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Numerical study of an effective interface model for the growth of wetting layers

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We present results from a numerical study of an effective interface model introduced by Lipowsky for the growth of wetting layers under complete wetting conditions. Both the equilibrium and the dynamical properties of the model are studied. The values of the scaling exponents are computed when the bulk dimension of the system is either above or below the upper critical dimension. In each case, we find good agreement with the theoretical predictions.

I. INTRODUCTION

The growth of wetting layers has received considerable attention in recent years.[1–8] Much of the effort has been devoted to study the properties of wetting layers in thermal equilibrium. More recently, however dynamical properties of the layers, i.e., how the thickness of such layers approach equilibrium from an initial nonequilibrium state, are also generating a lot of interest.[9–15]

In this paper, we numerically study the equilibrium and dynamical properties of an effective interface model introduced by Lipowsky.[9,10] In this model, a coarse-grained description of the wetting layer is presented by neglecting the intrinsic structure of the interface. On this coarse-grained scale, the wetting layer is described by a single variable l which measures the distance between the solid-liquid and liquid-vapor interfaces. In general, this distance deviates from its mean value due to thermal fluctuations, and depends on the coordinates $\mathbf{x}$ parallel to the substrate surface. Thus, $l=l(x_1,x_2,---,x_{d-1})$ is the distance between $(d-1)$-dimensional interfaces and d is the bulk dimension.

We consider the model in both two and three bulk dimensions such that the interfaces are of dimension one or two. The parameters of the model are chosen such that the bulk dimensionality can be either above or below the upper critical dimension d^*. When $d>d^*$, the system is said to be in the mean-field (MF) regime, otherwise the system is in the fluctuation (FL) regime. We calculate the corresponding scaling exponents in both the MF and the FL regimes, and find good agreements with the theoretical calculations in both the cases. The numerical determination of the MF exponents serves the purpose of checking the validity and the feasibility of the numerical procedures employed. The values of the scaling exponents calculated in the FL regime give strong support to the scaling ideas used in their analytical evaluations.

The rest of the paper is organized as follows. In Sec. II we discuss the effective interface model of Lipowsky in more detail and give a summary of the theoretical predictions of the model. In Section III we discuss the numerical procedures employed to calculate various quantities. We present our results for both equilibrium and nonequilibrium scaling exponents in Sec. IV and finally conclude with a brief summary and a conclusion in Sec. V.

II. THE EFFECTIVE INTERFACE MODEL

In the effective interface model, one starts with the free-energy functional (in units of k_BT) as

$$F\{l\}=\int d^{d-1}x\left[\tfrac{1}{2}\sigma(\nabla l)^2+V(l)\right], \tag{1}$$

where $l(x_1,x_2,---,x_{d-1})$ is the distance between the $d-1$)-dimensional interfaces which bind the wetting layer, σ is the interfacial tension, and $V(l)$ is an effective interface potential. In general, $V(l)$ consists of a repulsive part and an attractive part. For complete wetting, one considers

$$V(l)=Wl^{-p}+(\delta\mu)l\ , \tag{2}$$

where W is a positive (Hamaker) constant and $\delta\mu$ is the deviation of the chemical potential from its value at coexistence. The dynamical model is then defined in terms of a Langevin equation,

$$\frac{\partial l(\mathbf{x},t)}{\partial t}=-\Gamma\frac{\delta F\{l\}}{\delta l}+\eta\ , \tag{3}$$

where Γ is an Onsager coefficient and η is a Gaussian noise given by

$$\langle\eta(\mathbf{x},t)\eta(\mathbf{x}',t')\rangle=2\Gamma\delta(\mathbf{x}-\mathbf{x}')\delta(t-t')\ . \tag{4}$$

The theoretical predictions of the model are the following.

