The role of degenerate mobilities in Cahn-Hilliard models

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The present work provides an insight into the role of degenerate mobilities in phase field models and in particular their influence on the evolution of the interface. The equation of interest is the Cahn-Hilliard equation (in two space dimensions) with a polynomial double well free energy and different order-parameter dependent, degenerate mobilities. According to the preliminary work [1], considering an anisotropic version of the equation, the asymptotic sharp interface limit subtly depends on the degeneracy of the mobility. Whilst a quadratic degenerate mobility leads to a sharp interface model where bulk diffusion is present at the same asymptotic order as surface diffusion, a bi-quadratic degenerate mobility leads to a sharp interface model where bulk diffusion is subdominant. The present study continues the preliminary work and shows that the type of the degeneracy has a qualitative impact on the evolution: Considering numerical simulations of the dewetting process of a thin solid film with four-fold anisotropic surface energy, the evolution with bi-quadratic degenerate mobility turns out to be more effective for film pinch-off than with quadratic degenerate mobility. An extension to the isotropic Cahn-Hilliard equation ensures that the characteristic difference in the pinch-off behavior is in fact mobility-dependent.

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1 Motivation: An anisotropic Cahn-Hilliard model for surface diffusion dewetting

When a thin solid film is heated to sufficiently high temperatures, but well below the melting temperature of the material, it may retract, pinch-off and evolve similar as in the liquid state - while it still remains solid. This surface diffusion driven phenomenon is called solid state dewetting and modeling it mathematically was the initial motivation for the present study.

In our preliminary work [1] we introduced the following anisotropic version of the two-dimensional Cahn-Hilliard equation for solid state dewetting

$$\partial_t u = \nabla \cdot (m(u) \nabla \mu), \quad \mu = 2(u^3 - u) - \varepsilon^2 \nabla \left[ \gamma(\theta) \gamma'(\theta) \left( \frac{-u_{yy}}{u_x} \right) + \gamma(\theta)^2 \nabla u \right],$$

(1)

for a conserved order parameter $u(x, y, t)$ and $\gamma(\theta)$ in a domain $\Omega \subset \mathbb{R}^2$ for time $t > 0$, where $\gamma$ is the anisotropic surface energy, $-\pi < \theta \leq \pi$ is the angle between $-\nabla u$ and the x-axis and $m(u)$ a degenerate mobility. It is well known that Cahn-Hilliard equations with degenerate mobility approximate interface motion by surface diffusion on the slowest time scale $O(\varepsilon^{-2})$ but still, due to the diffuse character of the model, it is not obvious which explicit representation for $m(u)$ in (1) recovers motion by pure surface diffusion. In particular, it was shown in [3] that the mobility $m(u) = |1 - u^2|$ in the isotropic version of (1) (i.e. with $\gamma \equiv 1$) is not sufficient for this purpose: the sharp-interface limit, i.e. the limit equation when the width $\epsilon$ of the diffuse interface tends to zero, contains, besides surface diffusion, a contribution from porous-medium type bulk diffusion. Motivated by the reference paper [3], we chose $m(u) = (1 - u^2)^2$ to increase the suppression of the flux from the bulk and showed in [1] that for this choice the limit equation corresponds to the sharp interface model

$$\nu_n = \left( \frac{2}{3} \right)^2 \partial_s \left( \gamma_0 \partial_s \left( (\gamma_0 + \gamma_0^s) \kappa \right) \right), \quad \mu_1 = \left( \frac{2}{3} \right)^2 (\gamma_0 + \gamma_0^s) \kappa,$$

(2)

which, according to [4], correctly describes the anisotropic evolution due to surface diffusion.

2 Numerical simulations: $m(u) = |1 - u^2|$ vs. $m(u) = (1 - u^2)^2$

Fig. 1: Numerical comparison (showing the zero-level set of $u$) between the evolution with mobility $m(u) = (1 - u^2)^2$ and $m(u) = 1 - u^2$. where $\epsilon = 0.02, dx = dy = 0.002$ and $\tau = 0.001$ at a) $t = 0, b) t = 5$ and c) $t = 20$.

