J. Halpin-Healy, Troisième Cycle de la Physique en Suisse Romande, 29 October 1992.
(+ 5 November)

3d CRITICAL WETTING

1. RELATED EXPERIMENTS
2. MEAN-FIELD THEORY ⇝ SEMI-INFINITE ISING MODEL

   ↓

   INTERFACE DISPLACEMENT MODEL

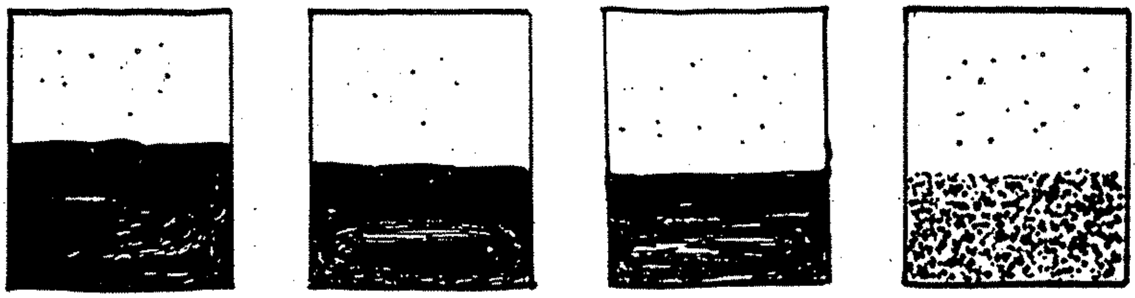
   ↓

   UCD = 3
3. NUMERICAL VERIFICATION OF CLASSICAL BEHAVIOR
   (BINDER, LANDAU + KROLL)
4. CAPILLARY WAVE FLUCTUATIONS -
   RENORMALIZATION OF 2d FIELD THEORIES
   MODELS I, II, III ⇝ NONUNIVERSAL CRITICALITY
5. GINZBURG CRITERIAN / CROSSOVER PHENOMENA
6. MONTE CARLO ⇝ INTERFACE (GOMPPER + KROLL)
7. EFFECTIVE EXPONENTS ~ APPROACH TO ASYMPTOPIA.
8. → FUNCTIONAL RENORMALIZATION GROUP

EXPT: SCHMIDT + MOLDOVER (1983) ⟶ PERFLUOROMETHYLCYCLOHEXANE / ISOPROPANOL BINARY MIXTURE

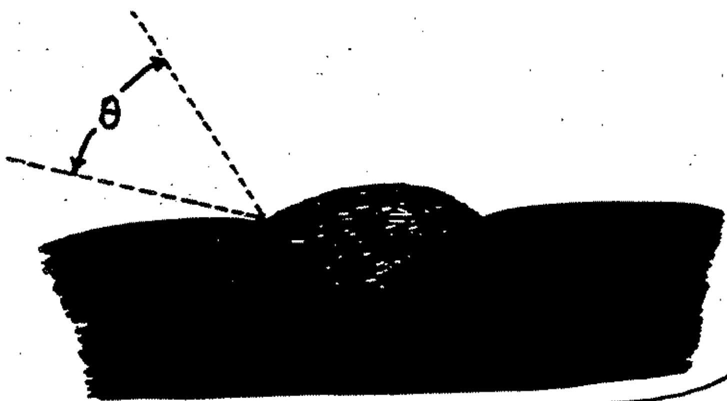
see also O'D. Kwon, PRL 48, 185 (1982).

CONTACT ANGLE MEASUREMENT



$T \ll T_W$ $T \lesssim T_W$ $T_W < T < T_c$ $T > T_c$

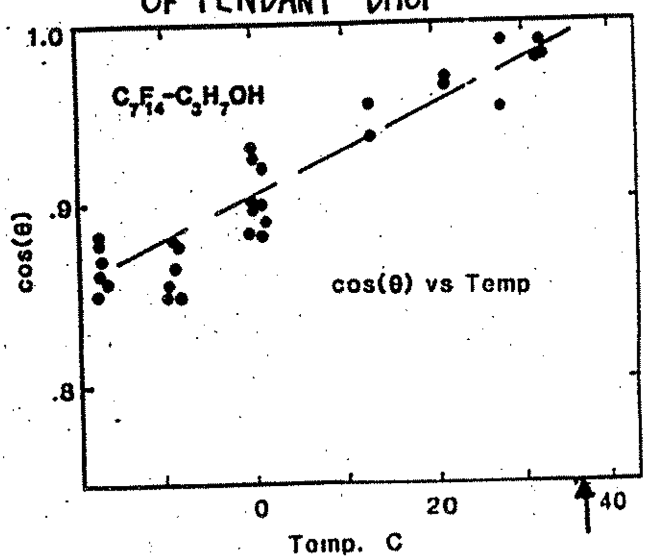
"PARTIAL WETTING"   "COMPLETE WETTING"   "MISCIBLE"



repeat expt without pendant drop

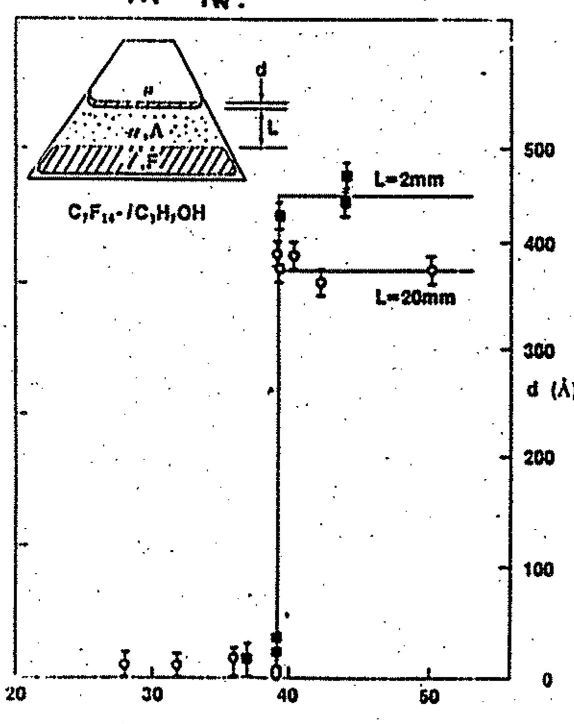
* INTERFACIAL PHASE TRANSITION INDICATED BY ⟶ VANISHING CONTACT ∡ OF PENDANT DROP

** ELLIPSOMETRY ⇒ SUDDEN APPEARANCE OF INTRUDING LAYER AT T_W.



$T_W = 38.0 \pm 0.1\ °C$

$T_c = 90.5 \pm 0.5\ °C$



$T \approx T_W$

i) THERMAL UNBINDING OF LIQUID-LIQUID INTERFACE

ii) THIN FILM - THICK FILM TRANSITION

iii) INTERFACE DELOCALIZATION

* CRITICAL WETTING ~ MEAN-FIELD THEORY

Motivated by thermally-driven wetting transitions observed in binary fluid mixtures near the consolute temperature, we examine interfacial critical phenomena within the context of a "SEMI-INFINITE" ISING MODEL with various surface terms. Our immediate goals are three-fold:

i) determination of MFT exponents
ii) ascertain upper critical dimension (UCD) of model, above which the MFT treatment is valid
iii) derivation of an effective "INTERFACE DISPLACEMENT" MODEL which allows us to concentrate entirely on the interface degrees of freedom & relieve ourselves of all excess baggage associated with the original Ising magnet formulation. Fruit of our labors = MF localization potential for the interface, appropriate for systems where underlying forces are SHORT-RANGED.

→ the classic reference for this material is

E. Brézin, B. Halperin, & S. Leibler, J. Physique 44, 775 (1983).

OK, off we go ~~> our starting point is the Landau Hamiltonian:

"OLD" NEWS

"NEW" NEWS

$$A = \int_{\substack{\text{BULK}\\ z>0}} d^d x \left\{ \frac{1}{2}(\nabla\varphi)^2 - \frac{\tau}{2}\varphi^2 + \frac{g}{4!}\varphi^4 \right\} + \int_{\substack{\text{SURFACE}\\ z=0}} d^{d-1}\rho \left\{ \frac{1}{2}c\varphi^2 - h_1\varphi \right\}$$

$\tau = \dfrac{T_c - T}{T_c}$ ← T_c = BULK CURIE TEMP

c: "SURFACE TEMPERATURE" (spins along edge have fewer neighbors ⟹ disorder sooner)

h_1: SURFACE "MAGNETIC FIELD" (acts only on spins in the surface)

with BOUNDARY CONDITION:

$$\varphi(z=\infty) = -M = -\sqrt{\frac{6\tau}{g}}$$ ← SPINS DOWN DEEP IN THE BULK.....

$$\frac{\delta A}{\delta \varphi} = 0 \Rightarrow \text{EQUATIONS OF MOTION}$$

$$-\nabla^2\varphi - r\varphi + \frac{g}{6}\varphi^3 = 0 \quad \text{AND} \quad \left.\frac{\partial \varphi}{\partial z}\right|_{z=0} = c\varphi - h_1$$

(in the bulk!) (at the surface)

At the MF level, we follow the tried & true strategy of searching for a FLUCTUATIONLESS solution $\varphi_c(z)$:

$$\frac{d^2\varphi_c}{dz^2} = -r\varphi_c + \frac{g}{6}\varphi_c^3$$

A "first integral" of the equations of motion permits us to write

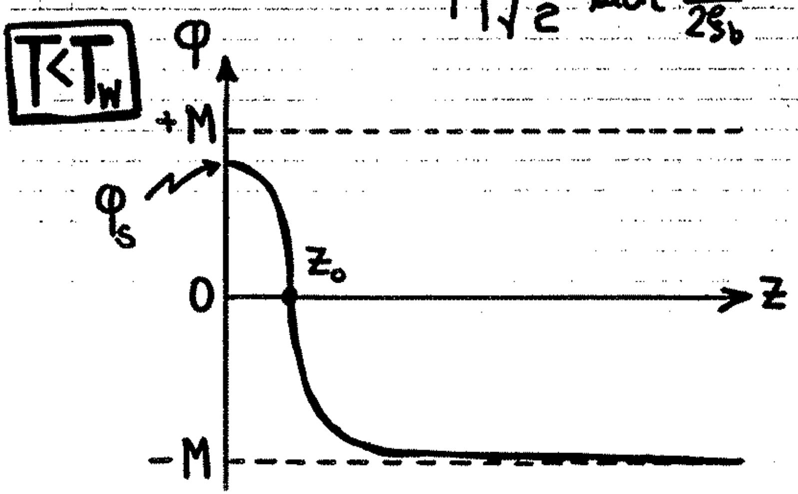
$$\left(\frac{d\varphi_c}{dz}\right)^2 = \frac{g}{12}\left(\varphi_c^2 - M^2\right)^2$$

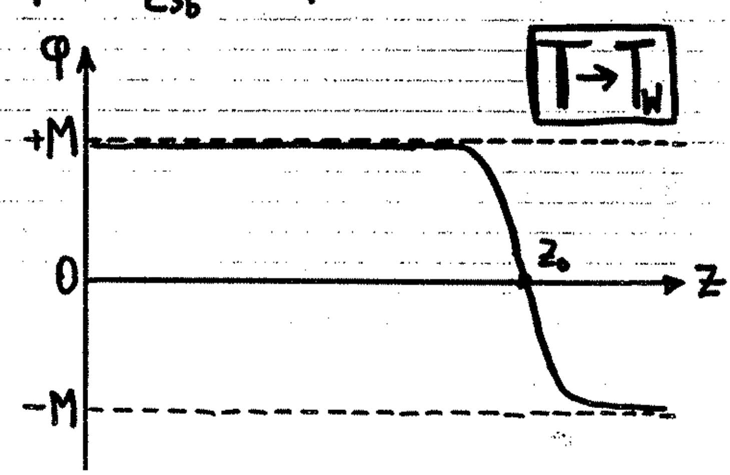
where we've made use of the BC as $z \to \infty$. The solution to this equation is the well known SOLITON/KINK:

$$\boxed{\varphi_c(z) = -M \tanh\left[(z - z_0)/2\xi_b\right]}$$

Note that the bulk correlation length $\xi_b = 1/\sqrt{2r}$ has been substituted, providing us, in a very natural way, with a MICROSCOPIC lengthscale. In an infinite system the domain wall, imposed by the BCs, could be anywhere (z_0 arbitrary, TRANSLATION SYMMETRY), but for the case at hand = SEMI-INFINITE ISING MODEL, z_0 is fixed by the BC at the surface (TRANSLATION SYMMETRY BROKEN):

$$-M\sqrt{\frac{r}{2}}\,\mathrm{sech}^2\frac{z_0}{2\xi_b} = cM\,\mathrm{th}\frac{z_0}{2\xi_b} - h_1$$





Now as the "WETTING TRANSITION" is approached ($T \to T_W$), the domain wall separating up and down spins is liberated ($z_0 \to \infty$, RESTORATION OF BROKEN TRANSLATIONAL SYMMETRY).

Note that $z_0 \to \infty$ implies sech$^2 \to 0$, th $\to 1$, so that $M \to \frac{h_1}{c}$. Indeed, this condition fixes the wetting transition temperature in terms of the phenomenological parameters of the semi-infinite Ising model:

$$M\Big|_{T=T_W} = \sqrt{\frac{6\tau_W}{g}} = \frac{h_1}{c} \quad \Rightarrow \quad \boxed{\frac{T_W}{T_c} = 1 - \frac{g h_1^2}{6c^2}}$$

WETTING TEMPERATURE

If one takes the BC at the surface and expands the hyperbolic trig functions to leading order in e^{-z_0/ξ_b}, dropping higher terms, it is straightforward to show that the mean interface position diverges LOGARITHMICALLY:

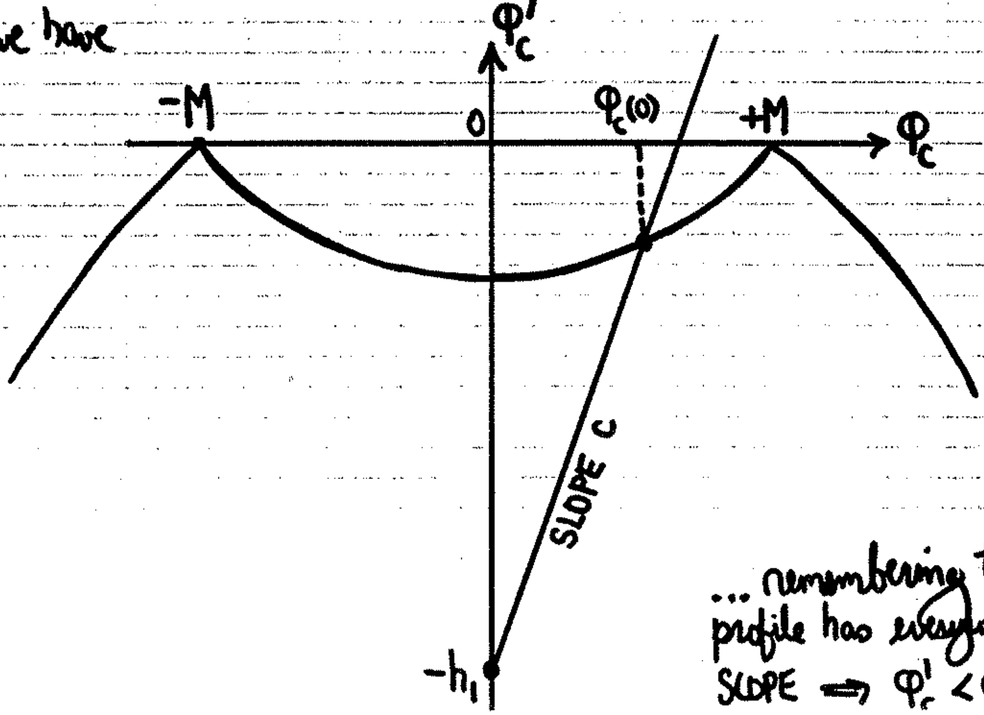
$$\boxed{z_0 \sim \xi_b \ln\left(\frac{1}{T_W - T}\right)}$$

