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Effect of Roughness Differences on the Unbinding of Interfaces[1]

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In recent years there has been considerable interest in the effect of disorder on the nature and universality of wetting transitions. One of the most frequently studied systems is that in which geometrical disorder is present in the form of substrate roughness. In $2D$ there is compelling evidence that the critical wetting transition found for a flat substrate may become first order when surface roughness is included. In particular, if the roughness exponent of the wall exceeds the anisotropy index of interface fluctuations in the bulk, then first-order wetting is found. Here we extend the investigation of roughness-induced effects to the situation in which we have unbinding of two fluctuating interfaces characterized by different roughness exponents ζ_1 and ζ_2 (e.g., a fluid membrane depinning from a liquid–vapor interface) in the absence of quenched disorder. In this case symmetry prevents a change in order of the unbinding transition as the roughnesses are varied; however, the critical behavior is again found to be controlled by the larger of ζ_1 and ζ_2. In addition, our results depend quantitatively on a nonuniversal parameter related to the relative curvature of the two interfaces whenever $\zeta_1 \neq \zeta_2$.

KEY WORDS: fluctuating interfaces; roughness; unbinding transitions.

1. INTRODUCTION

In this paper we present the results of an analytic study into the effect of relative roughnesses on the nature and universality of the unbinding transition between two fluctuating interfaces in three dimensions. This study is

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motivated by intriguing recent results on the importance of geometric disorder in $2D$ upon the critical wetting transition [1–3], and hence, we begin by providing a brief summary of the pertinent results of those studies here.

The wetting transition refers to the situation in which an interface between two coexisting phases unbinds from an attractive substrate. The transition may be continuous (or *critical*) or first-order depending on the dimensionality, disorder, and strength of the substrate forces. For the moment we consider the case of short-range substrate forces in $2D$, for which it is known that generally only continuous wetting transitions are predicted both in the absence of disorder and in the presence of bulk disorder (for a review, see Ref. 4). The results which interest us arise when geometrical disorder is present via the inclusion of a rough substrate with self-affine geometry, as has been observed in experimental situations [5]. The roughness is characterized by the exponent ζ_W such that transverse displacements of the wall profile, denoted l_W, have an average width $\overline{|l_W(x) - l_W(x')|} \propto |x - x'|^{\zeta_W}$ with $0 < \zeta_W < 1$. A bulk interface is known to display a similar scaling with roughness, or anisotropy exponent ζ_0—in $2D$, $\zeta_0 = \frac{1}{2}$ if the bulk is ordered and $\zeta_0 = \frac{2}{3}$ in the case of random bonds in the bulk [4].

Direct competition between the roughnesses of the wall and the fluctuating interface has led to the prediction of roughness induced first-order wetting transitions. In particular, numerical studies based on transfer matrix calculations for a model on a square lattice have shown that the wetting transition in a pure system is first-order for ζ_W sufficiently larger than $\frac{1}{2}$ but remains continuous and in the same universality class as the flat-wall case for low enough values of ζ_W [1]. Similar results have been found in the presence of bulk disorder with first-order wetting if ζ_W exceeds $\frac{2}{3}$ and critical wetting when $\zeta_W < \frac{2}{3}$ [2]. This behavior has been further elucidated using replica and functional renormalization group methods, where analysis of the fixed points clearly indicates that the crossover from continuous to first-order wetting occurs precisely at a threshold given by ζ_0 [3].

It is interesting to speculate whether the same behavior holds in $3D$, where for a pure system $\zeta_0 = 0$ so that any surface roughness (which would surely be present in an experimental system) would lead to first-order transitions. The studies described above cannot be easily extended to the $3D$ case, so in this paper we consider the related phenomena of the unbinding of two fluctuating interfaces in $3D$ to gauge the importance of roughness effects. The remainder of the paper is arranged as follows. In Section 2 we introduce our two-interface model and briefly present a functional renormalization group treatment which we analyze analytically and numerically. Section 3 is dedicated to conclusions and future avenues of research.

