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# Breakdown of the long-wavelength limit of the filling transition

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## Abstract

The mean-field analysis of the filling transition is based on the simple effective Hamiltonian. It is valid only in the long-wavelength limit and the transition occurs in the temperature regime where the behaviour of the interface is dominated by fluctuations. We evaluate the correlation function and the roughness of the interface in the Ornstein–Zernike approximation. With the help of the Ginzburg criterion we prove that the mean-field filling transition breaks down in this temperature range. We propose the replacement of the simple effective Hamiltonian with a more complex Hamiltonian evaluated using Landau theory. This Hamiltonian can be used in the temperature regime where fluctuations are negligible and the mean-field analysis is correct.

## 1. Introduction

The corrugation of the substrate can significantly influence fluid adsorption on a solid substrate. When a planar substrate exhibits continuous wetting, a weak corrugation of the substrate does not change the wetting temperature but a new first-order transition preceding the wetting transition, called the *filling* or *unbending* transition, can appear at the liquid–gas coexistence. It can occur when the corrugation amplitude exceeds a critical value. The filling transition is usually studied with the help of mean-field theory based on the effective interfacial Hamiltonian. Different shapes of the substrate have been discussed: sinusoidal [1–3], saw-shaped [5] or piecewise circular [6]. While saw-shaped and piecewise circular substrates allow for analytical results, the calculations for a sinusoidal substrate need some approximations. Moreover, the effective Hamiltonian adopted in these studies can be used only when the system is near the wetting point. In this case the interface strongly fluctuates, and the mean-field analysis can break down. In section 2 we briefly describe the interfacial model and the analysis of the filling transition for a sinusoidal substrate. In sections 3 and 4 we evaluate the interface correlation function in the Ornstein–Zernike approximation, and the roughness of the interface. We prove that mean-field theory cannot be used due to the divergence of the roughness of the interface. In section 5 we argue that a more complex effective Hamiltonian evaluated using Landau theory (relevant not only in the long-wavelength limit), can be adopted to the analysis of the filling transition not only in the vicinity of the wetting point but also far from the wetting temperature. In the second case the mean-field theory works well, and the phase diagram

obtained by minimization of the effective Hamiltonian displays a more complex structure, as the phase diagram obtained previously [1–3].

## 2. Mean-field filling transition

We discuss the periodically corrugated, one-dimensional substrate described by the function

$$b(x) = A(1 - \cos qx), \quad -\frac{N\pi}{q} \leq x \leq \frac{N\pi}{q}. \quad (2.1)$$

$A$  is called the corrugation amplitude of the substrate and  $q$  is the wavenumber of the substrate. The substrate contains a large number  $N$  of segments; each one has the length  $2\pi/q$ . The half space  $z > b(x)$  is occupied by the fluid at the bulk liquid–gas coexistence, or more precisely, infinitesimally close to the coexistence line on the gaseous side of the bulk phase diagram. In the absence of the substrate, the gaseous phase is the only thermodynamically stable bulk phase. In the presence of the substrate the quasi-liquid film can appear on the solid, due to the interactions with the substrate, but far away from the wall, i.e. for large  $z$  the fluid is still in the gaseous phase. When increasing the temperature to the wetting temperature  $T_W$  along the bulk coexistence line, the thickness of the liquid film grows to infinity. For the corrugated substrate an additional thin–thick transition (called the filling or the unbending transition) can appear at the specific temperature  $T_F(q, A)$  less than the wetting temperature. When discussing the filling transition much below the bulk critical point, one uses the standard effective Hamiltonian which can be used when the corrugation of the substrate is small, i.e. when  $qA \ll 1$

$$\mathcal{H}[f] = \int_{-N\pi/q}^{N\pi/q} dx \left[ \frac{\sigma}{2} f_x^2 + \omega(l) \right], \quad (2.2)$$

where  $f(x)$  denotes the position of the interface,  $l(x) = f(x) - b(x)$  denotes the liquid film thickness and  $\sigma$  is the surface tension of the free liquid–gas interface. Hamiltonian (2.2) is valid only in the asymptotic, wetting regime, i.e. when  $l(x)$  is very large. In consequence it can be adopted only near the wetting point.

