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FORCE CONVERGENCE FOR THE DE GENNES-CAHN-HILLIARD ENERGY

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Abstract. The degenerate de Gennes-Cahn-Hilliard (dGCH) equation is a recent phase field model that may more accurately approximate surface diffusion. After establishing the Gamma convergence of the dGCH energy in [10], in this paper, we study the convergence of boundary force. This is done by carefully crafting a nonlinear transformation that transforms the dGCH energy into a Cahn-Hilliard-type energy with a non-smooth potential. We carry out explicit computations and analysis to this new system, which in turn enables us to establish the convergence of boundary force for the dGCH energy.

Key words. de Gennes-Cahn-Hilliard energy, Gamma convergence, force convergence.

1. Introduction

In material science applications, especially in solid-state dewetting, motion by surface diffusion is governed by the surface Laplacian of mean curvature [24]. In general, diffuse interface approximations based on fourth-order nonlinear Cahn-Hilliard equations are widely used, and they formally converge to sharp interface models as the interface thickness approaches zero, see the classical paper [20] and later developments in various settings [1, 3, 4, 5, 13, 18, 21, 25, 27, 28]. While it was formally shown that the Cahn-Hilliard equation with a degenerate mobility may converge to surface diffusion for the case of a double barrier potential or the case of a logarithmic potential with the temperature also approaching zero [3], it is not so in the case of a polynomial potential. In fact, there are unintended bulk diffusions if the degeneracy in the mobility is not strong enough [4, 5, 15, 16, 26]. See also related theoretical and numerical results [6, 7].

The diffuse interface model for surface diffusion proposed in [21], known as the doubly degenerate Cahn-Hilliard (DDCH) equation, introduces an additional degeneracy similar to approaches used in classical phase-field models for solidification [14], improving the accuracy of surface diffusion approximations without altering the asymptotic limit [2, 27]. However, this model is non-variational, lacking a known free energy dissipation, which complicates the analysis of solution properties, numerical stability, and its extension to complex multi-physics applications [21]. In [23], the variational model was proposed together with the free energy $E^{\varepsilon}_{\text{dGCH}}$. This model has also recently attracted attention, in particular about questions related to its Gamma convergence [10] and the characterization of the minimizers [9]. In this work, we are concerned with force convergence of $E^{\varepsilon}_{\text{dGCH}}$.

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The degenerate de Gennes-Cahn-Hilliard (dGCH) equation

$$\partial_t u = \frac{1}{\varepsilon}\nabla \cdot (M_0(u)\nabla \mu), \tag{1}$$

$$\mu = -\varepsilon\nabla \cdot \left(\frac{\nabla u}{g(u)}\right) + \frac{1}{\varepsilon g(u)}W'(u) - \frac{g'(u)}{g^2(u)}\left(\frac{\varepsilon}{2}|\nabla u|^2 + \frac{1}{\varepsilon}W(u)\right) \tag{2}$$

is a variational diffuse interface model that may more accurately approximate surface diffusion [23]. It can formally be interpreted as a weighted H^{-1} gradient flow for the dGCH energy

$$E^{\varepsilon}_{\mathrm{dGCH}}(u) := \int_\Omega \frac{1}{g(u)}\left(\frac{\varepsilon}{2}|\nabla u|^2 + \frac{1}{\varepsilon}W(u)\right)dx, \quad \text{for all } u \in H^1(\Omega). \tag{3}$$

Here u is the relative concentration of the two phases, and $\mu = \delta_u E^{\varepsilon}_{\mathrm{dGCH}}$ is the chemical potential, defined by the variational derivative of $E^{\varepsilon}_{\mathrm{dGCH}}$ with respect to u. The double well potential W is taken to be smooth with two equal minima at $u^{\pm}$, corresponding to the two "pure" phases. In this paper we concentrate on the following smooth quartic potential

$$W(u) = (u - u^+)^2(u - u^-)^2. \tag{4}$$

The parameter $\varepsilon > 0$ is proportional to the thickness of the transition region between the two phases. The mobility $M_0(u)$ is degenerate at $u^{\pm}$.

This energy functional included a singularity due to the de Gennes coefficient $\frac{1}{g}$, where g is a function that is degenerate at $u^{\pm}$ (see, e.g., [11, 19]). A natural choice is the form

$$g(u) = |(u - u^-)(u - u^+)|^p, \quad p > 0. \tag{5}$$

Intuitively, the singularities at $u^{\pm}$ may help to keep solutions confined in $[u^-, u^+]$. But the validity of this argument remains open.

To theoretically explore the systemic properties of the dGCH model, as a first step, we have studied the sharp interface limit of the dGCH energy as the thickness of the transition region goes to zero, by establishing its Gamma limit under the strong $L^1(\Omega)$ topology [10]. To be more precise, by extending the definition of $E^{\varepsilon}_{\mathrm{dGCH}}$ to all $u \in L^1(\Omega)$ by defining

$$E^{\varepsilon}_{\mathrm{dGCH}}(u) := \begin{cases} \int_\Omega \frac{1}{g(u)}\left(\frac{\varepsilon}{2}|\nabla u|^2 + \frac{1}{\varepsilon}W(u)\right)dx, & \text{if } u \in H^1(\Omega), \\ \infty & \text{otherwise,} \end{cases} \tag{6}$$

we proved that for $0 < p \leq 1$, $E^{\varepsilon}_{\mathrm{dGCH}}$ Γ-converges to

$$E^{0}_{\mathrm{dGCH}}(u) := \begin{cases} \sigma(p)\mathrm{Per}(A) & \text{if } u = u^- + (u^+ - u^-)\chi_A \in BV(\Omega), \\ \infty & \text{otherwise} \end{cases} \tag{7}$$

as $\varepsilon \to 0$. Here χ_A is the characteristic function of a set A of finite perimeter, $\mathrm{Per}(A)$ is the perimeter of A, and

$$\sigma(p) = \sqrt{2}\int_{u^-}^{u^+} |(s - u^-)(s - u^+)|^{1-p}\,ds.$$

In other words, the Γ-limit of $E^{\varepsilon}_{\mathrm{dGCH}}$ is a multiple of the perimeter of the set A on which u takes the value u^+.

In this paper, we will introduce a nonlinear transformation to build a connection between the dGCH energy and a Cahn-Hilliard energy with a non-smooth double well potential, and state and prove Γ-convergence and force convergence of the new