Systematic smoothing of constrained interface profiles

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We introduce a family of crossing constraints for defining an interface Hamiltonian that yield order-parameter profiles of any desired smoothness. The usual local crossing criterion is generalized to include integral constraints. Application to short-range critical wetting allows us to demonstrate that fundamental predictions from the local crossing criterion are robust under a change of constraint. Further, interface Hamiltonians derived from any member of the family are shown to reproduce exact results for order-parameter correlation functions. [S1063-651X(97)02711-6]

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For critical wetting transitions in systems with short-range forces the upper critical dimension is $d=3$ [1]. At this dimension renormalization effects can be important and indeed striking nonuniversal behavior has been predicted [2]. Renormalization-group studies of wetting rely on the introduction of an effective interfacial Hamiltonian, which is a functional of the thickness l of the adsorbed layer. This Hamiltonian typically takes the form [3,4]

$$H_l[l]=\int d\mathbf{y}\left\{\frac{\Sigma_\infty}{2}(\nabla l)^2+W(l)\right\}, \tag{1}$$

where $W(l)$ is the binding potential and Σ_∞ is the stiffness or surface tension of a free interface. This Hamiltonian is derived from an underlying noncritical bulk order-parameter theory, typically a Landau-Ginzburg-Wilson Hamiltonian of the form

$$H[m]=\int d\mathbf{y}\left\{\left[\frac{K}{2}(\nabla m)^2+\phi(m)\right]dz+\phi_1(m_1)\right\}, \tag{2}$$

where $m_1\equiv m(\mathbf{y},z=0)$ is the surface order parameter or ''wall value.''The bulk free-energy density $\phi(m)$ is assumed to take the form $\phi(m;T,h)=\phi_0(m;T)-hm$, where ϕ_0 has two equal minima and h is the bulk ordering field. At $h=0$ two phases, α (corresponding to down spins, say, in a magnetic notation) and β (up spins), coexist. With this notation we denote the minima of ϕ by $m_{\alpha\infty}$ and $m_{\beta\infty}$. We assume that the wall in the plane $z=0$ is wet by the β phase at some subcritical temperature T_W so that for $T>T_W$ the $\alpha\beta$ interface is delocalized at a macroscopic distance from the wall. The surface potential ϕ_1 is modeled by the truncated expansion $\phi_1(m_1)=-h_1m_1-gm_1^2/2$, where h_1 is the surface field ($h_1>0$ for our analysis) and $g<0$ is the surface enhancement.

The derivation of Eq. (1) can be achieved by first determining the order-parameter profile with a given (fixed) wall value. The interface location is given implicitly by, for example, defining l as the position where this profile crosses some reference value. Clearly, l depends on the wall value so that exploring the full range of wall values allows the derivation of an effective Hamiltonian [3,4]. Recently, this approach was criticized by Fisher and Jin (FJ) [5], who have reanalyzed the problem, finding two modifications to the effective Hamiltonian (1). First, the binding potential W for large l should have the expansion

$$W(l;T,h)=\overline{h}l+w_1(l)e^{-\kappa l}+w_2(l)e^{-2\kappa l}+\cdots, \tag{3}$$

where the reduced ordering field $-\overline{h}\propto h$ and $\kappa\equiv 1/\xi_\beta$ is the inverse correlation length of the wetting phase. The coefficients of the exponentially decaying terms, $w_n(l)$ were found to be polynomials in l of order n rather than being l independent as had previously been believed. Second, the stiffness coefficient Σ_∞ in Eq. (1) should be replaced by a position-dependent stiffness $\Sigma(l)$ with an expansion similar to Eq. (3). Although the presence of a position-dependent contribution to the stiffness coefficient is also visible in [4], this was not utilized at the time.

