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Optimal profiles in a phase-transition model with a saturating flux

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ABSTRACT

It is well known that for the Allen–Cahn equation, the minimizing transition in an infinite cylinder $\mathbb{R} \times \omega$ is one-dimensional and unique up to a translation in the first variable. We analyze in this paper the existence and symmetry of optimal profiles for transitions in a similar phase-separation model with a saturating flux. This amounts to consider transitions in the space of BV functions as we consider the area integral instead of the Dirichlet energy to penalize the creation of wild interfaces.

1. Introduction

A classical model in phase-transition modeling is given by the so-called Allen–Cahn energy functional

$$\frac{\varepsilon}{2}\int |\nabla u|^2\,dx + \frac{1}{4\varepsilon}\int (|u|^2-1)^2\,dx \tag{1}$$

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where u is a scalar function taking values between -1 and $+1$. This energy functional is used to describe the pattern and the separation of the (stable) phases ± 1 of a substance or a material within the van der Waals–Cahn–Hilliard gradient theory of phase transitions [15]. For instance, it has important physical applications in the study of interfaces in both gasses and solids, e.g. for binary metallic alloys [2] or bi-phase separation in fluids [41]. In this model the function u describes the pointwise state of the material or the fluid. The constant equilibria corresponding to the global minimum points ± 1 of the potential $\frac{1}{4}(|u|^2-1)^2$ are called the pure phases, whereas other configurations u represent mixed states and, if asymptotic to ± 1, they describe phase transitions.

Let us mention that the Allen–Cahn energy functional is relevant too in the theory of superconductors and superfluids where it appears as a Ginzburg–Landau free energy functional, u being then a complex-valued function, see e.g. [11], as well as in cosmology [29] where the motivation is the detection of the shape of the interfaces which "separate" the different regions of the universe which possibly arose from the big-bang.

The classical van der Waals–Cahn–Hilliard theory postulates that interface formation is driven by a variational principle, namely the pattern is the outcome of the minimization of the potential energy. This is clearly not satisfactory since any pattern that takes the values ± 1 only minimizes the potential energy $\frac{1}{4\varepsilon}\int(|u|^2-1)^2\,dx$ so that the separation between the two phases could be as complicated as we want and dramatically non-smooth patterns occur. Since such wild patterns are not observed in experiments, one has to modify the model and a classical way consists in penalizing the creation of unnecessary interfaces by adding a gradient term such as $\frac{\varepsilon}{2}\int|\nabla u|^2\,dx$. The parameter ε accounts somehow for the thickness of the interface. A function u which minimizes the full energy functional now tries to minimize the potential energy without creating too many interfaces since this would increase the gradient term. So basically, the presence of the gradient term has a smoothing effect on the phase separation. To recover the van der Waals–Cahn–Hilliard theory, one then let ε go to zero. It has been shown that the level sets of the minimizers then approach (in a suitable way) hypersurfaces of least possible area [36,34,35,13], meaning that the optimal profiles tend to minimize the potential energy and the area of the interfaces.

In a series of papers (see, e.g., [37,12,32]) it was pointed out that, in some realistic diffusion processes, characterized for small gradients by linear gradient–flux relations, the flux response to an increase of gradients is expected to slow down and ultimately to approach saturation at large gradients. Accordingly, it was proposed in these contexts to penalize interfaces by a gradient term which is still quadratic for small values of the norm of the gradient but asymptotically linear. A simple model is given by the area integral

$$\int\sqrt{1+|\nabla u|^2}\,dx.$$

When the saturation of the diffusion flux is incorporated into these processes, it may cause a fundamental change in the morphology of the ensuing response. It may happen in particular that transitions connecting the equilibrium states may, when the potential exceeds a critical threshold, exhibit one or more discontinuities. In [32] a detailed numerical analysis of the morphology of the responses was performed for the Euler–Lagrange equation of the one-dimensional model

$$\left(u'/\sqrt{1+u'^2}\right)' = F'(u), \tag{2}$$

where F is a potential with several states at the lower energy level. At this stage, it is worth mentioning closely related models of flux limited diffusion equations studied in [5,16] and the references therein.

Apart from its physical relevance, the Allen–Cahn energy functional presents interesting mathematical features. The stationary Allen–Cahn equation in $\mathbb{R}^N$, namely

$$\Delta u = F'(u), \tag{3}$$

where F is the double-well potential

$$F(s) = \tfrac{1}{4}(1-s^2)^2, \tag{4}$$