

LETTER TO THE EDITOR

Intermediate fluctuation regime for wetting transitions in two dimensions

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Abstract. The intermediate fluctuation regime for wetting transitions is studied for $(1+1)$ -dimensional systems. This regime is found to consist of three different subregimes resulting from the competition between the short-range part and the long-range part of the direct interaction between the interfaces. In subregime A, the short-range part is irrelevant, which leads to a wetting transition of infinite order. In subregime B, both parts are relevant and the critical behaviour is non-universal. In these two subregimes, all critical singularities can be expressed in terms of a single length scale. This scaling breaks down in subregime C for which the interfacial fluctuations are strongly non-Gaussian.

The critical behaviour at wetting can be understood in terms of the effective interactions between the two interfaces bounding the wetting layer (for a review, see Fisher 1986). Two types of interactions can be distinguished: (i) direct interactions, V , between two planar interfaces which arise from the microscopic forces between the molecules or atoms and (ii) fluctuation-induced interactions, V_{FL} , arising from the roughness of the interfaces. The competition between these two types of interactions leads to various scaling regimes (Lipowsky and Fisher 1987 and references therein). Apart from a mean-field regime, two regimes have been studied in which the critical behaviour is governed by the interfacial fluctuations: (i) a weak fluctuation (wFL) and (ii) a strong fluctuation (sFL) regime. In this letter, we investigate a third fluctuation regime which lies at the borderline between the wFL and sFL regimes. Within this intermediate fluctuation (iFL) regime, we determine three different subregimes for space dimensionality $d = 2 = 1 + 1$: (i) subregime A consisting of wetting transitions of infinite order; (ii) subregime B for which the wetting transition is of second order but characterised by non-universal critical behaviour with parameter-dependent critical exponents and (iii) subregime C which has rather unusual critical properties: on the one hand, the interfacial fluctuations are strongly non-Gaussian and lead to an infinite number of distinct critical exponents, and, on the other hand, the interfacial energy is discontinuous which usually implies a first-order transition.

First, consider two planar interfaces with constant separation l . Their direct interaction, $V(l)$, typically contains both an attractive and a repulsive part. Furthermore, these parts may consist of short-range and long-range contributions. Now, the fluctuations or undulations of these interfaces can be characterised by their roughness, ξ_{\perp} . This gives rise to the fluctuation-induced repulsion, $V_{FL}(\xi_{\perp})$, with $V_{FL}(\xi_{\perp}) \sim 1/\xi_{\perp}^2$ for

$d = 2$ (Prokovsky and Talapov 1980). Then the mean-field and the wFL regimes in $d = 2$ are defined by (Lipowsky and Fisher 1986a)

$$1/\xi_{\perp}^2 \ll |V(l)| \quad \text{for large } l \sim \xi_{\perp}. \quad (1)$$

In this case, the interfaces undergo a discontinuous or a continuous unbinding transition if the tails of $V(l)$ are repulsive or attractive, respectively (Kroll *et al* 1985, Zia *et al* 1987). In the latter case, the associated critical behaviour is, in fact, determined by the long-range attraction. In contrast, one has

$$|V(l)| \ll 1/\xi_{\perp}^2 \quad \text{for large } l \sim \xi_{\perp} \quad (2)$$

for the sFL regime in $d = 2$ (Lipowsky and Fisher 1986a). Then the unbinding transition is always continuous (Kroll *et al* 1985, Zia *et al* 1987) and the critical behaviour is governed by a non-trivial renormalisation group fixed point (Lipowsky and Fisher 1986b, 1987) for which the long-range tails of $V(l)$ represent an irrelevant perturbation.

In the iFL regime, studied here,

$$V_{\text{FL}}(\xi_{\perp}) \sim 1/\xi_{\perp}^2 \sim |V(l)| \quad \text{for large } l \sim \xi_{\perp}. \quad (3)$$

As shown below, both the long-range part and the short-range part of $V(l)$ can now affect the critical behaviour. If the short-range part of $V(l)$ is irrelevant, the wetting transition is of infinite order. On the other hand, if the short-range part is relevant the critical behaviour is found to be non-universal.