2. UNBINDING OF TWO FLUCTUATING INTERFACES

2.1. Background

We consider the case of two interfaces unbinding in a d-dimensional system in the absence of bulk disorder. The location of the interfaces is denoted by $l_i(\mathbf{x})$, $i=1,2$, where $\mathbf{x}$ represents the $d-1$ directions in a plane approximately parallel to the interfaces. Ignoring interface overhangs, we can describe this situation using an effective Hamiltonian,

$$\mathscr{H}[l_1, l_2] = \int \mathrm{d}\mathbf{x} \{ \tfrac{1}{2} K_1 (\nabla^{\beta_1} l_1)^2 + \tfrac{1}{2} K_2 (\nabla^{\beta_2} l_2)^2 + U(l_2 - l_1) \} \tag{1}$$

where the β_i are related to the anisotropy exponent of the relevant interface via the relationship $(\beta_i - \zeta_i) = (d-1)/2$, $i=1,2$. For example, for a pure system a simple fluid interface is characterized by $\beta=1$ [or $\zeta=(3-d)/2$], while a tensionless membrane has $\beta=2$ [or $\zeta=(5-d)/2$]. The K_i are stiffness or rigidity coefficients, and the potential $U(l_2-l_1)$ models the interactions of the two interfaces. A further interaction term describing the coupling of corrugations of the two interfaces may also be included. This can be incorporated into Eq. (1) via the inclusion of a term $K_3(\nabla^{\beta_1} l_1) \cdot (\nabla^{\beta_2} l_2)$ in the Hamiltonian density; however, the relevant stiffness coefficient (K_3) must be zero since the two interfaces completely decouple in the limit of $l_2 - l_1 \to 0$. If one allows position-dependent contributions in the stiffness coefficients (which is beyond the scope of this paper), then K_3 should no longer be ignored, and one may anticipate that its inclusion may tend to drive the unbinding transition first-order [6].

In this study of unbinding it is the relative displacement $l_2 - l_1$ which is of interest, and so we aim to introduce a linear transformation which will isolate the behavior of the interfacial separation from the remaining coordinates. To this end we rewrite the kinetic (or gradient) terms in Eq. (1) using a momentum space representation,

$$\mathscr{H}_t[l_1, l_2] = \int \frac{\mathrm{d}\mathbf{p}}{(2\pi)^{d-1}} \left\{ \frac{1}{2} K_1 p^{2\beta_1} |\tilde{l}_1(\mathbf{p})|^2 + \frac{1}{2} K_2 p^{2\beta_2} |\tilde{l}_2(\mathbf{p})|^2 \right\} \tag{2}$$

where we use tildes to denote a Fourier-transformed function. In this formulation we identify the appropriate linear transformation [7]

$$\begin{aligned} \tilde{l}_1(\mathbf{p}) &= \tilde{L}(\mathbf{p}) - \frac{K_2 p^{2\beta_2}}{K_1 p^{2\beta_1} + K_2 p^{2\beta_2}} \tilde{l}(\mathbf{p}) \\ \tilde{l}_2(\mathbf{p}) &= \tilde{L}(\mathbf{p}) + \frac{K_1 p^{2\beta_1}}{K_1 p^{2\beta_1} + K_2 p^{2\beta_2}} \tilde{l}(\mathbf{p}) \end{aligned} \tag{3}$$

where $l \equiv l_2 - l_1$, and the new coordinates l and L are completely separated in the effective Hamiltonian. We observe that for two identical interfaces (when $\beta_1 = \beta_2$), the transformation [Eq. (3)] reduces to that found in the study of binary mixtures, where L may be identified as the "center of mass" coordinate [8]. Upon integrating out this coordinate, we are left with an effective interface model for the interfacial separation of the form

$$\mathscr{H}[l] = \int \frac{\mathrm{d}\mathbf{p}}{2(2\pi)^{d-1}} \left\{ \frac{K_1 p^{2\beta_1}}{[1 + (K_1/K_2)\, p^{2(\beta_1 - \beta_2)}]} |\tilde{l}(\mathbf{p})|^2 \right\} + \int \mathrm{d}\mathbf{x} \{ U(l) \} \tag{4}$$

Without loss of generality, we, henceforth, assume that $\beta_1 \geqslant \beta_2$ and define

$$\varepsilon = \beta_1 - \beta_2 \geqslant 0 \tag{5}$$

as a measure of the relative roughness difference of the two interfaces. A typical example would be the unbinding of a fluid membrane ($\beta_1 = 2$) from a liquid–vapor interface ($\beta_2 = 1$ and hence $\varepsilon = 1$) in $d = 3$ as is observed in the preparation of membranes for biological applications. However, we need not restrict ourselves to a specific value of ε at this stage.