INTERFACE LIBERATED

AN ASIDE - actually, the model is quite rich $\Rightarrow$ phase diagram possesses TRICRITICAL PT separating continuous (which we've been discussing) and 1$^{\text{ST}}$ order wetting transitions.
To understand the mechanism, recall the "first integral" and BC:

$$(\varphi_c')^2 = \frac{g}{12}(\varphi^2 - M^2)^2 \qquad \varphi_c' = c\varphi_c - h_1$$

graphically, we have



... remembering that the magnetization profile has everywhere a NEGATIVE SLOPE $\Rightarrow$ $\varphi_c' < 0$

From this vantage point, we see there are 2 distinct ways to incur the transition –

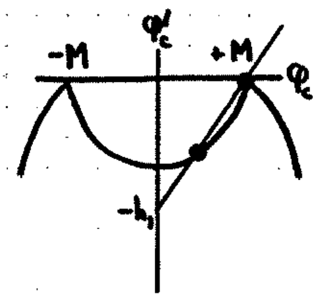
FIELD-DRIVEN WETTING: T fixed, $h_1 \uparrow \rightsquigarrow h_{1c} = cM$

** THERMALLY-DRIVEN WETTING: h_1 fixed, $T \uparrow$, $M \to 0$

intercept $(0 = cM_w - h_1) \Rightarrow$

$$\tau_w = 1 - \frac{T_w}{T_c} = \frac{g h_1^2}{6c^2}$$

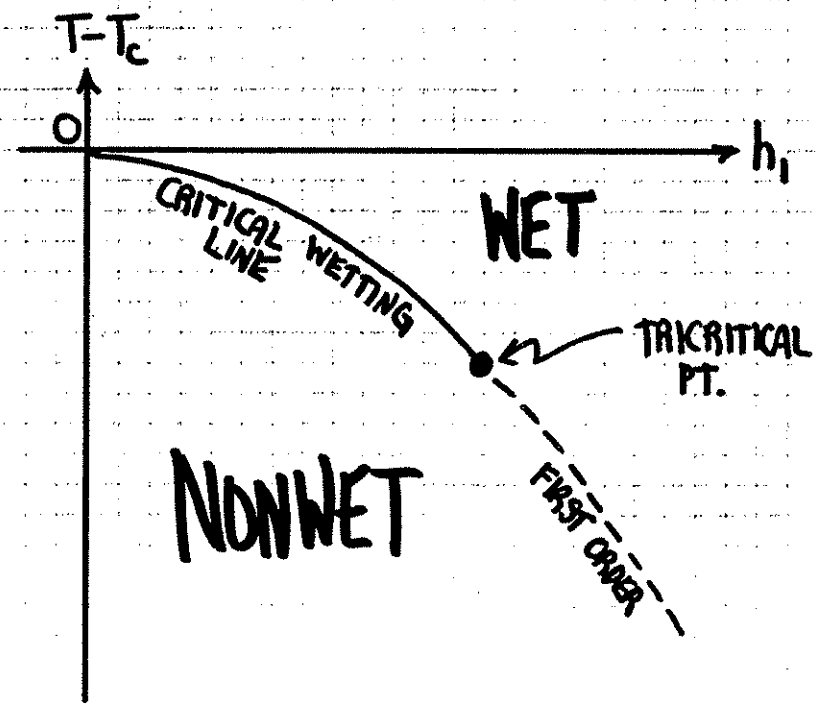
as above. However, one needs to take care because if c is too small it happens that the thickness of the wetting layer will jump **DISCONTINUOUSLY**, signature of a 1st order wetting transition $\rightsquigarrow$



To have a continuous transition it is necessary that the slope of the straight line $\varphi' = c\varphi - h_1$ exceed the slope of the parabolic arc $\varphi' = \sqrt{\frac{g}{12}}\,(\varphi^2 - M^2)$ at $\varphi(0) = M_\omega$

$$\Rightarrow \quad c > \sqrt{\frac{g}{12}}\cdot 2M_\omega = \sqrt{\frac{g}{3}}\sqrt{\frac{6\tau_\omega}{g}} = \sqrt{2\tau_\omega}$$

With this last bit of information, as well as our result from above for τ_ω, we can sketch the **PHASE DIAGRAM** in the h_1-T plane:



$\rightsquigarrow$ from this point on, we will concentrate only on CRITICAL WETTING

→ Let us now calculate the SPECIFIC HEAT EXPONENT that follows from this MFT of critical wetting. To do so, we need to isolate the "singular part of the free energy". In the present context, it is apparent that this quantity is nothing other than the BINDING ENERGY of the (still flat - remember we haven't allowed any fluctuations yet!) interface to the bounding wall/edge. In other words, we need to consider the energy difference between bound and unbound interfaces - Returning to our Landau Hamiltonian, we find

$$\delta\sigma \equiv \frac{A[\varphi_c]-A[M]}{L^{d-1}} = -\frac{1}{3}\sqrt{\frac{g}{12}}\left(\varphi_s^3-3M^2\varphi_s+2M^3\right) + \frac{1}{2}c\left(\varphi_s^2-M^2\right)-h_1\left(\varphi_s-M\right)$$

where $\varphi_s = M\,\mathrm{th}\,\frac{z_0}{2\xi_b}$ ← "MAGNETIZATION AT WALL"

Near the critical wetting transition, $\varphi_s \to M$. One can show, with some tedious algebra, that this "EXCESS SURFACE TENSION" vanishing quadratically

$$\delta\sigma \sim -(T_W-T)^2 \Rightarrow \alpha_{MF}=0$$ SPECIFIC HEAT EXPONENT

We are now in a position to derive the effective theory alluded to earlier -

INTERFACE DISPLACEMENT MODEL

A moment's reflection reveals that the essential physics of the wetting transition is tied up with the liberation of the up-down interface at T_W. As mentioned previously, one would like to dispense with the unnecessary, excess baggage associated with the semi-infinite Ising model picture, and concentrate on the statistical mechanics of the interface as it becomes depinned. Near the transition, the functional form of this pinning potential is easily determined - one simply expands

$$\varphi_s(z_0) = M\,\mathrm{th}\,\frac{z_0}{2\xi_b} \approx M\left(1-2e^{-z_0/\xi_b}\right)$$

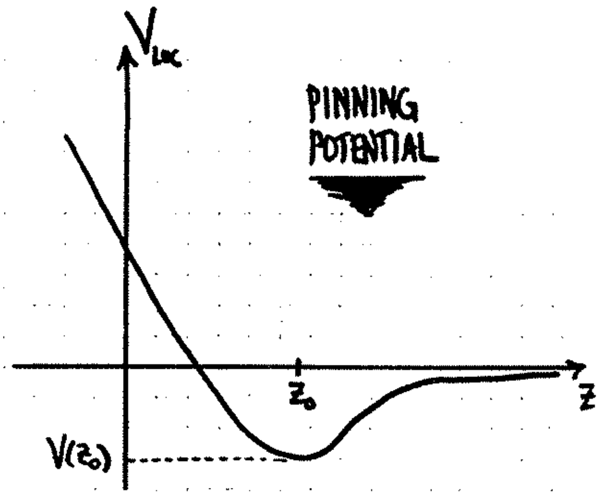
which implies that, when the interface is far from the wall (z_0 large), the BINDING ENERGY can be written asymptotically as

$$\delta\sigma(z_0) = -a e^{-z_0/\xi_b} + b e^{-2z_0/\xi_b} + \ldots..$$

where $a \sim (cM - h_1) \sim (T_W - T)$ and $b > 0$. In this fashion, one obtains a pinning potential

$$V_{loc}(z) = -a e^{-\alpha z} + b e^{-2\alpha z} \qquad \alpha = 1/\xi_b$$

that is the sum of attractive and repulsive exponentials. The position of the interface is given at the MF level by the MINIMUM of the potential. At the wetting transition, $a = 0$ $\Rightarrow$ the attractive piece vanishes, the repulsive part remains and the interface is liberated ($z_0 \to \infty$). The economy of this formulation is immediately apparent – knowledge of the pinning potential V gives easy access to the MF behavior



$$V'(z_0) = 0 \implies z_0 \sim \ln 1/a$$

$$V(z_0) = -\frac{a^2}{2b} \implies \text{SPECIFIC HEAT EXPONENT} \quad \alpha = 0$$

$$\xi_{\parallel}^{-2} = V''(z_0) \implies \frac{\alpha^2 a^2}{2b} \implies \text{CORRELATION LENGTH EXPONENT} \quad \nu_{\parallel} = 1$$

The first two results confirm earlier findings, while the last is new. It is the exponent characterizing the decay of correlations WITHIN the interface; i.e., PARALLEL TO THE WALL. The critical behavior of the interfacial correlation length $\xi_{\parallel}$ is quite distinct from that of the bulk correlation length ξ_b. The former diverges at T_W, the latter at T_c. Moreover, the interface index $\nu_{\parallel} = 1$ suggests that the UPPER CRITICAL DIMENSION of the wetting problem is three. This follows from the hyperscaling relation relevant for a $(d-1)$ dimensional interface, $2 - \alpha = \nu_{\parallel} d_{\parallel}$, in light of the above MF exponents. The analogous calculation for the BULK Ising problem, with $\alpha = 0$ and $\nu = \frac{1}{2}$, gives $d_c = 4$. Hence, we find ourselves in the rare situation (other examples include UNIAXIAL DIPOLAR FERROMAGNETS & ISING TRICRITICALITY) that for critical wetting phenomena, the real world of three bulk dimensions corresponds to a marginal dimension.

HYPERSCALING:

$$2 - \alpha = \nu_{\parallel}(d-1)$$

$$\Downarrow$$

$$d_c^{\text{WETTING}} = 3$$

** another route $\rightarrow \nu_{\parallel}$ for MF CRITICAL WETTING (using ISING MODEL)

One can derive the correlation length exponent directly within the semi-infinite Ising model context by considering gaussian fluctuations about the flat magnetization profile –

$$\varphi(z,\vec{\rho}) = \varphi_c(z) + \chi(z,\vec{\rho}) \qquad \text{BC at wall} \Rightarrow \frac{\partial \chi}{\partial z}(z,\vec{\rho})\Big|_{z=0^+} - c\,\chi(0,\vec{\rho}) = 0$$

The action to $\mathcal{O}(\chi^2)$ reads

$$A = A_c + \frac{1}{2}\int \chi(z_1,\vec{\rho}_1)\, A^{(2)}(z_1,z_2;\vec{\rho}_1-\vec{\rho}_2)\,\chi(z_2,\vec{\rho}_2)$$

where

$$A^{(2)} = \frac{\delta^2 A}{\delta\varphi\,\delta\varphi} = \delta(z_1-z_2)\,\delta^{d-1}(\vec{\rho}_1-\vec{\rho}_2)\left[-\frac{\partial^2}{\partial z_1^2} - \nabla_{\parallel}^2 - \frac{3\tau}{\cosh^2\sqrt{\frac{\tau}{2}}(z-z_0)} + 2\tau\right]$$

Our interest, of course is in the MF correlation function

$$G(x_1,x_2) = \langle \varphi(x_1)\varphi(x_2)\rangle - \langle\varphi(x_1)\rangle\langle\varphi(x_2)\rangle = \left[A^{(2)}\right]^{-1}$$

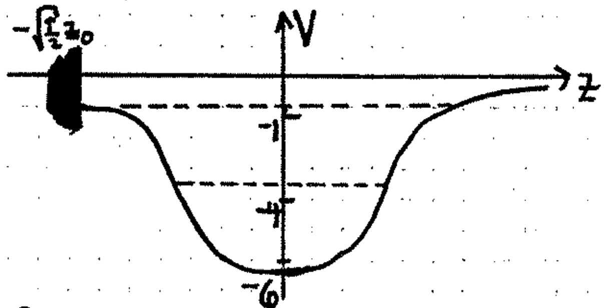
Best to Fourier transform parallel coords & look for eigenmodes of the operator $A^{(2)}$:

$$\left[-\frac{d^2}{dz^2} - \frac{3\tau}{\cosh^2\sqrt{\frac{\tau}{2}}(z-z_0)} + q_{\parallel}^2 + 2\tau\right]\psi_n(z) = \varepsilon_n(q)\,\psi_n(z)$$

Change of variables, $y = \sqrt{\frac{\tau}{2}}(z-z_0)$, with substitution $\varepsilon_n(q) = q_{\parallel}^2 + 2\tau\left(1-\frac{K_n^2}{4}\right)$, implies

$$\text{Schrodinger eq} \Rightarrow \left(-\frac{d^2}{dy^2} - \frac{6}{\cosh^2 y}\right)\psi_n = -K_n^2\psi_n$$

$$\text{BC} \Longrightarrow \left(c\psi_n - \sqrt{\frac{\tau}{2}}\frac{d\psi_n}{dy}\right)\Big|_{y_0=-\sqrt{\frac{\tau}{2}}z_0} = 0$$



In the limit $z_0\to\infty$, the TWO BOUND STATES ARE $K_0\approx 2$, $K_1\approx 1$, so that

$$\varepsilon_0(q_{\parallel}) \xrightarrow[T]{T_W} q_{\parallel}^2 + \frac{3}{2}\frac{c^2}{c^2-2\tau_W}\frac{1}{\left(1-\frac{T_W}{T_c}\right)}\left(\frac{T_W-T}{T_c}\right)^2$$

Need to be far from tricritical pt ($c^2 > 2\tau_W$) and away from Curie temp. LONG-RANGE CORRELATIONS induced by this $n=0$ mode for $q_{\parallel}$ small and $T\to T_W$.

$$G(z,z';q_{\parallel}) \approx \frac{\psi_0(z)\psi_0(z')}{\varepsilon_0(q_{\parallel})} \Longrightarrow \langle\varphi(z,\vec{\rho}_1)\varphi(z',\vec{\rho}_2)\rangle_{\text{CONN}} \approx \psi_0(z)\psi_0(z')\,\frac{e^{-\rho(T_W-T)}}{\rho^{(d-2)/2}}$$

* NUMERICAL VERIFICATION OF CLASSICAL BEHAVOR

Before moving on to the very important question of fluctuation effects in 3d critical wetting, we pause here to discuss some very nice Monte Carlo simulations that confirm, entirely, the MF picture. The standard references are

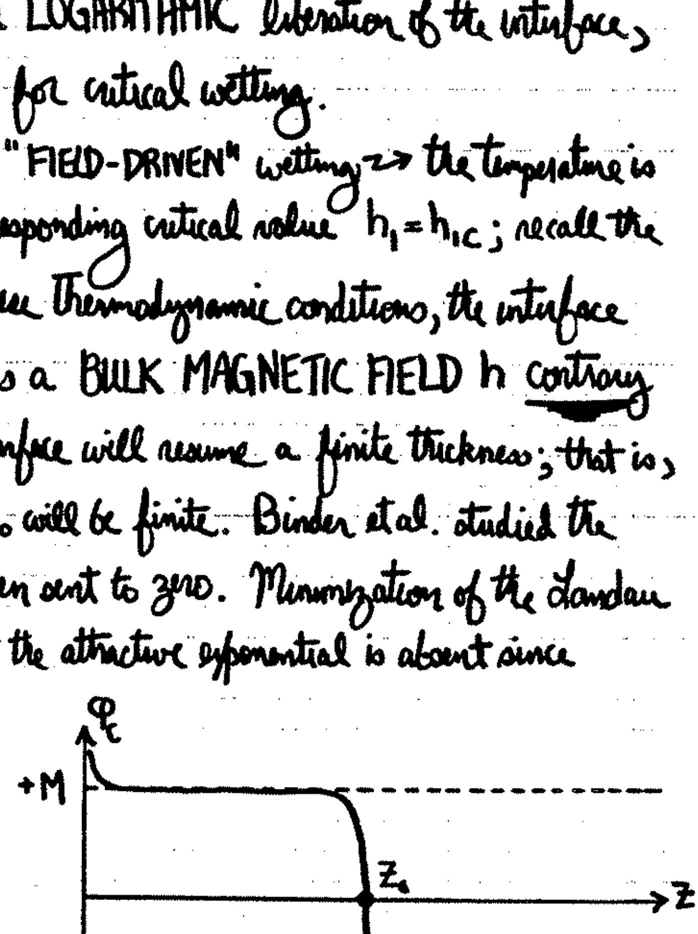
- K. Binder, D.P. Landau, & D.M. Kroll, PRL 56, 2272 (1986).
- K. Binder & D.P. Landau, Phys. Rev. B37, 1745 (1988).