The scheme that FJ prescribe for deriving $H_l[l]$ relies on introducing a suitable constraint in order to define the collective coordinate l. In particular they impose the ''local''crossing criterion $m(y,z=l(\mathbf{y}))=m^X\ \forall\mathbf{y}$ to *define* l, where m^X is a fixed reference level. The constraint consists of *fixing* l and then minimizing the free energy exactly. In a suitably generalized form effective Hamiltonians derived using this criterion have been shown to correctly rederive the correlation function structure associated with the underlying Landau-Ginzburg-Wilson model and provide quantitative predictions that are in agreement with Monte Carlo simulations of wetting [6,7]. However, as noted by FJ, the imposition of the local constraint naturally leads to a discontinuity in the first derivative of the corresponding constrained magnetization profile, m_Ξ say, at the position where $m_\Xi=m^X$.

A method of smoothing this discontinuity within the crossing criterion was suggested but not carried out in view of its computational complexity [5]. Instead, other criteria were explored. A natural alternative definition of the wetting layer thickness is the *adsorption* of phase β on the wall. Surprisingly, FJ showed that the integral constraint on the adsorption is insoluble and were led to consider other nonlocal constraints. A different approach was considered by Bukman *et al.*, who allowed magnetization profiles with a discontinuous *second* derivative at $z=\hat{z}$ and imposed $m(\hat{z})=m_{\alpha\infty}$ [8]. Further analysis aimed at minimizing the resulting free energy by varying $m_s\equiv m(\hat{z})$ for fixed adsorption [9]. However, this procedure leads to a trivial minimum independent of l.

Here we propose a soluble constraint that naturally leads to smoother profiles, within the crossing criterion framework. To define the constraint we first choose some fixed magnetization m^X. We are primarily interested in surfaces of fixed magnetization that lie in the interface, typified by $m^X=0$. Second, we define l in the same way that FJ do. However, we do not impose the constraint of fixed l, but leave l to be determined self-consistently by (in general) a different constraint. This *freedom of choice of constraint* is a key tool hitherto not utilized. The constraints we impose are of the form, with q a non-negative integer,

$$\int_0^{\hat{z}(\mathbf{y})}\left[\frac{m(\mathbf{y},z)-m^X}{m_{\beta\infty}-m^X}\right]^q dz=\Gamma^{(q)}(\mathbf{y}) \tag{4}$$

for some fixed $\Gamma^{(q)}$. The upper limit $\hat{z}(\mathbf{y})$ is defined by the crossing criterion so that, for fixed $\mathbf{y}$,

$$\hat{z}\equiv m^{-1}(m^X). \tag{5}$$

We thus obtain a family of constraints parametrized by the exponent q.

We define the collective coordinate $l(\mathbf{y};\Gamma^{(q)})$ as the value of $\hat{z}(\mathbf{y})$ that minimizes the free energy subject to the constraint (4). First consider $q=0$. In this case we see from Eq. (4) that our procedure simply corresponds to fixing $\hat{z}(\mathbf{y})$, which then equals $l(\mathbf{y})$. Consequently, we recover the *local* crossing criterion of FJ. For $q=1$ our constraint is akin to the *integral constraint on the adsorption*, while for $q\to\infty$ we reproduce features of the fixed-wall constraint as employed in [3,4] (see further).

For brevity we restrict our attention to planar magnetization profiles, $m_\pi(z;\Gamma^{(q)})$ say, which for convenience we write as $m(z)$. These profiles are associated with a fixed $\Gamma^{(q)}$ and we now describe how to obtain the profile that solves the free-energy minimization exactly. For later use we note that after minimization, each choice $\Gamma^{(q)}$ corresponds to a unique value of $l\equiv l^{(q)}$. We do not further consider the case $q=0$, which has been extensively treated in [5]. It follows from Eq. (4) that the Euler-Lagrange equation found from minimizing the free energy subject to the generalized constraint is

$$K\frac{d^2m}{dz^2}=\phi'(m)+\Theta(l-z)\lambda q\frac{[m(z)-m^X]^{q-1}}{[m_{\beta\infty}-m^X]^q}, \tag{6}$$

where Θ is the Heaviside step function, λ is a Lagrange multiplier, and primes always denote differentiation with respect to argument. The first integral of Eq. (6) is

