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Dynamics of evolving surfaces with small corner energy regularization

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Abstract

To overcome the backward parabolic behavior of geometric evolution laws based on non-convex interfacial energies a corner energy regularization is used. Anisotropic mean curvature flow and surface diffusion are addressed with such a regularization term in one space dimension. The resulting problems are fourth, respectively sixth order. A long-wave approximation is performed for both equations resulting in the Cahn–Hilliard equation for the fourth-order problem and a higher order Cahn–Hilliard equation for the sixth-order problem.

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1. Introduction

The equilibrium shape of a particle in two dimensions is defined as the shape of minimum surface free energy $F = E\int_\Gamma \gamma\,\mathrm{d}s$ under the constraint of fixed particle number and volume [7]. In this equation $\gamma = \gamma(\theta)$ is the surface free energy density parametrized by the angle θ and E a constant which sets the scale of energy per unit length. The equilibrium shape can then be constructed via the geometric interpretation of the Wulff theorem [12]: At each point of the polar plot of the free energy density $\gamma(\theta)$, a straight line perpendicular to the normal direction at that point is drawn; the inner envelope of the resulting family of lines

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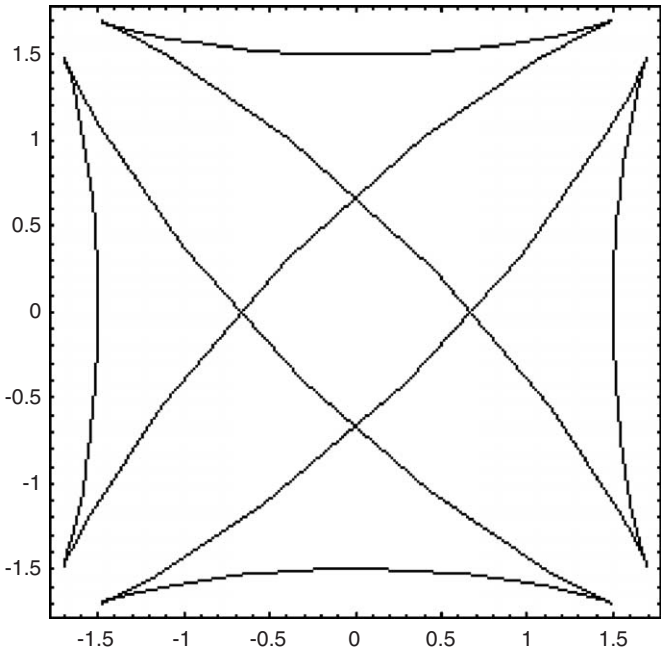

Fig. 1. Wulff shape for $\gamma(\theta) = 1 + \alpha\cos(k\theta + \beta)$ with $k = 4$, $\alpha = 0.5$ and $\beta = 0$. The unphysical "ears" correspond to a negative stiffness and have to be truncated to determine the equilibrium shape.

is then geometrically similar to the equilibrium shape. Depending on the details of γ the equilibrium shape can have corners, facets and wrinklings.

While the equilibrium problem is today well understood, the dynamics creates several difficulties. We concentrate here on the ill posedness for a negative surface stiffness $\tilde{\gamma}=\gamma+\gamma''$. Such a negative surface stiffness excludes high-energy orientations and leads to corners in the corresponding Wulff shape. Fig. 1 shows a corresponding equilibrium shape.

One way to overcome the resulting inherently unstable behavior of the dynamics problem is to regularize the equation by adding a curvature-dependent term to the interface energy density. This was already proposed on physical grounds in [6], and later mathematically introduced in [2,3]. Such a curvature-dependent term introduces a new length scale in which sharp corners are rounded. In two-dimensions the penalized interfacial energy density reads

$$\gamma_\alpha = \gamma + \tfrac{1}{2}\alpha^2\kappa^2,$$

with $\alpha > 0$ setting the length scale of the rounded corner, and κ denoting the curvature. Minimizing the surface energy $F_\alpha = E\int_\Gamma \gamma_\alpha \,\mathrm{d}s$ is therefore a compromise between a large curvature at the corner, which decreases orientations with large surface energy but increases the regularization term, and small curvature at the corner which decreases the regularization term but increases orientations with large surface energy. The amount of corner rounding is therefore determined by these two competing energy terms. The plausibility of such a regularization is clear, but its effect on the equilibrium shape was only recently analyzed.