The predominance of discontinuous wetting transitions in binary fluid mixtures, due to the presence of long-range van der Waals forces, has rendered moot for the most part the issue of experimental determination of wetting exponents in traditional systems. Nonetheless, numerical simulations, inspired by the marginal dimensionality of the problem, have recently studied in detail the wetting transitions exhibited by the discrete, semi-infinite short-range Ising model. Most pertinent is the work of Binder, Landau & Kroll, who established the LOGARITHMIC liberation of the interface, in addition to the correlation length exponent $\nu_{\parallel} = 1$ for critical wetting.

Their Monte Carlo simulations examined so-called "FIELD-DRIVEN" wetting $\Rightarrow$ the temperature is fixed and the surface magnetic field is set at the corresponding critical value $h_1 = h_{1c}$; recall the CRITICAL WETTING LINE in the $h_1 T$ plane. Under these thermodynamic conditions, the interface would be depinned ($z_0 = \infty$). However, if one imposes a BULK MAGNETIC FIELD h contrary to that at the surface, the layer of spins wetting the surface will resume a finite thickness; that is, the interface will be pushed back towards the wall and z_0 will be finite. Binder et al. studied the singularities of critical wetting as the bulk field h was then sent to zero. Minimization of the Landau hamiltonian appropriate to field-driven wetting (note that the attractive exponential is absent since $h_1 = h_{1c} \Rightarrow a = 0$),

$$V(z) = -\cancel{a e^{-\alpha z}} + b e^{-2\alpha z} + hz$$

$$V'(z_0) = 0 \;\Rightarrow\; \boxed{z_0 \sim \ln 1/h}$$



reveals the anticipated MF behavior, characterized by a LOGARITHMICALLY DIVERGENT interface position. Below, we show the numerical data of Binder et al which corroborate this theoretical result.

The convincing linearity of the plot, for a variety of lattice sizes, suggests that the behavior is indeed logarithmic for dimensionless fields $h = H/J$ as small as 10^{-3}.

To extract the interface correlation length exponent $\nu_{\parallel}$, Binder et al studied two separate thermodynamic quantities –

i) SURFACE SUSCEPTIBILITY $\chi_1 = \frac{\partial m_1}{\partial h}$ ← measures the response of the surface magnetization m_1 to changes of the bulk field h

ii) EXCESS MAGNETIZATION $\Delta m_1(h) = m_1(h) - m_1(0)$ ← difference between the surface magnetization in the presence & absence of h.

Consideration of phenomenological scaling laws for the singular part of the surface free energy suggests that

$$f_s(a,h) = a^{2\nu_{\parallel}} F(h a^{-2\nu_{\parallel}})$$

where we've invoked interface hyperscaling to write $2-\alpha = d_{\parallel}\nu_{\parallel} = 2\nu_{\parallel}$ and fixed the argument of F by using the fact that we expect f_s LINEAR in h for vanishing a. As above, $a = h_1 - h_{1c}$. Calculation of the resulting scaling form for the surface susceptibility is straightforward –

$$\chi_1(h) = \lim_{a \to 0} \frac{\partial^2 f_s}{\partial h \partial h_1} = \lim_{a \to 0} a^{-1} F'(h a^{-2\nu_{\parallel}}) \sim h^{-\frac{1}{2\nu_{\parallel}}}$$

With the MF exponent $\nu_{\parallel} = 1$, one therefore expects the surface susceptibility to diverge as $\chi_1 \sim h^{-1/2}$ as the bulk field vanishes. Likewise,

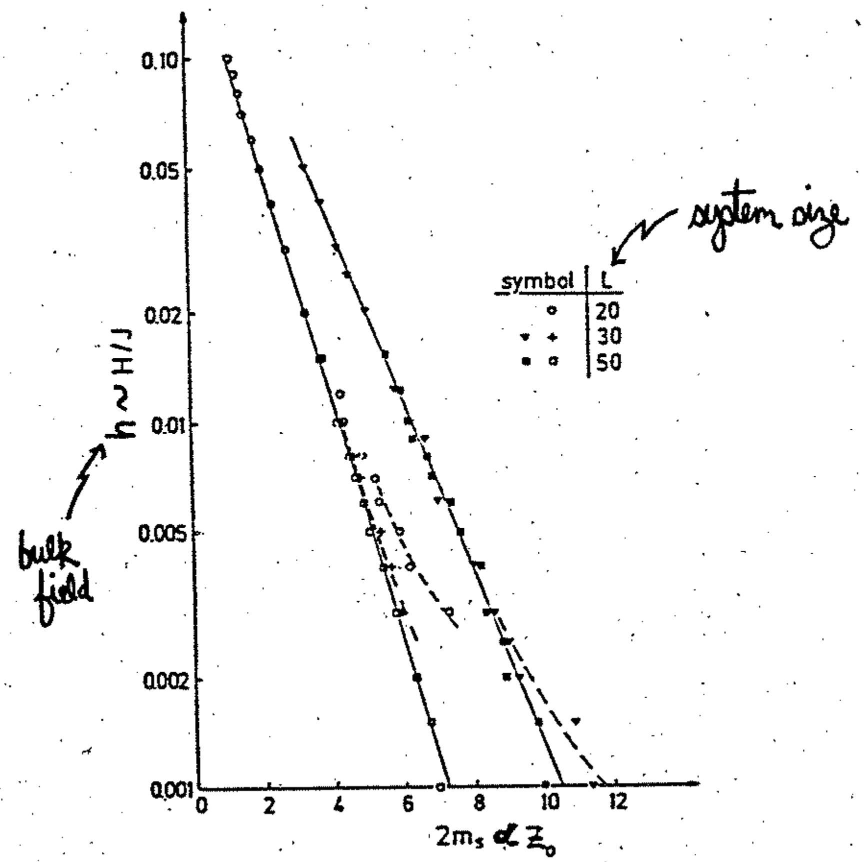
$$\Delta m_1(h) = \int_0^h \chi_1(h)\, dh \sim h^{1-\frac{1}{2\nu_{\parallel}}}$$

so the excess magnetization ought to go to zero as $\Delta m_1 \sim h^{1/2}$. Phenomenology notwithstanding, a complete, more firm theoretical justification of these scaling laws employed to extract $\nu_{\parallel}$ from the numerical data can be made [see Brézin & Halpin-Healy, J. Physique 48, 757 (1987)].
In any case, the Monte Carlo work of Binder, Landau, & Kroll found precisely these classical behaviors for χ_1 and Δm_1, providing a startling confirmation of the MFT of critical wetting.

Monte Carlo data – Binder, Landau & Kroll, PRL 56, 2272 (1986)

LOGARITHMIC DIVERGENCE OF MEAN INTERFACE POSITION:

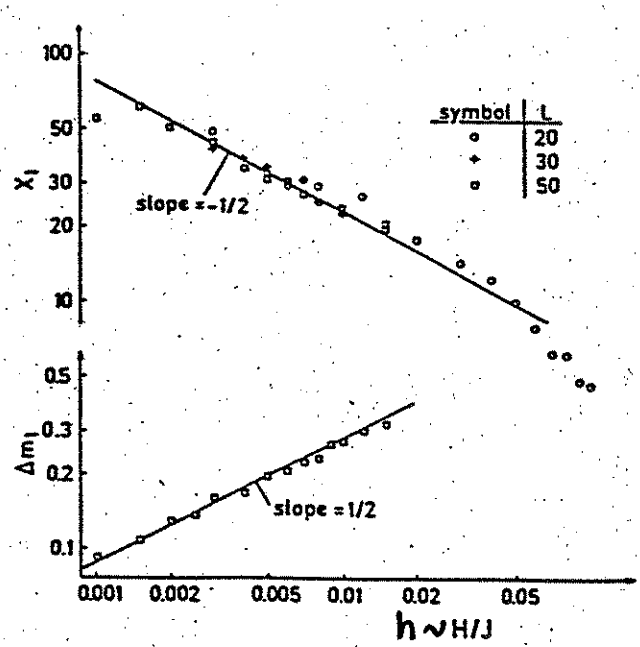
$Z_0 \sim \ln \frac{1}{h}$



SURFACE SUSCEPTIBILITY & EXCESS MAGNETIZATION:

$\chi_1 \sim h^{-1/2}$

$\Delta m_1 \sim h^{1/2}$



* 3d – THE ROLE OF CAPILLARY WAVE FLUCTUATIONS

reference → E. Brézin, B. Halperin, & S. Leibler, PRL 50, 1387 (1983) ← "BHL"

Our discussion thus far of critical wetting has been strictly at the MF level, with no explicit mention, whatsoever, of fluctuations about the planar configuration of the interface. However, like all critical phenomena, the wetting transition can be viewed as the restoration of a broken symmetry. For $T<T_W$, a finite value of z_0 – that is, an interface pinned to the wall – represents a breaking of translational symmetry that gives rise to gapless Goldstone modes. For the wetting problem, these Goldstone modes are just the familiar capillary wave fluctuations about a flat interface. Above T_W, the interface is liberated and the symmetry is restored. In the interest of determining what are the fluctuation-induced corrections to MFT in $d_c = 3$, BHL considered an action of the form –

MODEL I (details later)

$$\mathcal{A} = \int d^2\rho \left\{ \frac{1}{2}(\nabla z)^2 + V^{I}_{loc}(z) \right\}$$

where the gradient term discourages deviations from planar (the units are such that the SURFACE TENSION satisfies $\frac{\sigma}{k_B T} = 1$) and

$$V^{I}_{loc}(z) = -a e^{-\alpha z} + b e^{-2\alpha z} \qquad \alpha = 1/\xi_b$$

is the pinning potential derived earlier within the context of the semi-infinite Ising model. Capillary wave fluctuations induce RENORMALIZATIONS of the coefficents a and b. These renormalizations are, in fact, known exactly for this 2d field theory, provided one neglects the restriction $z>0$ imposed by the presence of the wall. BHL used this knowledge to write down an effective potential

$$V_\xi(z) = -a\,\xi^{\frac{\alpha^2}{4\pi}} e^{-\alpha z} + b\,\xi^{\frac{\alpha^2}{\pi}} e^{-2\alpha z}$$

obtained by integrating out large wavenumber fluctuations on length scales shorter than ξ. Setting $V'_\xi(z_0)=0$, $\xi^{-2} = V''_\xi(z_0)$ and solving for the thermal behavior of the interfacial correlation length produced the surprising result that the associated exponent was NONUNIVERSAL:

$$\xi \sim a^{-\nu} \quad \text{with} \quad \nu = \frac{1}{1-\frac{\alpha^2}{4\pi}}$$

though the mean interface position diverged logarithmically

$$\alpha z_0 = \left(1 + \frac{\alpha^2}{2\pi}\right) \ln \xi$$

as before. A worry soon presented itself to BHL, however, who realized that as the interface became liberated, its thickness δ, due to wandering, also diverged, though somewhat more slowly than z_0. A simple calculation permitted them to show that, in a first approximation, $\delta^2 \approx \frac{1}{2\pi} \ln \xi$. Nevertheless, they feared that interfacial collisions with the wall might invalidate their field theoretic approach. To check that their renormalization procedure was self-consistent, despite the presence of the wall, they proposed a straightforward, physically appealing test — convolute the potential with a gaussian of width δ:

$$V(z) \longrightarrow \tilde{V}(z) = \int_0^\infty dz'\, V(z')\, \frac{e^{-(z-z')^2/2\delta^2}}{\sqrt{2\pi\delta^2}}$$

to see if the rare (remember — the interface is being liberated!) collisions with the wall were relevant or not. For exponential interactions, they found

$n=1,2$

$$e^{-n\alpha z} \longrightarrow e^{-n\alpha z}\, \underbrace{e^{n^2\alpha^2\delta^2/2}}_{=\,\xi^{\frac{n^2\alpha^2}{4\pi}}} \int_{n\alpha\delta^2 - z_0}^{\infty} ds\, \frac{e^{-s^2/2\delta^2}}{\sqrt{2\pi\delta^2}}$$

just the "MULTIPLICATIVE" RENORMALIZATION from before...

The important point, of course, is the lower limit of this integral, which can be rewritten

$$\frac{1}{\alpha}\left[(n-1)\frac{\alpha^2}{2\pi} - 1\right] \ln \xi$$

For collisions with the wall to be IRRELEVANT — that is, to leave unaltered the simple multiplicative renormalizations of the exponentials in our interfacial pinning potential, this quantity must go to $-\infty$ in the scaling limit. For $n=2$, this necessitates $\frac{\alpha^2}{4\pi} < \frac{1}{2}$. Returning to physical units, we note that

$$\frac{\alpha^2}{4\pi} = \frac{k_B T}{4\pi \xi_b^2 \sigma} \equiv \omega \leftarrow \text{STIFFNESS PARAMETER}$$

serves as a dimensionless measure of the "stiffness" of the interface, so that for sufficiently stiff interfaces ($\omega < \frac{1}{2}$), collisions with the wall are irrelevant and the correlation length exponent is $\nu^{I} = 1/(1-\omega)$. By contrast, for $\omega > \frac{1}{2}$, the ad hoc convolution procedure of BHL indicated that renormalization of the repulsive exponential was dramatically affected by such collisions. They argued that the physics of these important collisions could be captured by replacing the repulsive exponential with a short-ranged, gaussian centered at the wall, giving rise to MODEL II potential:

$\frac{1}{2} < \omega < 2$:

$$V_{II}(z) = -a e^{-\alpha z} + \frac{c}{\delta_0} e^{-z^2/2\delta_0^2}$$

The repulsive gaussian was chosen for technical convenience since 2d field theory $\Rightarrow$ renormalization of a gaussian leads to a gaussian with a rescaled width $\delta^2(\lambda) = \delta_0^2 - \frac{1}{2\pi}\ln\lambda$. Following the same method as for MODEL I, one finds $z_0 = \sqrt{\frac{2}{\pi}}\ln\xi$ where

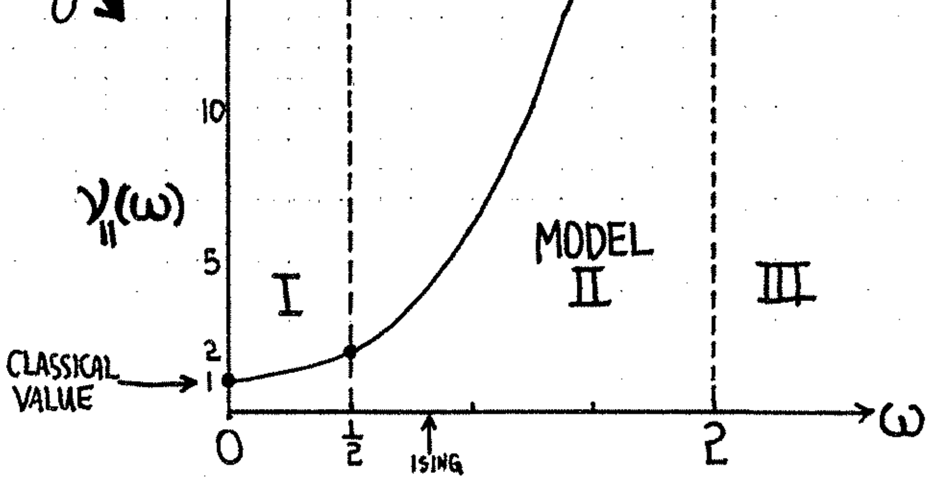
$$\xi \sim a^{-\nu}\left(\ln\frac{1}{a}\right)^{-\nu\sqrt{\frac{\omega}{8}}} \quad \underline{\text{with}} \quad \nu^{II} = \frac{1}{(\sqrt{2}-\sqrt{\omega})^2}$$

a check reveals, however, that simple multiplicative renormalization of the attractive exponential remains consistent only for $\omega < 2$.