Let us first consider the situation where $\delta\mu\to 0$. Then the effective interface potential $V(l)$ [Eq. (2)] has only a repulsive part and hence the mean thickness $l_{\rm eq}$ of the layer diverges as

$$l_{\rm eq}\sim(\delta\mu)^{\beta_s}\ . \tag{5}$$

The value of the exponent β_s is different for spatial dimensions above or below the upper critical dimension $d^*(p)$. The upper critical dimension $d^*(p)$ depends only on the repulsive part of the interface potential [Eq. (2)]

and is given by

$$d^*(p)=\frac{2+3p}{2+p} \ . \tag{6}$$

For example, when $p=2$, $d^*=2$ and when $p=3$, $d^*=2.2$. One usually defines two scaling regimes: a mean-field regime for which $d>d^*(p)$ and a fluctuation regime for which $d\leq d^*(p)$. In the MF regime one has

$$\beta_s=-\frac{1}{(p+1)} \tag{7}$$

independent of d, and in the FL regime one has

$$\beta_s=-\frac{3-d}{d+1} \tag{8}$$

independent of p. The same values of β_s have been obtained by several other methods.[16–18]

In order to study the dynamics of the growth of the wetting layers, one considers a different situation. In this case, the wetting layer has a small but finite thickness to start with. The scaling field $\delta\mu$ is then turned off at $t=0$. Since, again, the interface potential contains only repulsive terms in l, the thickness of the wetting layer $\langle l(t)\rangle$ grows with time as

$$\langle l(t)\rangle \sim t^n \ . \tag{9}$$

For $d>d^*(p)$, a MF approximation to Eq. (3) provides

$$n=\frac{1}{2+p} \tag{10}$$

independent of the spatial dimension d. For short-range forces, however, the interface potential has the form

$$V(l)=We^{-l/\xi}+(\delta\mu)l \ , \tag{11}$$

where ξ is the bulk correlation length. The corresponding MF approximation yields

$$\langle l(t)\rangle \sim \ln t \ . \tag{12}$$

In order to calculate n in the FL regime, one uses a scaling argument for the long-time behavior and finds[10]

$$n=\tfrac{1}{4}(3-d) \tag{13}$$

independent of all p, including the short-range interactions in Eq. (11) for which $p=\infty$. In particular then, for $d=2$ and $p\geq 2$, the wetting layer grows as t^n with the universal value $n=\frac{1}{4}$. We intend to check some of these predictions in our numerical calculations.

III. NUMERICAL PROCEDURE

We consider the Langevin equation (3) for $l(\mathbf{x},t)$ with the free-energy $F\{l\}$ given by Eq. (1). For the interface potential $V(l)$, we consider both the forms given by Eqs. (2) and (11). We set $\sigma=1$, $W=1$, $\xi=1$, and $\Gamma=1$ in the above equations. Thus, one gets the following equation:

$$\frac{\partial l(\mathbf{x},t)}{\partial t}=\nabla^2 l-\frac{\partial V}{\partial l}+\eta \tag{14}$$

for the evolution of $l(\mathbf{x},t)$. In order to integrate Eq. (14), we employ a finite-difference scheme for both the spatial and temporal derivatives. As mentioned earlier, Eq. (14) is defined over a $d'=(d-1)$-dimensional interface, where

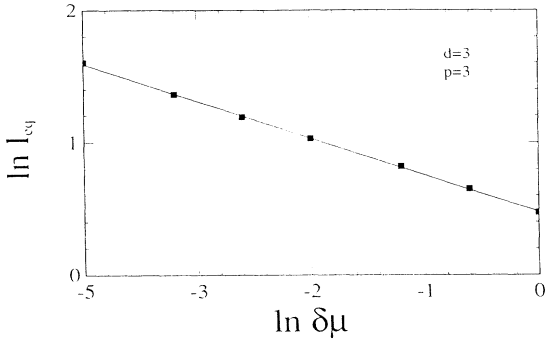

FIG. 1. $\ln l_{\rm eq}$ v $\ln\delta\mu$ for $d=3$ ($d'=2$) and $p=3$. The slope of the straight line is $\beta_s=-0.25\pm0.01$. The corresponding MF value for β_s is $\frac{1}{4}$.

