$\frac{\partial}{\partial t}\Delta\tilde{\Sigma}^{(t)}(l)=\zeta l\frac{\partial\Delta\tilde{\Sigma}^{(t)}}{\partial l}+\omega\xi_\beta^2\frac{\partial^2\Delta\tilde{\Sigma}^{(t)}}{\partial l^2} , \tag{2.10}$$

$$\frac{\partial}{\partial t}W^{(t)}(l)=(d-1)W+\zeta l\frac{\partial W^{(t)}}{\partial l}+\omega\xi_\beta^2\frac{\partial^2 W^{(t)}}{\partial l^2} +\omega\xi_\beta^2\Lambda^2\Delta\tilde{\Sigma}^{(t)} . \tag{2.11}$$

Note that if the bare stiffness $\tilde{\Sigma}(t)$ is constant, so that $\Delta\tilde{\Sigma}^{(0)}=0$, the first flow equation merely conserves $\Delta\tilde{\Sigma}=0$, while the second reduces to the equation derived by FH. The pair of equations are exact to linear order.

B. Solution of the flow equations

The flow equations are linear partial differential equations and may, hence, be solved in closed form in various ways. It is most convenient to decouple them by defining

$$U^{(t)}(l)\equiv W^{(t)}(l)+[\omega\xi_\beta^2\Lambda^2/(d-1)]\Delta\tilde{\Sigma}^{(t)}(l) , \tag{2.12}$$

whereupon, dropping the superscripts (t) for convenience, one finds, with $d'\equiv d-1$,

$$\frac{\partial U}{\partial t}=d'U+\zeta l\frac{\partial U}{\partial l}+\omega\xi_\beta^2\frac{\partial^2 U}{\partial l^2} . \tag{2.13}$$

But this is just the wall-potential flow equation solved by FH, for which they found

$$U^{(t)}(l)=\frac{e^{d't}}{\sqrt{2\pi}\delta(t)}\int_{-\infty}^{\infty}dl'\,U^{(0)}(l')e^{-(x-l')^2/2\delta^2(t)} , \tag{2.14}$$

where, reflecting the wave-function rescaling, it is convenient to introduce

$$x\equiv x(t,l;d)=le^{\zeta(d)t} , \tag{2.15}$$

while the width of the Gaussian convolution is given by

$$\delta^2(t;d)=2\omega(d)\xi_\beta^2(e^{(3-d)t}-1)/(3-d) . \tag{2.16}$$

For $d=3$ this reduces to $\delta^2=2\omega(d)\xi_\beta^2 t$; however, for $d<3$ one has $\delta^2\sim e^{(3-d)t}$, whereas $d>3$ yields $\delta^2(t)\to 2\omega\xi_\beta^2/(d-3)>0$ when $t\to\infty$. These differences reveal, in fact, how the marginality of $d=3$ arises.

It is also evident that the solution of (2.10) for the stiffness can be found simply by replacing U by $\Delta\tilde{\Sigma}$ and $d'=d-1$ by zero in (2.14). Evidently, then, $\Delta\tilde{\Sigma}^{(t)}(l)$ evolves in a purely diffusive way and decays to the limit $\Delta\tilde{\Sigma}^{(\infty)}=0$ when $t\to\infty$ for any initial condition or bare stiffness variation that is bounded and vanishes when $|l|\to\infty$.

If this solution for $\Delta\tilde{\Sigma}^{(t)}(l)$ is substituted in (2.11) and (2.13) one sees that the wall potential $W^{(t)}(l)$ renormalizes precisely as in the original constant stiffness ($\Delta\tilde{\Sigma}=0$) case, but as if the initial bare potential had been replaced by the *modified form*

$$\check{W}(l)=W(l)+(\omega\xi_\beta^2\Lambda^2/d')[1-e^{-d't}]\Delta\tilde{\Sigma}(l) . \tag{2.17}$$

For $d>1$ and large t, which is what is relevant near critical wetting, the dependence on t here may be dropped. Thus, in essence, $\check{W}(l)$ differs from $W(l)$ only by a fixed term proportional to $\Delta\tilde{\Sigma}(l)$. This immediately reveals how negative terms in the stiffness can compete with positive terms in $W(l)$ and thence alter the shape of the modified (renormalized) wall potential. This mechanism is, we will see, what leads to the destabilization of wetting criticality for large enough q.

C. Form of the potential and stiffness

The solutions (2.13), etc., obtained for the linearized flow equations for $W(l)$ and $\Delta\tilde{\Sigma}(l)$, depend on values specified over the whole domain $-\infty < l < \infty$. On the other hand, as the wetting problem is normally posed, $W(l)$ and $\Delta\tilde{\Sigma}(l)$ are given only for $l \geq 0$; the region z (or l) <0 is regarded as filled with an inert wall which totally excludes the interface. Such an infinite barrier lies outside the domain of a linearized RG theory. Hence, following FH, we employ a "soft wall" of finite strength $w_0 > 0$. Specifically, we extend the wall-interface potential to the full domain $-\infty < l < \infty$ by taking the bare/initial potential to be

$$W^{(0)}(l) = w_0 \Theta(-l) + W(l)\Theta(l) \ , \tag{2.18}$$

where $\Theta(z) = \frac{1}{2}(z + |z|)/z$ is the unit step function. As shown by FH, the interplay of w_0 with the parameters controlling the decay of $W(l)$ for positive l plays a basic role in delimiting the three critical wetting regimes. Furthermore, FH discuss the possible inadequacies of this approach and conclude that it is unlikely to be misleading: see also Ref. 8, where an approximate but nonlinear RG approach is studied.

In the present case the same issue arises in the specification of $\tilde{\Sigma}^{(0)}(l)$. We follow the spirit of FH by adopting the choice

$$\Delta\tilde{\Sigma}^{(0)}(l) = \Delta\tilde{\Sigma}(l)\Theta(l) \ . \tag{2.19}$$

In other words, the bare interface is assigned a fixed stiffness $\tilde{\Sigma}_\infty$ for $l<0$ but varies in the way discussed above for positive l. Of course other possibilities could be entertained: e.g., one might assign some other fixed value, say $\tilde{\Sigma}(0)$, for $l<0$. However, it hardly seems profitable to explore such options since, in the first place, the RG evolution of $\Delta\tilde{\Sigma}(l)$ *per se* is found to play an inconsequential role in determining the nature of critical wetting. Second, as shown in (2.17), any such changes in $\Delta\tilde{\Sigma}(l)$ for $l<0$ eventually merely amount to modifications of the wall term $w_0\Theta(-l)$ in $W^{(0)}(l)$. Such changes will not be significant unless they are unbounded or diverge in some way when $l \to -\infty$. We hence believe that the assignment (2.19) provides no grounds for further concern.

We may now utilize the explicit results (1.6) and (1.7) for the bare wall potential and stiffness. Combining these in (2.17)–(2.19), we can write

$$\check{W}^{(t)}(l) = \check{W}_\omega^{(t)}(l) + [\bar{h}l]^{(t)} + \sum_{k \leq j = 1}^{\infty} \check{W}_{jk}^{(t)} \ . \tag{2.20}$$

On performing the integrals in (2.14) in terms of the error function $\mathrm{erf}(u) = \int_0^u 2\, dv\, e^{-v^2}/\sqrt{\pi}$, we find

$$\check{W}_\omega^{(t)} = \tfrac{1}{2} w_0 e^{d't}\{1 - \mathrm{erf}[x/\sqrt{2}\delta(t)]\} \ , \tag{2.21}$$

where $x(t,l;d)$ and $\delta(t;d)$ were defined in (2.15) and (2.16), and

$$[\bar{h}l]^{(t)} = \bar{h}e^{d't}\{\tfrac{1}{2}x[1+\mathrm{erf}(x/\sqrt{2}\delta)] + (\delta/\sqrt{2\pi})e^{-x^2/2\delta^2}\} \ , \tag{2.22}$$

$$\check{W}_{j0}^{(t)} = \tfrac{1}{2}\check{w}_{j0}^{(t)} e^{d't + j^2\kappa^2\delta^2/2 - j\kappa x}\left[1 + \mathrm{erf}\left[\frac{x - j\kappa\delta^2}{\sqrt{2}\delta}\right]\right] \ , \tag{2.23}$$

with parallel expressions for $\check{W}_{jk}^{(t)}$ for $k=1,2,\ldots$ having only more complicated terms in the square brackets. The modified wall-interface coefficients are

$$\check{w}_{jk}^{(t)} = w_{jk} + (\omega\xi_\beta^2\Lambda^2/d')(1-e_t)s_{jk} \ , \quad e_t = e^{-d't} \ , \tag{2.24}$$

for $k \leq j = 1,2,\ldots$.

When, near critical wetting, $T \to T_{cW}^0$ and $h \to 0$, we can combine the results (1.8)–(1.11) and write

$$\bar{h} \approx -c_0 h \to 0 \ , \qquad \check{w}_{10}^{(t)} \equiv \tilde{\tau}^{(t)} \equiv \tilde{\tau}(1+c_1e_t) \sim \tau \to 0- \ , \tag{2.25}$$

$$\check{w}_{20}^{(t)} = p^{(t)} \equiv p(1+c_2e_t) > 0 \ , \qquad \check{w}_{21}^{(t)} = -q^{(t)} \approx -q(1-e_t) < 0 \ , \tag{2.26}$$

etc., where the c_i, p, and q are constants. In what follows we will frequently drop the terms e_t since they vanish rapidly when t becomes large in the regime of interest. Evidently $\tilde{\tau}$ acts as the temperature deviation, varying like $T - T_{cW}^0$. The parameters $\tilde{\tau}$, $\bar{h}$, and p are essentially those entering the previous FH analysis (see also I). The new feature here is the negative term $\check{w}_{21}$, which arises from the anomalous stiffness variation proportional to $le^{-2\kappa l}$: specifically, we have

$$q = |s_{21}|(\omega\xi_\beta^2\Lambda^2/d') \ , \tag{2.27}$$

where explicit expressions for s_{21} in terms of the parameters of the underlying LGW Hamiltonian (1.5) are given in I and in the Appendix below: see also Ref. 3. These show that one can also write

$$q = \omega\tilde{\Sigma}_\infty\xi_\beta^2\Lambda^2\tilde{\mathcal{G}}(T;d) = k_BT\Lambda^{d'}\tilde{\mathcal{G}}/(4\pi)^{d'/2}\Gamma(d'/2) \ , \tag{2.28}$$

where $\tilde{\mathcal{G}}(T;d) \lesssim 3/d'$ ($d' = d-1$) is slowly varying.

D. Matching procedures

As explained by FH, because there is no nontrivial fixed point of the RG transformation representing the wetting transition, it is necessary to adopt a matching technique. For completeness we recapitulate the procedure here.

Note, first, that if the interface is bound to the wall the renormalized potential $W^{(t)}(l)$ should exhibit a global minimum at some $l_0(t) < \infty$. If this minimum is sufficiently narrow and deep, one may expand the potential about it and use mean-field theory to estimate the interfacial correlation length $\xi_{\parallel}(T,h,\dots)$. In fact, this procedure will be valid provided $\xi_{\parallel}$ is of order ξ_β, the noncritical bulk correlation length. Accordingly, the recursion relations are integrated up to a point $t^{\dagger}(T,h,\dots)$, chosen so that

$$\partial^2 W^{(t^{\dagger})}/\partial l^2|_{l=l^{\dagger}}=\tilde{\Sigma}^{(t^{\dagger})}(l^{\dagger})/\xi_\beta^2 , \tag{2.29}$$

where $l^{\dagger}=l_0(t^{\dagger})<\infty$ represents the global minimum of $W^{(t^{\dagger})}(l)$ and $\tilde{\Sigma}^{(t^{\dagger})}(l^{\dagger})$ is supposed positive. Using mean-field theory at the matching point yields a renormalized interfacial thickness $l^{\dagger}$, a renormalized interfacial correlation length $\xi_{\parallel}\simeq\xi_\beta$, and a renormalized singular part of the interface-wall free energy $F_s\simeq W^{(t^{\dagger})}(l^{\dagger})$. Via the rescaling relations (2.6), etc., one obtains the original properties

$$\langle l\rangle(T,h,\dots)\approx e^{-(d-3)t^{\dagger}(T,h,\dots)/2}l^{\dagger}(T,h,\dots)<\infty , \tag{2.30}$$

$$\xi_{\parallel}(T,h,\dots)\approx e^{t^{\dagger}(T,h,\dots)}\xi_\beta , \tag{2.31}$$

$$F_s(T,h,\dots)\approx e^{-(d-1)t^{\dagger}}W^{(t^{\dagger})}(l^{\dagger}) . \tag{2.32}$$

If, on the other hand, the global minimum of $W^{(t)}(l)$ corresponds to $l^{\dagger}=\infty$ for t large, the interface is *delocalized* with original properties $\langle l\rangle(T,h,\dots)=\xi_{\parallel}(T,h,\dots)=\infty$ and $F_s(T,h,\dots)=0$.