2.2. The Functional Renormalization Group

In this section we apply the techniques of the functional renormalization group (RG) to analyze the unbinding behavior in our model [4, 9]. Here we provide only a sketch of the main ideas and results; a more detailed treatment is given in Ref. 7.

First, we note that the effective model [Eq. (4)] contains an implicit momentum cutoff, e.g., Λ. The RG procedure consists of integrating out Fourier modes of the field l with wave numbers in the range $\Lambda/b < |p| < \Lambda$ for some $b > 1$ and then rescaling $x \to bx$ to bring the cutoff back to its original value. In addition, we must rescale l in such a way that the RG transformation can reach a fixed point. Typically the scaling factor is simply the anisotropy exponent, but in our system this is not uniquely defined and some care is required. Analysis shows that to avoid the presence of a dangerous irrelevant variable [10] in the scheme, we must use the rescaling $l \to l b^{\zeta_1}$ [7]. With this rescaling in place, the stiffness K_1 is an invariant under the RG transformation, while K_2 is subject to the following flow equation ($b = e^t$):

$$\frac{\mathrm{d}\ln(K_2)}{\mathrm{d}t} = 2\varepsilon \tag{6}$$

The growth of K_2 under RG flow is not a deficiency of the approach since, as we shall see, this parameter appears only in the combination $1/K_2$ in the analysis that follows.

The flow of K_2 is coupled with that of the interface potential $U(l)$. In particular, if we work only to first-order in U, then we can perform an exact linear functional RG which yields the flow equation

$$\frac{\partial U}{\partial t} = (d-1)\, U + \zeta_1 l \frac{\partial U}{\partial l} + \Omega \left(\frac{1}{K_1} + \frac{\Lambda^{2\varepsilon}}{K_2} \right) \frac{\partial^2 U}{\partial l^2} \tag{7}$$

where $\Omega = \Lambda^{-2\zeta_1}/[(4\pi)^{(d-1)/2}\, \Gamma((d-1)/2)]$. At this stage we can already deduce some key features of the unbinding behavior. First, we note that in the limit of large t which is appropriate for considering fixed point behavior, the factor $1/K_2 \to 0$ and the flow equation (7) reduces to that found when considering the unbinding of a fluctuating interface (with stiffness K_1 and anisotropy exponent ζ_1) from a planar wall (see, e.g., Refs. 4 and 11). Consequently we might reasonably expect critical behavior in the same universality class as that of unbinding from planar substrates.

The dominance of ζ_1 over ζ_2 is a direct consequence of the assumption $\varepsilon > 0$ [recall Eq. (5)]. If instead $\beta_2 > \beta_1$, then a similar analysis would result in the unbinding behavior being controlled by the properties of interface "2." Hence, in general, the important anisotropy exponent for the transition is $\max(\zeta_1, \zeta_2)$, in complete analogy with unbinding from rough surfaces discussed earlier. This behavior is also the one suggested by physical intuition since the anisotropy exponent of the relative coordinate $l = l_2 - l_1$ must be dominated by $\max(\zeta_1, \zeta_2)$.

To provide a more quantitative analysis, it is convenient to also discuss the RG transformation beyond linear order in the interface potential. Such schemes are approximate and a number of variations are possible but here we concentrate on the nonlinear functional RG developed by Lipowsky and Fisher [11] based on Wilson's approximation scheme of expanding the fast modes in the fluctuating field in terms of a complete set of localized wavefunctions. This approach has proved to be particularly well suited to treating interface problems (see also Ref. 12).