In this paper we discuss a system with short range interactions exhibiting continuous wetting. We take into consideration the effective potential of the form

$$\omega(l) = tW \exp(-p_\beta l) + U \exp(-2p_\beta l), \quad (2.3)$$

where  $p_\beta$  is the inverse correlation length in the bulk liquid phase and  $t = \frac{T-T_W}{T_W}$  is the reduced temperature. For the wet state of the system  $t \geq 0$ , and for the partially wet state  $t < 0$ .  $U$ ,  $W$  are (positive) amplitudes of the repulsive and attractive part of the potential, respectively.

The mean-field approach consists of minimization of the effective Hamiltonian (2.2) in the appropriate class of functions representing the film thickness. We represent it in a simple way

$$l(x) = l_0 + B \cos qx, \quad (2.4)$$

where  $l_0$  and  $B$  has to be determined, when minimizing the effective Hamiltonian. The effective Hamiltonian (2.2) supplemented by the interfacial shape (equation (2.4)) has the following form

$$\begin{aligned} \mathcal{H}(p_\beta l_0, p_\beta B) &= \frac{\pi \sigma q}{2 p_\beta^2} (p_\beta B - p_\beta A)^2 \\ &+ \frac{2\pi}{q} [tW \exp(-p_\beta l_0) \Phi(p_\beta B) + U \exp(-2p_\beta l_0) \Phi(2p_\beta B)], \end{aligned} \quad (2.5)$$

where

$$\Phi(p_\beta B) = \frac{1}{\pi} \int_0^\pi \exp(-p_\beta B \cos t) dt, \quad (2.6)$$

is the Bessel function  $I_0(p_\beta B)$ . Minimization of this Hamiltonian with respect to  $l_0$  gives the  $B$ -dependent function  $l_0(p_\beta B)$

$$l_0(p_\beta B) = l_\pi + p_\beta^{-1} \ln \left( \frac{\Phi(2p_\beta B)}{\Phi(p_\beta B)} \right), \quad (2.7)$$

where  $l_\pi = \ln \left( \frac{-2U}{tW} \right)$  is the mean-field equilibrium film thickness on the planar substrate. Substituting  $l_0(p_\beta B)$  into the Hamiltonian (2.5) we obtain a Hamiltonian of the form

$$\mathcal{H}(p_\beta B) = \frac{\pi \sigma q}{p_\beta^2} \left[ \frac{1}{2} (p_\beta B - p_\beta A)^2 - \frac{1}{(q\xi_{\parallel\pi})^2} \Psi(p_\beta B) \right], \quad (2.8)$$

where  $\xi_{\parallel\pi} = -\frac{\sqrt{2\sigma U}}{tW p_\beta}$  is the parallel correlation length of the interface for the planar substrate and

$$\Psi(p_\beta B) = \frac{\Phi^2(p_\beta B)}{\Phi(2p_\beta B)}. \quad (2.9)$$

Minimizing Hamiltonian (2.8) we obtain the equation which determines the equilibrium value of the undulation amplitude  $\bar{B}$

$$p_\beta \bar{B} - p_\beta A = \frac{1}{(q\xi_{\parallel\pi})^2} \Psi'(p_\beta \bar{B}). \quad (2.10)$$

Hamiltonian (2.8) can display two minima, depending on the parameters of the model. The filling transition occurs provided the amplitude of the corrugation exceeds the critical value [1–3]. The corrugation amplitude  $A$  determines the value of  $q\xi_{\parallel\pi}$  at the transition;  $\xi_{\parallel\pi}$  denotes the correlation length for planar substrate (it diverges at the wetting point). The value of  $q\xi_{\parallel\pi}$  at the filling transition determines two undulation amplitudes  $\bar{B}$  and mean thicknesses of the interface  $l_0(\bar{B})$  of coexisting films. The analysis based on Hamiltonian (2.2) is, however, very doubtful due to the form of the phenomenological Hamiltonian (2.2). It is only an asymptotic form of a more exact expression, which can be evaluated using a more fundamental theory (for example Landau theory [4]). It can be used only when the adsorbed film thickness is very large, i.e. when the temperature is very close to the wetting temperature  $T_w$ , and in consequence when  $\xi_{\parallel\pi}$  is very large too. To keep a constant value of  $q\xi_{\parallel\pi}$ ,  $q$  has to be very small. The mean-field transition based on Hamiltonian (2.2) occurs near the wetting point where the interface strongly fluctuates, and in consequence the mean-field theory breaks down. It is evident when one compares the difference in thickness of the adsorbed liquid layers at the mean-field transition with the roughness of the interface.