This completes the RG framework: subsequent sections are devoted to analyzing the consequences.

III. CRITICAL WETTING AWAY FROM MARGINALITY

Our main focus in this article is on the marginal critical dimensionality $d=3$, which is unaltered by the stiffness terms. It is instructive, however, to examine the cases $d>3$ and $d<3$. The former shows that RG theory has something significant to say even above marginality; the latter case reveals the shortcomings of the linearized functional RG treatment. We will confine attention to $h=0-$, i.e., just *on* the phase boundary, but vary $\tilde{\tau}$ for given p and q: see (2.25) and (2.26).

A. Dimensionality exceeding $d=3$

Note, first, from (2.9) that the capillary parameter

$$\omega(d)=\frac{\Lambda^{d-3}}{(4\pi)^{d'/2}\Gamma(d'/2)}\frac{k_BT}{\tilde{\Sigma}_\infty\xi_\beta^2} \tag{3.1}$$

vanishes when $d\to\infty$ as also does the stiffness parameter $q=(\omega\xi_\beta^2\Lambda^2/d')|s_{21}|$: see (2.28). Furthermore, from (2.16) the basic RG convolution width $\delta(t;d)$ for $d>3$ behaves as

$$\delta(t;d)\to[2\omega(d)/(d-3)]^{1/2}\xi_\beta\equiv\delta_\infty(d)<\infty , \tag{3.2}$$

when $t\to\infty$. Evidently $\delta_\infty(d)$ also vanishes when $d\to\infty$. These results imply, as is to be expected, that all fluctuation effects may be neglected when $d\to\infty$ so that mean-field theory with the simple wall-interface potential

$$W(l)\approx\tilde{\tau}e^{-\kappa l}+pe^{-2\kappa l} \quad (d=\infty) \tag{3.3}$$

suffices to yield all transition behavior.

We conclude that for $d=\infty$ a critical wetting transition occurs at $T=T_{cW}^0$ with layer thickness and interfacial correlation length diverging when $\tilde{\tau}\sim T-T_{cW}^0\to 0-$ in the standard mean-field way as

$$\langle\kappa l\rangle\approx\ln(2p/|\tilde{\tau}|)+3\omega/(d-3) , \tag{3.4}$$

$$\kappa\xi_{\parallel}\approx(2p\tilde{\Sigma}_\infty)^{1/2}e^{\omega/(d-3)}/|\tilde{\tau}| , \tag{3.5}$$

where ω is to be set to 0 when $d\to\infty$. When $d<\infty$ fluctuation effects do play a role even if $d>3$ and $q=0$; indeed, the critical amplitudes are then found to change as shown by the ω-dependent terms in these expressions.

To justify these claims, we implement the RG procedure using (2.20)–(2.24) for the wall-interface potential. We first observe that near criticality both

$$x^{\dagger}\equiv le^{\zeta t^{\dagger}}\approx\langle l\rangle \text{ and } t^{\dagger}\approx\ln(\xi_{\parallel}/\xi_\beta) \tag{3.6}$$

must become large so that in view of (3.2) the condition

$$y_j\equiv[x(t,l)-j\kappa\delta^2(t)]/\sqrt{2}\delta(t)\gg 1 , \tag{3.7}$$

for $j=0,1,2$, becomes valid in the region of the minimum of $\check{W}^{(t)}(l)$ for any weakly bound interface. One can thus use the large argument expansions

$$\mathrm{erf}(y)=\mathrm{sgn}(y)-(e^{-y^2}/\sqrt{\pi}y)[1-\tfrac{1}{2}y^{-2}+\cdots] \tag{3.8}$$

$(|y|\to\infty)$ to estimate the terms (2.22), (2.23), etc. We conclude that

$$e^{-d't}\check{W}^{(t)}(l)\approx w_0\delta_\infty e^{-x^2/2\delta_\infty^2}/\sqrt{2\pi}x+\tilde{\tau}e^{\kappa^2\delta_\infty^2/2}e^{-\kappa x}+[p-q\kappa(x-2\kappa\delta_\infty^2)]e^{2\kappa^2\delta_\infty^2}e^{-2\kappa x} \tag{3.9}$$

describes the renormalized wall-interface potential near the minimum at large x. Since the direct wall contribution proportional to w_0 exhibits a rapid Gaussian decay it may be dropped. The result then closely mirrors (3.3). Note that this form for $\check{W}^{(t)}(l)$ corresponds to Regime I of FH in that the wall term (2.21) plays no asymptotic role while the attractive or w_{10} and repulsive or w_{20} parts of the potential retain exponential forms.

If the stiffness term proportional to q in (3.9) is now ignored and the matching procedure is carried through, the results (3.4) and (3.5) follow straightforwardly.

When the stiffness cannot be neglected graphical analysis of (3.9) immediately reveals the destabilizing influence of the $-q\kappa le^{-2\kappa le^{\zeta t}}$ contribution. For $T<T_{cW}^0$, i.e., $\tilde{\tau}<0$, the potential $\check{W}^{(t)}(l)$ displays a single minimum at finite l_0 with $\check{W}_{\min}<0$. However, since $q>0$ this minimum remains present even at $T=T_{cW}^0$ ($\tilde{\tau}=0$). When T increases above T_{cW}^0 ($\tilde{\tau}\gtrsim 0$), the minimum moves further out and $\check{W}_{\min}\to 0$ but a new (local) minimum appears at $l=\infty$. Eventually at $T=T_{0W}>T_{cW}^0$ one achieves $\check{W}_{\min}(T_{0W})=0$ with $l_{0W}<\infty$; this represents a point of *first-order transition* since for $T\gtrsim T_{0W}$ one has $\check{W}_{\min}>0$ and this finite-l_0 minimum becomes unstable relative to the (now global) minimum at $l=\infty$.

When q is small this new wetting transition is only weakly first order and one can show

$$T_{0W}-T_{cW}^0\sim\tilde{\tau}_0\approx qe^{-p/q-1-\omega/(d-3)} , \tag{3.10}$$

while just on the point of transition one has

$$\langle \kappa l \rangle_0 = p/q + 1 + 4\omega/(d-3) + O(e^{-p/q}) , \qquad (3.11)$$

$$\kappa\xi_{\parallel 0} \approx (e^2\tilde{\Sigma}/q)^{1/2} e^{p/q+2\omega/(d-3)} \quad (d>3) . \qquad (3.12)$$

Some of the details can be seen from the case $d=3$ discussed in Sec. IV A below. As expected, one sees that $\langle l \rangle_0$ and $\xi_{\parallel 0}$ diverge when $q \to 0$. Note that various terms also diverge when $d \to 3+$; however, we will see below that first-order behavior remains at $d=3$ when ω is small enough.

B. Dimensions below $d=3$

When $d<3$ the convolution width $\delta(t)$ increases exponentially with t as $e^{(3-d)t/2}$. This leads directly to failure of the condition (3.7) and, hence, indicates the inadequacy of the exponential form of the renormalized potential (3.9) for describing the renormalized potential minimum for weakly bound interfaces ($\langle \kappa l \rangle \approx \kappa x \sim e^{(3-d)t/2}$, $\kappa\xi_{\parallel} \sim e^{t^\dagger} \gg 1$). Indeed, one evidently has $x/\delta \sim O(1) \ll \kappa\delta$ in the relevant region.

Now, as shown by FH and seen again below, the condition $1 \ll x/\delta \ll \kappa\delta$ takes one into Regime III for wetting when $d=3$ (which then corresponds to $\omega>2$). In that regime all components of $\check{W}^{(t)}(l)$ are smeared to Gaussian forms and compete strongly in determining the minimum. We will study this behavior for $d=3$, following FH. The analysis fails, however, when $\delta^2(t)/t \to \infty$ as happens here: it then proves impossible to find a bounded value for $\tilde{\tau}_c$ (even with $q=0$).[7] In fact, it becomes clear that nonlinear terms are needed to locate a proper matching point. This surmise is confirmed by the approximate nonlinear functional RG studied by Lipowsky and Fisher, which is exact in linear order:[8] that yields fixed-point potentials describing critical wetting for all $1<d<3$ (with $q \equiv 0$).

As shown below, the stiffness variation (with $q>0$) generates first-order transitions in Regime III ($\omega>2$) when $d=3$ and $\omega<\omega_t(q)$. By continuity in d, therefore, we expect first-order transitions to persist for $d=3-\epsilon$ with $\epsilon \ll 1$ for all $\omega \lesssim \omega_t(q>0)$. However, for $d \gtrsim 2$ we expect only continuous and universal critical wetting (at least for q not too large) in accord with exact results[1(b),15] for $d=2$ and the approximate functional RG studies[8] for $d \gtrsim 2$.

IV. CRITICAL WETTING IN $d=3$ DIMENSIONS

In this section we restrict attention entirely to $d=3$, for which we have

$$x \equiv l , \quad \kappa^2\delta^2(t) = 2\omega t . \qquad (4.1)$$

For simplicity we again consider only $h \equiv 0$. We will regard the wall parameter w_0 and the repulsion amplitude $p \approx \check{w}_{20} > 0$ as fixed and examine the phase space (T,ω,q) or $(\tilde{\tau},\omega,q)$ considering all $\omega \geq 0$ and all values $q \lessgtr 0$: see Fig. 1. If one also regards ξ_β, Λ, and s_{21} as fixed,[3] then a "physical subspace" is specified by the planes $q=c\omega$, where c is a system-dependent constant: see (2.27). This viewpoint was implicitly adopted in Ref. 3 and is illustrated in Fig. 1. More generally, however, in a given system, such as a simple cubic Ising model, only Λ is fixed and $\omega(T_{cW})$ and $q(T_{cW})$ vary more or less independently: compare (1.3) and (2.28). Normally, though, both parameters increase[11(a)] with T_{cW} which can, in turn, be tuned by varying the properties of the wall: see I and Refs. 9–11.

The phase diagram we find is illustrated in Fig. 1. When $q \leq 0$ the wetting transition is always critical but, as in previous studies,[5,7] the behavior is separated into three regimes by "multicritical lines" P at $\omega=\frac{1}{2}$ and Q at $\omega=2$, about which crossover regions are found.[7] These lines demarcate the three critical regimes according to the behavior of the arguments

$$y_j = (\kappa l - 2j\omega t)/2\sqrt{\omega t} \qquad (4.2)$$

in the region of the potential minimum at matching: compare with (3.7). Specifically, one finds the Regimes

$$\begin{aligned} &\text{I:} \quad y_0, y_1, y_2 \gg 1 && \text{when } \omega < \tfrac{1}{2} , \\ &\text{II:} \quad y_0, y_1 \gg 1 , \quad y_2 \ll -1 && \text{when } \tfrac{1}{2} < \omega < 2 , \\ &\text{III:} \quad y_0 \gg 1 , \quad y_1, y_2 \ll -1 && \text{when } \omega > 2 . \end{aligned} \qquad (4.3)$$

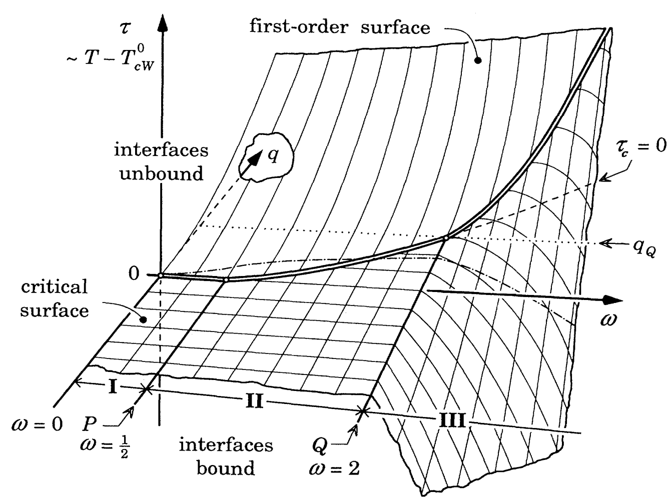

FIG. 1. Schematic view of the extended phase diagram for short-range wetting transitions in $d=3$ dimensions showing the effects of a generalized stiffness variation decaying near T^0_{cW} as $-qle^{-2\kappa l}$; the reduced temperature deviation is τ, while ω is the capillary parameter. The doubled curve represents the *tricritical wetting locus* $q=q_t(\omega)$, $\tau=\tau_t(\omega)$ that separates the critical wetting surface (cross ruled) at $q<q_t$ from the fluctuation-induced first-order wetting surface at $q>q_t$. Two multicritical lines, labeled P and Q, at $\omega=\frac{1}{2}$ and $\omega=2$, separate the three critical wetting regimes I, II, and III. In all regimes the critical wetting temperature never increases when ω increases at fixed q. For various walls bounding a given bulk system the physical subspace corresponds, roughly, to $q \propto \omega$ as suggested by the dot-dashed locus drawn on the transition surface. Note that the transition is first order for $\omega<\omega_t$ but becomes critical for $\omega>\omega_t$. However, the value of ω_t, etc., depends on the details of the system.

