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LETTER TO THE EDITOR

The problem of uniqueness in the reduced description of adsorption on the wedge-shaped substrate

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Abstract. In the reduced one-dimensional description of the adsorption on the wedge-shaped substrate the mid-point interface height serves as the order parameter. We point out the ambiguity which appears in the transfer-matrix approach to this problem. We also propose how to avoid this problem by introducing the appropriate order parameter.

1. Introduction

One of the possible scenarios of adsorption on the wedge-shaped substrate (see figure 1) is via the so-called critical filling transition [1–6]. In this transition the central part of the interface (separating the phases β and α) positioned above the edge of the wedge is shifted continuously to infinity while those parts of the interface corresponding to $|x| \to \infty$ remain pinned to the substrate. The filling transition takes place at the temperature T_φ, which depends on the wedge opening angle 2φ and which is smaller than the wetting temperature T_w on the planar substrate.

The critical filling transition was analysed recently [7] via the transfer-matrix approach. Due to the strong anisotropy of the interfacial fluctuations the order parameter corresponding to the height of the interface $\ell(x, y)$ above the substrate $z = |x| \cot\varphi$ can be effectively replaced by the mid-point height $\ell(y) = \ell(0, y)$. The corresponding one-dimensional Hamiltonian has the following form [7, 8]:

$$H[\ell(y)] = \int \mathrm{d}y\, \mathcal{H} = \int \mathrm{d}y \frac{\Sigma}{\alpha} \left[\ell(y) \left(\frac{\mathrm{d}\ell}{\mathrm{d}y} \right)^2 + (\Theta^2 - \alpha^2)\ell(y) \right] \tag{1.1}$$

where Σ is the α–β surface tension and the planar substrate *contact angle* Θ is defined via the Young equation. We consider a very open wedge and thus we have put $\alpha = \cos\varphi \approx \cot\varphi$.

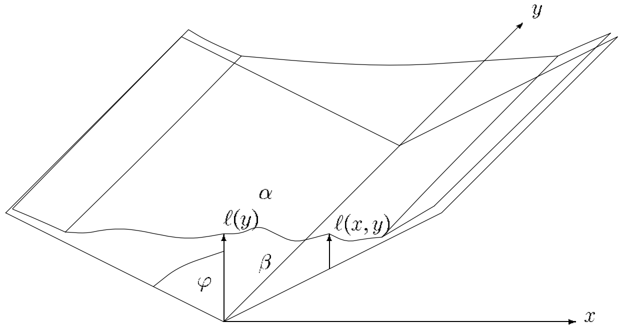

Figure 1. The wedge geometry and the fluctuating α–β interface.

Actually the factor $\Theta^2 - \alpha^2$ in equation (1.1) measures the dimensionless deviation from the filling temperature because $\Theta(T_\varphi) = \alpha$. The above one-dimensional Hamiltonian can be further simplified by introducing the rescaled variables Y and L:

$$\alpha y = \Sigma^{-1/2}((\Theta/\alpha)^2 - 1)^{-3/4} Y \qquad \ell = \Sigma^{-1/2}((\Theta/\alpha)^2 - 1)^{-1/4} L. \tag{1.2}$$

Then the Hamiltonian becomes free from any parameters and has the form

$$H[L(Y)] = \int \mathrm{d}Y\, L[(L'(Y))^2 + 1]. \tag{1.3}$$

This scaling property leads straightforwardly to the critical behaviour of the mean mid-height $\langle \ell \rangle \sim (\Theta/\alpha - 1)^{-1/4}$ and the correlation length $\xi_y \sim (\Theta/\alpha - 1)^{-3/4}$ [7].

2. The propagator

To solve the model described by the Hamiltonian in equation (1.3) one introduces the propagator [9]

$$V(L_2, L_1, Y_2, Y_1) = \int \mathcal{D}L \exp(-H[L])|_{L(Y_1)=L_1}^{L(Y_2)=L_2} \tag{2.1}$$

where the measure $\mathcal{D}L$ is given by $\mathcal{D}L = \prod_Y L^{1/2}(Y)\,\mathrm{d}L\,(Y)$. Actually it is the form of this measure which prohibits one from deriving the equation for the propagator in an unambiguous way. The problem encountered here is similar to the well known Itô–Stratonovich dilemma in the theory of stochastic processes [10].