### 3. Correlations in the Ornstein–Zernike approximation

In this section we evaluate the correlation function of the interface in the Ornstein–Zernike approximation. We include both: short- and long-wavelength fluctuations. We rewrite the film thickness in the following way

$$l(x) = l_\pi + \delta l(x). \quad (3.1)$$

Next, we express  $\delta l(x)$  as the Fourier series expansion

$$\delta l(x) = \frac{1}{2} B_0 + \sum_{k=1}^M B_k \cos kqx + \sum_{k=1}^M Q_k \sin kqx \quad (3.2)$$

$$+ \sum_{n=1}^{N-1} C_n \cos \frac{nqx}{N} + \sum_{n=1}^{N-1} R_n \sin \frac{nqx}{N}. \quad (3.3)$$

Amplitudes  $\{B_k, Q_k\}$  describe the short-wavelength fluctuations,  $M$  is the short-wavelength cut-off. We do not discuss the value of  $M$ , for our purpose it is not important. We will show that the short-wavelength fluctuations do not influence correlations in the thermodynamic limit. Amplitudes  $\{C_n, R_n\}$  describe long-wavelength fluctuations. The Ornstein–Zernike Hamiltonian has the following form

$$\mathcal{H}_{\text{OZ}}[\delta l] = \frac{\sigma}{2} \int_{-N\pi/q}^{N\pi/q} dx (f_x^2 + \xi_{\parallel\pi}^{-2}(\delta l)^2). \quad (3.4)$$

It is a function of Fourier amplitudes

$$\begin{aligned} \mathcal{H}_{\text{OZ}}(\{B_k, Q_k\}, \{C_n, R_n\}) &= \frac{\pi\sigma N}{q} \left[ \frac{1}{4}\xi_{\parallel\pi}^{-2} B_0^2 + \frac{1}{2}(q^2 + \xi_{\parallel\pi}^{-2})B_1^2 - q^2 A B_1 \right. \\ &\times \frac{1}{2} \sum_{k=2}^M (k^2 q^2 + \xi_{\parallel\pi}^{-2}) B_k^2 + \frac{1}{2} \sum_{k=1}^M (k^2 q^2 + \xi_{\parallel\pi}^{-2}) Q_k^2 \\ &\left. + \frac{1}{2} \sum_{n=1}^{N-1} \left( \frac{n^2}{N^2} q^2 + \xi_{\parallel\pi}^{-2} \right) C_n^2 + \frac{1}{2} \sum_{n=1}^{N-1} \left( \frac{n^2}{N^2} q^2 + \xi_{\parallel\pi}^{-2} \right) R_n^2 \right]. \end{aligned} \quad (3.5)$$

The partition function

$$\begin{aligned} \mathcal{Z}(T, q, A, N) &= \int dB_0 \prod_k d\{B_k dQ_k\} \prod_n d\{C_n dR_n\} e^{-\beta \mathcal{H}_{\text{OZ}}(\{B_k, Q_k\}, \{C_n, R_n\})}, \end{aligned} \quad (3.6)$$

is a product of the partition functions of all modes

$$\mathcal{Z}(T, q, A, N) = \mathcal{Z}_0^B \prod_{k>0} \mathcal{Z}_k^B \mathcal{Z}_k^Q \prod_n \mathcal{Z}_n^C \mathcal{Z}_n^R. \quad (3.7)$$