The asymptotic forms (3.8), etc., then determine the behavior of the various terms in $\check{W}^{(t)}(l)$. In Regimes I and II one has $T_{cW}=T_{cW}^{0}$ ($\tilde{\tau}_c=0$) but in Regime III the transition occurs below T_{cW}^{0} ($\tilde{\tau}_c<0$).[4,7]

By contrast, for stiffness parameter $q>0$ the wetting transition is always first order when $\omega<\frac{1}{2}$ and occurs at a temperature $T_{0W}>T_{cW}^{0}$ ($\tilde{\tau}>0$), as shown in Fig. 2(a). Evidently the locus $q=\tilde{\tau}=0$ for $\omega\le\frac{1}{2}$ corresponds to a *tricritical line* in the full phase space of Fig. 1. In Regime II this locus departs from the $q=0$ axis and $q_t(\omega)$ increases monotonically with ω; however, the tricritical temperature T_{tW} remains fixed at T_{cW}^{0} [i.e., $\tilde{\tau}_t(\omega)=0$]: see Fig. 2(b). Finally, in Regime III the strong capillary fluctuations raise the tricritical locus *above* the plane $T=T_{cW}^{0}$ ($\tilde{\tau}=0$): see Fig. 2(c).

To establish the various scenarios just outlined and to discover the detailed transition behavior in each situation we analyze the three wetting regimes in order of increasing ω.

A. Weak fluctuations: Regime I

To proceed we first adopt the ansatz $y_0, y_1, y_2 \gg 1$ and then check, recognizing (4.1), that a suitable minimum of $W^{(t)}(l)$ can, in fact, be found satisfying the ansatz: this yields the condition $\omega<\frac{1}{2}$. As in (3.9), the wall contribution ($\propto w_0$) can be dropped and we are left with the exponential form

$$\check{W}^{(t)}(l)\approx\tilde{\tau}e^{(2+\omega)t-\kappa l}+[p-q(\kappa l-4\omega t)]e^{(2+4\omega)t-2\kappa l}\,, \tag{4.4}$$

valid as $\tilde{\tau}\to 0-$. On using the matching formulas (2.29)–(2.32) we obtain from $\partial\check{W}/\partial l$, $\partial^2\check{W}/\partial l^2$, and $\check{W}$, respectively, the equations

$$\tilde{\tau}\approx-2[p-q(\kappa l^{\dagger}-4\omega t^{\dagger}-\tfrac{1}{2})]e^{3\omega t^{\dagger}-\kappa l^{\dagger}}\,, \tag{4.5}$$

$$\tilde{\Sigma}_{\infty}\approx 2[p-q(\kappa l^{\dagger}-4\omega t^{\dagger}-\tfrac{3}{2})]e^{(2+4\omega)t^{\dagger}-2\kappa l^{\dagger}}\,, \tag{4.6}$$

$$F_s\approx-[p-q(\kappa l^{\dagger}-4\omega^{\dagger}-1)]e^{4\omega t^{\dagger}-2\kappa l^{\dagger}}\le 0\,, \tag{4.7}$$

which determine $l^{\dagger}$, $t^{\dagger}$, and F_s.

For $q\le 0$ and $\omega<\frac{1}{2}$ one can now show that $F_s\le 0$ for $\tilde{\tau}\le 0$ and hence see that critical wetting occurs at $\tilde{\tau}_c=0$. Further analysis yields the various critical singularities of which we quote only

$$\langle \kappa l\rangle\approx\frac{1+2\omega}{1-\omega}\ln\left[\frac{p}{|\tilde{\tau}|}\right]+\frac{2+\omega}{2(1-\omega)}\ln\left[1+\frac{1-2\omega}{1-\omega}\frac{q}{p}\ln\left[\frac{|\tilde{\tau}|}{p'}\right]\right]\,, \tag{4.8}$$

as $\tilde{\tau}\to 0-$ where $p'=p\sqrt{(8p/\tilde{\Sigma}_{\infty})}$. See also Sec. VII of I. Note that the stiffness only introduces a subsidiary $\ln\ln|\tilde{\tau}|$ singularity.[2,4]

When $q>0$, on the other hand, the analysis closely mirrors that discussed for $d>3$: one finds that $F_s\to 0-$ only for $\tilde{\tau}=\tilde{\tau}_0>0$: see Fig. 2(a). In principle (4.5) and (4.6) yield the full behavior of $l^{\dagger}\approx\langle l\rangle(\tau,q)$ and $e^{t^{\dagger}}\approx\xi_{\parallel}(\tau,q)/\xi_{\beta}$ but explicit expressions are difficult to obtain so we content ourselves with results for small q close to the transition. On setting $F_s=0$ in (4.7) we find[3] just at the point of transition

$$\langle \kappa l\rangle_0\approx\frac{1+2\omega}{1-2\omega}\left[\frac{p}{q}+1\right]+\frac{2\omega}{1-2\omega}\ln\left[\frac{\tilde{\Sigma}_{\infty}}{q}\right]\,, \tag{4.9}$$

$$\kappa\xi_{\parallel 0}\approx(e^2\tilde{\Sigma}_{\infty}/q)^{1/2(1-2\omega)}e^{p/q(1-2\omega)}\,, \tag{4.10}$$

as $q\to 0+$. Using (4.5) then yields the transition surface for small q as

$$T_{0W}(q,\omega)-T_{cW}^{0}\sim\frac{\tilde{\tau}_0}{\tilde{\Sigma}_{\infty}}\approx e^{-\vartheta_1}\left[\frac{q}{\tilde{\Sigma}_{\infty}}\right]^{\vartheta_2}e^{-\vartheta_1 p/q}\,, \tag{4.11}$$

where $\vartheta_1=(1-\omega)/(1-2\omega)$ and $\vartheta_2=(1-\frac{3}{2}\omega)/(1-2\omega)$.

It is instructive to compare these results with the parallel expressions (3.10)–(3.12) for $d>3$ and all ω: the leading dependence on q is similar but the corrections differ. Note, furthermore, that both exponents ϑ_1 and ϑ_2 in (4.11) diverge to ∞ when $\omega\to\frac{1}{2}-$; this is, of course, indicative of the necessary restriction $\omega<\frac{1}{2}$. Similar divergences are evident in (4.9) and (4.10). In fact, as shown by Fisher and Huse[7] *on* the borderline P: $\omega=\frac{1}{2}$, a new form of (multi)critical behavior arises. For $q=0$ this dominates when[7]

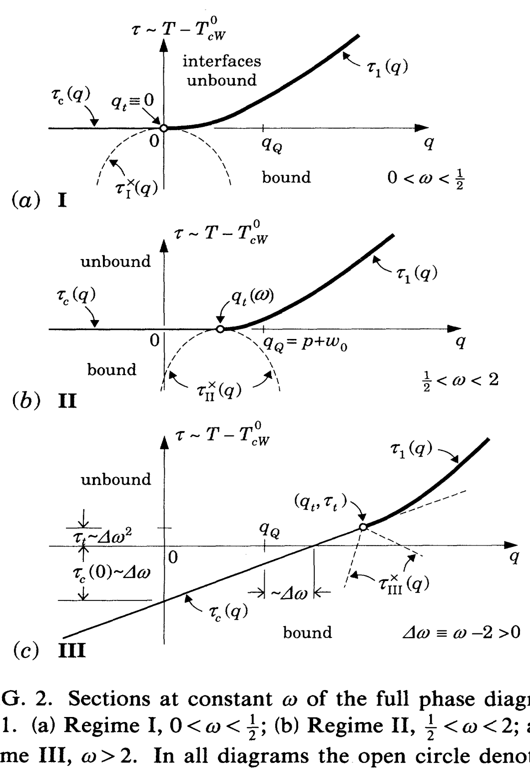

FIG. 2. Sections at constant ω of the full phase diagram of Fig. 1. (a) Regime I, $0<\omega<\frac{1}{2}$; (b) Regime II, $\frac{1}{2}<\omega<2$; and (c) Regime III, $\omega>2$. In all diagrams the open circle denotes the *tricritical wetting point*. The loci of critical and first-order wetting transitions τ_c and τ_1 are shown as light and bold lines, respectively. Dashed curves labeled $\tau_{\mathrm{I}}^{\times}$, etc., delineate crossover regimes within which, on approaching the wetting transitions from below, behavior characteristic of the tricritical point is found.

$$|\tilde{\tau}| \gtrsim \tilde{\tau}_P^{\times} \approx \sqrt{(8p^3/\tilde{\Sigma}_\infty)}e^{-2/(1-2\omega)^2} . \quad (4.12)$$

Equally we can identify a crossover value $q_P^{\times}(\omega)\approx p|\frac{1}{2}-\omega|$ such that when $|q|\gtrsim q_P^{\times}$ the critical behavior as $\tilde{\tau}\to 0$ follows that for $\omega=\frac{1}{2}$.

Whenever $q>0$ the point $T=T_{cW}^0$ ($\tilde{\tau}=0$) lies below the transition and, by (4.5) and (4.6), the interface is bound with

$$\langle \kappa l\rangle(T_{cW}^0)\approx\langle \kappa l\rangle_0-\frac{1+2\omega}{2(1-2\omega)}-\frac{2\omega}{1-2\omega}\ln 2 , \quad (4.13)$$

$$\xi_\parallel(T_{cW}^0)\approx\xi_{\parallel 0}/(2e)^{1/2(1-2\omega)} , \quad (4.14)$$

$$F_s(T_{cW}^0)\approx -f_1(qe^{-2p/q}/\tilde{\Sigma}_\infty)^{1/(1-2\omega)} , \quad (4.15)$$

where $f_1=2^{1+2\omega}e^{-1/(1-2\omega)}\tilde{\Sigma}_\infty$. These results can be extended to yield a power series in $\tilde{\tau}$ but the expressions are very cumbersome.

However, when q is small but $|\tilde{\tau}|$ exceeds a certain crossover value, $\tilde{\tau}_I^{\times}(q)$, one should see the same behavior as found for $q=0$: see I, FH, etc. This tricritical crossover locus is indicated in Fig. 2(a). Its behavior as $q\to 0$ can be gauged from (4.5)–(4.7) since q is significant only when

$$\kappa l^\dagger-4\omega t^\dagger\gtrsim p/|q| \quad (\tilde{\tau}=\tilde{\tau}_I^{\times}) . \quad (4.16)$$

For $q=0$ the left side behaves as

$$(1-2\omega)t^\dagger\approx[(1-2\omega)/2(1-\omega)]\ln(8p^3/\tilde{\Sigma}_\infty\tilde{\tau}^2) , \quad (4.17)$$

which leads to

$$\tilde{\tau}_I^{\times}(q)\approx\sqrt{(8p^3/\tilde{\Sigma}_\infty)}e^{-(1-\omega)p/(1-2\omega)q} . \quad (4.18)$$

This behavior can also be read off from (4.8). Finally, on the crossover locus one finds

$$\langle \kappa l\rangle^{\times}\simeq(1+2\omega)p/(1-2\omega)q , \quad (4.19)$$

$$\kappa\xi_\parallel^{\times}\simeq e^{p/q(1-2\omega)} . \quad (4.20)$$

We could now examine the special multicritical limit P: $\omega=\frac{1}{2}$, which has been studied by Fisher and Huse[7] for $q=0$. However, at this point the labor does not seem worthwhile so we proceed directly to the next regime.