To proceed, introduce cartesian coordinates x and z and consider two interfaces which are, on average, parallel to the x axis. Their local separation is denoted by $l(x)$. As usual, only interfacial configurations without overhangs will be taken into account. Then, the effective Hamiltonian, \mathcal{H} , has the generic form (Lipowsky and Fisher 1987 and references therein)

$$\mathcal{H}\{l\} = \int dx \left[\frac{1}{2} \tilde{\Sigma} (\nabla l)^2 + V(l) \right] \quad (4)$$

where $\tilde{\Sigma}$ is the effective interfacial stiffness and $V(l)$ is the direct interaction between the interfaces. A high-momentum cutoff, Λ , is implicitly contained in (4).

One may now use the usual rules of statistical mechanics in order to express thermodynamic quantities and expectation values in terms of Feynman path integrals. In $d = 1 + 1$, as studied here, l depends only on one spatial coordinate and these path integrals can be evaluated via transfer matrix methods. For finite small-distance cutoff $1/\Lambda$, one has to determine the eigenvalues and eigenfunctions of the transfer matrix from an integral equation (e.g. Burkhardt 1981). In the limit $1/\Lambda \rightarrow 0$, this integral equation reduces to the Schrödinger-type equation (e.g. Kroll and Lipowsky 1983)

$$\left\{ -\frac{1}{2} [(k_{\text{B}} T)^2 / \tilde{\Sigma}] \partial^2 / \partial l^2 + V(l) \right\} \phi_n(l) = E_n \phi_n(l). \quad (5)$$

In the following, we will focus on a specific interaction within the iFL regime defined by (3). This interaction is given by

$$V(l) = \begin{cases} \infty & l < 0 \\ -U & 0 < l < l_0 \\ -W/l^2 & l_0 < l \end{cases} \quad (6)$$

The special case $U = -\infty$ has been studied before (Kroll and Lipowsky 1983, Chui and Ma 1983). For $W < 0$ and $U > 0$, some scaling relations between the critical exponents have been obtained previously (Zia *et al* 1987). In this letter, we will

determine the global phase diagram in the (W, U) plane, show that the critical behaviour exhibits three different subregimes and determine the critical exponents within the various regimes.

In order to simplify the notation, let us introduce the rescaled variables $z \equiv l/l_0$, $u \equiv 2\tilde{\Sigma}l_0^2 U/(k_B T)^2$, $w \equiv 2\tilde{\Sigma}W/(k_B T)^2$ and the rescaled energies $\varepsilon_n \equiv 2\tilde{\Sigma}l_0^2 E_n/(k_B T)^2$. Then the Schrödinger-type equation (5) becomes

$$[-\partial^2/\partial z^2 + v(z)]\phi_n(z) = \varepsilon_n\phi_n(z) \tag{7}$$

with

$$v(z) = \begin{cases} \infty & z < 0 \\ -u & 0 < z < 1 \\ -w/z^2 & 1 < z. \end{cases} \tag{8}$$

Within the transfer matrix formalism, the unbinding of the interfaces is given by the unbinding of the ground state, ϕ_0 , which undergoes a transition from a bound to a scattering state. The ground-state energy, ε_0 , is obtained from the usual matching condition that $\phi_0(z)$ and $\partial\phi_0/\partial z$ are continuous at $z = 1$. It is convenient to distinguish two cases: (i) $-\infty < w \leq \frac{1}{4}$ and (ii) $\frac{1}{4} < w < \infty$.