$\omega > 2$: MODEL III $\rightarrow$ DOUBLE GAUSSIAN POTENTIAL $\rightarrow \xi \sim \exp\left(\frac{c}{\tau}\ln\frac{1}{\tau}\right) \Rightarrow \nu^{III} = \infty$

(for these very supple interfaces, the correlation length diverges exponentially!)

In summary, BHL discovered three distinct types of nonuniversal asymptotic wetting criticality ↘



"NONUNIVERSAL" CORRELATION LENGTH EXPONENT 3d CRITICAL WETTING

nb $\omega(\text{3d Ising}) \approx 0.8$

* 3d CRITICAL WETTING – GINZBURG CRITERION

reference → J. Halpin-Healy & E. Brézin, PRL 58, 1220 (1987). ← attached

For the 3d Ising model, it is known that the interfacial stiffness parameter is very nearly temperature independent and has the value $\omega \approx 0.8$ [see Moldover, Phys. Rev. A 31, 1022 (1985) for expt'l results; Brézin & Feng, Phys. Rev. B 29, 472 (1984) for related theoretical work], so one expects a correlation length exponent $\nu_{\parallel} \approx 4$. Nevertheless, this scaling property may be observable only in the immediate vicinity of the wetting transition. How close must one be to see deviations from classical, MF type behavior $\nu_{\parallel} = 1$? This question is best addressed within the context of a Ginzburg criterion formulated for the critical wetting problem by the above authors. There, we integrate explicitly the gaussian capillary wave fluctuations about the MF solution to obtain the fluctuation correction to the classical action. The relevant quantity then becomes the effective action, which is the sum of the mean-field and fluctuation contributions. Derivatives of this effective action with respect to the appropriate thermodynamic fields yield the fluctuation correction to the critical quantity of interest. The Ginzburg criterion predicts that as the classical and fluctuation contributions become comparable, deviations from MF behavior can be expected. In this rough, order of magnitude fashion, the Ginzburg criterion fixes the crossover from classical criticality. Our results here suggest a possible explanation as to why Binder, Landau & Kroll observe only MF behavior, even for bulk fields as low as $h = 10^{-3}$. It is our feeling that they need somewhat smaller fields to be confident that they are truly in the critical regime. Worse still, one will need substantially smaller fields, $h \approx 10^{-10}$, with correspondingly greater system sizes to accommodate a diverging ξ, to see the NONUNIVERSAL exponent $\nu_{\parallel}(\omega \approx 0.8) \approx 4$ alluded to above.

Having given you the punchline, I sketch out in the next few pages, calculation of the Ginzburg criterion and the various crossovers –

First, we recall the MF results

$$V_{MF} = -ae^{-\alpha z} + be^{-2\alpha z}$$

$$\left.\begin{array}{lll} V'(z_0) = 0 & \Longrightarrow & e^{-\alpha z_0} = \dfrac{a}{2b} \\ \xi^{-2} = V''(z_0) & \Longrightarrow & \xi^{-2} = \dfrac{a^2\alpha^2}{2b} \end{array}\right\} \Longrightarrow \alpha z_0 = \ln \xi + \text{constant}$$

$$\Downarrow$$

$$\boxed{\frac{d\xi}{dz_0} = \alpha\xi}$$

To calculate the fluctuation correction to MFT, we need to determine the effective action to 1-loop order –

$$V_{eff}(z_0) = \underbrace{V(z_0)}_{\text{MFT}} + \underbrace{\tfrac{1}{2}\int\!\!\!\!\!\!\;\;\;\; k \ln\left(k^2 + V''(z_0)\right)}_{\text{FLUCTUATIONS}}$$

nb $\int_k \Rightarrow \int_0^{\Lambda} \frac{d^2k}{(2\pi)^2}$ — Λ: UV cutoff; 0: our interest is in the infrared behavior

taking two derivatives $\Rightarrow$

$$\xi_{eff}^{-2} = \xi^{-2} + \frac{1}{2}\frac{d^2}{dz_0^2}\int_k \ln\left(k^2 + V''(z_0)\right)$$

$$\frac{d\xi}{dz_0}\frac{d}{d\xi}\left(\frac{d\xi}{dz_0}\frac{d}{d\xi}\int_k \ln\left(k^2+\xi^{-2}\right)\right) = \alpha\xi\frac{d}{d\xi}\left(\alpha\xi\frac{d}{d\xi}\int_k \ln\left(k^2+\xi^{-2}\right)\right)$$

$$= 4\alpha^2\xi^{-2}\left[\int_k \frac{1}{k^2+\xi^{-2}} - \xi^{-2}\int_k \frac{1}{(k^2+\xi^{-2})^2}\right]$$

Which shows again, somewhat formally, that $d_c = 3$. Performing the integrals, remembering that $\alpha^2 = 4\pi\omega$, and setting the lattice cutoff equal to unity $(\Lambda \sim \frac{1}{a_0} \sim 1)$, we have

$$\xi_{eff}^{-2} = \xi^{-2}\Big[\underset{\text{MF}}{1} + \underbrace{2\omega\left\{\ln(1+\xi^2) + \frac{1}{1+\xi^2} - 1\right\}}_{\text{FLUCTUATION CORRECTION}}\Big]$$

we expect CROSSOVER from classical criticality when the MF and fluctuation contributions become comparable $\Rightarrow$

$$1 = 2\omega\left\{\ln(1+\xi^2) + \frac{1}{1+\xi^2} - 1\right\}$$

$\xi_{MF\to I}$

One can obtain similar results for the specific heat C, excess magnetization ΔM_1, and surface suscept χ_1.

If $\frac{1}{2}<\omega<2$, the asymptotic criticality will be that of MODEL II. One needs a more powerful formalism to pin down on what lengthscale this will happen, but a crude estimate can be made by considering the gaussian convolution used by Brezin, et.al –

CROSSOVER: MODEL I $\rightarrow$ MODEL II

Recall that MODEL II is characterized by non-trivial renormalization of the REPULSIVE exponential –

$$e^{-2\alpha z} \longrightarrow e^{-2\alpha z} \exp(2\alpha^2\delta^2) \int_{2\alpha\delta^2 - z}^{\infty} \frac{e^{-s^2/2\delta^2}}{\sqrt{2\pi\delta^2}}\, ds$$

where our attention was focused on the importance of the lower limit

$$2\alpha\delta^2 - z_0 = \frac{1}{\sqrt{4\pi\omega}}\left[2\omega - 1\right] \ln \xi$$

Of course when $\xi \to \infty$, one has achieved asymptotic criticality, but an approximate determination of the crossover I $\rightarrow$ II can be made by setting

$$\text{LOWER LIMIT} = -\delta = -\left(\frac{1}{2\pi} \ln \xi\right)^{\frac{1}{2}}$$

$\Longrightarrow$

CROSSOVER LENGTH-SCALE $\quad \xi_{\mathrm{I}\rightarrow\mathrm{II}} = \exp\left\{\frac{2\omega}{(2\omega-1)^2}\right\}$

For $\omega>2$, the system will eventually exhibit MODEL III criticality –

CROSSOVER: MODEL II $\rightarrow$ MODEL III

MODEL III arises because the ATTRACTIVE exponential is no longer simply multiplicatively renormalized:

$$e^{-\alpha z} \rightarrow e^{-\alpha z} \exp\left(\tfrac{1}{2}\alpha^2\delta^2\right) \int_{\alpha\delta^2 - z}^{\infty} \frac{e^{-s^2/2\delta^2}}{\sqrt{2\pi\delta^2}}\, ds$$

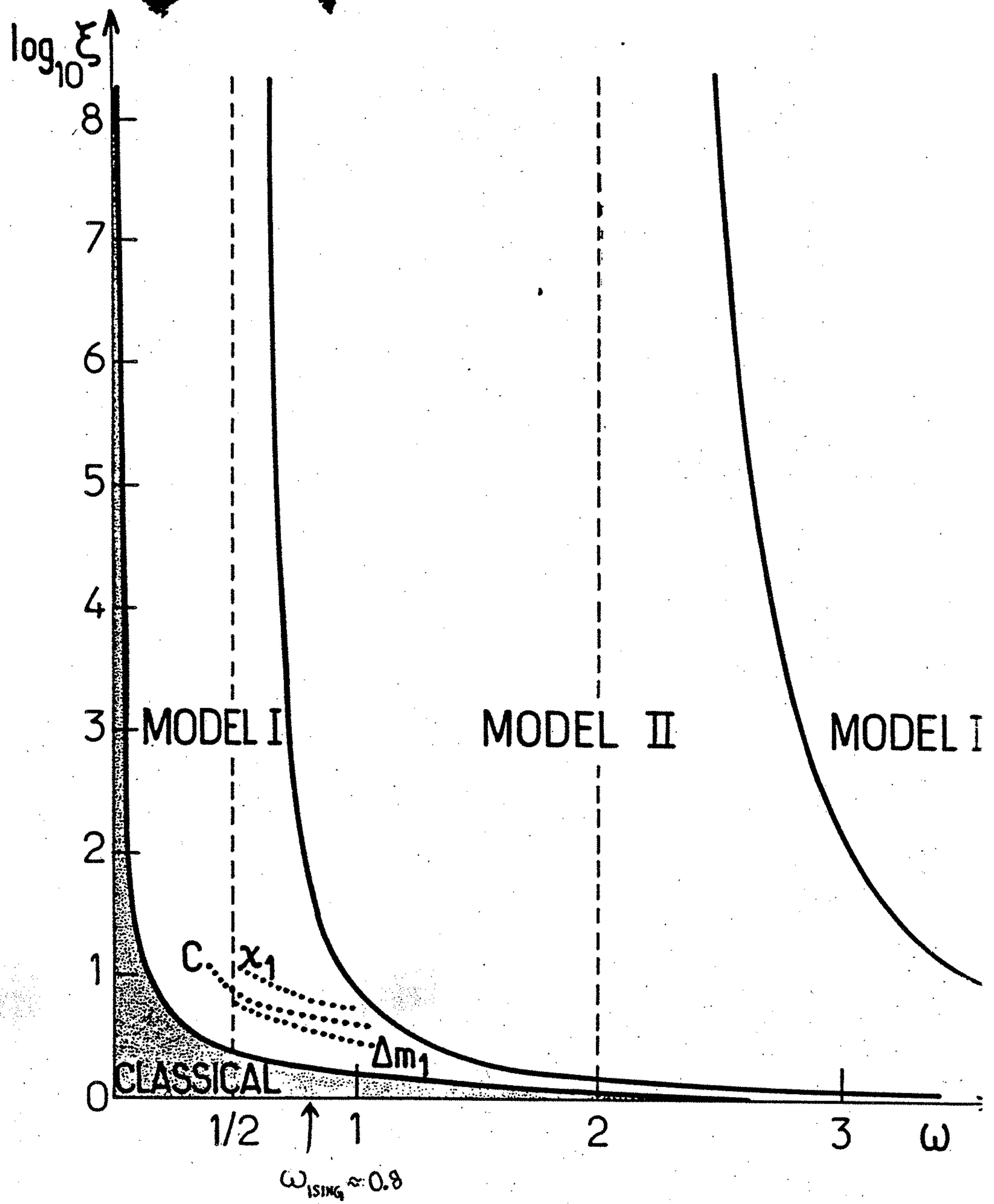
set lower limit: $\quad \alpha\delta^2 - z_0 = \frac{1}{\sqrt{\pi}}\left[\sqrt{\omega} - \sqrt{2}\right] \ln \xi = -\delta$

$\Longrightarrow$

ANOTHER CROSSOVER LENGTH-SCALE $\quad \xi_{\mathrm{II}\rightarrow\mathrm{III}} = \exp\left\{\frac{1}{(\sqrt{2\omega} - 2)^2}\right\}$

but things are a little bit more complicated ....

GINZBURG CRITERION



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Critical Wetting in Three Dimensions: A Ginzburg Criterion

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The crossover from mean-field to nonclassical (model I) criticality for 3D critical wetting with short-range forces is derived via an appropriately formulated Ginzburg criterion. Subsequent crossovers to models II and III are also discussed. Although the domain of classical behavior is found to be small, we suggest that recent numerical simulations have failed to venture outside this regime. Pure, asymptotic nonuniversal critical behavior may be inaccessible to presently available experimental systems.

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Below the consolute point T_c of a binary fluid mixture, a thin microscopic layer, perhaps a few angstroms thick, will coat the container because of its preferential adsorption by the walls. As the temperature is raised it may happen that the thickness of this adsorbed layer diverges, becoming a film of macroscopic size. In describing this transition, one can say that the interface between the two fluids has become liberated or delocalized from the wall. The temperature at which this occurs is known as the wetting transition temperature T_w and the transition may be first[1] or second order,[2,3] depending on the specific properties of the system. The latter case, known as critical wetting, has been the object of recent theoretical[4] scrutiny. Indeed, rather spectacular behavior is expected of critical wetting in 3D, the upper critical dimension for systems possessing only short-range forces. Renormalization-group studies[5-7] predict that the interface correlation-length exponent ν is *nonuniversal,* depending continuously on the dimensionless parameter $\omega = k_BT/4\pi\xi_b^2\sigma$, where ξ_b is the *bulk* correlation length of the system and σ the surface tension of a free interface between the two coexisting phases. In particular, $\nu = (1-\omega)^{-1}$ for $\omega < \frac{1}{2}$, while for $\frac{1}{2} < \omega < 2$, $\nu = (\sqrt{2} - \sqrt{\omega})^{-2}$, and finally $\nu = \infty$ for $\omega > 2$. These distinct asymptotic behaviors define models I, II, and III,[6] there being a different fixed-point potential associated with each. Of course, any given system is characterized by a single value of ω and it is presently believed, for example, that those belonging to the universality class of the 3D Ising model (ferromagnets, binary fluid mixtures, liquid-gas critical point) possess $\omega \simeq 0.8$,[8] which suggests that model II is the physically relevant one. The bizarre criticality described above provides a striking contrast to the simple mean-field (MF) behavior exhibited by critical wetting above three dimensions, for which it is known that $\nu = 1$.[4] In ordinary bulk critical phenomena,[9] the situation is more mundane at the upper critical dimension—one retrieves universal MF exponents, though the scaling functions are modified by logarithmic corrections.