B. Intermediate fluctuations: Regime II

Even in the case $q=0$ the FH analysis of Regimes II and III is algebraically involved; the complications increase for $q\neq 0$. Accordingly it is useful at the outset to introduce scaled space and renormalization parameters via

$$X=\frac{\kappa l}{2\omega t} , \quad \eta=\frac{\xi_B^2}{\delta^2}=\frac{1}{2\omega t}\ll 1 , \quad (4.21)$$

where the inequality applies near matching in the critical and tricritical neighborhoods. The condition (4.3) for Regime II then reads

$$1+\sqrt{2\eta}<X<2-\sqrt{2\eta} . \quad (4.22)$$

The wall and repulsive parts of $\check{W}^{(t)}(l)$ now become Gaussian in form; only the attractive term remains exponential. Asymptotically one obtains

$$e^{\kappa l-(2+\omega)t}\check{W}^{(t)}\approx\sqrt{\eta}\Omega(X)e^{-\omega t(X-1)^2}+\tilde{\tau} , \quad (4.23)$$

where, extending FH, the crucial factor is

$$\sqrt{2\pi}\Omega(X;w_0,p,q)=\frac{w_0}{X}+\frac{p}{2-X}-\frac{q}{(2-X)^2} . \quad (4.24)$$

The minimum and curvature matching conditions now read

$$\sqrt{\eta}\Omega_1(X,\eta)e^{-\omega t(X-1)^2}+\tilde{\tau}=0 , \quad (4.25)$$

$$e^{\kappa l-(2+\omega)t}\tilde{\Sigma}_\infty\approx\sqrt{\eta}\Omega_2(X,\eta)e^{-\omega t(X-1)^2}+\tilde{\tau} , \quad (4.26)$$

where, with $\Omega'(X)=\partial\Omega/\partial X$, and $\Omega''(X)=\partial^2\Omega/\partial X^2$, one has

$$\Omega_1(X,\eta)=X\Omega-\eta\Omega' , \quad (4.27)$$

$$\Omega_2(X,\eta)=X^2\Omega-\eta\Omega-2\eta X\Omega'+\eta^2\Omega'' . \quad (4.28)$$

If one eliminates $\tilde{\tau}$ between (4.25) and (4.26) and takes logarithms one can obtain the relation

$$X^2=(2/\omega)+\eta\ln[\eta(\Omega_2-\Omega_1)^2/\tilde{\Sigma}_\infty^2] . \quad (4.29)$$

When $t\to 0$, this yields $X\to X_t\equiv\sqrt{2/\omega}$. The condition (4.22) then implies $\frac{1}{2}<\omega<2$ as was anticipated. Now criticality requires $\ln(\kappa\xi_\parallel)\approx t^\dagger\to\infty$ and so $\eta^\dagger\to 0$. Provided $\Omega_1(X_t,0)=X_t\Omega(X_t)>0$ the condition (4.25) then implies criticality at $\tilde{\tau}_c=0$. Since $X_t<2$ we thus see from (4.24) that critical wetting still occurs at $T=T_{cW}^0$ provided q is not too large.

On the other hand, for $q>q_t(\omega)$, we anticipate a first-order transition. In this case, as seen in Sec. IV A, the wall-interface potential must exhibit a minimum at $l_0<\infty$ even when $\tilde{\tau}=0$. For such a minimum (4.25) and (4.27) imply

$$\eta=X\Omega(X)/\Omega'(X) . \quad (4.30)$$

But, on approach to tricriticality $\ln(\kappa\xi_{\parallel 0})$ diverges as does $t^\dagger$, so, again, $\eta^\dagger\to 0$ and $X^\dagger\to X_t$. Finally, then, the equation

$$\Omega(X_t;w_0,p,q_t)=0 \quad \text{with } X_t=\sqrt{2/\omega} , \quad (4.31)$$

determines the *tricritical locus* in the plane $\tilde{\tau}=0$. One finds directly

$$q_t(\omega)=\sqrt{2/\omega}[p+(\sqrt{2\omega}-1)w_0](\sqrt{2\omega}-1)>0 , \quad (4.32)$$

for $2>\omega>\frac{1}{2}$. Evidently q_t increases monotonically with ω from $q_t(\frac{1}{2})=0$ to $q_Q\equiv q_t(2)=p+w_0$, the limiting ω derivatives being $q_t'(\frac{1}{2}+)=2p$ and $q_t'(2-)=\frac{1}{4}(p+3w_0)$.

For $q<q_t(\omega)$ one finds critical behavior which is unchanged from the original $q=0$ Regime II situation[2,4,7] except for modifications of the nonuniversal amplitudes. For example, one has

$$\xi_\parallel(T)\approx\xi_0(\omega,q)[|\tilde{\tau}/p|(\ln|p/\tilde{\tau}|)^{\sqrt{(\omega/8)}}]^{-\nu_\parallel} , \quad (4.33)$$

where $\nu_\parallel=1/(2-\sqrt{8\omega}+\omega)$ and ξ_0 depends on ω and q (and on p and w_0).

By using (4.31) and (4.24)–(4.29) one can determine the jumps in the first-order region

$$\Delta q \equiv q - q_t(\omega) > 0 \; . \tag{4.34}$$

For the layer thickness we can write

$$\langle \kappa l \rangle_0 \approx \frac{3}{2}\left[\frac{\bar{p}}{\Delta q} - \left[\frac{\omega}{2}\right]^{1/2}\right] \times \left[\ln\left[\frac{E\bar{p}}{\Delta q}\right] + \ln\ln\left[\frac{E\bar{p}}{\Delta q}\right] + o(1)\right] + \frac{\sqrt{\omega}}{\sqrt{2}-\sqrt{\omega}} + o(1) \; , \tag{4.35}$$

where $\bar{p} = p + (2\omega - 1)w_0$, while

$$E^{3/2} = \sqrt{27\pi}\, e^{1/(1-\sqrt{\omega/2})} \frac{(\sqrt{2\omega}-1)^2}{(\sqrt{2\omega}-\omega)} \left[\frac{\omega}{2}\right]^{3/4} \frac{\tilde{\Sigma}_\infty}{\bar{p}} \; . \tag{4.36}$$

Similarly for the correlation length we find

$$\ln \kappa \xi_{\parallel 0} \approx \frac{3}{4\sqrt{2\omega}} \frac{\bar{p}}{\Delta q}\left[\ln\left[\frac{E\bar{p}}{\Delta q}\right] + \ln\ln\left[\frac{E\bar{p}}{\Delta q}\right] + o(1)\right] . \tag{4.37}$$

The first-order transition surface for small q [see Fig. 2(b)] can be found by setting $\check{W}^{(t)} = 0$ in (4.23) and using the other results. This yields

$$T_{0W} - T_{cW}^0 \sim \tilde{\tau}_0 \sim e^{-\vartheta_3 \langle \kappa l \rangle_0} / \langle \kappa l_0 \rangle^{\sqrt{(9\omega/8)}} \; , \tag{4.38}$$

where $\vartheta_3 = (2+\omega)/\sqrt{8\omega} - 1 > 0$.

If one approaches the tricritical locus from $T < T_{cW}^0$ but with $q = q_t(\omega)$, i.e., $\Delta q = 0$, one should expect pure tricritical singularities differing somewhat from those on the critical surface where $q < q_t(\omega)$. Following the standard line of argument and using

$$\Omega[X; q_t(\omega)] \approx \Omega'(X_t)(X - X_t) \to 0- \; , \tag{4.39}$$

one obtains

$$\xi_\parallel(T) \sim \left[\frac{(\ln\ln|\bar{p}/\tilde{\tau}|)^{\sqrt{(\omega/2)}}}{|\tilde{\tau}/\bar{p}|(\ln|\bar{p}/\tilde{\tau}|)^{3\sqrt{(\omega/8)}}}\right]^{\nu_\parallel} \quad (q = q_t) \; , \tag{4.40}$$

where $\nu_\parallel$ was defined after (4.33). Comparison with (4.33) shows that while the leading behavior is the same, the confluent tricritical singularities diverge more strongly than those at criticality. The same is true for the layer thickness, for which we find

$$\langle \kappa l \rangle \approx A_t \ln\left|\frac{\bar{p}}{\tilde{\tau}}\right| + \vartheta_4\left[3\ln\ln\left|\frac{\bar{p}}{\tilde{\tau}}\right| - 2\ln\ln\ln\left|\frac{\bar{p}}{\tilde{\tau}}\right| + O(1)\right] \tag{4.41}$$

($q = q_t$), where $A_t = \sqrt{8\omega}\,\nu_\parallel$ while $\vartheta_4 = \omega\nu_\parallel + \sqrt{\omega/8}$.

One may also determine the crossover region controlled by the tricritical behavior: see Fig. 2(b). For Δq small this is given by

$$|T_{\rm II}^\times - T_{tW}| \sim \tilde{\tau}_{\rm II}^\times(q) \sim \exp(-|\vartheta_5\bar{p}/\Delta q|\ln|\vartheta_5\bar{p}/\Delta q|) \; , \tag{4.42}$$

where $\vartheta_5 = 3(\sqrt{2}-\sqrt{\omega})^2/\sqrt{2\omega}$ and, as above, $\bar{p} = p + (2\omega - 1)q$. On this crossover locus one has

$$\langle \kappa l \rangle^\times \approx \sqrt{8\omega}\ln(\kappa\xi_\parallel^\times) \approx \frac{A^\times}{|\Delta q|}\left[\ln\left|\frac{B^\times}{\Delta q}\right| - \ln\ln\left|\frac{B^\times}{\Delta q}\right|\right] , \tag{4.43}$$

where the amplitudes are given by

$$A^\times = 6\Omega'(X_t; q_t)/\partial\Omega(X_t; q_t)/\partial q \; , \tag{4.44}$$

$$B^\times / A^\times = [4\sqrt{2\pi}\omega\tilde{\Sigma}_\infty / X_t(X_t - 1)\Omega'(X_t; q_t)]^{2/3} \; . \tag{4.45}$$

Finally we note that the multicritical crossover from $\omega > \frac{1}{2}$ is still determined by (4.12) and $q_P^\times(\omega) \approx p|\frac{1}{2} - \omega|$. As shown by FH, crossover also occurs when $\omega \to 2-$ and one has $\tilde{\tau}_{Q-}^\times \sim (2-\omega)$.[7]

C. Strong fluctuations: Regime III

With the definitions (4.21) the condition (4.3) for Regime III becomes

$$\sqrt{2\eta} < X < 1 - \sqrt{2\eta} \; , \tag{4.46}$$

while all parts of $W^{(t)}(l)$ take a Gaussian form so that asymptotically one has

$$\check{W}^{(t)}(l) \approx \sqrt{\eta}[\Omega(X) + \tilde{\tau}\Psi(X)]e^{2t - \omega t X^2} \; , \tag{4.47}$$

with $\Psi(X) = 1/\sqrt{2\pi}(1-X)$ and $\Omega(X)$ still defined by (4.24). Then the minimum and matching conditions are

$$\Omega_1(X,\eta) + \tilde{\tau}\Psi_1(X,\eta) = 0 \; , \tag{4.48}$$

$$e^{-2t}\tilde{\Sigma}_\infty = \sqrt{\eta}[\Omega_2(X,\eta) + \tilde{\tau}\Psi_2(X,\eta)]e^{-\omega t X^2} \; , \tag{4.49}$$

where the definitions of Ψ_1 and Ψ_2 precisely parallel those of Ω_1 and Ω_2 in (4.27) and (4.28). Eliminating $\tilde{\tau}$ as in Sec. IV B yields

$$X^2 = (2/\omega) + \eta\ln[\eta(\Omega_2\Psi_1 - \Omega_1\Psi_2)^2/\Psi_1^2\tilde{\Sigma}_\infty^2] \; , \tag{4.50}$$

which again, as did (4.29), implies $X \to X_t \equiv \sqrt{2/\omega}$ when $t \to \infty$; but now (4.46) requires $\omega > 2$.