First, consider the case $w \leq \frac{1}{4}$. Then, the ground-state energy ε_0 is found to vanish along the phase boundary $u = u_c(w)$ which is given by

$$S(u_c) \equiv \sqrt{u_c} \cot(\sqrt{u_c}) - \frac{1}{2} = -(\frac{1}{4} - w)^{1/2}. \tag{9}$$

This implies $u_c(w) \approx \pi^2$ for $w \rightarrow -\infty$ and $u_c(0) = \frac{1}{4}\pi^2$. As $w \rightarrow \frac{1}{4}^-$, the critical value $u_c(w)$ approaches the limit $u_c(\frac{1}{4}) = u_{mc} = 1.358$. This locus of the phase boundary corresponds to a multicritical point (see (19) below). In the vicinity of the transition line given by (9), the ground-state energy behaves as

$$|\varepsilon_0| \sim \begin{cases} \exp(C/\Delta u) & \text{for } \mu = 0 \\ \Delta u^{1/\mu} & \text{for } 0 < \mu < 1 \\ \Delta u/|\ln \Delta u| & \text{for } \mu = 1 \\ \Delta u & \text{for } \mu > 1 \end{cases} \tag{10}$$

with $\mu \equiv (\frac{1}{4} - w)^{1/2}$ as $\Delta u \equiv u - u_c(w) \rightarrow 0^+$ while $\varepsilon_0 = 0$ for $\Delta u < 0$. The second case includes the situation without long-range forces for which $w = 0$ and $\mu = \frac{1}{2}$.

Next, consider $w > \frac{1}{4}$. In this case, we used the procedure described by van Haering (1978). As a result, the asymptotic behaviour is found to be

$$\ln(q/2) \approx \begin{cases} -\pi n/\lambda - \gamma + 1/S(u) & \text{for } u \neq u_{mc} \\ -(\pi/\lambda)(n - \frac{1}{2}) - \gamma & \text{for } u = u_{mc} \end{cases} \tag{11}$$

$$\tag{12}$$

with $q \equiv |\varepsilon_0|^{1/2}$ as $\lambda \equiv (w - \frac{1}{4})^{1/2} \rightarrow 0$ where $\gamma = 0.5772$ is Euler's constant and n is an integer which is not determined by the matching conditions. Now, negative values of n are unphysical since they lead to a divergence of $|\varepsilon_0| = q^2$ as $\lambda \rightarrow 0$. Therefore, the ground state must correspond either to $n = 0$ or to $n = 1$. If it corresponds to $n = 0$, one has $|\varepsilon_0| \rightarrow \text{constant}$ as $w \rightarrow \frac{1}{4}^+$. This applies to $u > u_{mc}$ for which a bound state exists even for $w < \frac{1}{4}$. If the ground-state energy is given by $n = 1$, one has $|\varepsilon_0| \rightarrow 0$ as $w \rightarrow \frac{1}{4}^+$ which applies to $u \leq u_{mc}$. In the latter case, one finds from (11) and (12) that

$$|\varepsilon_0| \approx \exp[-2\pi/(\Delta w)^{1/2} + 2/S(u) + 2(\ln 2 - \gamma)] \tag{13}$$

for $u < u_{mc}$ and

$$|\varepsilon_0| \approx \exp[-\pi/(\Delta w)^{1/2} + 2(\ln 2 - \gamma)] \tag{14}$$

for $u = u_{mc}$ as $\Delta w \equiv w - \frac{1}{4} \rightarrow 0^+$.

Within the transfer matrix formalism, the interfacial free energy is given by $f_1 = E_0$ and the longitudinal correlation length by $\xi_{||} = k_B T / (E_1 - E_0)$. The mean separation of the two interfaces is

$$\bar{l} \equiv \langle l \rangle \equiv \int_0^\infty dl l \phi_0(l)^2 \tag{15}$$

where ϕ_0 is the ground state. Likewise, the interfacial roughness is $\xi_{\perp} \equiv \langle (l - \langle l \rangle)^2 \rangle^{1/2}$. We will also discuss the length scales $\xi_m \equiv \langle (l - \langle l \rangle)^m \rangle^{1/m}$ where m is taken to be positive and real.