The mean values of the amplitudes and the product of the amplitudes are very easy to evaluate in the Ornstein–Zernike approximation

$$\begin{aligned} \langle B_k \rangle|_{k \neq 1} &= 0, & \langle B_1 \rangle &= A \frac{(q\xi_{\parallel\pi})^2}{1 + (q\xi_{\parallel\pi})^2} \\ \langle C_k \rangle &= \langle Q_n \rangle = \langle R_n \rangle = 0, \\ \langle B_l B_l \rangle &= B_k^2 \delta_{k,l}, & \langle C_n C_m \rangle &= C_n^2 \delta_{k,l}, & \langle B_k C_n \rangle &= 0, \end{aligned} \quad (3.8)$$

and

$$\begin{aligned} \langle B_0^2 \rangle &= \frac{2k_B T (q\xi_{\parallel\pi})}{\pi\sigma N} \xi_{\parallel\pi}, \\ \langle B_1^2 \rangle &= \frac{k_B T (q\xi_{\parallel\pi})}{\pi\sigma N} \frac{\xi_{\parallel\pi}}{1 + (q\xi_{\parallel\pi})^2} + \frac{A^2 (q\xi_{\parallel\pi})^4}{(1 + (q\xi_{\parallel\pi})^2)^2}, \\ \langle B_1^2 \rangle - \langle B_1 \rangle^2 &= \frac{k_B T (q\xi_{\parallel\pi})}{\pi\sigma N} \frac{\xi_{\parallel\pi}}{1 + (q\xi_{\parallel\pi})^2}, \\ \langle B_k^2 \rangle|_{k \neq 1} &= \langle Q_k^2 \rangle = \frac{k_B T (q\xi_{\parallel\pi})}{\pi\sigma N} \frac{\xi_{\parallel\pi}}{1 + k^2 (q\xi_{\parallel\pi})^2}, \\ \langle C_n^2 \rangle &= \langle R_n^2 \rangle = \frac{k_B T (q\xi_{\parallel\pi})}{\pi\sigma N} \frac{\xi_{\parallel\pi}}{1 + \frac{n^2}{N^2} (q\xi_{\parallel\pi})^2}. \end{aligned} \quad (3.9)$$

From equation (3.8) we obtain

$$\langle \delta l(x) \rangle = \frac{(q\xi_{\parallel\pi})^2}{1 + (q\xi_{\parallel\pi})^2} A \cos qx, \quad (3.10)$$

$$\langle f(x) \rangle = l_\pi - \frac{A \cos qx}{1 + (q\xi_{\parallel\pi})^2}. \quad (3.11)$$

Equations (3.10) and (3.11) show that near the wetting temperature the mean interface position is almost the same as the mean-field interface position over the planar substrate. At depinning, the interface is very weakly influenced by the corrugation of the substrate.

The correlation function  $C_N(x, y)$  is defined as

$$C_N(x, y) = \langle (l(x) - \langle l(x) \rangle)(l(y) - \langle l(y) \rangle) \rangle. \quad (3.12)$$

With the help of equation (3.9) we obtain

$$C_N(x, y) = \xi_{\parallel\pi} \frac{k_B T (q\xi_{\parallel\pi})}{\pi \sigma N} \left( \frac{1}{2} + \sum_{k=1}^M \frac{\cos kq(x-y)}{1 + k^2 (q\xi_{\parallel\pi})^2} \right) + \xi_{\parallel\pi} \frac{k_B T (q\xi_{\parallel\pi})}{\pi \sigma} \left( \sum_{n=1}^{N-1} \frac{\cos \frac{nq(x-y)}{N}}{N \left[ 1 + \frac{n^2}{N^2} (q\xi_{\parallel\pi})^2 \right]} \right). \quad (3.13)$$

The first contribution to the correlation function vanishes in the thermodynamic limit  $N \rightarrow \infty$ . In the second contribution the sum over  $n$  is replaced by the integral, therefore we obtain

$$C_\infty(x, y) = \xi_{\parallel\pi} \frac{k_B T}{\pi \sigma} \int_0^{q\xi_{\parallel\pi}} dt \frac{\cos \left( t \frac{(x-y)}{\xi_{\parallel\pi}} \right)}{1 + t^2}. \quad (3.14)$$