The most natural question that arises in light of these extraordinary predictions for 3D critical wetting is whether or not they can be observed experimentally. The importance of long-range forces in traditional experimental systems, such as binary fluid mixtures, suggests that this may not be the most appropriate domain to search for such effects.[10] Nevertheless, recent numerical simulations of critical wetting in the 3D Ising model by Binder, Landau, and Kroll[11] have proven quite fruitful in this regard, as the authors confirm many aspects of the predicted MF behavior. To their great surprise, though, they noted no anomalous critical behavior. Perhaps the numerical experiments had not yet explored the critical regime. To test this hypothesis, we formulated a Ginzburg criterion[12] for the 3D critical-wetting problem to determine explicitly, by traditional means, the domain of validity of MF theory. A fundamental issue concerning the nature of this crossover quickly followed our completed Ginzburg criterion. For example, in the 3D Ising model, it is far from clear whether one would immediately see model-II behavior or whether there would be an intermediate regime for which the system exhibited type-I criticality. Furthermore, it is important to know how close to the wetting transition one must be in order to see an unadulterated model-II exponent for the 3D Ising model. It is our belief that a clear understanding of these various crossovers is crucial to an appreciation of the validity of past, as well as the limitations of future, numerical simulations of 3D critical wetting. In this paper we discuss in detail these crossovers.[7]

Crossover MF→ model I.—The 3D critical-wetting transition is most conveniently discussed by use of the language of interface delocalization, with associated Landau-Ginzburg-Wilson Hamiltonian[4-7]:

$$\beta H = \int d^2x[\tfrac{1}{2}(\nabla z)^2 + V(z)].$$

Here $z(\mathbf{x})$ gives the mean position of the interface, which is bound to the wall via the pinning potential $V(z)$. The system of units is such that $\sigma/k_BT = 1$. Brézin, Halperin, and Leibler,[4] starting from a semi-infinite Ising-model formulation of the wetting transition, derived the following form for the MF potential:

$$V_{\mathrm{MF}}(z) = -ae^{-\alpha z} + be^{-2\alpha z},$$

where $a \sim T_w - T$, and to the attractive part of the potential vanishes at the transition. With the units as above, the relation $\xi_b^{-1} = a = (4\pi\omega)^{1/2}$ holds. The MF exponents for critical wetting are easily retrieved by means of this potential: $V'(z_0) = 0 \rightarrow az_0 \sim \ln(1/a)$, $V(z_0) \sim a^2$, so that the specific-heat exponent $\alpha = 0$. Also, $\xi^{-2} = V''(z_0) \sim a^2 \rightarrow$ correlation-length exponent $\nu = 1$. These results, together with the hyperscaling relation $2 - \alpha = \nu(d-1)$, suggest that the upper critical dimension is 3, as will be made explicit in what follows. To determine how close to the transition one must be in order to observe behavior that is no longer classical, we consider, as Ginzburg did, the Gaussian fluctuations about the MF solution. In the critical-wetting problem, these correspond to capillary-wave excitations about the flat interface. In field-theoretic language, our formulation of the Ginzburg criterion amounts to calculating the effective action to one-loop order:

$$V_{\text{eff}}(z_0) = V_{\text{MF}}(z_0) + \tfrac{1}{2}\,\text{Tr}\ln[k^2 + V''_{\text{MF}}(z_0)].$$

Of course, by Tr we mean $\int d^{d-1}k/(2\pi)^{d-1}$. Derivatives of the effective action result in a Ginzburg criterion for the specific thermodynamic quantity of interest. It is important to realize that each physical observable has its unique region of criticality, though we expect the crossover from MF to occur at roughly the same point for all. To illustrate, we proceed with the calculation for the interface correlation length. We have

$$\xi_{\text{eff}}^{-2} = \xi^{-2} + \tfrac{1}{2}\, d^2\{\text{Tr}\ln[k^2 + \xi^{-2}(z_0)]\}/dz_0^2.$$

Recall that $az_0 \sim \ln\xi \rightarrow d\xi/dz_0 = a\xi$, and so

$$\xi_{\text{eff}}^{-2} = \xi^{-2}\left\{1 + 2a^2(2\pi)^{1-d}\left[\int_0^\Lambda d^{d-1}k/(k^2+\xi^{-2}) - \xi^{-2}\int_0^\Lambda d^{d-1}k/(k^2+\xi^{-2})^2\right]\right\}.$$

Here, the uv cutoff $\Lambda = 1/a_0$, where a_0 is the lattice spacing. For $d > 3$, the integrals associated with the fluctuation corrections converge, merely altering the amplitude, but nonetheless testifying to the validity of mean-field theory. Furthermore, since $a^2 \sim \omega$, it is clear that there are not fluctuation corrections if $\omega = 0$. This makes physical sense since $\omega = 0$ corresponds to an interface of infinite surface tension. At $d_c = 3$, the first integral diverges logarithmically at the transition—for T close enough to T_w, the fluctuation contribution will exceed that of MF. Concentrating on this physically relevant dimension, we evaluate the integrals and find that the crossover from MF to nonclassical criticality occurs when the interface correlation length has reached a value such that

$$1 = 2\omega[\ln(1+\xi^2) + 1/(1+\xi^2) - 1],$$

where ξ is measured in units of the lattice spacing. In Fig. 1, we have drawn this curve for arbitrary ω, though one should keep in mind that the physical value is nearly 0.8. This preliminary finding suggests that the regime in which one expects to observe purely MF behavior for 3D critical wetting is quite small. A mathematically similar calculation of the fluctuation corrections to the specific heat is obtained if we set $V_{\text{MF}} = -a^2/4b$, $\xi^{-2} = a^2a^2/2b$ and take two derivatives with respect to temperature. Our Ginzburg criterion for this quantity results in the curve

$$1 = 2\omega[\tfrac{1}{2}\ln(1+\xi^2) + 1/(1+\xi^2) - 1],$$

the physically relevant piece of which is part of the figure. Apparently, the specific heat exhibits purely classical behavior over a slightly larger regime than the interface correlation length. Anticipating, as well, our findings for χ_1 and Δm_1 (see Fig. 1), we suggest that once the interface correlation length exceeds $\sim$5–6 lattice spacings, capillary-wave fluctuations become important.

Crossover model I → model II—Suppose one is work-

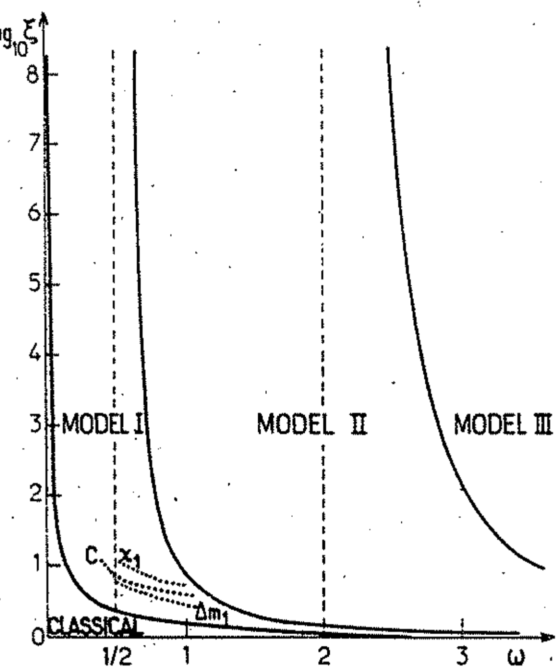

FIG. 1. The various crossovers exhibited by 3D critical wetting, plotted as functions of ω, the dimensionless parameter that measures the stiffness of the free interface. ξ is the characteristic length describing the capillary-wave correlations within that interface. For Ising systems ($\omega = 0.8$), the region of MF behavior is small, but asymptotic nonuniversal model-II criticality is not obtained until ξ is quite large. Models I, II, and III correspond to the different accessible fixed-point potentials. The dotted lines follow from a Ginzburg criterion formulated for the specific heat (C), surface susceptibility (χ_1), and excess magnetization (Δm_1).

ing with a system, such as the 3D Ising model, for which we expect $\omega \simeq 0.8$. At the wetting transition, $T = T_w$, theory[6,7] predicts that the critical behavior will be strictly that of model II. Nonetheless, for a finite range of temperatures sufficiently distant from T_w, the important fluctuations that bring the interface in contact with the wall and are ultimately responsible for the behavior unique to model II will be inactive, and we expect the system to exhibit model-I criticality. The underlying belief here is that a model-II system will cross over first from MF to model I and then only when ξ is sufficiently large will it make the crossover I $\rightarrow$ II. But how does one calculate this second crossover? We recall that the mean position of a model-I interface increases as $z_0 = (4\pi\omega)^{-1/2}(1+2\omega)\ln\xi$, while the thickness of that interface diverges as $\delta = [(\frac{1}{2}\pi)\ln\xi]^{1/2}$. Of course, since $\delta/z_0 \rightarrow 0$ as $T \rightarrow T_w$, the interface remains well defined. As shown first by Brézin, Halperin, and Leibler, the renormalization of model I is self-consistent, provided that the interface is stiff enough ($\omega < \frac{1}{2}$). This was established via a simple, physically appealing procedure. One convolutes the repulsive piece of the model-I potential with a Gaussian of width δ, obtaining

$$e^{-2az} \rightarrow e^{-2az}\exp(2a^2\delta^2)\int_{2a\delta^2 - z_0}^{\infty}\exp(-s^2/2\delta^2)ds/\delta(2\pi)^{1/2},$$

and examines the scaling behavior of the lower limit. For $\omega < \frac{1}{2}$, this quantity goes to $-\infty$ as $T \rightarrow T_w$, and so the functional integrity of the repulsive exponential is maintained with there being a simple renormalization of the coefficient b. If $\omega > \frac{1}{2}$, the repulsive exponential is renormalized to zero in the limit $\xi \rightarrow \infty$ and one is led to model II. To ascertain the crossover from model I to model II, we set the lower limit equal to $-\delta$. The physics here is quite simple—if the coefficient in the lower limit is negative (large ω) and of large absolute value, the crossover should occur rather early on (small ξ). On the other hand, if $\omega = \frac{1}{2}+$, there is no doubt that model-II criticality will be obtained eventually, but one will have to go very close to T_w (large ξ) to see it. Implementing the above procedure, we obtain the crossover line

$$\xi_{\mathrm{I}\rightarrow\mathrm{II}} = \exp[2\omega/(2\omega-1)^2],$$

which is included in Fig. 1. The steepness of the crossover suggests that, for 3D Ising critical wetting, one needs interface correlations extending over a distance $\sim 10^4$ lattice spacings before one can honestly expect to observe pure model-II critical behavior. This requirement may prove a bit too taxing for presently working numerical experimenters.

Crossover model II $\rightarrow$ model III.—Renormalization-group work predicts that for $\omega > 2$, the renormalization of model II at T_w is no longer self-consistent, with the fixed-point potential being the sum of two Gaussians, which Brézin, Halperin, and Leibler called model III. The exponentially divergent correlation-length characteristic of this model should be observed within a small neighborhood of T_w, but is first preceded by a series of crossovers: MF $\rightarrow$ I $\rightarrow$ II $\rightarrow$ III. Using the fact that the model-II interface has mean position $z_0 = (2/\pi)^{1/2}\ln\xi$ and thickness $\delta = [(1/2\pi)\ln\xi]^{1/2}$, we proceed precisely as in the previous section and obtain the crossover line

$$\xi_{\mathrm{II}\rightarrow\mathrm{III}} = \exp[1/(\sqrt{2\omega}-2)^2],$$

which is our final addition to Fig. 1. A quick glance at the figure reveals that if one could, by some artificial means, create a short-range system with sufficiently supple interfaces ($\omega \gtrsim 3$), the size constraints alluded to above could be ameliorated and unadulterated nonuniversal behavior (in this case, model III) might be observable.

Thermal Ginzburg criterion.—We chose to present the results summarized in Fig. 1 as we did because ξ, the capillary-wave correlation length, is a convenient and physically appealing variable to use. This differs somewhat from the usual Ginzburg criterion which determines, for example, the particular value of the reduced temperature at which crossover from classical to nonclassical criticality occurs. An entirely similar procedure is possible in the present context, but requires a bit more work since one must resurrect the original Ising system used to derive the interface-displacement model. Nonetheless, one can show that

$$\xi^2 = [(a_0^3\Delta C)4\pi\omega]^{-1}t_w t^{-2}.$$

Here, $a_0^3\Delta C$ is the dimensionless universal specific-heat discontinuity[13] associated with the bulk consolute point and $t_w = (T_c - T_w)/T_c$ measures the temperature difference between wetting and bulk critical phenomena. This result is of interest because it suggests that the range of validity of mean-field theory grows ($t_{\mathrm{MF}\rightarrow\mathrm{I}} \sim t_w^{1/2}$) as one considers systems with $T_w \sim T_c$.

Numerical experiments.—Presently, the most convenient testing ground for the predictions of 3D wetting with short-range forces is Monte Carlo computer simulations of the semi-infinite Ising model. Thus far, Binder, Landau, and Kroll have managed to confirm the elaborate MF phase-diagram topology, including critical, tricritical, and first-order transitions, elucidated first by Nakanishi and Fisher.[3] More recently, however, they have attempted to explore the nonclassical behavior expected of 3D critical wetting—in particular, the nonuniversal properties of the correlation-length exponent ν. For technical reasons, it was most convenient for them to simulate fixed-temperature, field-driven wetting in which the surface magnetic field is set at its critical value $(h_1 = h_{1c})$ and the interface is liberated as an opposing bulk magnetic field $h \to 0$. Under these conditions, it can be shown that the interface position is given by $z_0 \sim \ln(1/h)$, while the surface-layer susceptibility $\chi_1 = \partial m_1/\partial h$ and magnetization excess $\Delta m_1 = m_1 - m_1(h=0)$ have the scaling forms[14]

$$\chi_1 \sim h^{-1/2\nu}, \ \Delta m_1 \sim h^{1-1/2\nu},$$

where $\nu = \nu(\omega)$ is the correlation exponent. With $\omega = 0.8$, we would expect to see $\nu \sim 4$ for sufficiently small h. Nonetheless, using a bulk field as low as 10^{-3}, Binder, Landau, and Kroll see only the mean-field behavior $\nu = 1$. It is our belief that not only are they quite distant from pure asymptotic model-II critical behavior, but, in fact, they have not even made the first crossover, from MF to model-I criticality. A Ginzburg criterion formulated for χ_1 leads to the crossover line

$$1 = (\omega/2)[\ln(1+\xi^2) + 1/(1+\xi^2) - 1],$$

which suggests a classical region even larger than that for the specific heat discussed earlier. Given the temperature of the simulation $(J/k_BT = 0.35)$, as well as the results of Tarko and Fisher[15] $(\xi_0^+ = 0.48a_0)$ and Brézin, Le Guillou, and Zinn-Justin[16] $(\xi_0^+/\xi_0^- = 1.95)$, we can estimate the field dependence of the correlation length: $\xi = \xi_b/(2ah)^{1/2} = 0.15/\sqrt{h}$. This leads to a crossover at a field strength $h_{\mathrm{MF}\to\mathrm{I}} \sim 7\times 10^{-4}$, somewhat less than the smallest field used by Binder, Landau, and Kroll. Furthermore, we do not expect pure model-II behavior until one employs very small fields of the order $h \sim 10^{-1}$. A similar procedure applied to the magnetization excess leads to the MF $\to$ Model I line $\xi = (e^{2/\omega} - 1)^{1/2}$, and so for the simulation at $J/k_BT = 0.25$, we find crossover at $h_{\mathrm{MF}\to\mathrm{I}} \sim 6\times 10^{-2}$. These rough calculations suggest that the numerical simulations have barely approached the first crossover. It is our belief that one must employ smaller fields $(h \lesssim 10^{-3})$ to see a nonclassical correlation-length exponent.