Arguing as in Sec. IV B, criticality is associated with $t^\dagger \to 0$, $\eta^\dagger \to 0$, and hence $X^\dagger \to X_t$. Thus (4.48) yields the critical locus

$$\begin{aligned}\tilde{\tau}_c &= -\Omega_1(X_t,0)/\Psi_1(X_t,0) \\ &= -\Omega(X_t)/\Psi(X_t) \\ &= -\frac{1-X_t}{2-X_t}\left[p + \left[\frac{2}{X_t} - 1\right]w_0\right] + \frac{(1-X_t)}{(2-X_t)^2}q \; ,\end{aligned} \tag{4.51}$$

so that one can write

$$\tilde{\tau}_c(\omega; q) = (q - q_Q)\Delta X(1 - 2\Delta X) - (p + 3w_0)\Delta X^2 + O(\Delta X^3) \; , \tag{4.52}$$

where $q_Q \equiv p + w_0 = q_t(2)$ [see (4.32) and Fig. 1] and

$$\Delta X \equiv 1 - X_t = \tfrac{1}{4}(\omega-2) - \tfrac{3}{32}(\omega-2)^2 + \cdots \geq 0 \ . \qquad (4.53)$$

Evidently, as found by FH, the critical locus $T_{cW}(\omega,q)$ in Regime III departs from the plane $T = T^0_{cW}$. In these circumstances, as also noted by FH, the analysis is no longer accurate since higher-order terms in $W(l)$, such as $w_{30}e^{-3\kappa l}$, etc., will start to play a quantitative role. However, the qualitative behavior, including the linear departure from $\tau_c = 0$ for $q < q_Q$ $(= p + w_0)$, will remain correct. Furthermore, $T_{cW}(\omega,q)$ remains below T^0_{cW} for

$$q < q_0(\omega) = (2 - X_t)[p + w_0 + 2(X_t^{-1} - 1)w_0]$$
$$= q_Q + \tfrac{1}{4}(p + 3w_0)(\omega - 2) + \cdots \ , \qquad (4.54)$$

see Fig. 2(c). However, T_{cW} increases linearly with q and rises above T^0_{cW} when q exceeds $q_0(\omega)$: see Fig. 1. Comparison with (4.32) shows that the locus $q_0(\omega)$ for $\omega \geq 2$ smoothly continues the tricritical locus $q_t(\omega)$ in Regime II $(\omega < 2)$.

To ensure that criticality is actually attained one must check $W^{(t^\dagger)}(l^\dagger) < 0$ using (4.47). Conversely, we may locate the *tricritical locus* by requiring that $W^{(t^\dagger)}$ vanish at the minimum. By (4.47) and (4.48) this yields the condition $\Omega\Psi_1 = \Omega_1\Psi$, which, however, on using (4.27) and its analog for Ψ_1 reduces to the relation

$$\Psi'(X_t)\Omega(X_t; q_t) = \Psi(X_t)\Omega'(X_t; q_t) \ . \qquad (4.55)$$

This is readily solved to yield the locus

$$q_t(\omega) = (\sqrt{2\omega} - 1)p + (\sqrt{2\omega} - 1)^3 w_0$$
$$= q_Q + 2(p + 3w_0)\Delta X + O[(\Delta X)^2] \qquad (4.56)$$

for $\Delta X \geq 0$. Comparison with (4.32) for Regime II shows that $q_t(\omega)$ is continuous at $\omega = 2$ but the slope $q_t'(2+)$ just above $\omega = 2$ is twice as large as in Regime II.

The *tricritical temperature* can now be found by setting $q = q_t$ in (4.51), which leads to

$$T_{tW} - T^0_{cW} \sim \tilde{\tau}_t(\omega) = \frac{\tfrac{1}{2}(\omega-2)^2}{3\omega + \sqrt{2\omega^3} - 2}[p + (2\omega - 1)w_0] \ . \qquad (4.57)$$

Evidently T_{tW} rises quadratically above T^0_{cW} when ω increases beyond the borderline $\omega = 2$: see Fig. 2(c). From (4.51) one can readily compute $\dot{\tau}_c \equiv (\partial \tilde{\tau}_c / \partial X_t)_q \sim (\partial T_{cW}/\partial \omega)_q$; one then finds that the locus $\dot{\tau}_c = 0$ *coincides* with the tricritical locus (4.56). In other words, the slope of the critical locus $T_{cW}(\omega,q)$ in a plane of constant $q > q_Q$ *vanishes at the tricritical* point $T_{tW}(q)$ and is always negative for $\omega > \omega_t(q)$: this is illustrated in Fig. 1.

One can also check that for $T_{cW}(\omega) < T_{tW}(\omega)$ or $q < q_t(\omega)$ one has $\check{W}_{\min} < 0$ as $T \to T_{cW}-$. Indeed it is easily seen that for all $q < q_t$ the criticality is as found by FH for $q = 0$. Thus from (4.50) one obtains

$$X^\dagger - X_t \approx -\tfrac{3}{2}\ln(Ct^\dagger)/\sqrt{8\omega}\,t^\dagger \sim \Delta\tilde{\tau} \equiv \tilde{\tau}_c - \tilde{\tau} \to 0+ \ , \qquad (4.58)$$

where C is a nonuniversal amplitude depending on ω, q, p, and w_0. This leads to the *critical behavior*[7,2,4]

$$\kappa\xi_\parallel \sim \exp\left\{\frac{D}{\Delta\tilde{\tau}}\left[\ln\frac{D}{\Delta\tilde{\tau}} + \ln\ln\frac{D}{\Delta\tilde{\tau}} + O(1)\right]\right\} \ , \qquad (4.59)$$

$$\langle \kappa l \rangle \sim \sqrt{8\omega}[\ln(\kappa\xi_\parallel) - \tfrac{3}{8}\ln\ln(\kappa\xi_\parallel) + O(1)] \ , \qquad (4.60)$$

as $\tilde{\tau} \to \tilde{\tau}_c-$, where D is another nonuniversal amplitude.

The *tricritical behavior* for $\tilde{\tau} \to \tilde{\tau}_t-$ at $q = q_t$ follows similarly. The $\tfrac{3}{2}\ln(Ct^\dagger)$ factor in (4.58) becomes, instead, $\tfrac{5}{2}\ln C't^\dagger - \ln\ln C't^\dagger$, which then leads to

$$\kappa\xi_\parallel \sim \exp\left\{\frac{D'}{\Delta\tilde{\tau}}\left[\ln\frac{D'}{\Delta\tilde{\tau}} - \tfrac{3}{5}\ln\ln\frac{D'}{\Delta\tilde{\tau}} - \tfrac{2}{5}\ln\ln\ln\frac{D'}{\Delta\tilde{\tau}} O(1)\right]\right\} \ , \qquad (4.61)$$

$$\langle \kappa l \rangle \approx \sqrt{8\omega}[\ln(\kappa\xi_\parallel) - \tfrac{5}{8}\ln\ln(\kappa\xi_\parallel) + \tfrac{1}{4}\ln\ln\ln(\kappa\xi_\parallel) + O(1)] \qquad (4.62)$$

$(q = q_t)$, where C' and D' are further nonuniversal amplitudes. Evidently crossover from tricritical behavior is only weakly visible.

To proceed further and examine the first-order region a more delicate analysis near tricriticality is needed. We introduce the offset

$$\delta\tilde{\tau}_0(q,\omega) \equiv \tilde{\tau}_0(q,\omega) - \tilde{\tau}_c(q,\omega) \qquad (4.63)$$

between the first-order transition point $\tilde{\tau}_0(q,\omega)$ and the *extended* critical locus $\tilde{\tau}_c(q,\omega)$ obtained by analytically continuing (4.51). Then we can expand about tricriticality as

$$\Omega + \tilde{\tau}\Psi \approx K_1\delta\tilde{\tau}_0 + K_2(q - q_t)(X^\dagger - X_t) + K_3(X^\dagger - X_t)^2 + \cdots \ , \qquad (4.64)$$

as $q \to q_t+$ and $X^\dagger \to X_t$: the coefficients $K_{i=1,2,3}$ prove to be positive. On substituting in (4.47)–(4.49) one obtains

$$\delta\tilde{\tau}_0 \approx \tfrac{1}{2}(K_2^2/K_1K_3)(q - q_t)^2 > 0 \ , \qquad (4.65)$$

so that, as expected, the first-order transition locus $T_{0W}(q)$ rises above the extended critical locus $T_{cW}(q)$: see Fig. 2(c). In addition one finds, on the point of the first-order wetting transition, the limiting values

$$\langle \kappa l \rangle_0 = \sqrt{8\omega}\ln(\kappa\xi_{\parallel 0}) - O[\ln\ln(\kappa\xi_{\parallel 0})]$$
$$\approx \frac{\sqrt{8\omega}D''}{q - q_t}\left[\ln\frac{D''}{q - q_t} - O\left[\ln\ln\frac{D''}{q - q_t}\right]\right] \ , \qquad (4.66)$$

where D'' is a further nonuniversal amplitude.

Finally, one can use the expansion (4.64) with (4.58) and its tricritical counterpart to see that *crossover* from the tricritical behavior (4.61) and (4.62) sets in only for

$$\tilde{\tau}_c - \tilde{\tau} \ , \quad \tilde{\tau}_0 - \tilde{\tau} \lesssim \tilde{\tau}^\times_{\rm III} \sim |q - q_t(\omega)| \ , \qquad (4.67)$$

as indicated in Fig. 2(c).

As regards the critical crossover $\omega \to 2+$ with $q < q_Q$ we recall the result of FH to the effect that the multicritical behavior for Q ($\omega=2$) remains controlling until $(\tau_c-\tau)$, $(\tau_0-\tau)\lesssim\tilde{\tau}^{\times}_{Q+}\sim(\omega-2)^2$; only then does Regime III critical behavior set in. This contrasts with the crossover relation $\tilde{\tau}^{\times}_{Q-}\sim|\omega-2|$ applicable below $\omega=2$.

This completes our analytical study of critical, tricritical, and near-critical wetting in $d=3$ dimensions on the basis of the linearized functional renormalization group. We have already commented that in Regime III terms in $W(l)$ and $\tilde{\Sigma}(l)$ not considered will contribute quantitatively to various amplitudes, critical loci, etc., although they will not change qualitative behavior, critical exponents, etc. Beyond that, of course, one must bear in mind the effects of the linearization. The presence of the wall-potential amplitude w_0 in various expressions already in Regime II serves as a reminder that although, as FH argue,[7,8] a more realistic "nonlinear" wall should not alter any qualitative behavior, most numerical values must change. Indeed, the actual magnitude of the tricritical locus for $\omega>\frac{1}{2}$ depends not only on w_0 but also on the cutoff Λ via $q\propto s_{21}$, so one must recognize again that the nonuniversal amplitudes calculated here should be regarded only as approximations for the corresponding parameters in more realistic models. Nevertheless it is worthwhile making some numerical estimates as we now attempt to do.

V. QUANTITATIVE ESTIMATES AND DISCUSSION

Having characterized the form of the phase diagram in the space (T,ω,q) we are ready to assess the implications for real systems or, at least, for three-dimensional Ising models. Their wetting transitions have been intensively studied by simulations[9–11] and have yielded quantitative results at variance with the original RG calculations,[5,7] which, however, neglected the l dependence of the interfacial stiffness. In making numerical estimates, we must bear in mind the limitations of our theoretical treatment as discussed in the previous section. Nevertheless some progress can be made.

A. Nature of the wetting transition

The primary issue is whether or not the simple cubic (sc) Ising models simulated[9–11] fall within the region where first-order wetting transitions are to be expected. We may consider only T exceeding the roughening temperature $T_R\simeq0.54T_c$, where T_c is the bulk critical temperature. Now the capillary parameter $\omega(T)$ is a continuous function of T rising sharply from[11(a)] $\omega(T_R)\simeq0.51_2$. The relevant values are $\omega(T_{cW})$, where the supposed wetting critical points T_{cW} (which might, in fact, turn out to be weak first-order transition points T_{0W}) depend on the surface field h_1 and the surface couplings (which influence g: see I). These, in turn, are assigned by the simulator, who then "measures" T_{cW} using the Monte Carlo (MC) data. In the work to date,[9–11] the wetting transitions studied fell in the range $(0.6–0.93)T_c$. The best current estimates[11(a)] indicate $0.70<\omega(t)\lesssim0.87$ for $T>0.6T_c$: this places the sc Ising model firmly in Regime II: $\frac{1}{2}<\omega<2$. By contrast, the *fits* of the MC data to the previous ($q\equiv0$) RG theory required $\omega_{\rm fit}<0.25$ (and were even consistent with $\omega_{\rm fit}\simeq0$).[9,10] The discrepancy of a factor of $\gtrsim2.8$ is clearly serious.