The correlation function depends on the difference  $x - y$ . It can be expressed by integral sine and integral cosine functions

$$C_\infty(x, y) = \xi_{\parallel\pi} \frac{k_B T}{2\pi \sigma} \times \left\{ - \left[ \text{Si} \left( \frac{x-y}{\xi_{\parallel\pi}} (q\xi_{\parallel\pi} + i) \right) + \text{Si} \left( \frac{x-y}{\xi_{\parallel\pi}} (q\xi_{\parallel\pi} - i) \right) \right] \sinh \left( \frac{x-y}{\xi_{\parallel\pi}} \right) + i \left[ \text{Ci} \left( \frac{x-y}{\xi_{\parallel\pi}} (q\xi_{\parallel\pi} + i) \right) - \text{Ci} \left( \frac{x-y}{\xi_{\parallel\pi}} (q\xi_{\parallel\pi} - i) \right) + \text{Ci} \left( -i \frac{x-y}{\xi_{\parallel\pi}} \right) - \text{Ci} \left( i \frac{x-y}{\xi_{\parallel\pi}} \right) \right] \cosh \left( \frac{x-y}{\xi_{\parallel\pi}} \right) \right\}. \quad (3.15)$$

The correlation function decays with the same correlation length  $\xi_{\parallel\pi}$  as the correlation length for the planar substrate. Functions Si and Ci oscillate, and in consequence the correlation function oscillates too. If  $q\xi_{\parallel\pi}$  increases, the amplitude and the wavelength of the oscillations decreases (see figures 1 and 2).

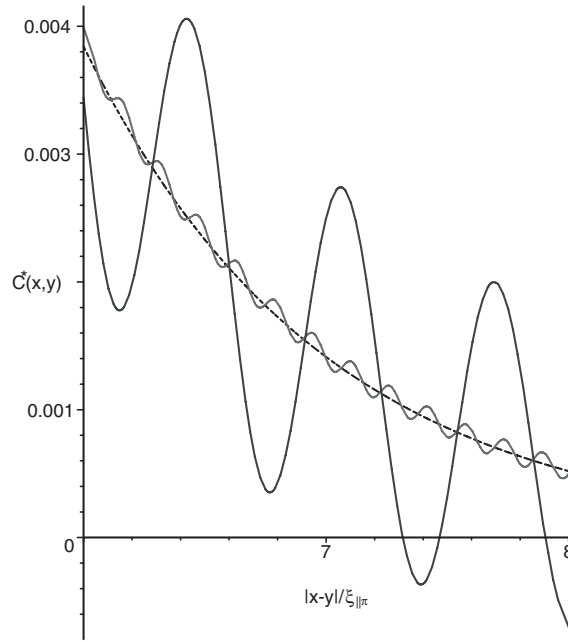
#### 4. Roughness of the interface and the filling transition

The roughness of the interface  $\xi_\perp$  is defined as

$$\xi_\perp^2 = \langle (l(x) - \langle l(x) \rangle)^2 \rangle. \quad (4.1)$$

It can be expressed by the correlation function

$$\xi_\perp^2 = C_\infty(x, x) = \xi_{\parallel\pi} \frac{k_B T}{\pi \sigma} \arctan(q\xi_{\parallel\pi}). \quad (4.2)$$



**Figure 1.** The correlation function  $C^*(x, y) = \xi_{\parallel\pi}^{-1} \frac{\pi\sigma}{k_B T} C(x, y)$  for two different values of  $q\xi_{\parallel\pi}$ . The correlation function decays exponentially with the same correlation length  $\xi_{\parallel\pi}$  as for a planar substrate, and oscillates. The greater  $q\xi_{\parallel\pi}$ , the smaller the amplitude and wavelength of the oscillations. The curve with large oscillations corresponds to  $q\xi_{\parallel\pi} = 10$  and the curve with small oscillations corresponds to  $q\xi_{\parallel\pi} = 40$ . Both curves correspond to the regime  $q\xi_{\parallel\pi} > (q\xi_{\parallel\pi})_{CF}$ , where the mean-field filling transition does not appear. The exponential decay with the correlation length  $\xi_{\parallel\pi}$  is plotted in the background as the dashed line.