In summary, we have presented an analysis of the various crossover phenomena expected of critical wetting in three dimensions. It was our intention to elucidate the relationship of MF to the anticipated nonuniversal asymptotic criticalities. Furthermore, our discussion has been quantitatively explicit in an effort to inform future numerical simulators properly of the challenging task that lies before them.

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* MONTE CARLO ⇝ INTERFACE DISPLACEMENT MODEL

Binder, Landau and Kroll worked strictly within the context of the semi-infinite Ising model with surface fields – aside from the excess baggage mentioned earlier, they were stuck with an interface with fixed $\omega \approx 0.8$. Much is gained by simulating the interface model directly including the freedom to vary ω at will. See–

- G. Gompper + D.M. Kroll, Europhys. Lett. 5, 49 (1988).
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These authors managed to observe various manifestations of nonuniversal behavior characteristic of 3d critical wetting. For example–

$\omega = \frac{1}{4}$

→ FIXED TEMP, FIELD-DRIVEN ($h \to 0$) CRITICAL WETTING

$$\beta \mathcal{H} = \int d^2\rho \left\{ \frac{1}{8\pi\omega} (\nabla z)^2 + V(z) \right\}$$

with
$$V(z) = \begin{cases} B e^{-2z} - A e^{-z} + hz, & z>0 \\ 0 & , z<0 \end{cases}$$

For MODEL I, one expects

$$\langle z \rangle \approx \tfrac{1}{2}(1+2\omega) \ln h^{-1}$$

$$\Delta m_1 = m_1 - m_1(h=0) = h^{\beta_1 = \frac{1}{2}(1+\omega)}$$

" $\langle e^{-z} \rangle$

$$\chi_1 = \frac{\partial m_1}{\partial h} = h^{-\gamma_1 = -\frac{1}{2}(1-\omega)}$$

for $\omega = \frac{1}{4}$, expect $\beta_1 = \frac{5}{8}$ and $\gamma_1 = \frac{3}{8}$.

Confirmed, at least for $B = 1.0$. Not so for other values of B.

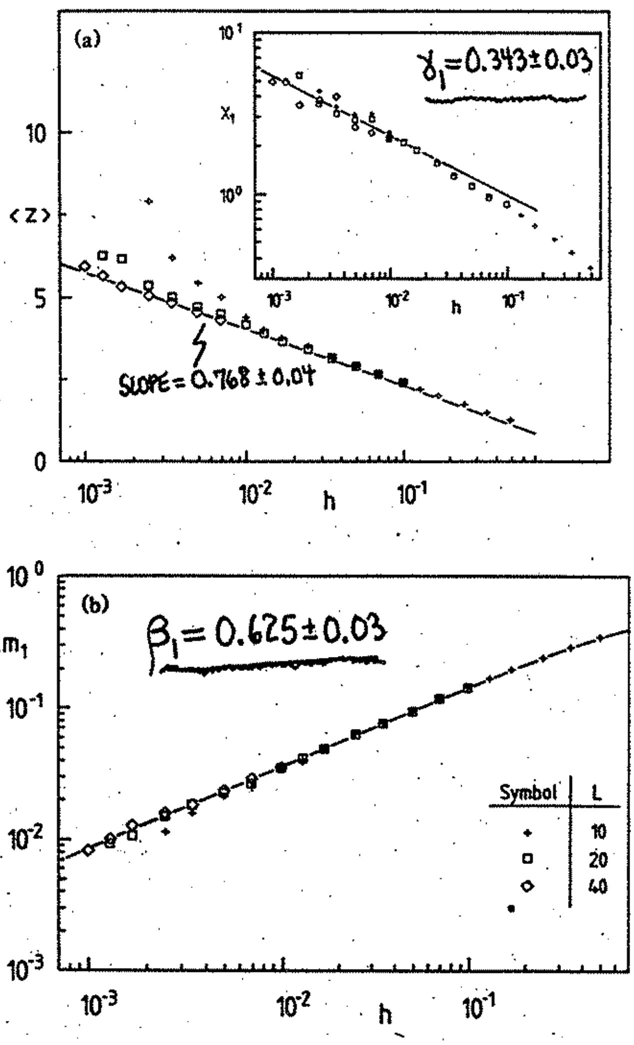

FIG. 1. (a) Coverage $\langle z \rangle$ and (b) excess surface order parameter Δm_1 for $\omega = 0.25$ and $B = 1.0$ plotted vs h. The solid lines are obtained by integrating the linear RG flow equations as described in the text with $g = 2.0$ and $x_m = 5.0$. The deviations of the data from the RG curves for small h are due to finite-size effects. The inset in (a) shows the surface susceptibility χ_1; the straight line is the asymptotic RG prediction.

MORAL: APPROACH TO ASYMPTOPIA DEPENDS STRONGLY ON BARE PARAMETERS! J.Z.J. Phys. Rev. B40

Effective exponents for critical wetting: The approach to the asymptotic region

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Motivated by recent, apparently conflicting, Monte Carlo simulations of three-dimensional critical wetting in Ising systems and interface displacement models, we employ a linear functional renormalization group to calculate explicitly the effective surface magnetization exponent in fixed-temperature, field-driven wetting. Our results indicate, for some values of the parameters, a quick exit from the classical regime, followed by a slow, very broad crossover to pure unadulterated nonuniversal criticality that requires a many-decade decrease of the magnetic field.

Placing a two-phase system within the confines of a container can lead to a novel surface critical phenomenon known as wetting,[1] in which the component preferentially adsorbed by the bounding walls undergoes a thin-film–thick-film transition as the thermodynamic parameters are varied. The characteristic feature of this transition is the fluctuation-induced delocalization of the interface separating adsorbed and bulk phases. Depending on the details of the system, wetting or interfacial depinning transitions can be first or second order. The latter case, particularly in those circumstances where the underlying microscopic forces are short ranged, has received much theoretical attention because renormalization-group (RG) analyses[2–4] suggest that three-dimensional (3D) critical wetting is highly nonuniversal. Scaling indices such as the excess surface magnetization exponent β_1 depend continuously on the interfacial stiffness parameter $\omega = k_B T/4\pi\sigma\xi_b^2$, where ξ_b is the bulk correlation length in the adsorbed phase and σ the surface tension of the free interface. Specifically, the predictions are that $\beta_1 = \frac{1}{2}(1+\omega)$ for $\omega \le \frac{1}{2}$, while for $\frac{1}{2} \le \omega \le 2$, $\beta_1 = \sqrt{2\omega} - \omega/2$, and finally, $\beta_1 = 1$ for $\omega \ge 2$; the classical mean-field result $\beta_1 = \frac{1}{2}$ is, of course, retrieved in the limit $\omega \to 0$, corresponding to very great surface tensions.

Monte Carlo simulations have proved to be the most appropriate testing ground for these extraordinary predictions of 3D critical wetting with short-range forces. Nevertheless, the various studies to date have yielded results that appear, at first glance, contradictory. Binder, Landau, and Kroll[5] (BLK), examining this phenomenon within the context of a discrete semi-infinite Ising system with surface fields, observed strictly mean-field behavior. By contrast, subsequent work by Gompper and Kroll[6] (GK), performed directly on a continuum interface model itself, noted the near absence of a classical regime and a broad crossover towards nonuniversal criticality. Since the two simulations appeared to cover the same range of scaling fields, this discrepancy posed a mild dilemma to theorists eager to declare confirmation of critical-wetting nonuniversality. It is the purpose of this Brief Report to clarify these issues by presenting a functional RG calculation of effective exponents for critical wetting, thereby allowing an explicit measure of the approach to nonuniversal criticality. The results, complementary to an earlier Ginzburg criterion by Halpin-Healy and Brézin[7] and taken in light of a more recent Ising simulation of Binder and Landau,[8] indicate a possible resolution of the controversy.

Our starting point is the free-energy functional describing interfacial delocalization,

$$\beta H = \int d^2x \left[\frac{1}{8\pi\omega} (\nabla z)^2 + V(z) \right],$$

where $z(\mathbf{x})$ is the local distance of the interface from the wall ($z=0$) and $V(z) = Be^{-2z} + hz$ is the pinning potential appropriate to fixed-temperature, field-driven critical-wetting in systems with underlying microscopically short-ranged forces. The repulsive ($B>0$) exponential and "magnetic" field terms compete in such a manner that the interface is liberated from the wall in the limit $h \to 0$. A functional RG treatment of the critical-wetting problem, which follows from an investigation of the general scaling properties of V taken in conjunction with fluctuations induced at the one-loop level, yields a partial differential equation for the renormalized potential,

$$\dot{V}_l(z) = 2V_l + \ln(1 + 2\omega V_l''),$$

where l is the logarithm of the spatial rescaling factor, dots and primes denoting derivatives with respect to l and z, respectively. This nonlinear equation is difficult to manage, so one linearizes and obtains a diffusion equation with the solution,

$$V_l(z) = \frac{e^{2l}}{(4\pi\omega l)^{1/2}} \int_{-\infty}^{+\infty} dz' \, V_0(z') e^{-(z-z')^2/4\omega l}.$$

Here, V_0 is just the bare pinning potential discussed above. The critical behavior is determined by renormalizing the potential until the curvature at its minimum is of order 1. Since the linear RG cannot handle a hard wall, one cuts off the bare potential at the origin and considers a soft wall ($V_0 = g$) for $z<0$. The critical object studied most extensively in the simulations is the so-called excess surface magnetization $\Delta m_1(h) = m_1(h) - m_1(0) = \langle e^{-z} \rangle$, which vanishes at the wetting transition with an exponent β_1.

Let us consider first a reasonably stiff interface, one characterized by the parameter $\omega = 0.25$, as well as a pinning potential constant, $B = 1.0$. In their Monte Carlo simulation of the critical-wetting transition exhibited in just this situation, GK (Ref. 6) noted that for small fields

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($h \lesssim 10^{-3}$), a best fit to the excess magnetization Δm_1 data indicated an asymptotic exponent $\beta_1 = 0.625 \pm 0.03$. This state of affairs led them to remark that the asymptotic critical regime was "very wide." In an effort to quantify such a statement, we have employed the previously discussed functional RG to calculate the effective exponent,

$$\beta_1^{\rm eff}(h) = \frac{\partial \ln \Delta m(h)}{\partial \ln h},$$

in terms of the field h. The results, incorporated into Fig. 1, confirm the suspicion of GK that they are observing essentially unadulterated nonuniversal asymptotic criticality for $h \approx 10^{-3}$. Indeed, our analysis yields $\beta_1^{\rm eff}(h=10^{-3}) = 0.623$, with the exact asymptotic value, $\frac{5}{8}$, being obtained to three digits for all fields smaller than $h \approx 2\times 10^{-4}$. Even for fields as large as $h \approx 0.1$, the effective exponent has only dropped to 0.592, the data of GK being fairly well fit by a single straight line over nearly two decades ($h = 10^{-3}$–10^{-1}). For $h \approx 0.2$, the decline continues to 0.574. Nonetheless, the startling fact, first suggested by the GK simulation and explicitly confirmed here, is the complete absence for these fields of a mean-field regime in which the excess surface magnetization exhibits classical criticality ($\beta_1^{\rm MF} = \frac{1}{2}$).

The above situation changes dramatically when one looks at the same interface in a slightly different pinning potential, $B = 0.1$, also examined by GK.[6] A glance, with

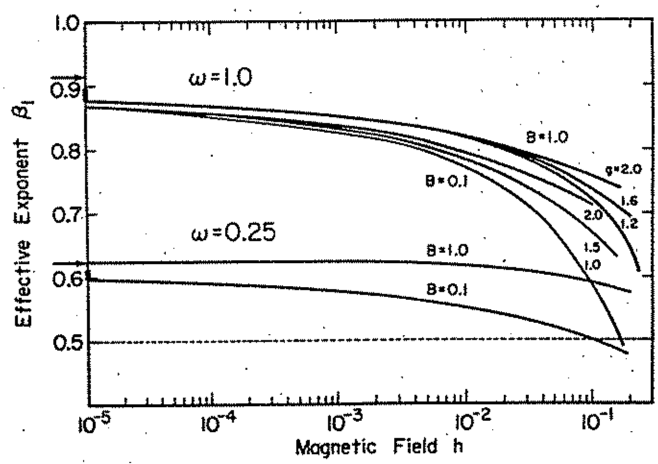

FIG. 1. The effective exponent $\beta_1^{\rm eff}$ for critical wetting, which describes the vanishing of the excess surface magnetization $\Delta m_1(h) = m_1(h) - m_1(0) = \langle e^{-z}\rangle$, as a function of the external driving field h. The curves were generated using a linear functional renormalization group, assuming a soft-wall potential of strength g. The bottom two correspond to a relatively rigid interface, characterized by the dimensionless stiffness parameter $\omega = 0.25$. The values chosen for B, the coefficient of the repulsive exponential in the pinning potential, correspond to those used by Gompper and Kroll (Ref. 6) in their simulations. The nonuniversal asymptotic exponent $\beta_1^{\rm asym}(\omega = 0.25) = \frac{5}{8}$ is indicated, as is the evolution of the effective exponent for successive decades beyond $h = 10^{-5}$. The upper curves ($\omega = 1.0$, $B = 0.1$, and 1.0, various values of g) may shed light on issues surrounding critical-wetting behavior in Ising systems. Note the rather rapid exit from classical criticality ($\beta_1 = \frac{1}{2}$) and the slow, very broad crossover towards the unadulterated, nonuniversal asymptotic exponent $\beta_1^{\rm asym}(\omega = 1) = 0.914$.

ruler in hand, at Fig. 2 of their paper makes it quite clear that the data for $h \approx 10^{-3}$ cannot possibly be fit with a straight line of the correct asymptotic slope. GK were clearly aware of this fact, mentioning that for $B = 0.1$, the asymptotic critical regime is "smaller than for $B = 1.0$." Furthermore, though extending perhaps for only a single decade, a convincing line of slope $\frac{1}{2}$ could be passed through the data in the neighborhood of $h \approx 0.1$. Our explicit computation of the field-dependent effective exponent reveals this to be precisely the case; see Fig. 1. For $h = 10^{-1}$, we find $\beta_1^{\rm eff} = 0.497$, though the less than leisurely rise of the effective exponent for decreasing field insures that any mean-field region is certainly short lived. Indeed, just a decade later at $h = 10^{-2}$, $\beta_1^{\rm eff}$ has already reached the value 0.550. However, as the driving field goes to zero, there is a slow and very labored approach to the asymptotic exponent $\frac{5}{8}$, a behavior quite distinct from that of $B = 1.0$. For the smallest field considered by GK, one has $\beta_1^{\rm eff}(h = 10^{-3}) = 0.570$. At $h = 10^{-5}$, $\beta_1^{\rm eff} = 0.596$, indicating that one still has a long way to go before closing in on the unadulterated nonuniversal exponent. To keep measure of the lengthy crossover of this critical wetting phenomena, the figure has dots to mark the effective exponent for successive decades of the vanishing external field. To reiterate, there is an abrupt, quick exit from a brief mean-field regime at moderately large fields ($h \approx 0.1$), followed by a long winded, gradual crossover to asymptopia. This appears to be a characteristic feature of the interface displacement model for some values of the parameters. For others, the classical regime is lost entirely.