From Figs. 1 and 2(b) we see that the criterion for a first-order transition in Regime II is

$$q>q_t(\omega)\approx2p\Delta\omega[1+O(\Delta\omega w_0/p)]\ , \tag{5.1}$$

where (4.32) has been expanded for small $\Delta\omega\equiv\omega-\frac{1}{2}$. In the present case we have $\Delta\omega=0.20–0.37$ which justifies neglecting the correction factor in (5.1) unless $w_0/p\gg1$. Note, from (4.32), that q_t rises only to $p+w_0$ at $\Delta\omega=1.5$. Now since w_0 enters the linearized RG as a measure of the wall influence, its magnitude is hard to gauge with confidence; but it is most reasonable to suppose that w_0 is only a relatively small multiple of $p=O(\tilde{\Sigma}_\infty)$.

Now from (2.24), (2.26) and the relation (2.27), which states $q/|s_{21}|=\frac{1}{2}\omega\xi_\beta^2\Lambda^2$, we obtain

$$p\simeq w_{20}+s_{20}q/|s_{21}|\ . \tag{5.2}$$

The explicit calculations of I for the parabolic models with the crossing constraint yield (for $T\to T^0_{cW}$) $w_{20}=K\kappa\mathcal{G}m^2_{\beta\infty}$, and

$$s_{21}=-2w_{20}\ ,\quad s_{20}\simeq c_{20}w_{20}\quad \text{with } c_{20}=O(1)\ . \tag{5.3}$$

The calculations also show that these relations should change relatively little for more realistic order-parameter models. (See also the Appendix and I for the integral-constraint results.) We can thus rewrite the first-order criterion (5.1) as

$$(\Lambda\xi_\beta)^2\omega/(2\omega-1)>f_1\simeq1+\tilde{c}\Delta\omega\ ,\quad \tilde{c}=O(c_{20},w_0/p)\ . \tag{5.4}$$

In this form we believe the criterion may have fairly general applicability to fluids and model fluids.

Now for $T=T_R$ the factor $\omega/(2\omega-1)$ in the sc Ising model is about 21; it falls rapidly to around 1.75 at $T=0.6T_c$ but never drops below about 1.15 for $T\leq T_c$. If a is the simple cubic lattice spacing it is appropriate to take $\Lambda=\pi/a$, i.e., to use a lattice cutoff. One might imagine adopting a *smaller* cutoff but, for simple nearest-neighbor Ising models we see no compelling grounds for doing so. To evaluate the true correlation length $\xi_\beta(T)$ we can employ, with considerable confidence, low-temperature Ising-model series: see Refs. 11(a) and 16. For $T=T_R$ we thus find $(\Lambda\xi_\beta)^2\simeq0.95$: clearly the first-order condition is well satisfied!

At $T=0.6T_c$ we obtain $(\Lambda\xi_\beta)^2\simeq1.3$: multiplying by $\omega/(2\omega-1)$ gives 2.3, which, unless c_{20} or w_0/p are large, still meets the criterion safely, say, by a margin of 1.7 if we suppose $\tilde{c}\lesssim2$. When $T=0.7T_c$ we find $(\Lambda\xi_\beta)^2\simeq2.1$ and $\omega/(2\omega-1)\simeq1.28$; thus, allowing for an increasing right-hand side of (5.3), we have an almost identical margin of safety. Thereafter $(\Lambda\xi_\beta)^2$ increases rapidly since $\xi_\beta(T)$ diverges at T_c, but $\Delta\omega$ changes only slightly. We therefore conclude, with reasonable confidence, that the sc Ising model above T_R is *always* in a region of *first-order wetting transitions.* However, in the vicinity of $T_{cW}/T_c\simeq0.65$, where many of the simulations were performed, the model would seem to be relatively close to critical wetting. Indeed we cannot definitively rule out critical wetting in this region although we judge a weak first-order transition as significantly more likely.

B. Magnitude of first-order discontinuities

How strong are the expected first-order transitions? To answer this let us suppose, first, that the system could be realized in Regime I ($\omega < 0.5$), as suggested by some of the MC fits. Then a first-order transition is *always* expected and we can estimate the layer thickness just below the transition point via

$$\left\langle \frac{l}{a} \right\rangle_0 \simeq \frac{1+2\omega}{1-2\omega}\left[\frac{\Lambda\xi_\beta}{\pi}\right]\left[\frac{1}{\omega(\Lambda\xi_\beta)^2}+\frac{3}{2}\right] + \frac{2\omega}{1-2\omega}\ln\left[\frac{1/\mathcal{G}}{\omega(\Lambda\xi_\beta)^2}\right] . \quad (5.5)$$

If we evaluate this assuming $\omega \simeq 0.25$, $\mathcal{G} \simeq \frac{3}{4}$, and use $\Lambda\xi_\beta \simeq 1$ (for $T \simeq T_R$) we find $\langle l \rangle_0 \simeq 7a$. A jump of $\langle l \rangle_0$ from $7a$ to ∞ is on the borderline of current simulation capabilities but perhaps not beyond what might be observed. The correlation length at the transition follows similarly from (4.10); this yields $\xi_{\parallel 0}/a \simeq 2.5\times 10^4$, which, in the eyes of any plausible simulations, will surely appear as infinity!

Of course, this example is purely illustrative since we believe $\omega \gtrsim 0.7$ for the sc Ising model and should thus use the results (4.34)–(4.36) for Regime II to estimate $\langle l \rangle_0$. The relevant parameters are then the amplitude

$$\bar{p} = p[1+2\Delta\omega(w_0/p)] \equiv f_2 p , \quad (5.6)$$

which involves, as previously, the wall amplitude; the ratio

$$\bar{p}/\tilde{\Sigma}_\infty \simeq f_2 \mathcal{G}[\omega(\Lambda\xi_\beta)^2 + \tfrac{1}{2}] , \quad (5.7)$$

where we have used (5.2), (5.3), and (2.27); and the tricritical deviation, which we write

$$\Delta q = q - q_t(\omega) \equiv \epsilon q_t(\omega) , \quad (5.8)$$

that, clearly, is the most uncertain parameter although the numerical estimates of the previous subsection suggest $\epsilon \lesssim 0.7$. (Of course, it is not even certain that ϵ is positive.)

If, for concreteness, we now suppose that $\omega \simeq 0.75$ (as in the main simulation region), we may estimate the layer thickness at the point of transition via

$$\frac{\langle l \rangle_0}{a} \simeq \frac{3\Lambda\xi_\beta}{2\pi}\left[\frac{f_1}{2\epsilon\Delta\omega} - 0.61\right] \times \left[\ln\left[\frac{\tilde{E}}{\epsilon}\right] + \ln\ln\left[\frac{\tilde{E}}{\epsilon}\right]\right] + 1.6 , \quad (5.9)$$

where taking $\mathcal{G} \simeq 1$ gives $\tilde{E} \simeq 16 f_2^{1/3}/f_1[(\Lambda\xi_\beta)^2 + \frac{2}{3}]^{2/3}$. (Actually one has $\tilde{E} \sim \Delta\omega^{1/3}$ for $\Delta\omega \to 0$.) One may reasonably guess $f_1 \simeq 1.5$, $f_2 \simeq 2$, and use $\Lambda\xi_\beta \simeq 1.67$ to obtain the rough estimate $\tilde{E} \simeq 6.0$. Fortunately, however, this value enters only logarithmically. For deviations $\epsilon = 0.7$, 0.4, and 0.2 we thence obtain the estimates $\langle l \rangle_0 \simeq 10a$, $22a$, and $55a$, respectively. These values are, again, sufficiently large that the wetting transitions could be hard to distinguish numerically from critical transitions in which $\langle l \rangle_0$ truly diverged. As in Regime I, the values of $\xi_\parallel$ at the transition are vastly larger: e.g., for $\epsilon \simeq 0.7$ we obtain via (4.37) the estimate $\xi_{\parallel 0} \simeq 1100a$.

C. Discussion

We conclude, despite the evident quantitative uncertainties, that wetting transitions in the simple cubic Ising model are likely to be weakly first order as a result of destabilizing fluctuations induced by the wall-dependent interfacial stiffness. Of course, this conclusion applies only to systems infinite in all dimensions. In a finite system, as necessarily involved in simulations, both critical and weakly first-order transitions will be rounded. It is most plausible, we believe, that such a rounded weakly *first-order* transition will resemble quite closely a rounded *critical* transition but one with a *weaker* singularity than would be displayed in the absence of the instability (since underlying incipient divergences are prevented from growing). This mechanism may well, therefore, account for the reports[9,10] of critical wetting transitions consistent with the original $q \equiv 0$ RG theory but with anomalously low values of $\omega_{\rm fit}$ (corresponding to weaker apparent critical singularities).

To substantiate this explanation in more detail one would like an improved theory able to deal directly with the RG nonlinearities and one which could be applied more quantitatively to specific Ising models. Progress may be possible using approximate interfacial functional renormalization groups[8] adapted to allow for a varying stiffness $\tilde{\Sigma}(l)$. Nevertheless it may be overoptimistic to expect this route to lead to a fully convincing quantitative assessment of the Ising models. On the other hand, improved simulations, designed specifically to detect weak first-order transitions, perhaps via some hysteresis in the dynamics, might confirm our scenario. Unfortunately, though, such transitions are notoriously hard to establish definitively in Monte Carlo studies. By going to lower temperatures, closer to T_R smaller values of ω are relevant which, by our analysis, should enhance the first-order character of the transition.

In summary, our long and necessarily rather detailed analysis has unambiguously revealed the importance of the stiffness variation in short-range wetting in $d=3$ dimensions. First-order transitions may be induced in place of nonuniversal critical behavior. This is very likely the explanation of the serious discrepancies between the original RG theories[5–7] and the simulations designed to test them.[9,10] However, extended simulations and new theoretical analyses more closely linked to the specific lattice systems observed are desirable. In the future one may hope that appropriate experimental systems will be available for study although the ubiquitous presence of van der Waals forces makes this problematical.

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APPENDIX: INTERFACIAL STIFFNESS USING THE INTEGRAL CRITERION

The analysis presented in this paper relies heavily on the specific form (1.7) for the wall stiffness $\tilde{\Sigma}(l)$ with bare coefficients s_{jk} behaving either as in (1.10) or, alternatively, as in (1.12). The first set of expressions was derived explicitly in **I** (i.e., Ref. 4) via perturbative calculations using a *crossing criterion.* Here, we derive the second set of coefficients (1.12) following the *integral-criterion* formulation developed in Sec. VI of **I** and using notations explained there.

1. Foundations of the derivation revisited

We recall, first, from **I** that our derivation of the effective interface Hamiltonian (1.1) is based on an underlying bulk order-parameter theory reflecting short-range interactions between a planar wall at $z=0$ and a noncritical, bulk medium occupying the half-space ($\mathbf{y}$, $z>0$) with two near-coexisting phases, the wetting phase β and the stable phase α: see Fig. 1 of **I**. Explicit calculations then rely on the systematic implementation of suitable constraints on the bulk interfacial profile specifying $l(\mathbf{y})$, the wetting-layer thickness, regarded as a collective coordinate. Following this procedure we derived in Sec. II of **I** a compact general expression for the wall stiffness as

$$\tilde{\Sigma}(l)\equiv\tilde{\Sigma}_\infty+\Delta\tilde{\Sigma}(l)=K\int_0^\infty dz\left[\frac{\partial m_{\Pi}(z;l)}{\partial l}\right]^2 . \quad \text{(A1)}$$

Here K is the coefficient of the $\frac{1}{2}(\nabla m)^2$ term in the underlying order-parameter theory [see (1.5)], while $m_{\Pi}(z;l)$ is the *constrained planar profile* that minimizes the order-parameter Hamiltonian *under the restriction* that the interfacial profile satisfies $l(\mathbf{y})=l_\pi=l$, fixed, for all $\mathbf{y}$ at given temperature T, ordering field h, etc.