The critical behaviour of the correlation length, $\xi_{||} \sim 1/|\varepsilon_0|$, can be obtained directly from (10), (13) and (14). Then one finds that the locus of the wetting transitions is composed of three different subregimes A, B, and C, as shown in figure 1. In subregime A with $w = \frac{1}{4}$ and $-\infty < u < u_{mc}$, the correlation length exhibits an essential singularity:

$$(A) \quad \xi_{||} \sim \exp[2\pi/(w - \frac{1}{4})^{1/2}] \tag{16}$$

where the next-to-leading corrections are $O(1)$ (see (13)). This behaviour has been obtained previously for the special case $u = -\infty$ (Kroll and Lipowsky 1983, Chui and Ma 1983). In subregime B with $-\frac{3}{4} < w < \frac{1}{4}$ and $u_{mc} < u_c(w) < u_c(-\frac{3}{4}) \equiv \bar{u} = 3.737$ as given by (9), one has

$$(B) \quad \xi_{||} \sim (u - u_c)^{-\nu_{||}} \quad \text{with} \quad \nu_{||} = (\frac{1}{4} - w)^{-1/2}. \tag{17}$$

Thus, the critical behaviour is non-universal in this case. Finally, in subregime C with $-\infty < w < -\frac{3}{4}$ and $\bar{u} < u_c(w) < \pi^2$, one finds the simple behaviour

$$(C) \quad \xi_{||} \sim (u - u_c)^{-\nu_{||}} \quad \text{with} \quad \nu_{||} = 1. \tag{18}$$

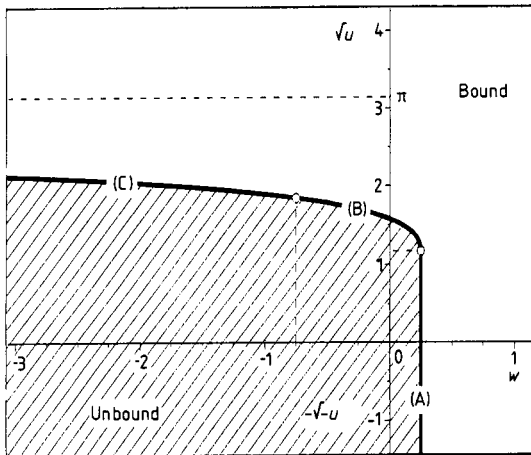


Figure 1. Global phase diagram for the direct interaction given by (8). The phase boundary between the bound and the unbound states of the interfaces consists of three distinct subregimes A, B and C. The locus of transitions within subregime A is given by the curve which extends from $(w, u) = (\frac{1}{4}, -\infty)$ to $(\frac{1}{4}, u_{mc} = 1.358)$; the curve for B extends from $(\frac{1}{4}, u_{mc})$ to $(-\frac{3}{4}, \bar{u} = 3.737)$ and the curve for C from $(-\frac{3}{4}, \bar{u})$ to $(-\infty, \pi^2)$.

The regimes A and B are separated by the multicritical point at $(w, u) = (\frac{1}{4}, u_{mc})$. At this point, the correlation length, ξ_{\parallel} , behaves as

$$\xi_{\parallel} \sim \exp[\Delta u^{-1} \Omega(\Delta w / \Delta u^2)] \quad (19)$$

where the shape function, Ω , goes as

$$\Omega(0) = \text{constant} \quad (20)$$

and

$$\Omega(x) \approx \pi/x^{1/2} \quad \text{for} \quad x \rightarrow \infty. \quad (21)$$

Between the subregimes B and C, one has the special point $(w, u) = (-\frac{3}{4}, \bar{u})$. At this point

$$\xi_{\parallel} \sim |\ln(\Delta u)| / \Delta u \quad (22)$$

as follows from (10) for $\mu = 1$. In all cases, the hyperscaling relation, $f_1 \sim 1/\xi_{\parallel}$, is valid. This implies that the interfacial energy, $\partial f_1 / \partial T$, is continuous in the subregimes A and B including the point $(w, u) = (-\frac{3}{4}, \bar{u})$, but is discontinuous in subregime C.