We have also studied in great detail the case of a slightly more supple interface, $\omega = 1.0$, since there are various indications that this value of the dimensionless stiffness parameter might be appropriate to a description of critical wetting phenomena in discrete Ising models. GK performed simulations of this interface subject to a pinning potential with $B = 1.0$, observing good agreement with the theoretical predictions of the linear RG when using $g = 2.0$. We confirm this and explicitly calculate $\beta_1^{\rm eff}$ as before. For large $h \approx 0.1$, where it appears quite difficult if not impossible to fit the GK data to a line of mean-field slope $\frac{1}{2}$, our analysis yields $\beta_1^{\rm eff} \approx \frac{3}{4}$. Interestingly, though, we find that by decreasing g, smaller and smaller values of the effective exponent are had for a given large magnetic field, without seriously spoiling the agreement with Δm_1 data in the regime considered by GK. Altering g seems to have very little effect on the asymptotics, however, since all values yield $\beta_1^{\rm eff}(h = 10^{-3}) = 0.849$, corroborating the fact which is obvious from the GK data that one is quite distant from $\beta_1^{\rm asym} = 0.914$. Indeed, even for $h = 10^{-5}$, one has only $\beta_1^{\rm eff} = 0.876$, successive dots in Fig. 1 indicating the evolution with later decades. To complete the picture, we include results for $B = 0.1$. As for $\omega = 0.25$, we note that a decrease in B incurs a less rapid approach to nonuniversal asymptotic criticality, while the effect of diminishing g is further magnified. In particular, for $g = 1.0$, $\beta_1^{\rm eff}$ passes through $\frac{1}{2}$ for $h \approx 0.1$, leading to the appearance of an ephemeral mean-field regime. It is apparent that, within the context of the interface displacement model and its simulation, increasing ω exacerbates the brevity of the classical regime, eventually resulting in its complete absence. This was first suggested on theoretical grounds,[7] being observed subsequently by GK at $\omega = 3$ and in a separate study[9] for $\omega = 5$.

Our results for $\omega = 1.0$ make quantitative the recent controversy arising from seemingly inconsistent Monte Carlo simulations of continuum interface displacement models and Ising critical-wetting phenomena. Whereas GK, in the former, note the near absence of a mean-field regime and the quick crossover towards nonuniversal exponents, BLK observe strictly classical criticality in the latter. The dilemma arises because both simulations involve roughly the same range of scaling field. Thus, it is a bit surprising that BLK manage to fit their excess magnetization data to a line of slope $\frac{1}{2}$. Nevertheless, as a practical first step to estimate the size of the asymptotic regime for 3D critical wetting, a Ginzburg criterion suggested[7] that BLK were on the verge of exiting the mean-field region. They needed merely to consider slightly smaller fields, in order that the interfacial correlation length exceed 5–6 lattice spacings, to see deviations from classical criticality. Indeed, a later, somewhat more thorough examination of Ising model critical wetting by Binder and Landau[8] is not at all inconsistent with this notion. Their fixed-temperature (reduced coupling $J/k_BT = 0.25$), field-driven ($H \to 0$) wetting simulation extends down to $H/J = 5\times10^{-4}$ and the final four data points of their Δm_1 plot surely hint at a slope greater than $\beta_1 = \frac{1}{2}$. This departure from the mean-field behavior is quite explicit in a similar plot at a slightly different temperature ($J/k_BT = 0.35$). In fact, in both of these figures of Binder and Landau, it is crucial to observe that the data are convincingly fit to a line of mean-field slope for roughly a single decade at most. This might be related to the peculiar behavior of $\beta_1^{\rm eff}$ for smaller values of g, as documented by the linear RG. In any case, it is fairly clear that were the Ising simulations extended another decade or so, the mean-field slope would probably be lost.

Given the above comments, the dilemma formerly associated with the Ising wetting phenomena all but vanishes and the important task remaining for the theorist is to explain the rather more abrupt exit from classical criticality observed in the interface displacement simulations. It is our belief that, though the two models certainly share the same asymptotic criticality, their essential differences manifest themselves in a strong way for large fields ($h \approx 0.1$), where the mean interface position is not much greater than unity. Among these crucial differences is the anisotropic surface tension in the Ising system, the discrete versus continuous nature of z, as well as the distinct working definitions of Δm_1 in the various simulations. Apparently, it is not sufficient to note that the Ising and interface displacement model simulations covered nearly the same range of external magnetic field. This is certainly clear. BLK point out that in their work $\langle z\rangle \lesssim 5$ for $H/J = 10^{-3}$, while the figures of GK for $\omega = 1.0$ indicate $\langle z\rangle \gtrsim 10$ for the analogous h. Perhaps a smaller ω is appropriate for the Ising model. More likely, however, an explanation for the different crossovers can be found in very general considerations associated with the functional RG and Wilsonian ideas.[10] That is, although the two models become essentially identical following a sufficient number of renormalization transformations, *as bare entities they are quite distinct.* Hence, in the many-dimensional Wilson space of couplings, their initial starting points are also quite different and the functional RG takes them along differing trajectories on their trip to the inevitable fixed point function. Evidently, the trajectory followed by the Ising system manages a brief, but observable visit in the neighborhood of the Gaussian fixed point, while the interface displacement model sticks to a more direct route. The former would give rise to a brief exhibition of classical criticality, as seen in the simulations of Binder and co-workers,[5,8] who note agreement between their data and the mean-field slope over just a decade or so. Yet, as the previous work of Halpin-Healy and Brézin[7] suggested and the present calculation of $\beta_1^{\rm eff}$ confirms, this is quite a small regime indeed, and the complete crossover to unadulterated, nonuniversal, asymptotic criticality can require many, many decades. It is our hope that the Ising simulations will be revisited at smaller fields to verify these expectations.

The author would like to thank Martin Gelfand and Michael Fisher for helpful discussions regarding the many subtleties of 3D critical wetting. Financial support has been provided by the National Science Foundation through Grant No. DMR 87-16816.

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FUNCTIONAL RG ~ Interfacial Critical Phenomena

references ↳

D.S. Fisher & D.A. Huse, Phys. Rev. B32, 247 (1985) "LINEAR"

R. Lipowsky & M.E. Fisher, Phys. Rev. Lett. 57, 2411 (1986) } "NONLINEAR" INTERFACES

R. Lipowsky & M.E. Fisher, Phys. Rev. B36, 2126 (1987).

for related earlier work, using functional RG on bulk Ising criticality see Ma ~ Modern Theory of Critical Phenomena, sections 6.1, 6.2 & 7.1 of the celebrated Wilson & Kogut paper on the RG, Phys. Reports 12, 75 (1974), and more specifically

A. Hasenfratz & P. Hasenfratz, Nucl. Phys. B270 [FS16], 687 (1986). φ^4 THEORY

Recall that our starting point ~ role of capillary wave fluctuations in interfacial depinning / critical wetting phenomena –

$$\mathcal{Z} = \underbrace{\int \mathcal{D}z}_{\text{INTERFACE CONFIGURATIONS}}\, e^{-\int d^{d-1}x \left\{ \overbrace{\frac{\sigma}{2kT}}^{\text{"SURFACE TENSION"}} (\nabla z)^2 + \underbrace{V(z)}_{\text{"LOCALIZING POTENTIAL"}} \right\}}$$

Our goal will be to develop a functional renormalization group for $V(z)$, the localizing potential which keeps the interface NEAR THE WALL for temperatures well below T_W. The functional RG will be sufficiently powerful that it will tell us how the entire function, $V(z)$, gets renormalized upon rescaling and inclusion of capillary wave fluctuations. Ultimately, we will rederive the NONUNIVERSAL CRITICALITY characteristic of 3d critical wetting, but our understanding of these phenomena will be much deeper ~ based on a knowledge of the "FIXED POINT FUNCTIONS" that control the asymptotic scaling. We'll find, using the full non-linear functional RG, that for $d<3$ there are two nontrivial fixed pt functions – one for the critical manifold, the other associated with the completely delocalized phase. As the dimensionality is varied, these do not bifurcate from the Gaussian fixed pt at the upper critical dimension $d_c^{\text{WETTING}} = 3$ (remember that this is what happens for ordinary BULK Ising criticality at $d_c^{\text{ISING}} = 4$ ← STANDARD SCENARIO!), but rather mutually "annihilate" leaving behind what Lipowsky + Fisher refer to as a line of unusual "drifting" fixed points. The FALLOUT = "STRONG-FLUCTUATION" critical exponents that exhibit singular behavior as $d \to 3^-$. This was seen already by BHL, who discovered for $\omega > 2$ in 3d critical wetting, the interfacial correlation length exponent $\nu_{\parallel} = \infty$.

The basis of the functional RG is a 1-loop calculation of the effective action, see our earlier discussion of the Ginzburg Criterion ...., which implies

$$V_{1\text{-loop}} = V_{\substack{\text{MEAN}\\\text{FIELD}}} + \frac{1}{2} \int_q \log\left\{1 + \frac{k_B T}{\sigma q^2} V''\right\}$$

* nb) $\int_q = \int^{\Lambda} \frac{d^{d-1} q}{(2\pi)^{\frac{d-1}{2}}}$

where we have simply performed a Taylor-expansion of the localizing potential about its minimum (keeping only terms up to quadratic order) + performed the gaussian functional integral. If one RESCALES the coordinates according to the prescription

$$x \to x/b \qquad z \to z/b^{\varsigma = \frac{3-d}{2}}$$

where $b = 1 + \delta l$ will be our infinitesimal spatial rescaling factor and $\varsigma = \frac{3-d}{2}$ is the "roughness" exponent, introduced before, that describes the transverse, thermal fluctuations of the interface due to capillary waves ($\langle z_q z_{-q} \rangle = \frac{kT}{\sigma q^2} \Rightarrow$ interfacial width/diffuseness scales as $w \sim L^{\frac{3-d}{2}}$ for a given longitudinal length L : ). Of course, rescaling the coordinates will incur a change in the potential ~ this is a result of the length dimension of V itself, as well as its argument z :

$$\delta V = V(b^{\varsigma} z)/b^{1-d} - V(z)$$

$$\approx \left(1 + (d-1)\delta l\right) V(z + \varsigma z \delta l) - V(z) + \cdots$$

$$\delta V \approx \left[(d-1) V + \varsigma z \frac{\partial V}{\partial z}\right] \delta l + \cdots$$

these are the trivial contributions, due simply to the dimension dependences. The interesting piece comes from the fluctuation effects

$$\delta V_{\text{FLUC}} = \frac{1}{2}\int_{\Lambda}^{\overset{1+\delta l}{\Lambda b}} \frac{d^{d-1}q}{(2\pi)^{d-1}} \log\left\{1+\frac{k_BT}{\sigma q^2}V''\right\}$$

$\Longrightarrow$

$$\delta V_{\text{FLUC}} \approx \frac{1}{2}\frac{\Lambda^{d-1}}{(2\pi)^{d-1}}\log\left\{1+\frac{k_BT}{\sigma\Lambda^2}V''\right\}\ \delta l$$

Putting these two contributions together, we obtain a NONLINEAR, PARTIAL DIFFERENTIAL EQUATION of the form

$$\frac{\partial V_l(z)}{\partial l} = (d-1)V_l + \frac{(3-d)}{2}z\frac{\partial V_l}{\partial z} + \log\left\{1+\frac{\partial^2 V_l}{\partial z^2}\right\}$$

which describes the RG "flow" of the localizing potential $V(z)$. Note that the "INITIAL CONDITION" at $l=0$ corresponds to the "BARE POTENTIAL", while the solution to the PDE would give one an effective or "RENORMALIZED POTENTIAL" V_l, with fluctuations of the interface up to a longitudinal lengthscale l integrated out.

⇝ LINEAR TREATMENT (Fisher + Huse)

expand the logarithm to linear order in V'' $\Longrightarrow$ our functional RG flow equation becomes

$$\frac{\partial V}{\partial l} = (d-1)V + \underbrace{\frac{3-d}{2}}_{\zeta}z\frac{\partial V}{\partial z} + \frac{1}{\tilde\sigma}\frac{\partial^2 V}{\partial z^2} \qquad \tilde\sigma = \frac{\sigma}{k_BT}\frac{(4\pi)^{\frac{d-1}{2}}\Gamma\left(\frac{d-1}{2}\right)}{\Lambda^{d-3}}$$

which is nothing but a DIFFUSION EQUATION with rescaling. This PDE can be explicitly integrated, starting from an arbitrary bare potential $V_0(z)$ at $l=0$; one has

$$V_l(z) = \frac{e^{(d-1)l}}{\sqrt{2\pi S^2(l)}}\int_{-\infty}^{\infty}dz'\,V_0(z')\,e^{-(ze^{\zeta l}-z')^2/2S^2(l)}$$

← EFFECTIVE, RENORMALIZED POTENTIAL

where the width of the convolution is given by

INTERFACIAL DIFFUSENESS

$$S^2(l) = 2\left(e^{(3-d)l}-1\right)/(3-d)\tilde\sigma$$

It is crucial to keep in mind that the parameter l in this flow equation is the logarithm of the factor for which lengths PARALLEL to the interface have been rescaled, while the factor in the z-direction is $e^{\zeta l}$

Let us focus our attention on the marginal case $d=3$, where we anticipate NONUNIVERSAL CRITICALITY as discovered first by BHL. For this dimensionality, we find $\tilde{\sigma} = 4\pi\sigma/k_BT$, so if we agree to measure distances in the z-direction in units of the bulk correlation length ξ_b, then

DIFFUSION COEFFICIENT — GAUSSIAN CONVOLUTION OF BARE POTENTIAL (REMINISCENT OF BHL)

$$\boxed{\frac{\partial V}{\partial \ell} = 2V + \omega \frac{\partial^2 V}{\partial z^2}} \Rightarrow V_\ell(z) = \frac{e^{2\ell}}{\sqrt{2\pi\delta^2(\ell)}} \int_{-\infty}^{\infty} dz'\, V_0(z')\, e^{-(z'-z)^2/2\delta^2}, \text{ with } \delta^2(\ell) = 2\omega\ell$$

where, recall from before, $\omega = k_BT/4\pi\sigma\xi_b^2$ is a dimensionless measure of the interfacial stiffness. Within the linear functional RG treatment of 3d critical wetting, this parameter appears in a very natural way as a DIFFUSION CONSTANT! (small surface tension $\sigma \Rightarrow$ large diffusion const $\omega \Rightarrow$ substantial wandering of interface & vice versa)

RG STRATEGY: to determine critical behavior at wetting transition, rescale until a scale e^{ℓ^*} at which the curvature (n.b., $\xi^{-2} = V''$) of the renormalized potential V_{ℓ^*} is of order unity. At this scale, fluctuations not important because the interfacial correlation length is of order unity $\Rightarrow$ MF method applicable - minimization of potential works! The original parallel correlation length $\xi_\parallel \approx e^{\ell^*}$.

n.b.) everything checks with BHL. $\xi_\parallel = e^{\ell^*} \Rightarrow \ell^* = \ln \xi_\parallel$, so that

$$\left(\frac{\delta}{\xi_b}\right)^2 = 2\omega\ell \Rightarrow \delta^2 = 2\xi_b^2\left(\frac{kT}{4\pi\sigma\xi_b^2}\right)\ln\xi_\parallel = \left(\underbrace{\frac{kT}{\sigma}}_{\text{1 in notation of BHL}}\right)\frac{1}{2\pi}\ln\xi_\parallel = \underbrace{\frac{1}{2\pi}}_{\text{WIDTH OF AD HOC BHL CONVOLUTION}}\ln\xi_\parallel$$