In the integral-criterion approach, expounded in Sec. VI of **I**, the precise location of the interface is defined through an "adsorption thickness" $\bar{l}$ parametrized by an exponent $p>0$: see **I** (6.1). Adopting a standard m^4 LGW Hamiltonian and choosing $p=2$, the appropriate planar profile, denoted by $\overline{m}_{\Pi}(z;\bar{l})$, has been found in exact closed form. Specifically, after substituting for $\bar{l}$ in favor of the *corresponding crossing point* $z=l$, one finds that the *rescaled* profile

$$\rho\equiv[\overline{m}_{\Pi}(z;\bar{l}(l))-m_{\alpha\infty}]/(-2m_{\alpha\infty}) , \quad \text{(A2)}$$

with $m_{\alpha\infty}(T,h)$ being the order-parameter value in the pure α phase, is given explicitly by

$$\rho(z;l)=\frac{1+\mu}{1+F_+e^{\tilde{\kappa}(z-l)}+F_-e^{-\tilde{\kappa}(z-l)}} , \quad \text{(A3)}$$

with, however, coefficients $F_\pm(l)$, $\tilde{\kappa}(l)$, and $\mu(l)$ depending implicitly on l: see (6.18) of **I**.

Fortunately, subsequent manipulations in **I** Sec. VI allow the determination of these coefficients for large l near the mean-field critical wetting transition determined by $h\to 0$ and $\tilde{\tau}\sim(T-T_{cW}^0)\to 0-$. Indeed, collecting relevant results in **I** Sec. VI E yields the expansion

$$\mu(l)=\sum_{j=k+1}^{\infty}\sum_{k=0}^{\infty}\mu_{jk}(\kappa l)^k e^{-j\kappa l} , \quad \text{(A4)}$$

with leading coefficients $\mu_{jk}(T,h)$ given by

$$\mu_{10}=\frac{2}{1-\tilde{g}}\tilde{\tau} , \quad \mu_{20}=\mathcal{G}+O(\tilde{\tau}) , \quad \text{(A5)}$$

$$\mu_{21}=\frac{2}{(1-\tilde{g})^2}\tilde{\tau}^2 , \quad \mu_{32}=O(\tilde{\tau}^3) , \quad \mu_{31}=O(\tilde{\tau}), \quad \ldots , \quad \text{(A6)}$$

where, together with $\tilde{\tau}$, $\tilde{g}$ (<-1) and $\mathcal{G}$ ($0<\mathcal{G}<1$) are completely specified on the basis of the order-parameter model: see **I** Eqs. (6.28), (6.16), (4.6), (4.12), and related equations. Completing the story, one also has, directly from (6.19) and (6.20) of **I**, the relations

$$F_\pm(l)=\tfrac{1}{2}(1+2\mu)\pm\tfrac{1}{2}[(1+\mu)(1+4\mu)]^{1/2} , \quad \text{(A7)}$$

$$\tilde{\kappa}(l)=\kappa(1+\mu)^{1/2} , \quad \text{(A8)}$$

in terms of $\mu(l)$ and $\kappa(T,h)$ (the inverse of the true bulk correlation length).

To calculate the wall stiffness we use (A1) and focus on evaluating the integral

$$\tilde{\Sigma}(l)=4\Sigma_0\int_{-\tilde{\kappa}l}^{\infty}\frac{(\tilde{\kappa}\kappa)^{-1}f(x)dx}{[1+F_+e^x+F_-e^{-x}]^4} , \quad \text{(A9)}$$

where $\Sigma_0\equiv K\kappa m_{\alpha\infty}^2$ represents a convenient unit of stiffness, while

$$f(x)\equiv\left\{\left[(1+\mu)\frac{\partial\tilde{\kappa}}{\tilde{\kappa}\partial l}(F_-e^{-x}-F_+e^x)\right]x+\frac{\partial\mu}{\partial l}+\left[\frac{\partial\mu}{\partial l}F_+-(1+\mu)\left[\frac{\partial F_+}{\partial l}-\tilde{\kappa}F_+\right]\right]e^x+\left[\frac{\partial\mu}{\partial l}F_--(1+\mu)\left[\frac{\partial F_-}{\partial l}+\tilde{\kappa}F_-\right]\right]e^{-x}\right\}^2 . \quad \text{(A10)}$$

Unfortunately, the complexity of this expression and the presence of polynomial combinations like $x^2P_1(e^{\pm x})/P_2(e^{\pm x})$, in particular, have so far impeded the derivation of a closed expression for the wall stiffness. The following expansions, however, suffice for the extraction of all the leading terms needed for studying critical wetting.

2. Wall stiffness for critical wetting

It is appropriate to check first the limit $l\to+\infty$ for fixed T, h, etc. As for the crossing-criterion derivation discussed in **I**, the wall stiffness in this limit when $h=0$ must approach the standard surface-tension expression for a free $\alpha|\beta$ interface, namely, $\Sigma_{\alpha|\beta}=\frac{2}{3}\Sigma_0(T,h=0)$ in this isotropic model. This may be easily confirmed. Specifically, from (A6) and subsequently from (A3) and (A4), it is clear that

$$\mu(l\rightarrow+\infty)=0\ ,\quad \left.\frac{\partial\mu}{\partial l}\right|_{l\rightarrow+\infty}=0\ , \tag{A11}$$

$$F_{\pm}(l\rightarrow+\infty)=1,0\ ,\quad \tilde{\kappa}(l\rightarrow+\infty)=\kappa\ , \tag{A12}$$

and

$$\left.\frac{\partial F_{\pm}}{\partial l}\right|_{l\rightarrow+\infty}=\frac{\partial\tilde{\kappa}}{\partial l}=0\ . \tag{A13}$$

From (A9), one therefore simply gets

$$\tilde{\Sigma}(l\rightarrow+\infty)\equiv\tilde{\Sigma}_{\infty}=4\Sigma_0\int_{-\infty}^{\infty}\frac{e^{2x}dx}{[1+e^x]^4}=\tfrac{2}{3}\Sigma_0\ . \tag{A14}$$

For l large but finite, it is helpful, first, to simplify the denominator in (A9) by observing from (A3)–(A8) that, for $\tilde{\tau}$ and $X\equiv e^{-\kappa l}$ small, as needed for critical wetting, one has

$$\left|\frac{F_-e^{-x}}{1+F_+e^x}\right|\lesssim|O(\tilde{\tau})+O(X,\tilde{\tau}lX)|\ll 1 \tag{A15}$$

over the range of the integration $-\tilde{\kappa}l\le x<+\infty$. A straightforward expansion then leads to

$$\tilde{\Sigma}(l)=4\Sigma_0\sum_{k=0}^{2}\sum_{n=4}^{+\infty}\sum_{j=2-n}^{6-n}(\tilde{\kappa}\kappa)^{-1}\sigma_{jkn}R_{jkn}\ , \tag{A16}$$

where we have introduced the integrals

$$R_{jkn}(l;T,\dots)\equiv\int_{-\tilde{\kappa}l}^{\infty}\frac{x^ke^{jx}dx}{[1+F_+e^x]^n} \tag{A17}$$

and the corresponding coefficients $\sigma_{jkn}(l;T,\dots)$. In terms of the combinations,

$$\dot{\kappa}_{\pm}\equiv\mp\frac{(1+\mu)}{\tilde{\kappa}}\frac{\partial\tilde{\kappa}}{\partial l}F_{\pm}\ , \tag{A18}$$

$$E_{\pm}\equiv\frac{\partial\mu}{\partial l}F_{\pm}-(1+\mu)\left[\frac{\partial F_{\pm}}{\partial l}\mp\tilde{\kappa}F_{\pm}\right]\ , \tag{A19}$$

these coefficients can be read out directly as

$$\sigma_{224}=\dot{\kappa}_+^2\ ,\quad \sigma_{024}=2\dot{\kappa}_+\dot{\kappa}_-\ ,\quad \sigma_{(-2)24}=\dot{\kappa}_-^2\ ; \tag{A20}$$

$$\sigma_{214}=2\dot{\kappa}_+E_+\ ,\quad \sigma_{114}=2\dot{\kappa}_+\frac{\partial\mu}{\partial l}\ ,$$
$$\sigma_{014}=2\dot{\kappa}_+E_-+2\dot{\kappa}_-E_+\ ,$$
$$\sigma_{(-1)14}=2\dot{\kappa}_-\frac{\partial\mu}{\partial l}\ ,\quad \sigma_{(-2)14}=2\dot{\kappa}_-E_-\ ; \tag{A21}$$

$$\sigma_{204}=E_+^2\ ,\quad \sigma_{104}=2E_+\frac{\partial\mu}{\partial l}\ ,$$
$$\sigma_{004}=\left[\frac{\partial\mu}{\partial l}\right]^2+2E_+E_-\ ; \tag{A22}$$

$$\sigma_{(-1)04}=2E_-\frac{\partial\mu}{\partial l}\ ,\quad \sigma_{(-2)04}=E_-^2\ ; \tag{A23}$$

$$\sigma_{j-1,k,n+1}=\sigma_{jkn}(-4F_-)\ ;\quad \dots\ . \tag{A24}$$

In order to evaluate the integrals R_{jkn} for large l we set $x_0\equiv\tilde{\kappa}l$ and write

$$\frac{\partial R_{jkn}}{\partial x_0}=(-x_0)^ke^{-jx_0}[1-nF_+e^{-x_0}+\cdots]\ . \tag{A25}$$

When $x_0\rightarrow\infty$ three cases arise: (i) if $j>0$, one has

$$R_{jkn}=c_{jkn}+O(x_0^ke^{-jx_0})\ , \tag{A26}$$

with constants $c_{jkn}(T,h,\dots)\equiv R_{jkn}(l\rightarrow\infty)$; (ii) if $j=0$, one has

$$R_{jkn}=-\frac{(-x_0)^{k+1}}{k+1}+c'_{0kn}+O(x_0^ke^{-x_0})\ ; \tag{A27}$$

and (iii) when $j<0$, one finds

$$R_{jkn}=e^{|j|x_0}|j|^{-1}(-x_0)^k[1+k/jx_0+\cdots]$$
$$\times[1+O(e^{-x_0})]\ . \tag{A28}$$

Now, using (A4)–(A8), we can expand the factors $\dot{\kappa}_{\pm}$ and $E_{\pm}$ as

$$\dot{\kappa}_{\pm}=\tfrac{1}{2}\kappa[\mu_{10}+2(\mu_{20}+\mu_{21}\kappa l)X+\cdots]X\ , \tag{A29}$$

$$\dot{\kappa}_-=\tfrac{1}{8}\kappa[\mu_{10}^2+3\mu_{10}(\mu_{20}+\mu_{21}\kappa l)X+\cdots]X^2\ , \tag{A30}$$

$$E_+=\kappa[1+5\mu_{10}X+\tfrac{25}{4}(\mu_{20}+\mu_{21}\kappa l)X^2+\cdots]\ , \tag{A31}$$

$$E_-=-\tfrac{1}{4}\kappa(\mu_{20}+\mu_{21}\kappa l)X^2+\cdots\ , \tag{A32}$$

with $X\equiv e^{-\kappa l}$. These expressions, in turn, determine the expansions for all the coefficients (A20)–(A24) and, together with (A26)–(A28), yield the desired form for $\tilde{\Sigma}(l)$, namely,

$$\tilde{\Sigma}(l)=\sum_{j\ge k=0}^{\infty}s_{jk}^I(\kappa l)^ke^{-j\kappa l}\ , \tag{A33}$$

where the superscript I denotes the use of the integral criterion.