We leave aside the details of the calculation here (these can be found in Ref. 7) and concentrate on the main results. The flow equation [Eq. (6)] is accurate to all orders and is now supplemented by the following equation for the renormalized binding potential:

$$\frac{\partial U}{\partial t} = (d-1)\, U + \zeta_1 l \frac{\partial U}{\partial l} + \Omega \Lambda^{2\beta_1} \ln \left[1 + \frac{1}{\Lambda^{2\beta_1}} \left(\frac{1}{K_1} + \frac{\Lambda^{2\varepsilon}}{K_2} \right) \frac{\partial^2 U}{\partial l^2} \right] \tag{8}$$

where Ω is the constant given after Eq. (7). Once again, we observe that, for large t, the inverse stiffness $1/K_2 \rightarrow 0$ and the flow equation for U reduces to that found when studying the unbinding of an interface (with roughness exponent ζ_1 and stiffness K_1) from a flat substrate [11]. Hence the fixed-point potentials of the two systems must be the same.

However, we stress that this observation is *not sufficient* to determine the critical behavior. For example, for wetting in a system with short-range forces, it has been demonstrated that there exists a large class of fixed-point potentials [13] (the precise number depending on the dimensionality of space) but that typically only three have attractive manifolds: one describing pinned interface situations, one for the wet regime with unbound interfaces, and one between the domains of attraction of the previous two, describing the transition-point behavior. Most notably, ignoring position-dependent stiffness coefficients, this intermediate fixed-point potential always describes critical wetting if the initial (bare) potential models a continuous transition, and hence no fluctuation-induced first-order transitions can be predicted. In contrast, a recent study [12] has demonstrated that if an extra parameter representing an additional stiffness contribution is included in the RG flow, then additional fixed point potentials may have attractive manifolds. This occurs even though the additional parameter flows to zero and the binding potential flow equation reduces to its standard form for large t, just as we observe in the present study. Importantly, the outcome of the additional fixed points is a completely revised picture for the critical behavior with first-order wetting being observed.

Hence, it is clear that we must consider the transient behavior in the RG flow and not rely solely on the large-t behavior. Thus we present a more thorough investigation in the next subsection to determine properly the critical behavior when fluctuation effects are included.

2.3. Numerical Study

To study the RG flow numerically, it proves convenient to use the RG recursion relations for a fixed rescaling parameter b, rather than the flow equations, (6) and (8). Furthermore, because of the simple nature of the flow of K_2, it is straightforward to solve for this parameter analytically, and hence we need study only the recursion relation for the binding potential numerically. Finally, we introduce dimensionless variables via a simple rescaling [7] such that z represents the dimensionless interface separation, and $V(z)$ the dimensionless interface potential. With these variables the recursion relation takes the form [7]

$$V^{(N+1)}(z) = -b^{d-1} \ln\left[\frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\mathrm{d}y}{\sqrt{1+\mathscr{X}(b,N,d)}} \exp\left(\frac{-y^2}{1+\mathscr{X}(b,N,d)} \right) \right.$$
$$\left. \times \exp\left(\frac{-V^{(N)}(b^{\zeta_1}z+y) - V^{(N)}(b^{\zeta_1}z-y)}{2} \right) \right] \tag{9}$$

where we have introduced the nonuniversal function

$$\mathscr{X}(b,N,d) = \frac{K_1 \zeta_1 \Lambda^{2\varepsilon}}{K_2^{(0)} \zeta_2 b^{2\varepsilon N}} \left(\frac{b^{2\zeta_2}-1}{b^{2\zeta_1}-1} \right) \tag{10}$$

with $K_2^{(0)}$ being the initial bare value of K_2, and where the dimension dependence is implicit in the exponents ζ_i.

For concreteness here we specialize to the case $d=3$ and consider the situation of a fluid interface unbinding from a membrane as discussed earlier. Thus $\varepsilon=1$, $\zeta_1=1$, and $\zeta_2=0$, and the parameter $\mathscr{X}$ reduces to $\mathscr{X}_{m-i}(b,N) = [2K_1\Lambda^2/K_2^{(0)}]/[\ln b/(b^{2N}(b^2-1))]$. We compare this situation with the cases of a membrane with rigidity K_1 unbinding from a planar wall and two membranes, each of rigidity K_1, unbinding from one another. In both situations the RG flow is also modeled by the recursion relation, Eq. (9), but in the first case $\mathscr{X} \equiv \mathscr{X}_{m-w}(b,N)=0\ \forall N$, while in the second case $\mathscr{X} \equiv \mathscr{X}_{m-m}(b,N)=1\ \forall N$. Here, we take $K_1\Lambda^2/K_2^{(0)}=1$ (which is reasonable as an order-of-magnitude estimate), and hence, $\mathscr{X}_{m-i}(b\approx 1,N)$ interpolates between the two reference cases, starting at unity and reducing to zero for large N.