$$\frac{K}{2}\left(\frac{dm}{dz}\right)^2=\Delta\phi(m)+\Theta(l-z)\left(\lambda\left[\frac{m(z)-m^X}{m_{\beta\infty}-m^X}\right]^q+E\right), \tag{7}$$

where $\Delta\phi(m)=\phi(m)-\phi(m_{\alpha\infty})$ and E is an integration constant. Note that there is no integration constant in the region $z>l$ by virtue of the bulk condition $m(z)\to m_{\alpha\infty}$ for $z\to\infty$.

Extremization with respect to variations of the wall value m_1 leads to the familiar *boundary condition* $K(dm/dz)|_{z=0}=-h_1-gm_1$. It is important to consider also the variation of the crossing point $\hat{z}$, which leads to the extremality condition that the quantity $G(z)$, defined by

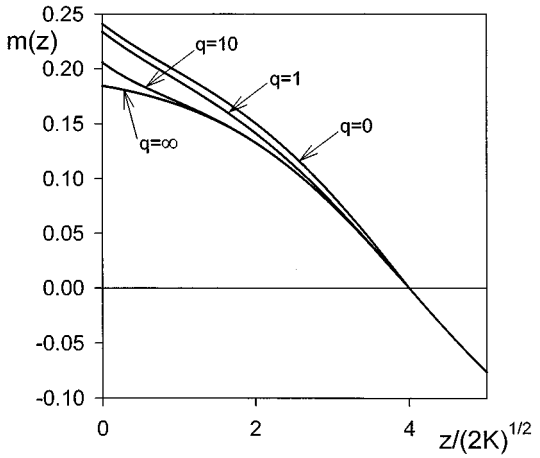

FIG. 1. Comparison of constrained order-parameter profiles $m(z)$ for $q=0$, 1, 10, and ∞. We have taken $m_{\beta\infty}=-m_{\alpha\infty}=0.2$, $\phi=(m-m_{\beta\infty})^2(m-m_{\alpha\infty})^2$, $h_1\approx 0.68\sqrt{2K}m_{\beta\infty}^2$, and $g=0$. For clarity, the value of the constraint $\Gamma^{(q)}$ is chosen so that for each q the same crossing point $l=4\sqrt{2K}$ is obtained. The profile for $q=0$ displays a discontinuous derivative at $m=m^X=0$. In general, $m\in C^q$, with a discontinuous $(q+1)$st derivative at $z=l$. The boundary condition at $z=0$ is satisfied for all *finite* q (see the text). For $q\to\infty$ the profile becomes coincident with the function $m(z)=m_{\alpha\infty}\tanh[m_{\beta\infty}\sqrt{2/K}(z-l)]$, which solves the fixed-wall-value problem.

$$G(z)\equiv\frac{K}{2}\left(\frac{dm}{dz}\right)^2-\Delta\phi(m(z))-\lambda\left[\frac{m(z)-m^X}{m_{\beta\infty}-m^X}\right]^q,$$

be *continuous* at $z=l$. This corresponds to a Weierstrass-Erdmann condition [9]. Utilizing the continuity of $m(z)$ and $G(z)$ at $z=l$ identifies the integration constant $E=0$. Thus we observe from Eq. (7) that the constrained profile will have a continuous first derivative for $q\geqslant 1$, in contrast to the $q=0$ criterion. It follows from Eq. (6) and its derivatives that, provided ϕ is suitably smooth, $m(z)\in C^q$. That is, $m(z)$ and its first q derivatives are continuous everywhere, but the $(q+1)$st derivative has a jump at $z=l$. Consequently, the criterion we have introduced provides a mechanism to smooth, in a controlled manner, the kink enforced by the local crossing criterion.