OK, let's put the linear functional RG to work -

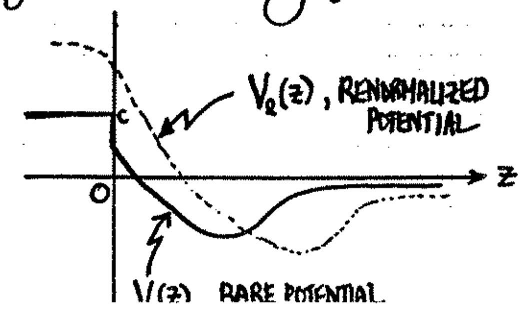
IMMEDIATE PROBLEM = cannot handle HARD WALL POTENTIAL

Replace by SOFT WALL; add in double exponential appropriate for system with short-range forces $\Rightarrow$

"BARE POTENTIAL"

$$V_0(z) = \underbrace{W_0(z)}_{\begin{cases} 0 & z>0 \\ c & z<0 \end{cases}} + \overbrace{\underbrace{A_0(z)}_{\begin{cases} -ae^{-z} & z>0 \\ 0 & z<0 \end{cases}} + \underbrace{R_0(z)}_{\begin{cases} be^{-2z} & z>0 \\ 0 & z<0 \end{cases}}}$$

undergoes functional renormalization:



because of the LINEAR treatment, we can consider the three contributions SEPARATELY. Recall from BHL that both mean interfacial position and width diverge as $\ln \xi_{\parallel}$, which is of order l $\Rightarrow$ makes good sense to scale z distances by l and evaluate gaussian convolution

$$V_l(\mu l) = \frac{e^{2l}\sqrt{l}}{\sqrt{4\pi\omega}} \int_{-\infty}^{\infty} d\mu' \, V_0(\mu' l)\, e^{-l(\mu-\mu')^2/4\omega}$$

by method of STEEPEST DESCENT (since $l \to \infty$ as $T \to T_W$). Let us proceed with pieces A, R, and W, in turn:

i) ATTRACTIVE EXPONENTIAL –

$$A_l(\mu l) = -a\sqrt{\frac{l}{4\pi\omega}}\, e^{2l} \int_0^{\infty} d\mu'\, e^{l[-\mu' - (\mu'-\mu)^2/4\omega]}$$

exponent is MAXIMIZED $\frac{d}{d\mu'}[-\mu' - (\mu'-\mu)^2/4\omega] = 0$ at $\mu'_S = \mu - 2\omega$

therefore, as $l \to \infty$, we need to distinguish the cases $\mu \gtrless 2\omega$. For $\mu > 2\omega$, the integral is dominated by the saddle pt at μ'_S, yielding

$$A_l(\mu l) \approx -a e^{l(2+\omega-\mu)} \qquad \mu > 2\omega$$

MULTIPLICATIVELY RENORMALIZED EXPONENTIAL

By contrast, for $\mu < 2\omega$, the steepest descent integral is dominated by μ' near zero (i.e., the LOWER LIMIT!), giving

$$A_l(\mu l) \approx -\frac{a}{\sqrt{4\pi\omega l}} \frac{1}{1-\mu/2\omega}\, e^{l(2-\mu^2/4\omega)} \qquad \mu < 2\omega$$

NEAR WALL COLLISIONS IMPORTANT $\rightarrow$ LOOKS GAUSSIAN

moral = the renormalized $A(z)$ is a Gaussian at short distances $z < 2\omega l$ and decays as a (multiplicatively renormalized $\rightarrow e^{\omega l} e^{-\mu l} = \xi^{\omega} e^{-z}$; e^{2l} is just the "SPATIAL RESCALING") exponential at large distances $z > 2\omega l$.

likewise –

ii) REPULSIVE EXPONENTIAL – again, there are two regimes

$$R_l(\mu l) \approx \begin{cases} b e^{l(2+4\omega-2z)} & \mu > 4\omega \\ \dfrac{b}{\sqrt{4\pi\omega l}} \dfrac{1}{2-\mu/2\omega}\, e^{l(2-\mu^2/4\omega)} & \mu < 4\omega \end{cases}$$

GAUSSIAN CHARACTER MANIFEST OVER GREATER RANGE OF z-VALUES COMPARED TO ATTRACTIVE PIECE.

iii) WALL CONTRIBUTION – dominated by small negative z parts of W_0 for all $\mu > 0$

$$W_l(\mu l) \approx \frac{c}{\sqrt{4\pi\omega l}}\, e^{l(2-\mu^2/4\omega)}\, \frac{2\omega}{\mu}$$

SOFT WALL RENORMALIZED TO REPULSIVE GAUSSIAN

FLUCTUATIONS $\Rightarrow$ minimum of the full renormalized potential moves to greater z ($\Rightarrow$ further from wall) and its value at the minimum changes under the action of the RG.

MODELS I, II, III correspond to potential minima with $\mu > 4\omega$, $2\omega < \mu < 4\omega$, and $\mu < 2\omega$, respectively. Here, we sketch the calculation for MODEL I, leaving the others as an exercise requiring a careful reading of the original paper of Fisher + Huse.

* MODEL I: $\mu > 4\omega \Rightarrow$ gaussian $W_\ell \ll$ exponential A_ℓ, B_ℓ for ℓ large.

Minimizing $V_\ell(z) \approx -a e^{2\ell + \omega\ell} e^{-z} + b e^{2\ell + 4\omega\ell} e^{-2z}$

w.r.t. z implies

$$z_{MIN} \approx 3\omega\ell + \ln(2b/a)$$

If we require the curvature of the renormalized, rescaled potential at z_{MIN} to be of order unity

$$\left.\frac{\partial^2 V_\ell}{\partial z^2}\right|_{z=z_{MIN}} \approx \frac{a^2}{2b} e^{(2-2\omega)\ell^*} \approx 1 \Longrightarrow \ell^* \approx \frac{1}{1-\omega} \ln\frac{1}{a}$$

Recall that $a \sim (T_W - T)$ marks the distance from the transition. Once we have ℓ^* as a function of this vanishing parameter, we're all set since

$$\xi_\parallel = e^{\ell^*} \approx a^{-\frac{1}{1-\omega}} \Longrightarrow \nu_\parallel = \frac{1}{1-\omega}$$

$$z^*_{MIN} \approx (1+2\omega)\ell^* \approx (1+2\omega)\ln \xi_\parallel$$

which are precisely the results of BHL for MODEL I asymptotic wetting criticality. Note, finally, that the assumption $\mu > 4\omega$ requires $z^*_{MIN} = \mu\ell^* > 4\omega\ell^*$. In other words,

$$(1+2\omega) > 4\omega \Rightarrow \omega < \tfrac{1}{2}.$$

which defines MODEL I.

* MODELS II, III follow similarly, but involve substantially more algebra

II: attractive exponential + repulsive gaussian (W+R)

III: double gaussian (BHL)

* transition occurs at finite value of a

strong fluctuations – TUNNELING

(similar to situation for 2d critical wetting)

instantons ?!

⇝ NONLINEAR FUNCTIONAL RG (Lipowsky + Fisher)

Using techniques very closely tied to Wilson's original approach, Lipowsky and Fisher developed a nonlinear functional RG specifically suited for interfacial critical phenomena. The fruit of their labors was a "RECURSION RELATION" for the renormalized pinning potential when the longitudinal dimensions are rescaled by finite b:

$$\mathcal{R}[V(z)] = -v b^{d-1} \log\left\{ \int_{-\infty}^{\infty} \frac{dz'}{\sqrt{2\pi a^2}}\, e^{-\frac{z'^2}{2a^2} - \frac{1}{2v}\left[V(b^{\varsigma}z - z') + V(b^{\varsigma}z + z')\right]} \right\}$$

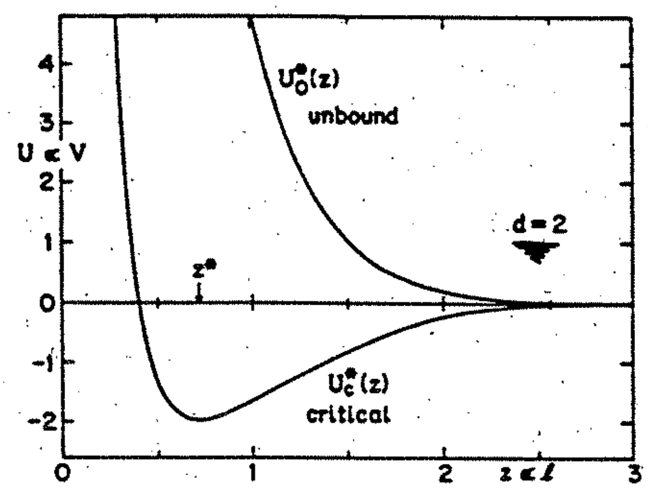
which, crudely speaking, represents a

⟶ "GAUSSIAN CONVOLUTION OF BOLTZMANN WEIGHT"

As such it can handle, without any difficulty, an infinite hard wall potential & is superior to the linear treatment of Fisher & Huse. If one considers a differential formulation of this nonlinear functional RG, one obtains the flow equation $\Downarrow b = 1 + \delta l$

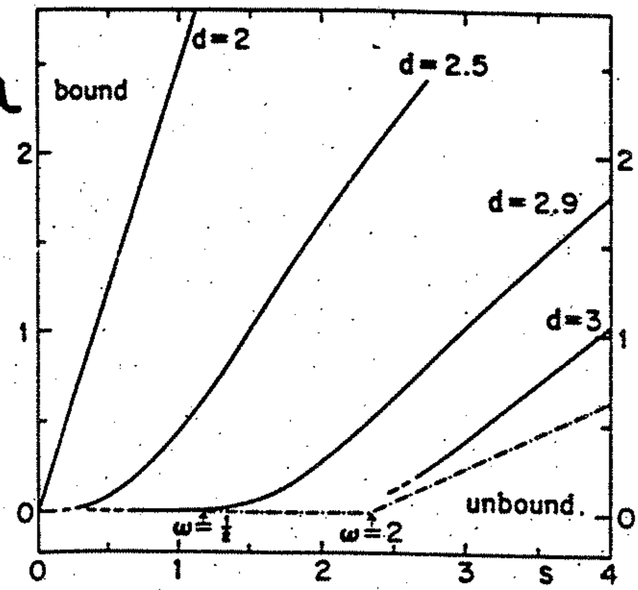
$$\frac{\partial V}{\partial l} = (d-1)V + \varsigma z \frac{\partial V}{\partial z} + \ln\left(1 + \frac{\partial^2 V}{\partial z^2}\right)$$

which was derived earlier via a 1-loop calculation of the effective action. Lipowsky & Fisher searched for "FIXED POINT FUNCTIONS" that were SCALE INVARIANT ($\partial_l V^* = 0$) under the RG –



(spatial rescaling factor b = 2 for both figures)

a



$\Downarrow$

✱ QUITE CLOSE TO THE RESULT EXPECTED FROM ABRAHAM'S EXACT SOL'N 2d CRITICAL WETTING

$$\nu_{\parallel} = 2.04 \pm 0.05 \quad ✓$$

PHASE TRANSITION LINES – VARIOUS DIMENSIONALIT

$$V_0(z) = \begin{cases} -a e^{-sz} + e^{-2sz} & z > 0 \\ 0 & z < 0 \end{cases}$$

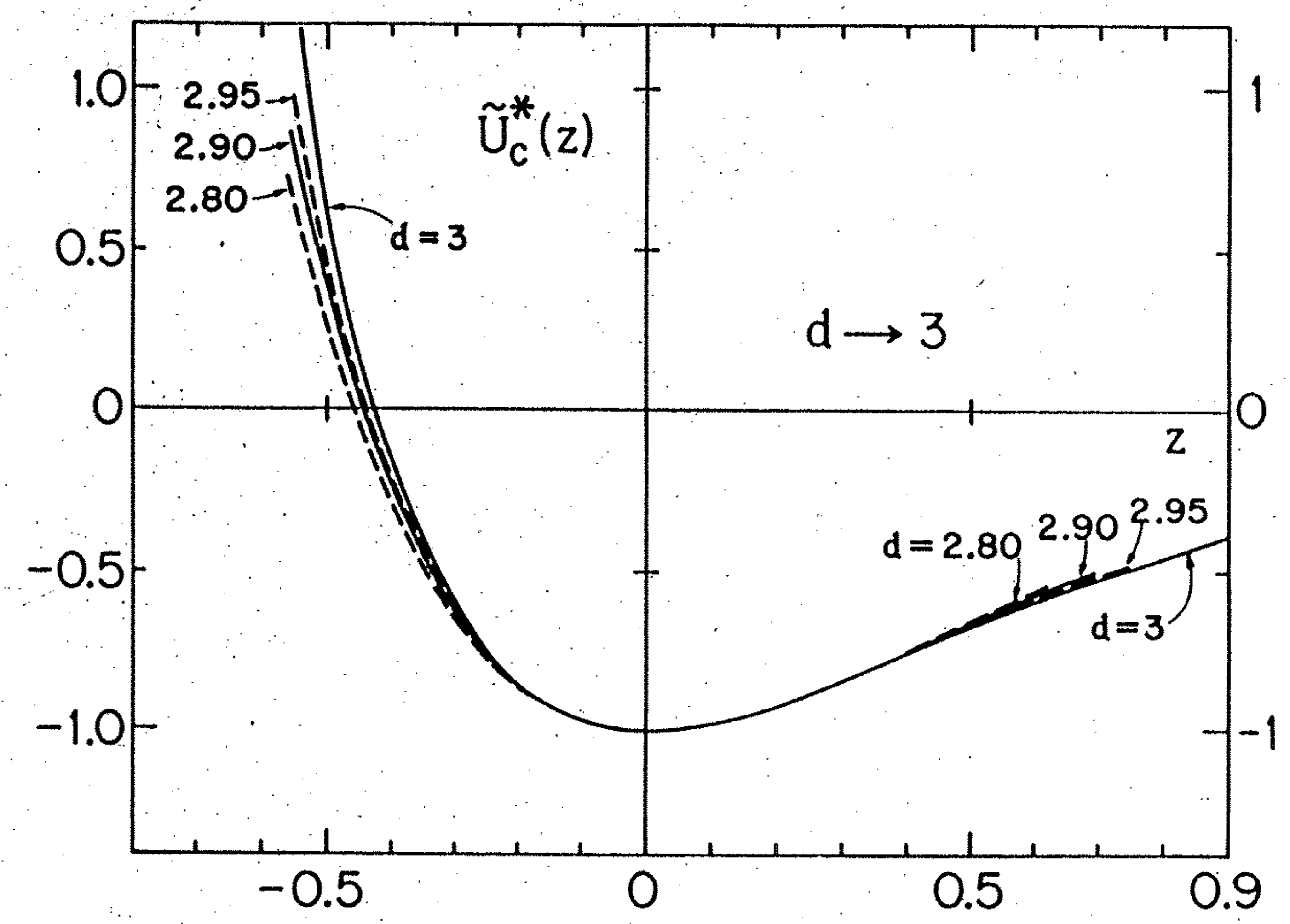


Fig. 7 Lipowsky & Fisher

RESCALED & SHIFTED CRITICAL FIXED POINT POTENTIALS FOR DIMENSIONALITIES APPROACHING d=3, FOR WHICH A DEFINITE LIMITING FORM APPEARS TO EXIST.