Filling and wetting transitions on sinusoidal substrates: a mean-field study of the double parabola model

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Wetting and related interfacial phenomena can be studied at different levels. From a microscopic point of view, they can be analysed by using models which account for the molecular structure of the fluid, including simplified versions as the lattice gas isomorphic to the Ising model, or coarse-grained microscopic models such as the Landau-Ginzburg (LG) model[1]. An alternative is the use of mesoscopic models where the free-energy cost of an interfacial configuration is modeled by an interfacial Hamiltonian model[2]. However, there is a gap between the microscopic and mesoscopic approaches, since usually the interfacial Hamiltonians are proposed in an ad hoc way by generalizing simpler situations such as the interfacial phenomena on planar substrates.

In our study[4], we have considered the mean-field study of the adsorption phase diagram on an array of infinite grooves of sinusoidal section within the double parabola model (DP). This model is interesting because can be regarded as an approximation to the LG model, but on the other hand it can be formally reduced to an interfacial Hamiltonian theory which reduces to the perturbative non-local models[3] in some limit. In this sense, our study may help to bridge the gap between the microscopic and mesoscopic descriptions of fluid adsorption on microstructured substrates. The sinusoidal section (Figure 1) is characterized by a period L and amplitud A and modeled by a double parabola functional, with a fluid-substrate coupling m_s (surface magnetization) that controls the wetting of the substrate. We have restricted our study to a substrate which undergoes critical wetting.

The method to minimize the free-energy functional for the DP model is related to the Boundary Element Method (BEM) used for engineering applications. We have obtained the interfacial phase diagram, and from a qualitatively point of view is quite similar to that obtained from the Landau-Ginzburg model (Figure 2), both for bulk coexistence $h = 0$ and in the single-phase region $h < 0$. When the results of the DP and the LG models are compared in terms of the fields $\cos\theta$, with θ being the contact angle, and the interfacial curvature R^{-1} , which are different functions of m_s and h for each model, we observe an agreement between them. Thus, we conclude that the DP model is a good approximation to the LG model[1]. When comparing our numerical calculations with the interfacial Hamiltonian predictions[2], we have observed (see the inset in Figure 2) similar discrepancies as for the LG model on the dependence of the rescaled temperature with L. However, we cannot rule out the possibility that they converge to the interfacial Hamiltonian prediction for low roughness substrates. If this is the case, the DP predictions are closer to this asymptotics than those obtained within the LG model.

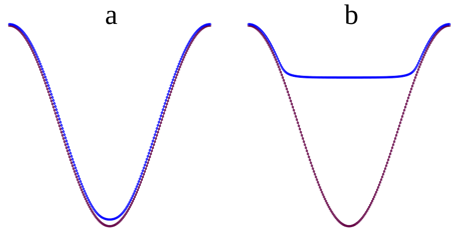

Figure 1: Liquid-vapour interfacial profile for: (a) the dry and (b) the filled states in coexistence at the filling transition, $A/L = 0.5$ and $L = 20$.

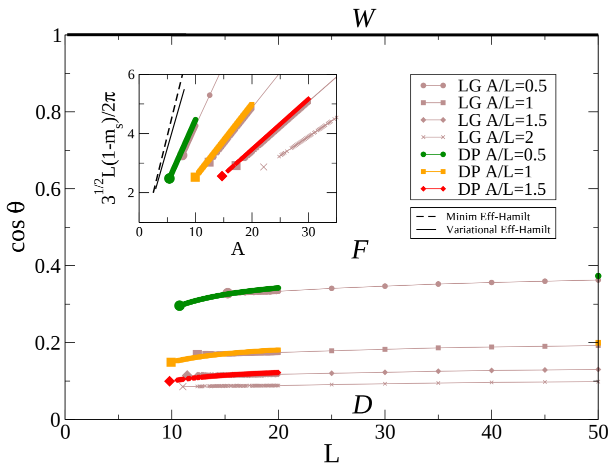

Figure 2: Adsorption phase diagram on a sinusoidal substrate at coexitence $h = 0$. The phase boundaries between Dry and Fill states (DP model) are plotted for $A/L = 0.5$ (green circles), $A/L = 1$ (orange squares), $A/L = 1.5$ (red diamonds), LG model (grey lines and symbols) (the lines serve only as guides for the eyes), and the big symbols to the filling transition critical points. wetting transition is represented by the thick continuous line for $m_s = 1$. Inset: plot of $\Delta T = \sqrt{3}L(1 - m_s)/(2\pi)$ as a function of the substrate amplitude A along the filling transition line. The black lines correspond to the predictions from interfacial Hamiltonian theories [2].

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