Next, consider the length scales \bar{l} , ξ_{\perp} and ξ_m . In the wFL and sFL regimes, these different length scales are not independent but satisfy the relation (Lipowsky and Fisher 1987 and references therein)

$$\bar{l} \sim \xi_{\perp} \sim \xi_m \sim \xi_{\parallel}^{\zeta} \quad \text{with} \quad \zeta = \frac{1}{2} \quad (23)$$

in $d = 2$. The same relation is found to apply in the subregimes A and B of the IFL regime studied here. Thus, to leading order, there is only *one* independent length scale in these cases. However, this scaling is no longer valid in subregime C with $w < -\frac{3}{4}$. First, consider the mean separation, \bar{l} , which is found to behave as

$$\bar{l} \sim \Delta u^{-\psi} \quad \text{with} \quad \psi = \frac{3}{2} - (\frac{1}{4} - w)^{1/2} \quad (24)$$

for $-2 < w < -\frac{3}{4}$ and $\bar{l} \sim O(1)$ for $w < -2$. Likewise, the roughness, ξ_{\perp} , goes as

$$\xi_{\perp} \sim \Delta u^{-\nu_{\perp}} \quad \text{with} \quad \nu_{\perp} = 1 - \frac{1}{2}(\frac{1}{4} - w)^{1/2} \quad (25)$$

for $-\frac{15}{4} < w < -\frac{3}{4}$ but $\xi_{\perp} \sim O(1)$ for $w < -\frac{15}{4}$. In general, one has

$$\xi_m \sim \Delta u^{-\nu_m} \quad \text{with} \quad \nu_m = \frac{1}{m} \left(\frac{m+2}{2} - (\frac{1}{4} - w)^{1/2} \right) \quad (26)$$

for $m > (1 - 4w)^{1/2} - 2 > 0$. Thus, subregime C is characterised by strongly non-Gaussian fluctuations and by a complete breakdown of scaling with a single length scale. This also shows up in the fact that the ratios $\nu_m / \nu_{\parallel} = \nu_m$ differ from $\zeta = \frac{1}{2}$ as has been shown previously (Zia *et al* 1987).

The critical exponents determined above depend only on the value of $w = 2\tilde{\Sigma} W / (k_B T)^2$, i.e. on the rescaled amplitude of the long-range tail $\sim -W/l^2$ of the direct interaction. The same behaviour should apply to a large class of direct interactions, $V(l)$, in the effective Hamiltonian (4). Indeed, it should apply to all $V(l)$ which have a long-range tail $\sim W/l^2$ and a short-range part which, by definition, falls off faster than $1/l^2$ for large l and which can be changed independently from the long-range part. A similar behaviour is expected to hold for sos models on a lattice for which the gradient term $(\nabla l)^2$ in (4) is replaced by $|l(x_i) - l(x_j)|$ and the direct interaction, $V(l)$, again has a long-range tail $\sim 1/l^2$. Such sos models have been previously studied for short-range $V(l)$ (e.g. Burkhardt 1981) and for $V(l) \sim 1/l$ (Privman and Švrakic 1987).

For wetting transitions in $d = 3 = 2 + 1$, all fluctuation regimes become degenerate. Then, one has a marginal scaling regime which consists of all direct interactions, $V(l)$, for which the tails decay faster than an inverse power of l . For example, for $V(l) \sim \exp(-l)$, various subregimes with different scaling properties have been found from functional renormalisation group calculations and from Monte Carlo simulations (Lipowsky *et al* 1983, Brézin *et al* 1983, Fisher and Huse 1985, Lipowsky and Fisher 1986b, 1987, Gompper and Kroll 1987). The associated critical behaviour is similar to the critical behaviour in the subregimes A and B of the intermediate fluctuation regime as determined in this letter. So far, a subregime such as subregime C, which is characterised by strongly non-Gaussian fluctuations and many independent length scales, has not been found in $d = 2 + 1$.

Intermediate fluctuation regimes can also be studied in the context of other physical systems. Two particularly interesting cases are: (i) wetting transitions in systems with quenched impurities and (ii) unbinding transitions of amphiphilic membranes. In both cases, different subregimes are expected which exhibit essential singularities or non-universal critical behaviour.

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