Furthermore, the $q\to\infty$ limit of the family is reminiscent of, but not identical to, the fixed-m_1 criterion discussed previously [3,4]. To see this consider some fixed wall value, $M_1<m_{\beta\infty}$ say. One can derive the corresponding magnetization profile simply by requiring that $m(z=0)=M_1$ and $m(z\to\infty)\to m_{\alpha\infty}$. The resulting profile $M(z)$ crosses m^X at some location l. Now for a given q we choose in our constraint (4) precisely the $\Gamma^{(q)}$ that ensures $l^{(q)}=l$. For $z>l$ the profiles $m(z;\Gamma^{(q)})$ and $M(z)$ are identical, while for $0<z<l$ one can consider a Taylor expansion of $m(z;\Gamma^{(q)})$ about l. From the discussion above we see that this series will differ from that of $M(z)$ only after $q+1$ terms. Thus, in the limit $q\to\infty$ the regular parts of the two functions have identical Taylor series and we verified numerically (see Fig. 1) that they coincide at all points including at the wall. However, $m(z;\Gamma^{(q)})$ and $M(z)$ have different first derivatives *at* the wall since, in general, $M(z)$ does not satisfy the boundary condition. Thus the $q\to\infty$ limit leads to profiles that are

singular at $z=0$, but smoothly converge to those obtained with the fixed-wall-value constraint for all $z>0$.

Concerning the binding potential $W(l)$, we remark that the constraint of fixed $\Gamma^{(q)}$ naturally leads to a potential as a function of this variable, i.e., $\widetilde{W}(\Gamma^{(q)})$. This potential gives the free-energy minimum for fixed $\Gamma^{(q)}$. Since the exact solution of the free-energy minimization provides a unique value of l for a given value of $\Gamma^{(q)}$, the potential $\widetilde{W}(\Gamma^{(q)})$ leads to an equivalent potential $W^{(q)}(l)$. Note that this function does not give the free-energy minimum for fixed l, except for $q=0$. In fact, for a given l, the values $W^{(q)}(l)$ increase as q is increased. (For simplicity, we will henceforth write W in place of $W^{(q)}$.)

One application of our smoothing procedure is to test the fundamental predictions of the $q=0$ criterion. Any physics that is not common with, for example, the choice $q=1$ cannot be considered robust but rather an artifact of imposing the constraint. First note that because all constraints in the family employ the crossing criterion $m(z=l)=m^X$, the expressions of FJ for $W(l)$ and $\Sigma(l)$ are valid for the effective Hamiltonian derived with any q. In particular, up to l-independent terms

$$W(l)=\int_0^\infty \left\{ \frac{K}{2}\left(\frac{\partial m}{\partial z}\right)^2+\Delta\phi(m)\right\} dz+\phi_1(m_1) \tag{8}$$

and

$$\Sigma(l)=K\int_0^\infty \left(\frac{\partial m}{\partial l}\right)^2 dz, \tag{9}$$

where in each case only planar profiles are involved. Explicit expressions for the binding potential and stiffness coefficient can be calculated within the double-parabola (DP) model used by FJ. Specifically, we consider the case $q=1$ since the DP model automatically forces a singularity in the second derivative of the magnetization profile, due to a discontinuity in $\phi_0'(m)$ [see Eq. (6)] countering the advantage of extra smoothness associated with larger q. We further choose $m^X=0$, allowing a direct comparison with existing $q=0$ results. The DP model, which assumes that $\phi_0(m)$ can be represented in a piecewise parabolic fashion, allows the calculation of (planar) magnetization profiles $m(z;l)$ by solving Eq. (6) in the regions $z>l$ and $z<l$. Expressions for $W(l)$ and $\Sigma(l)$ are found from substituting $m(z;l)$ into Eqs. (8) and (9), respectively.