It does not depend on  $x$ . The amplitude  $A$  of the substrate determines the value of  $q\xi_{\parallel\pi}$  at the filling transition (we denote it by  $q\xi_{\parallel\pi}(A)$ ), and therefore, when  $q$  is fixed, it determines the filling temperature. The roughness of the interface diverges with the same power law as in the planar case

$$\xi_{\perp} \sim \xi_{\parallel\pi}^{\zeta}, \quad (4.3)$$

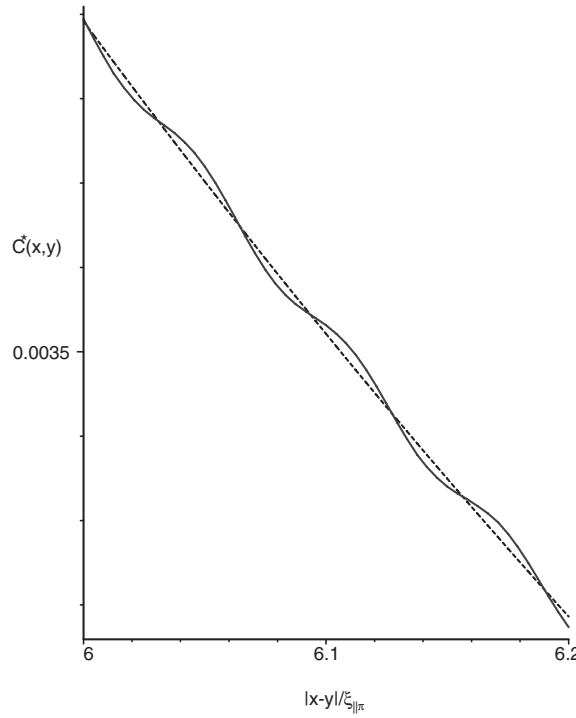
where  $\zeta = (3 - d)/2$  is the roughness exponent. (For  $d = 2$ , the roughness exponent is equal to  $1/2$ .) When the mean-field filling transition occurs near the wetting point, the transition is wiped out by interfacial fluctuations. We compare the difference in the thickness of coexisting films with the roughness of the interface

$$\bar{l}_1(x = 0, (q\xi_{\parallel\pi})(A)) - \bar{l}_3(x = 0, (q\xi_{\parallel\pi})(A)) = \xi_{\perp}. \quad (4.4)$$

If the temperature is greater than the temperature  $T_0$  determined by equation (4.4), the mean-field predictions break down. The left-hand side of equation (4.4) is determined unambiguously by the amplitude of the substrate; we denote it simply by  $\Delta\bar{l}(A)$ . Equation (4.4) can be rewritten in the explicit form

$$\frac{T_W}{T_0} - 1 = \frac{k_B T_W}{\pi p_{\beta} W} \sqrt{\frac{2U}{\sigma}} \frac{\arctan[(q\xi_{\parallel\pi})(A)]}{(\Delta\bar{l}(A))^2}. \quad (4.5)$$

Equation (4.5) represents the Ginzburg criterion which determines the applicability of the mean-field theory. If  $T$  is greater than  $T_0$  determined by equation (4.5), the roughness of the



**Figure 2.** The correlation function  $C^*(x, y)$  for  $q\xi_{\parallel\pi} = 100$ .

interface is greater than the difference in the thickness of coexisting films, and the mean-field theory breaks down. The value of  $q\xi_{\parallel\pi}$  at the filling transition is determined by the amplitude  $A$  of the corrugation of the substrate. Only when this amplitude becomes infinitely huge does the factor  $\arctan[(q\xi_{\parallel\pi})]$  vanish and temperature  $T_0$  tends to  $T_w$ . (The mean-field filling described in section 2 occurs when  $q\xi_{\parallel\pi} < (q\xi_{\parallel\pi})_{CF}$ , i.e. the factor  $\arctan[(q\xi_{\parallel\pi})] < 0.457 (\pm 0.001)$ .) Our statement does not mean that the filling transition does not exist at all, but rather that the model based on Hamiltonian (2.2) is wrong.