In [10] asymptotic analysis is performed which shows the convergence to the sharp-corner results as the regularization parameter $\alpha \to 0$, and therefore validates the use of such a regularization in numerical simulations and provides a mathematical basis for its use.

2. Dynamic problem

The surface chemical potential μ_α is defined by the variational derivative of F_α, namely

$$\mu_\alpha = \frac{\delta F_\alpha}{\delta \Gamma} = E\left(-\tilde{\gamma}\kappa + \alpha^2\left(\partial_{ss}\kappa + \frac{1}{2}\kappa^3\right)\right).$$

In the following we assume the evolution essentially interface-controlled and neglect any effect due to the bulk phases. The dynamics equations result from relating the normal velocity v to the chemical potential μ_α. For attachment kinetics as the dominant mass transport mechanism we get

$$\beta v = E(\tilde{\gamma}\kappa - \alpha^2(\partial_{ss}\kappa + \tfrac{1}{2}\kappa^3)),$$

with $\beta = \beta(\theta) > 0$ a kinetic coefficient and ∂_s denoting differentiation with respect to the arc length s. The resulting equation is a fourth-order parabolic geometric evolution law. For surface diffusion as the dominant mass transport mechanism we get

$$\beta v = E\partial_s(v\partial_s(-\tilde{\gamma}\kappa + \alpha^2(\partial_{ss}\kappa + \tfrac{1}{2}\kappa^3))),$$

with $v = v(\theta)$ the mobility of atoms diffusing along the surface. This is a sixth-order parabolic geometric evolution law.

3. Long-wave approximation

In order to derive a dimensionless form, we rescale $\hat{s} = s/\alpha$ and $\hat{t} = Et/\alpha\beta$ which leads to

$$\hat{v} = \tilde{\gamma}\hat{\kappa} - (\partial_{\hat{s}\hat{s}}\hat{\kappa} + \tfrac{1}{2}\hat{\kappa}^3) \tag{1}$$

and

$$\hat{v} = \partial_{\hat{s}}(v\partial_{\hat{s}}(-\tilde{\gamma}\hat{\kappa} + (\partial_{\hat{s}\hat{s}}\hat{\kappa} + \frac{1}{2}\hat{\kappa}^3))), \tag{2}$$

respectively. In the following we will drop the $\hat{}$ in the notation. Choosing γ such that the planar front $\theta = 0$ is thermodynamically unstable and a stable pair of facets with slope $\theta \sim \pm\eta$ exists ($0 < \eta \ll 1$), we can consider the evolution of a surface in the vicinity of the unstable planar front $\theta = 0$ and describe it by the graph $y = h(x, t)$. In the following we closely follow [11], who derived a long wave approximation for the driven system of (1), i.e.

$$\hat{v} = \tilde{\gamma}\hat{\kappa} - (\partial_{\hat{s}\hat{s}}\hat{\kappa} + \tfrac{1}{2}\hat{\kappa}^3) + c \tag{3}$$

with c the driving force. We expand $h=\eta h_1+\eta^2 h_2+\cdots$ and assume only $O(1)$ variations in x. These lead to the small slope condition $\partial_x h=\eta\partial_x h_1+O(\eta^2)$ and the following expansion:

$$v = \eta\partial_t h_1 + O(\eta^2),$$

$$\partial_s = \partial_x + O(\eta^2),$$

$$\theta = \eta\partial_x h_1 + O(\eta^2),$$

$$\kappa = \eta\partial_{xx} h_1 + O(\eta^2),$$

$$\partial_{ss}\kappa = \eta\partial_{xxxx} h_1 + O(\eta^2),$$

where $\kappa=\partial_s\theta$ was used. If we assume $\tilde{\gamma}(\theta)=\hat{\gamma}(\theta/\eta)$ we further get