In addition, we restrict our attention to the case of a bare potential which is strictly short-range and assume for $z \geqslant 0$,

$$V^{(0)}(z) = -we^{-sz} + e^{-2sz} \tag{11}$$

although the qualitative details of our results are unaffected by varying the form of the short-range potential [7]. Here w is a measure of the deviation from the mean-field unbinding temperature $w \propto T_u^{MF} - T$, and $s>0$. We further impose a “hard-wall” condition ($V(z<0)=\infty$) so that the interface and membrane cannot pass through one another. For our numerical study we have typically fixed the rescaling parameter to the value $b=2$, but we note that we have checked that the results described below are robust to other choices of b in the range $1.25 \leqslant b \leqslant 4$.

To study the model, we vary the initial parameters w and s in the potential and examine the development of $V(z)$ under the recursion relation, Eq. (9). The unbinding phase boundary is the locus of intermediate (unstable) fixed points which separates the stable regions governed by the “pinned interfaces" and "unbound interfaces" fixed points. We find that the transition *always remains second-order* with an unbinding temperature, T_u^{m-i}, shifted below T_u^{MF}. Furthermore, the unbinding temperature lies between that for the two reference cases (assuming that all transitions have the same mean-field unbinding temperature) such that $T_u^{m-m} < T_u^{m-i} < T_u^{m-w}$, and hence, the presence of additional roughness appears to aid the unbinding process and lower the transition temperature (see also Section 3).

Finally, we have examined the critical exponent governing the unbinding behavior using a numerical eigenperturbation analysis about the transitional fixed point [7]. We find strong evidence for an inverse linear relationship, in particular, we obtain $l \sim |T_u^{m-i} - T|^{-\psi}$ and $\psi = 0.99 \pm 0.02$ on the approach to unbinding. The same exponent is found for our reference cases, suggesting that all the transitions are in the same universality class when one considers purely short-range forces. Furthermore, Lipowsky and Leibler [14] find precisely the same result, $\psi \approx 1$, in their study of membrane–membrane unbinding of both charged and uncharged membranes, where long-range van der Waals forces have been included, indicating that the membrane anisotropy exponent ζ may play a particularly dominant role in determining the critical behavior in these systems.

3. DISCUSSION AND GENERALIZATIONS

In this paper we have applied RG techniques to study unbinding of two interfaces characterized by different roughness exponents. We have observed that the important parameter for describing the transition is the maximum roughness exponent. However, we have found no evidence for roughness-induced first-order transitions analogous to those found for unbinding from a rough substrate. This is almost certainly related to the extra symmetry in considering two fluctuating surfaces in comparison to one fluctuating and one fixed surface.

For simplicity we have concentrated on systems with purely short-range forces and shown that the behavior of a membrane unbinding from a fluid interface is, in some sense, intermediate between a membrane unbinding from a flat substrate and a membrane unbinding from another membrane. However, this result is sensitive to the value of the nonuniversal ratio $K = K_1 \Lambda^2 / K_2^{(0)}$. For $0 < K \leqslant 1$ the scenario above holds, while for $K \gg 1$ the transition temperature of the membrane–interface transition is lowered below that of the membrane–membrane transition (numerically the crossover seems likely to occur at $K \approx 1$, although the precise value has not been determined). Hence, the sequence of unbinding transitions that one would observe for a stack of membranes pinned at a liquid–vapor interface, as the temperature is increased, would be highly sensitive to this nonuniversal ratio. Prior to comparison with experimental results, however, it will be necessary to consider the wide range of longer-range interactions which may be present (see, e.g., Ref. 15).

Future work will be targeted at extending the analysis to unbinding of an interface of arbitrary roughness from a rough substrate in dimensions $d > 2$. Treatment of a self-affine substrate have proved problematic, but we are confident that the introduction of a deterministic rough substrate will allow progress to be made in this area.

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