d is the bulk dimension. The spatial discretization is achieved by replacing the continuous space of position vectors by a lattice of $N=L^{d'}$ sites and lattice spacing a. Periodic boundary conditions are assumed in order to avoid surface effects. We consider both $d'=1$ and 2 in our simulations and write the Laplacian operator as

$$\nabla^2 f(x)=\frac{1}{a^2}[f(x+a)+f(x-a)-2f(x)] \tag{15}$$

and

$$\nabla^2 f(x,y)=\frac{1}{a^2}[f(x+a,y)+f(x-a,y)+f(x,y+a)+f(x,y-a)-4f(x,y)] \tag{16}$$

for $d'=1$ and 2, respectively.

We employ a simple Euler scheme for the integration[19] with a time step Δt and write, at each lattice point i,

$$l_i(t+\Delta t)=l_i(t)+\Delta t\left[\nabla^2 l_i-\frac{\partial V(l_i)}{\partial l_i}\right]+\sqrt{\Delta t}\,\eta_i(t) \ . \tag{17}$$

The Gaussian random numbers η_i are generated by using the standard Box-Muller formula. We have considered $a=1$ and $\Delta t=0.01$ in our simulations. We have checked that smaller values of Δt do not change the measured quantities appreciably.

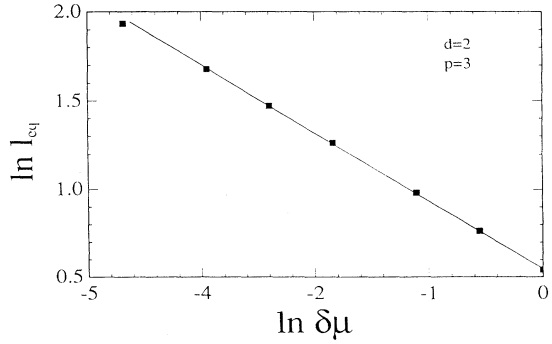

FIG. 2. $\ln l_{\rm eq}$ v $\ln\delta\mu$ for $d=2$ ($d'=1$) and $p=3$. The slope of the straight line is $\beta_s=-0.32\pm0.01$. The corresponding value of β_s in the FL regime is $\frac{1}{3}$.

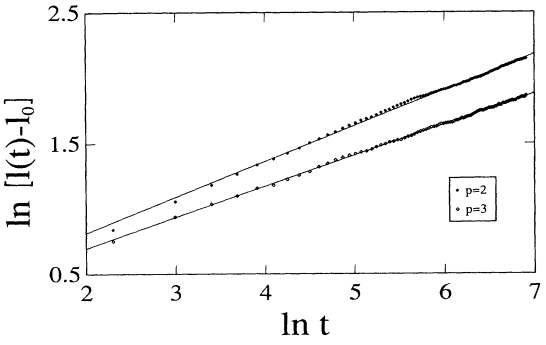

FIG. 3. $\ln[l(t)-l_0]$ v $\ln t$ for $d=3$ ($d'=2$) and $p=2$ (upper curve) and $p=3$. The lattice size is 32×32 and the data are averaged over 100 runs in each case. The slopes of the lines are given by 0.26 ± 0.01 and 0.21 ± 0.01, respectively, which compares favorably to the MF values of $\frac{1}{4}$ and $\frac{1}{5}$, respectively.