## 5. Beyond the critical region

The mean-field theory breaks down near the wetting point. Nevertheless it is still valid, when the temperature is sufficiently lower than the wetting temperature. In this case the thickness of the adsorbed film is finite, and the Hamiltonian (2.2) ceases to be adequate. Instead of Hamiltonian (2.2) it is necessary to use a more complex Hamiltonian, for example

$$\mathcal{H}[f] = \int_{-N\pi/q}^{N\pi/q} dx \left[ \frac{\Sigma_{\alpha\beta}(l)}{2} f_x^2 + \lambda(l) f_x b_x + \frac{\Sigma_{\beta w}(l)}{2} b_x^2 + \omega(l) \right]. \quad (5.1)$$

This Hamiltonian was previously evaluated using Landau theory [4].  $\Sigma_{\alpha\beta}(l)$  and  $\Sigma_{\beta w}(l)$  are the liquid–gas and liquid–substrate surface stiffness coefficients [7], respectively. Both stiffnesses are dependent on  $l$ . Only when  $l$  becomes infinite are they equal to the relevant surface tensions.  $\lambda(l)$  is the coefficient describing the coupling between undulations of the substrate and interface. It vanishes when the thickness of the liquid film grows to infinity. Hamiltonian (5.1) is valid for an arbitrary thickness of the adsorbed layer as opposed to the



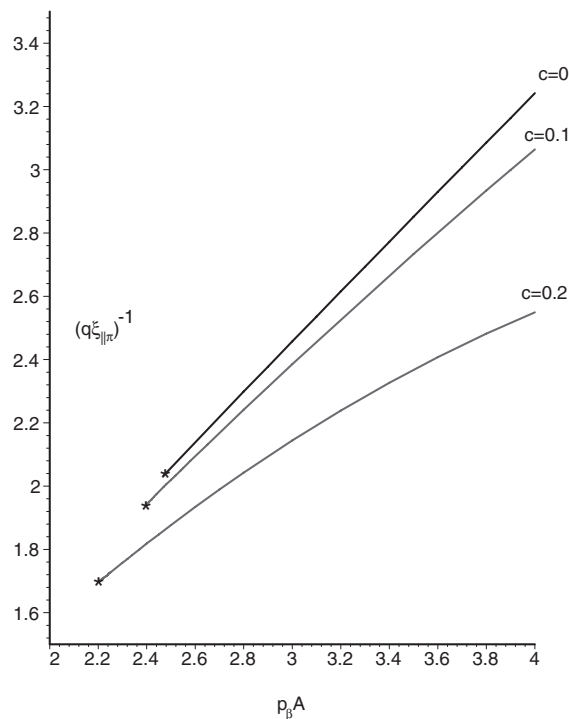
simplified form of Hamiltonian (2.2), which is restricted to the critical region only. When we substitute the ansatz defined in equation (2.4) into Hamiltonian (5.1) we obtain a function which depends explicitly on  $q/p_\beta$  [8]

$$\begin{aligned}
\mathcal{H}(p_\beta l_0, p_\beta B) = & \frac{\pi \sigma q}{2p_\beta^2} (p_\beta B - p_\beta A)^2 \\
& + \frac{2\pi}{q} \left\{ W t X_0 I_0(p_\beta B) + U X_0^2 I_0(2p_\beta B) \right. \\
& + \left( \frac{q}{p_\beta} \right)^2 p_\beta A (p_\beta B - p_\beta A) (2p_\beta l_0 - 1 - \mathcal{G}) \\
& \times \left( \frac{W t}{4} X_0 \frac{I_1(p_\beta B)}{p_\beta B} + U X_0^2 \frac{I_1(2p_\beta B)}{2p_\beta B} \right) \\
& + \left( \frac{q}{p_\beta} \right)^2 p_\beta A (p_\beta B - p_\beta A) \\
& \times \left( \frac{W t}{4} X_0 \left[ \frac{2I_1(p_\beta B)}{p_\beta B} - I_0(p_\beta B) \right] \right. \\
& \left. + U X_0^2 \left[ \frac{I_1(2p_\beta B)}{p_\beta B} - \frac{1}{2} I_0(p_\beta B) \right] \right) \left. \right\}, \tag{5.2}
\end{aligned}$$