For $Y_2 - Y_1 = \Delta Y \ll 1$ the discretization schemes applied to equation (2.1) can be parametrized by two parameters a and b ($a, b \in [0, 1]$). These two parameters reflect the freedom (or rather ambiguity) in: (i) defining the measure because of the factor $L^{1/2}(Y)$ present in the measure $\prod_Y L^{1/2}(Y)\,\mathrm{d}L\,(Y)$, a; and (ii) defining the discrete analogue of the term $L(Y)\,(\mathrm{d}L\,(Y)/\mathrm{d}Y)^2$ present in the Hamiltonian, b. In each of these cases the factor $L^{1/2}$ can be split into two factors $L^{c/2}$ and $L^{(1-c)/2}$, $c = a, b$, attached to the left and to the right end of the segment ΔY, respectively. In this way one obtains

$$V(L_2, L_1, \Delta Y) = L_2^{(1-a)/2} L_1^{a/2} \exp\left\{-[(1-b)L_2 + bL_1]\frac{(L_2 - L_1)^2}{\Delta Y} - L_2 \Delta Y\right\} \tag{2.2}$$

which leads to the following equation for the propagator (the Fokker–Planck equation) in the limit $\Delta Y \to 0$:

$$\frac{\partial V}{\partial Y} = -L_2 V + \frac{\partial^2 V}{4L_2 \partial L_2^2} - \frac{(3b - a)\partial V}{4L_2^2 \partial L_2} + \frac{(15b^2 - 6ab - a(2-a))V}{16L_2^3}. \tag{2.3}$$

We see that the form of this equation depends on the choice of parameters a and b. If one insists that the propagator is symmetric, i.e. invariant upon interchanging L_1 and L_2, then one obtains the condition $3b - a = 1$, which still leaves the equation for the propagator depending on one parameter.

The above ambiguity can be avoided by changing the variable in the one-dimensional Hamiltonian in equation (1). Instead of the variable L one introduces the new order parameter $\eta \equiv 2L^{3/2}/3$ and the Hamiltonian takes the form

$$H[\eta(Y)] = \int \mathrm{d}Y \left[(\eta'(y))^2 + \left(\frac{3\eta}{2}\right)^{2/3}\right]. \tag{2.4}$$

The corresponding propagator is defined as

$$\mathcal{V}(\eta_2, \eta_1, Y_2, Y_1) = \int \mathcal{D}\eta \exp(-H[\eta])|_{\eta(Y_1)=\eta_1}^{\eta(Y_2)=\eta_2} \tag{2.5}$$

where $\mathcal{D}\eta = \prod_Y \mathrm{d}\eta\,(Y)$. Now the equation for the propagator is obtained unambiguously:

$$\frac{\partial \mathcal{V}}{\partial Y} = \frac{\partial^2 \mathcal{V}}{4\partial \eta_2^2} - \left(\frac{3\eta_2}{2}\right)^{2/3} \mathcal{V}. \tag{2.6}$$

The propagators $\mathcal{V}(\eta_1, \eta_2, Y)$ and $V(L_1, L_2, Y)$ are related:

$$V(L_1, L_2, Y_1, Y_2) = (3/2)^{1/3}(\eta_1\eta_2)^{1/6}\mathcal{V}(\eta_1, \eta_2, Y_1, Y_2). \tag{2.7}$$

It is interesting to note that equation (2.3) for the 'symmetrical choice' $a = b = 1/2$ is not equivalent to equation (2.6).

3. The boundary condition

The equation for the propagator must be supplemented by appropriate boundary conditions at $\eta = 0$, i.e. at $L = 0$. In this letter we follow [9] and impose the following condition:

$$\left.\frac{\partial \mathcal{V}(\eta_2, \eta_1, Y_2, Y_1)}{\partial \eta_2}\right|_{\eta_2=0} = a\mathcal{V}(0, \eta_1, Y_2, Y_1). \tag{3.1}$$

This condition should not depend on $\Theta - \alpha$. Thus for the non-rescaled variable $\bar{\eta}$ defined as $\bar{\eta} = (\Theta/\alpha - 1)^{-3/8}\eta$ one must have

$$\partial_{\bar{\eta}_2} \ln \mathcal{V}|_{\bar{\eta}_2} = \bar{a} = \text{const}. \tag{3.2}$$

Therefore the parameter $a = \bar{a}(\Theta/\alpha - 1)^{-3/8}$ tends to ∞ upon approaching the filling temperature, from which one concludes that the correct boundary condition has the Dirichlet form:

$$\mathcal{V}(0, \eta_1, Y_2, Y_1) = 0. \tag{3.3}$$

In order to find the propagator explicitly we express it by eigenvalues E_n and eigenfunctions ψ_n of the equation

$$[-E_n + (3\eta/2)^{2/3} - \partial_\eta^2/4]\psi_n(\eta) = 0 \tag{3.4}$$

with boundary condition $\psi_n(0) = 0$. Then the propagator is written in the form

$$\mathcal{V}(\eta_2, \eta_1, Y_2, Y_1) = \sum_n \psi_n(\eta_2)\psi_n(\eta_1)\mathrm{e}^{-E_n(Y_2 - Y_1)}. \tag{3.5}$$

The first four eigenvalues are $E_0 \approx 1.751\,37$, $E_1 \approx 2.652\,89$, $E_2 \approx 3.320\,79$, $E_3 \approx 3.875\,86$ and the corresponding eigenfunctions obtained numerically [11] are shown in figure 2.