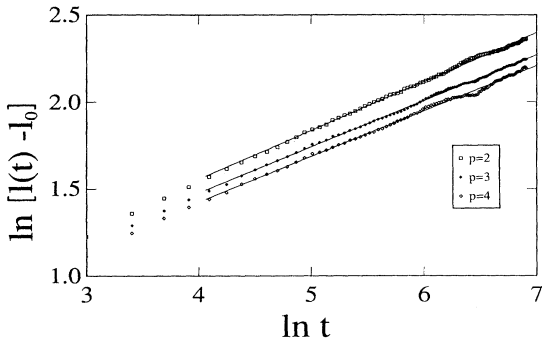

FIG. 5. $\ln[l(t)-l_0]$ vs $\ln t$ for $d=2$ ($d'=1$) and for $p=2$ (uppermost curve), 3, and 4, respectively. The lattice size is $L=500$ and the data are averaged over 100 runs in each case. The slopes of the straight lines are given by 0.26 ± 0.01, 0.25 ± 0.01, and 0.25 ± 0.01, respectively. The theoretical value of the exponent is $\frac{1}{4}$ independent of p.

IV. RESULTS

A. Equilibrium calculations

In order to calculate the exponent β_s in different dimensions d, we start with a small value of $\delta\mu$ run the Langevin equation (14) to equilibrium, and calculate the equilibrium value of the thickness of the wetting layer $l_{\rm eq}$ as

$$l_{\rm eq}=\left\langle \frac{1}{N}\sum_i l_i \right\rangle , \tag{18}$$

where N is the number of lattice sites considered in the simulation, and $\langle\cdots\rangle$ is the ensemble average. For $d=3$ (i.e., $d'=2$) the exponent β_s is expected to be given by mean-field calculations [Eq. (7)] for both $p=2$ and 3. In $d'=2$ we consider a 10×10 lattice for most of our calculations, although lattice sizes of 16×16 and 20×20 are also used in some runs to check possible finite-size effects. We always start with $l_i=l_{\rm MF}$ everywhere on the lattice and then equilibrate the system. Here $l_{\rm MF}$ is the mean-field value of the equilibrium thickness of the wetting layer, i.e.,

$$l_{\rm MF}=\left[\frac{pW}{\delta\mu}\right]^{1/(p+1)} . \tag{19}$$

Runs over the first 5000 time units are discarded and then $l_{\rm eq}$ is calculated over another $t=5000$. We computed $l_{\rm eq}$ for both $p=2$ and 3, although we show the results for $p=3$ only in Fig. 1. Good agreement with the MF results are found in each case.

For $d'=1$, the system is expected to be in the FL regime for both $p=2$ and 3 and the exponent β_s is equal to $-\frac{1}{3}$ [Eq. (8)] independent of p. We check this result by carrying out the numerical simulations in $d'=1$ for an $L=100$ lattice for several values of $\delta\mu$ and for both $p=2$ and 3. Again, good agreement with the theoretical calculation is found in each case. In Fig. 2 we show our results only for $p=3$, however.

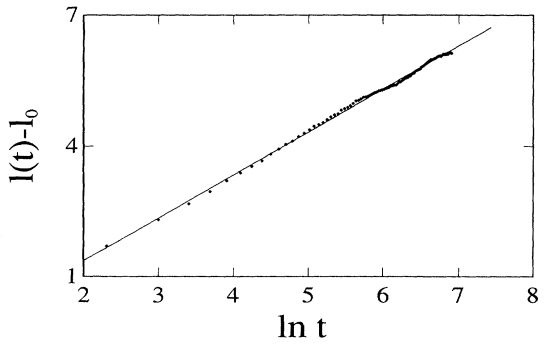

FIG. 4. $[l(t)-l_0]$ vs $\ln t$ for $d=3$ ($d'=2$) and for the interaction potential given by Eq. (11). The lattice size is 32×32 and the data are averaged over 100 runs. In this case a log-log plot shows considerable curvature.