Explicitly one finds (a) a constant piece $s_{00}^I\equiv\tilde{\Sigma}_{\infty}$, that comes only from the term involving $\sigma_{204}R_{204}$ so that $\tilde{\Sigma}_{\infty}=\Sigma_0c_{204}=\frac{2}{3}\Sigma_0$, as in (A14); (b) pieces decaying as $e^{-\kappa l}$ that can arise only from $\sigma_{204}R_{204}$, $\sigma_{105}R_{105}$, and $\sigma_{104}R_{104}$ so that

$$s_{10}^I=4\Sigma_0(10\mu_{10})c_{204}+4\Sigma_0(-2\mu_{10})c_{104}+4\Sigma_0\mu_{10}c_{105}$$
$$=10\Sigma_0\tilde{\tau}/(1-\tilde{g}) \tag{A34}$$

and also

$$s_{11}^I\equiv 0\ ; \tag{A35}$$

(c) many terms containing the factor $e^{-2\kappa l}$ but as $\tilde{\tau}\rightarrow 0$ all the leading contributions arise from $\sigma_{014}R_{014}$, $\sigma_{004}R_{004}$, $\sigma_{204}R_{204}$, $\sigma_{104}R_{104}$, $\sigma_{105}R_{105}$, and $\sigma_{(-2)04}R_{(-2)04}$ so that one has

$$s_{22}^I=95\Sigma_0\tilde{\tau}^2/(1-\tilde{g})^2\ , \tag{A36}$$

$$s_{21}^I=-2\Sigma_0\mathcal{G}+O(\tilde{\tau}^2),\quad s_{20}^I=O(\mathcal{G},\tilde{\tau}^2)\ ; \tag{A37}$$

and (d) many terms, such as $\sigma_{014}R_{014}$ and $\sigma_{024}R_{024}$, etc., which contribute to terms in $\tilde{\Sigma}(l)$ decaying faster than $e^{-2\kappa l}$; while generally (e) we surmise

$$s_{jk}^{I} \approx a_{jk}^{I} \tilde{\tau}^{\max\{2k-j,0\}}, \quad a_{jk}^{I} = O(1) , \tag{A38}$$

for $j \geq k \geq 3$.

These results are in complete accord with those from the crossing-criterion derivation. In particular one has

$$s_{21}^{I} / s_{21} = m_{\alpha\infty}^{2} / m_{\beta\infty}^{2} = 1 + O(h) \tag{A39}$$

for the *destabilizing* $\kappa l e^{-2\kappa l}$ variation of the bare wall stiffness. In addition, the calculation supports the surmise that s_{11} vanishes in the crossing-criterion derivation in *all* orders of perturbation about the parabolic limit.

Finally, for the sake of completeness, we reexpress the results in term of the adsorption thickness $\bar{l}$. The variational formulation outlined in *I* Sec. II justifies the relation

$$\underline{\tilde{\Sigma}}(\bar{l}; T, h, \ldots)(\nabla \bar{l})^2 = \tilde{\Sigma}(l; T, h, \ldots)(\nabla l)^2 \tag{A40}$$

for the stiffness expressed in terms of $\bar{l}$. To go further we use results in I Sec. VI such as (6.48) and (6.50) to get in leading order

$$X = \frac{2}{e}\bar{X}\left\{1 + \left[-\frac{2\tilde{g}}{1-\tilde{g}} + \frac{\tilde{\tau}}{1-\tilde{g}}\bar{\kappa}\bar{l}\right]\frac{2}{e}\bar{X} + \left[O(1) + \frac{2}{e^2}\mathcal{G}\bar{\kappa}\bar{l} + O(\tilde{\tau}^2)\bar{l}^2\right]\bar{X}^2 + \cdots\right\}, \tag{A41}$$

where $\bar{X} \equiv e^{-\bar{\kappa}\bar{l}}$ and $\bar{\kappa} = \kappa + O(h)$ as given by (6.26) of I. On taking gradients this yields

$$(\nabla l)^2 = (\nabla \bar{l})^2 \left\{1 + \left[-\frac{8\tilde{g}}{1-\tilde{g}} + \frac{2\tilde{\tau}}{1-\tilde{g}}\bar{\kappa}\bar{l}\right]\frac{2}{e}\bar{X} + [O(1) + 2\mathcal{G}\bar{\kappa}\bar{l} + O(\tilde{\tau}^2)\bar{l}^2]\left[\frac{2}{e}\bar{X}\right]^2 + \cdots\right\}, \tag{A42}$$

up to a factor $[1 + O(h, \tilde{\tau})]$. To the same precision one thus finds

$$\underline{\tilde{\Sigma}}(\bar{l}) = \left\{\tilde{\Sigma}_\infty + s_{10}^{I}\frac{2}{e}\bar{X} + [O(1) + s_{21}^{I}\bar{\kappa}\bar{l} + O(\tilde{\tau}^2)]\left[\frac{2}{e}\bar{X}\right]^2 + \cdots\right\}. \tag{A43}$$

Thus, evaluating (A40) generates the full expansion

$$\underline{\tilde{\Sigma}}(\bar{l}) = \sum_{j \geq k = 0}^{\infty} \bar{s}_{jk}^{I} (\bar{\kappa}\bar{l})^k e^{-j\bar{\kappa}\bar{l}} , \tag{A44}$$

with corresponding coefficients

$$\bar{s}_{00}^{I} = \tfrac{2}{3}\Sigma_0 + O(h), \quad \bar{s}_{11}^{I} = \frac{8}{3e}\frac{\Sigma_0}{1-\tilde{g}}\tilde{\tau} + O(h\tilde{\tau}) , \tag{A45}$$

$$\bar{s}_{10}^{I} = -\frac{32}{6e}\frac{\tilde{g}}{1-\tilde{g}}\Sigma_0 + O(h, \tilde{\tau}), \quad \bar{s}_{22}^{I} = O(\tilde{\tau}^2, \tilde{\tau}^2 h) , \tag{A46}$$

$$\bar{s}_{21}^{I} = -\tfrac{2}{3}\left[\frac{2}{e}\right]^2 \mathcal{G}\Sigma_0 + O(h, \tilde{\tau}), \quad \bar{s}_{20}^{I} = O(1), \ldots . \tag{A47}$$

It is evident from these results that the general functional form (1.7) is verified in terms of either l or $\bar{l}$ (for $\tilde{\Sigma}$ or $\underline{\tilde{\Sigma}}$). However, various coefficients s_{jk} ($j \geq k \geq 0$) evidently need not match: note, for example, $s_{11}^{I} = 0$ but $\bar{s}_{11}^{I} \sim \tilde{\tau}$. An exact treatment of the fluctuations should, of course, yield correct final results using either a formulation with l or with $\bar{l}$. However such an analysis is beyond present powers. On the other hand, for use in a renormalization-group treatment such as presented in the main body of this paper, general considerations suggest that one should use basic "field" variables which are defined as locally as possible. For the collective coordinate of the effective interface Hamiltonian the crossing criterion thus seems preferable. Note, indeed, that the absorption thickness $\bar{l}$ is essentially a *delocalized* quantity involving the varying profile near the wall as well as in the tail beyond the interfacial region (the latter contribution leading to the breakdown for $p = 1$: see I Sec. VI B). We conclude that one should choose the localized, crossing definition l and the corresponding results, $W(l)$ and $\tilde{\Sigma}(l)$ *or* $W^I(l)$ and $\tilde{\Sigma}^I(l)$ for the analysis of critical wetting, as we have done here and previously.[2–4]

As further commentary on our analysis we mention that Parry and Evans have shown,[17] using sum-rule arguments for appropriate microscopic Hamiltonians, that specific corrections to the leading-order singular behavior of the moments of the density-density correlation function exist near the *complete wetting transition*.[11(b)] Moreover, they have demonstrated fairly convincingly that those corrections can*not* be properly generated by the standard interfacial Hamiltonian (1.1) with (1.2). Thus on quite different grounds they also conclude that the standard interfacial Hamiltonian used in previous RG theory[5–8] is oversimplified.

Furthermore, Parry and Evans[17] have shown that the necessary corrections can be naturally accounted for by adopting the full interfacial Hamiltonian including the specific stiffness variation discussed here. In fact, by retaining the standard linear plus pure exponential form (1.2) (with no anomalous terms), they argued that the leading decay of the stiffness variation should be of the form $le^{-\kappa l}$. Since we found in I that $\underline{W}^I(\bar{l})$ had just the form (1.2), this conclusion corresponds precisely with the results of our *integral derivation* expressed in terms of the corresponding adsorption thickness $\bar{l}$, namely $W(\bar{l})$ given by (6.38)–(6.41) of I and $\tilde{\Sigma}(\bar{l})$ given by (A44)–(A47)!

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[1]For reviews focusing on *short-range* critical wetting, see (a) D. M. Kroll, J. Appl. Phys. **61**, 3595 (1987); (b) M. E. Fisher, in *Statistical Mechanics of Membranes and Surfaces,* edited by D. R. Nelson, T. Piran, and S. Weinberg (World Scientific, Singapore, 1988), p. 19. The inadequate justification available for expressing the wall-interface potential simply as a linear term plus a pure exponential was first emphasized here: see especially Sec. 1.6 and Chap. 3; (c) S. Dietrich, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, New York, 1988), Vol. 12, p. 1.

[2]M. E. Fisher and A. J. Jin, Phys. Rev. B **44**, 1430 (1991), and references therein. This article announced the presence of anomalous terms in the bare wall-interface potential *and,* in Footnote 12, noted the dependence of the interfacial stiffness on the wall-interface separation, subsequently found to be important.

[3]M. E. Fisher and A. J. Jin, Phys. Rev. Lett. **69**, 792 (1992). The detailed functional form of the interfacial stiffness variation and its role in critical wetting transitions was briefly reported here.

[4]A. J. Jin and M. E. Fisher, Phys. Rev. B **47**, 7365 (1993). This article will be denoted **I**. It presents a systematic formulation for deriving the effective interfacial Hamiltonian through suitable constraints on the collective coordinate describing the interface configuration and explains detailed calculations of both the wall-interface potential and the wall-interface stiffness for short-range critical wetting. The present article builds on and extends this work.

[5]E. Brézin, B. I. Halperin, and S. Leibler, J. Phys. (Paris) **44**, 775 (1983); Phys. Rev. Lett. **50**, 1387 (1983).

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

[7]D. S. Fisher and D. A. Huse, Phys. Rev. B **32**, 247 (1985), which presents the linearized functional renormalization-group method that we follow here. This paper will frequently be denoted FH.

[8]R. Lipowsky and M. E. Fisher, Phys. Rev. Lett. **57**, 2411 (1986); Phys. Rev. B **36**, 2126 (1987).

[9](a) K. Binder, D. P. Landau, and D. M. Kroll, Phys. Rev. Lett. **56**, 2272 (1986); (b) K. Binder and D. P. Landau, Phys. Rev. B **37**, 1745 (1988); (c) K. Binder, D. P. Landau, and S. Wansleban, *ibid.* **40**, 6971 (1989).

[10]A. O. Parry, R. Evans, and K. Binder, Phys. Rev. B **43**, 11 535 (1991), have reanalyzed the original data of Ref. 9; G. Gompper, D. M. Kroll, and R. Lipowsky, *ibid.* **42**, 961 (1990), simulated the solid-on-solid limit of the Ising model. Both works seem to suggest $\omega \simeq 0.25$ for the Ising model: see below.

[11](a) M. E. Fisher and H. Wen, Phys. Rev. Lett. **68**, 3654 (1992), show that the original estimate of the interfacial parameter $\omega(T)$ in Ref. 9(a) should be reduced by a factor of approximately 2 to $\omega(T) > 0.6$ for the temperatures simulated. The *true* correlation length must be used for ξ_β instead of the commonly quoted second moment correlation length; (b) R. Evans, D. C. Hoyle, and A. O. Parry, Phys. Rev. A **45**, 3823 (1992), have independently reached similar conclusions: see Refs. 3 and 4 for fuller discussions.

[12]The true correlation length specifies the leading exponential decay of the correlations and, hence, the decay of the order-parameter profile in the direction perpendicular to the wall. Its significance in the present context has been stressed recently: see discussions in Ref. 3 and Refs. 11.

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

[14]One might, heuristically, (i) note that the critical point-cum-fixed point corresponds to $l = \infty$, (ii) observe that $\tilde{\Sigma}(l)$ does not vanish when $l \to \infty$, and so (iii) argue that the variation $\Delta\tilde{\Sigma}$ cannot play a crucial role.

[15]D. B. Abraham, Phys. Rev. Lett. **44**, 1165 (1980); see also M. E. Fisher, Ref. 2 and J. Stat. Phys. **34**, 667 (1984) for reviews.

[16]H. B. Tarko and M. E. Fisher, Phys. Rev. B **11**, 1217 (1975); A. J. Liu and M. E. Fisher, Physica (Amsterdam) **156A**, 35 (1989).

[17]A. O. Parry and R. Evans, Mol. Phys. (to be published).