Here we present a summary of our results in the limit $l\to\infty$. For $W(l)$ we find

$$W(l)=\overline{h}l+\sum_{m=1}^{\infty}\sum_{n=0}^{m} w_{mn}(\kappa l)^n e^{-m\kappa l}, \tag{10}$$

where $-\overline{h}\propto h$. The leading-order coefficients w_{mn} are

$$\begin{aligned} w_{10}(T,h,h_1,g)&=2K\kappa m_{\beta\infty}\tau+O(h),\\ w_{20}(T,h,h_1,g)&=K\kappa\mathcal{G}m_{\beta\infty}^2+O(h,\tau^2),\\ w_{11}=O(h),\quad w_{21}&=O(h,\tau^2),\quad w_{22}=0, \end{aligned} \tag{11}$$

while $\tau=(h_1+gm_{\beta\infty})/(K\kappa-g)\propto T-T_W$ and $0<\mathcal{G}=(g+K\kappa)/(g-K\kappa)<1$. These results agree precisely with those found for $q=0$ in this model up to terms of $O(h,\tau^2)$. The key feature is that (for $h\to 0-$) the leading term w_{10} vanishes at mean-field wetting criticality, while w_{20} remains positive. We also note the presence of nonpure exponential contributions in $W(l)$ already at the level of the DP approximation.

For the stiffness coefficient we find a similar expansion

$$\Sigma(l)=\Sigma_\infty+\sum_{m=1}^{\infty}\sum_{n=0}^{m} s_{mn}(\kappa l)^n e^{-m\kappa l}, \tag{12}$$

where Σ_∞ is as defined earlier. The coefficients s_{mn} are

$$\begin{aligned} s_{10}(T,h,h_1,g)&=2K\kappa m_{\beta\infty}\tau+O(h),\\ s_{20}(T,h,h_1,g)&=K\kappa m_{\beta\infty}^2(\mathcal{G}^2+10\mathcal{G}-1)/2+O(h,\tau),\\ s_{21}=-2K\kappa\mathcal{G}m_{\beta\infty}^2+O(h,\tau),&\quad s_{11}=0,\quad s_{22}=0. \end{aligned} \tag{13}$$

Again these results are in close agreement with the $q=0$ analysis, with the two leading terms s_{10} and s_{21} matching identically up to $O(h)$. Of particular importance is the fact that at critical wetting the dominant contribution arises through s_{21}, which is negative and of order unity. This term leads to the so-called stiffness instability mechanism through which, under renormalization, a (bare) critical wetting transition may be driven weakly first order [5]. That is, under renormalization the presence of a term of $O(le^{-2\kappa l})$ in the stiffness expansion is found to destabilize the critical wetting transition. A recent nonlinear renormalization-group study strongly suggests that in three dimensions the transition *is* driven weakly first order for values of the stiffness strength s_{21} predicted from the $q=0$ analysis [10]. The above observation that s_{21} remains unchanged for $q=1$ implies that the same prediction of a fluctuation-induced first-order transition is appropriate with this criterion.

More generally, the existence of nonpure exponential contributions to the stiffness has been shown to be a vital ingredient in obtaining a thermodynamically consistent theory of correlation functions [11,6]. That analysis was based upon the $q=0$ criterion, but from the above we may anticipate that identical thermodynamically consistent results would be found using any member of our family of constraints. We conclude by showing that this is indeed the case.

An important success of the $q=0$ criterion has been the ability to rederive known mean-field expressions for the order-parameter correlation function $\mathcal{G}(\mathbf{r}_1,\mathbf{r}_2)=\langle m(\mathbf{r}_1)m(\mathbf{r}_2)\rangle_c$. From translational invariance this depends only on the normal distances z_1 and z_2 and relative parallel separation $|\mathbf{y}_{12}|$. Consequently, it is convenient to define the transverse structure factor and its moment expansion

$$\widetilde{\mathcal{G}}(z_1,z_2;Q)=\int d\mathbf{y}_{12}e^{iQy_{12}}\mathcal{G}(\mathbf{r}_1,\mathbf{r}_2)=\Sigma_{n=0}^{\infty}\widetilde{\mathcal{G}}_{2n}(z_1,z_2)Q^{2n}.$$