$$\tilde{\gamma}(\theta) = \hat{\gamma}(\partial_x h_1) + O(\eta).$$

Expanding (1) and (2) in powers of η yields for $O(\eta)$

$$\partial_t h_1 = \hat{\gamma}(\partial_x h_1)\partial_{xx} h_1 - \partial_{xxxx} h_1$$

and

$$\partial_t h_1 = \partial_x(v\partial_x(-\hat{\gamma}(\partial_x h_1)\partial_{xx} h_1 + \partial_{xxxx} h_1)),$$

respectively. Differentiating both equations with respect to x and setting $q=\partial_x h_1$ we get equations for the local slope

$$\partial_t q = \partial_{xx}(W'(q) - \partial_{xx} q) \tag{4}$$

and

$$\partial_t q = \partial_{xx}(v\partial_{xx}(-W'(q) + \partial_{xx} q)), \tag{5}$$

respectively, with $W''(q)=\hat{\gamma}(q)$. The fourth-order equation (4) is known as the Cahn–Hilliard equation and serves as a prototype equation for phase ordering systems. It was introduced as a model to describe spinodal decomposition of binary alloys under isothermal conditions [1]. In this context q is the phase fraction and $W(q)$ a symmetric double well with minima at $q=\pm 1$. In our context the Cahn–Hilliard equation describes a thermally annealed faceted surface with a hill/valley structure with a selected slope $q=\pm 1$. In thin film growth this equation can be derived from a different point of view. We represent the height of the film surface at time t in a co-moving frame by a height function h. Conservation of mass leads to

$$\partial_t h = -\partial_x j,$$

with j the surface current, depending on $\partial_x h$. If we assume isotropic surface diffusion and the current induced by the Ehrlich–Schwoebel effect as the main mechanisms of transport (see [8] for a detailed description of the physical phenomena), we have

$$j = j_{\mathrm{SD}} + j_{\mathrm{ES}},$$

where j_{SD} is the equilibrium surface current due to the adatom surface diffusion and j_{ES} is the kinetic surface current due to the Ehrlich–Schwoebel effect. j_{ES} is only present if the deposition flux, which is transformed into the moving frame, is nonzero. The equilibrium surface current in the linearized version read after appropriate rescaling $j_{SD} = \partial_{xxx} h$. For the derivation of j_{ES} we refer to [9]. After appropriate rescaling the kinetic surface current can be described by $j_{ES} = \partial_x h/(1 + (\partial_x h)^2)$. Both together result in the nonlinear diffusion equation

$$\partial_t h = -\partial_x \left(\frac{\partial_x h}{(1 + (\partial_x h)^2)} + \partial_{xxx} h \right).$$

If $\partial_x h$ is small, which is assumed in the linearization of the equilibrium surface current anyway, $1/(1 + (\partial_x h)^2) \approx 1 - (\partial_x h)^2$ and we obtain

$$\partial_t h = -\partial_x ((1 - (\partial_x h)^2)\partial_x h + \partial_{xxx} h).$$

Differentiating this equation with respect to x and setting $q = \partial_x h$ we again arrive at

$$\partial_t q = \partial_{xx} (W'(q) - \partial_{xx} q) \tag{6}$$

with $W'(q) = q^3 - q$. But even if the long-wave approximation (4) and the model for thin film growth (6) turns out to be the same, the physics behind them is different. The perspective in (4) is thermodynamic and in (6) kinetic. The first term in (4) results from the anisotropic free energy density γ, whereas the second term, indicating the stabilizing Mullins term, results from the regularization. In (6) the first term is purely kinetic resulting from the Ehrlich–Schwoebel current, whereas the second term describes isotropic surface diffusion. The sixth-order equation (5) serves as a long-wave approximation for regularized anisotropic surface diffusion. The first term in (5) results again from the anisotropic free energy density γ, whereas the second term is due to the corner regularization.

4. Numerical approaches

The geometric evolution laws (1) and (2) are treated numerically by parametric finite elements in [4,5], respectively. In both cases the equation is reformulated into a system of second-order equations and a variational formulation is derived which allows the use of linear finite elements within a semi-implicit scheme. The convergence to the Wulff shape is shown for both algorithms.

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