The question naturally arises if the choice of the degenerate mobility has a qualitative influence or if it only influences the characteristic time scale of the evolution. In order to answer this question for the present model, numerical simulations of (1)
with the quadratic degenerate mobility \( m(u) = |1 - u^2| \) and the bi-quadratic degenerate mobility \( m(u) = (1 - u^2)^2 \) were applied and compared concerning the evolution of a thin long film on a solid substrate \( \Gamma_w \). The model was completed by natural boundary conditions, i.e.

\[
\epsilon \, \mathbf{n} \cdot \left[ \gamma(\theta) \gamma'(\theta) \left( \frac{-u_u}{u_u} \right) + \gamma(\theta)^2 \nabla u \right] + \frac{f_{\text{adm}}}{\lambda} = 0 \quad \text{on } \Gamma_w, \quad \mathbf{n} \cdot \nabla u = 0 \quad \text{on } \partial \Omega \setminus \Gamma_w,
\]

where \( f_{\text{adm}} \) denotes the energy density at the substrate, and conservation of mass

\[
\mathbf{n} \cdot (m(u) \nabla \mu) = 0, \quad \text{on } \partial \Omega. \tag{3b}
\]

The finite element based simulation in MATLAB applies an operator splitting ansatz and a diffuse boundary approximation at the substrate (details of the numerical implementation are given in Chapter 5 of [2]). Considering a rectangular initial state and the fourfold anisotropic surface energy \( \gamma(\theta) = 1 + 0.05 \cos(4\theta) \), the simulation, Fig. 1, shows that the mobility in fact has a qualitative impact on the evolution: The film corresponding to \( m(u) = 1 - u^2 \) forms a single equilibrium crystal, whereas the film corresponding to \( m(u) = (1 - u^2)^2 \) pinches off and in the near term forms two equilibrium shapes. Note that, as long as \( \epsilon > 0 \), bulk transport of a subdiffusive character is expected to still be present which leads to coarsening on a very long time-scale, i.e. the two equilibrium shapes will merge to a single equilibrium shape for large time values. The Figure shows in addition the exact equilibrium shape, which is determined by the Winterbottom construction [5].

### 3 The role of degenerate mobilities in the (isotropic) Cahn-Hilliard equation

In order to exclude the impact of the anisotropy and energy at the substrate, the present sections extends the numerical study of Section 2 to the isotropic version of (1), i.e.

\[
\partial_t u = \nabla \cdot (m(u) \nabla \mu), \quad \mu = 2(u^3 - u) - \epsilon^2 \Delta u, \tag{4}
\]

with homogeneous Neumann- and conservation of mass boundary conditions. Since the boundary conditions now allow for the application of spectral methods, which have excellent error properties, the simulations in the present section are based on a Fast Fourier Transform algorithm together with an operator splitting ansatz. The corresponding numerical simulations, Fig.2, show that, considering a particular critical film length, the pinch-off behavior is in fact mobility dependent: While the film with constant mobility retracts to one circle, the quadratic degenerate mobility case leads to two and the bi-quadratic degenerate mobility case to even three (near-term) limit circles. This observation provides a new insight into the role and influence of degenerate mobilities in Cahn-Hilliard models and an analytical verification of the present film-breakup phenomenon is currently in progress.

![Fig. 2: Numerical comparison (showing the zero-level set of \( u \)) between the evolution with mobility \( m(u) = 1 \), \( m(u) = |1 - u^2| \) and \( m(u) = (1 - u^2)^2 \), where \( \epsilon = 0.05, \, dx = dy = 0.05 \) and \( \tau = 0.0001 \) at a) \( t = 0 \), b) \( t = 3.5 \) and c) \( t = 7 \).](image)

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