For the discussion presented here we restrict our attention to the zeroth moment $\widetilde{\mathcal{G}}_0(z,z)$. The mean-field expression for $\widetilde{\mathcal{G}}_0(z_0,z_0)$ can be derived from an interfacial Hamiltonian defined through a $q=0$ crossing constraint provided the ref-

erence value m^X is chosen such that $m^X = \check{m}(z=z_0)$, where $\check{m}(z)$ is the equilibrium magnetization profile found from minimizing the bulk Hamiltonian with no constraint on l [11]. The result is

$$\widetilde{\mathcal{G}}_0(z_0,z_0;m^X=\check{m}(z_0)) = \frac{\check{m}'(z=z_0)^2}{W''(l=z_0;m^X)}, \qquad (14)$$

where we have highlighted the implicit m^X dependence. The fundamental reason why at $q=0$ this expression recovers the known result is that for the choice of l involved ($l=z_0$) the planar magnetization profile is identically the equilibrium profile $\check{m}$ (which, recall, is everywhere smooth).

For $q>0$ a similar derivation leading to the formal expression (14) holds. Indeed, if we denote the equilibrium position of the surface of fixed magnetization m^X by $\check{l}$ and define $\check{\Gamma} = \int_0^{\check{l}} [\check{m}(z)-m^X]^q/[m_{\beta\infty}-m^X]^q dz$, then imposing the choice $\Gamma^{(q)}=\check{\Gamma}$ must, by consistency, yield the equilibrium profile, i.e., $m_\pi(z;\check{\Gamma})=\check{m}(z)$. As a result, provided we again make the local choice for the reference magnetization $m^X=\check{m}(z_0)$, the contribution of the binding potential to $\widetilde{\mathcal{G}}_0(z_0,z_0)$ is only dependent upon $\check{m}(z)$. In fact, in each case the appropriate constrained profile that is used to calculate the zeroth moment is exactly the equilibrium profile. Since the definition (8) for the binding potential has no explicit q dependence it follows that the local curvature $W''(l=z_0;m^X)$ is independent of q. Hence $\widetilde{\mathcal{G}}_0(z_0,z_0)$ is correctly derived via the interface Hamiltonian approach *with any choice of* q. Similar considerations apply to the higher moments of $\mathcal{G}$.

In conclusion, we have shown that the use of integral constraints within the crossing criterion $m(z=l)=m^X$ allows us to obtain order-parameter profiles of any desired smoothness. The key consideration is to split the crossing criterion into two steps. The first is the *definition* of l, given fixed m^X. The second is the *choice of constraint* that determines l self-consistently. This constraint need not be that of fixing l, but may be nonlocal. This freedom allows us to obtain a one-parameter family of soluble constraints.

As an application we have verified that the stiffness instability mechanism and the correlation function reconstruction scheme, previously derived using one particular constraint ($q=0$), are robust under a change of constraint from local to integral type.

The family of constraints provides a scheme in which the local constraint of FJ ($q=0$), the integral constraint *related to* fixed adsorption ($q=1$), and the constraint *reminiscent of* the traditional approach of Brézin *et al.* and Lipowsky *et al.* ($q\to\infty$) are brought together. From a laboratory viewpoint it is satisfactory that the adsorption is now involved in the framework of a soluble constraint. It is interesting that a preference for working with *differentiable* profiles can be met by the use of this constraint ($q=1$). We remark that for $q=1$ the approach of Bukman *et al.* [8] is reproduced for the special choice $m^X=m_{\alpha\infty}$ [12]. If, with this choice of m^X, we furthermore take the limit $\hat{z}(\mathbf{y})\to\infty$ in the integral in Eq. (4), we recover the insoluble constraint of fixed adsorption.

In practice, for smoothing the singularity in the interface arising from the local crossing criterion $q=0$ it is sufficient to work with $q=1$ or 2 since already for $q=1$ the profile appears smooth to the eye. On the other hand, large values of q are also interesting because they can be employed to smooth the $q=\infty$ singularity at the wall. Therefore, the high-q members of the family provide a means of reconciling the profiles of [3,4] with the boundary condition at the wall.

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