where  $X_0 = \exp(-p_\beta l_0)$ . Hamiltonian (5.2) is still a simplified form; it is valid for a finite, but large, value of  $l(x)$ . The phase diagram obtained when minimizing Hamiltonian (5.2) displays a more complex dependence on the wavelength of the substrate than the phase diagram obtained from the phenomenological Hamiltonian (2.2). The filling temperature depends not only on  $q\xi_{\parallel\pi}$  but also on  $c = q/p_\beta$ . Figure 3 presents the phase diagram for three different values of  $c$ . When  $c = 0$  we obtain the phase diagram based on the Hamiltonian (2.2) and, in consequence, on Hamiltonian (2.8).  $c = 0$  is the long-wavelength limit, i.e. the case of infinite wavelength of the substrate with respect to the parallel correlation length  $\xi_{\parallel\pi}$ . This second length itself becomes infinite in the fluctuation regime which is connected to the validity of Hamiltonian (2.2); in this regime the mean-field approach breaks down. In the mean-field regime, the locus of the filling transition on the  $(p_\beta A, (q\xi_{\parallel\pi})^{-1})$  plane is determined by the ratio  $q/p_\beta$ .

## 6. Conclusions

The simple mean-field analysis of the filling transition based on the Hamiltonian (2.2) [1–3] is inadequate. The corrugation amplitude of the substrate  $A$  unambiguously determines the value of  $q\xi_{\parallel\pi}$  at the transition. In consequence the transition temperature depends on the wavelength of the substrate through the ratio of the wavelength of the substrate and the parallel correlation length  $\xi_{\parallel\pi}$ . One obtains the same phase diagram for a wide range of temperature, including temperatures close to the wetting temperature. The starting point of this analysis, Hamiltonian (2.2), can be used only when the temperature is close to the wetting temperature of the substrate. This restricts the applicability of the model to the vicinity of the wetting point, and in consequence to a very large value of the wavelength of the substrate. From the other side the interface strongly fluctuates when the temperature approaches the (continuous) wetting temperature. We have evaluated the parallel correlation function and the roughness of the interface over the corrugated substrate for a two-dimensional system. The roughness of the interface diverges with the parallel correlation length  $\xi_{\parallel\pi}$  in the same way as in the case of a planar substrate. The Ginzburg criterion determines the critical region, where the behaviour



**Figure 3.** The phase diagram of the filling transition for  $c = 0, 0.1$  and  $0.2$ , respectively. The diagram is determined for  $\mathcal{G} = 0.5$ , and  $U/\sigma = 1$ . Stars denote the filling critical point.

of the interface is governed by fluctuations and the mean-field approach breaks down. The mean-field analysis is still valid when the temperature is sufficiently lower than the wetting temperature, but in this case Hamiltonian (2.2) must be replaced by Hamiltonian (5.1). It displays a more complex structure of the phase diagram. The locus of the filling transition is determined not only by the ratio of the parallel correlation length  $\xi_{||\pi}$  to the wavelength of the substrate but also by the ratio of the bulk correlation length to the wavelength of the substrate.

## References

- [1] Rascón C, Parry A O and Sartori A 1999 *Phys. Rev. E* **59** 5697
- [2] Rascón C and Parry A O 2000 *J. Phys.: Condens. Matter* **12** A369
- [3] Rejmer K 2002 *Phys. Rev. E* **65** 061606  
Rejmer K 2005 *Phys. Rev. E* **71** 011605
- [4] Rejmer K and Napiórkowski M 1997 *Z. Phys. B* **102** 101
- [5] Rejmer K and Napiórkowski M 2000 *Phys. Rev. E* **62** 588
- [6] Rejmer K 2004 *Fluid Phase Equilib.* **222/223** 169
- [7] Jin A J and Fisher M E 1993 *Phys. Rev. B* **47** 7365
- [8] Rejmer K 2006 *Physica A* doi:10.1016/j.physa.2006.05.051