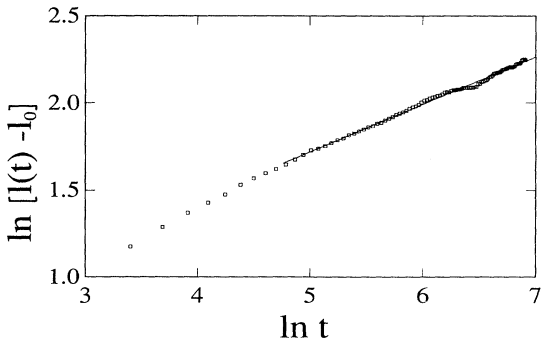

FIG. 6. $\ln[l(t)-l_0]$ vs $\ln t$ for $d=2$ ($d'=1$) and for the interaction potential given by Eq. (11). The lattice size is $L=500$ and the data is averaged over 100 runs. The slope of the straight line is 0.26 ± 0.01 whereas the theoretical value for the exponent in this case is $\frac{1}{4}$.

B. Dynamics of growth

As discussed earlier, the system is in the MF regime for $d=3$ and the growth exponent n is given by Eq. (10). Our results for $p=2$ and 3 are shown in Fig. 3. In all of these cases, we start with an $L=32\times32$ lattice, set $l_i(t=0)=l_0=1$ everywhere as our initial condition, and integrate Eq. (3) with $\delta\mu=0$. We then define the layer thickness at any time t as

$$l(t)=\left\langle \frac{1}{N}\sum_i l_i(t)\right\rangle , \tag{20}$$

where $\langle\cdots\rangle$ denotes an average over the noise. We then look for a growth exponent n by plotting $[l(t)-l_0]$ versus t in a log-log plot and finding the slope of the straight line. As can be seen in Fig. 3, our results agree very well with the MF results. For $d=3$ the system is in the MF regime even for $p=\infty$ (i.e., short-ranged interaction potential) and one expects a logarithmic growth with time. We show such a plot of $[l(t)-l_0)$ versus $\ln t$ in Fig. 4 for the interaction potential given by Eq. (11). In this case a log-log plot shows considerable curvature.

For $d'=1$ the system is in the FL regime and the growth-law exponent n is found to be $\frac{1}{4}$ independent of p. In order to study the growth in the FL regime we start with an $L=500$ lattice and set $\delta\mu=0$. We calculate the growth exponents for $p=2,3$ and 4 (Fig. 5) and $p=\infty$ (Fig. 6). In each case we get $n=\frac{1}{4}$ within our numerical accuracy.

V. SUMMARY AND CONCLUSIONS

We have studied the effective interface model for both $d=2$ and 3 and calculated the equilibrium and dynamical properties of the wetting films. We have calculated the scaling exponents under the condition of complete wetting in mean-field and fluctuation regimes. We have chosen the effective interface potentials $V(l)$ both of the type $V(l)\sim l^{-p}$ and $V(l)\sim e^{-l/\xi}$. The cases $p=2$ and 3 correspond to van der Waals and retarded van der Waals potentials and are of physical interest.

In equilibrium situations, we find that the thickness of the film $l_{\rm eq}$ scales as $(\delta\mu)^{-1/(p+1)}$ in the mean-field regime. In the fluctuation regime, the corresponding scaling behavior is given by $l_{\rm eq}\sim(\delta\mu)^{-3/d+1}$. For nonequilibrium situations, the thickness of the film scales t^n with time. In the mean-field regime we find $m=1/2+p$ for $p=2$ and 3. When the effective potential is given by $e^{-l/\xi}$ we find that the thickness of the film grows as $\ln t$ in the MF regime. In the fluctuation regime we study the growth behavior for several different interface potentials and find $n\sim\frac{1}{4}$ in each case. All of these results are in very good agreement with the theoretical predictions.[10]

In summary, then, we conclude that numerical simulation of Langevin-type models can be effectively used to calculate both equilibrium and nonequilibrium properties of wetting films in the complete wetting conditions. Langevin models to study critical wetting have also been proposed by Lipowsky.[10] Moreover, similar models have also been worked out[20,21] for the unbinding transition of polymerized membranes and these models are amenable to similar kinds of numerical studies. Works in these directions are already in progress and the results are planned to be published elsewhere.[22]

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