To calculate physical quantities one needs the multipoint probability distribution $p(Y_0, \eta_0, \ldots, Y_k, \eta_k)$. This distribution can be expressed as the product of propagators

$$p(Y_0, \eta_0, \ldots, Y_k, \eta_k) = \frac{\prod_{i=-1}^{k} \mathcal{V}(\eta_{i+1}, \eta_i, Y_{i+1}, Y_i)}{\mathcal{V}(\eta_{k+1}, \eta_{-1}, Y_{k+1}, Y_{-1})} \tag{3.6}$$

where (Y_{-1}, η_{-1}) and (Y_{k+1}, η_{k+1}) are coordinates of the boundary conditions.

4. Conclusions

We have pointed out that, although the transfer-matrix method seems to be applicable rather straightforwardly to the effective one-dimensional Hamiltonian describing the critical fluctuations at the filling transition, one is still left with the problem of the non-unique way of discretizing this problem. Thus the analogue of the Itô–Stratonovich dilemma appears in the transfer-matrix analysis of the critical interfacial fluctuations in the presence of a non-planar

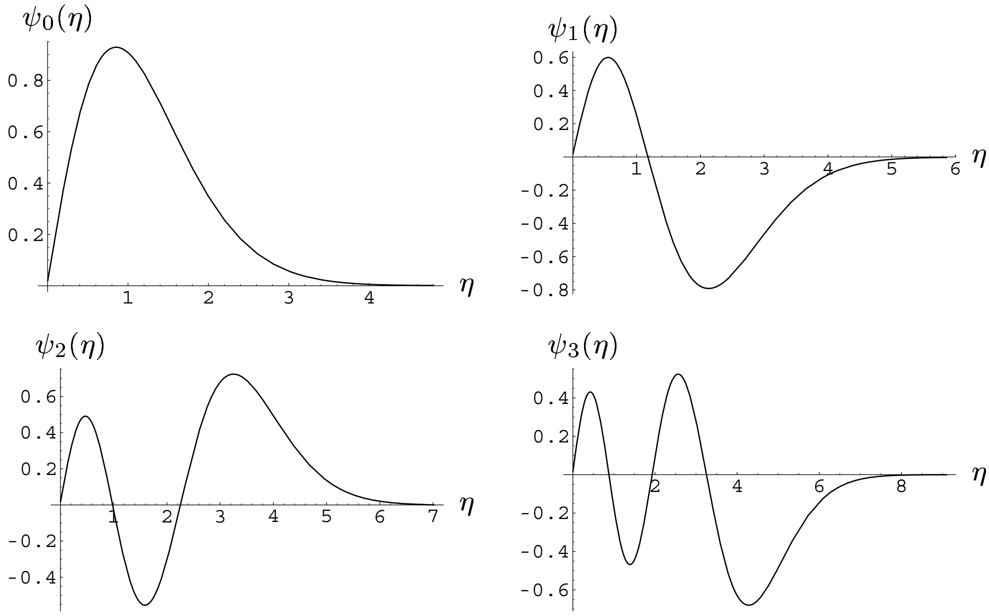

Figure 2. The eigenfunctions ψ_0, ψ_1, ψ_2 and ψ_3.

substrate. In order to avoid this problem we propose to find, first, the right order parameter and the corresponding space of functional integration. We show how such a choice leads to the disappearance of the ambiguity upon the discretization of the problem.

The above considerations show that, in order to get a hint about the right form of the Fokker–Planck equation, one should go back to the complete two-dimensional description and from there, deduce the correct values of a and b. Equation (2.3) becomes equivalent to equation (2.6) if the term $\epsilon\mathcal{V}/4\eta_2^2$ is added to the rhs of equation (2.3), where the coefficient ϵ depends on the parameters a and b. For a 'symmetrical choice' $\epsilon = -1/36$. We suspect that ϵ is, in fact, non-zero and finding its right value remains the challenge.

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