

Stability of the Semi-Implicit Method for the Cahn-Hilliard Equation with Logarithmic Potentials

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Abstract. We consider the two-dimensional Cahn-Hilliard equation with logarithmic potentials and periodic boundary conditions. We employ the standard semi-implicit numerical scheme, which treats the linear fourth-order dissipation term implicitly and the nonlinear term explicitly. Under natural constraints on the time step we prove strict phase separation and energy stability of the semi-implicit scheme. This appears to be the first rigorous result for the semi-implicit discretization of the Cahn-Hilliard equation with singular potentials.

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1 Introduction

Consider the 2D Cahn-Hilliard equation on $\Omega = \mathbb{T}^2 = [-\pi, \pi)^2$:

$$\begin{cases} \partial_t u = \Delta \mu = \Delta(-\nu \Delta u + F'(u)), & (t, x) \in (0, \infty) \times \Omega, \\ u|_{t=0} = u_0, \end{cases} \quad (1.1)$$

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where $u: \Omega \rightarrow (-1, 1)$ is the order parameter of a two-phase system such as a binary alloy, and the term μ denotes the chemical potential. The two end-points $u = \pm 1$ correspond to pure states. The coefficient $\nu > 0$ denotes mobility. In this paper we take it to be a constant parameter. The thermodynamic potential $F: (-1, 1) \rightarrow \mathbb{R}$ is given by

$$F(u) = \frac{\theta}{2} \left((1+u) \ln(1+u) + (1-u) \ln(1-u) \right) - \frac{\theta_c}{2} u^2, \quad 0 < \theta < \theta_c, \quad (1.2a)$$

$$f(u) = F'(u) = -\theta_c u + \frac{\theta}{2} \ln \frac{1+u}{1-u} =: -\theta_c u + \tilde{f}(u), \quad F''(u) = \frac{\theta}{1-u^2} - \theta_c, \quad (1.2b)$$

where the logarithmic part accounts for the entropy of mixing. The parameters θ and θ_c corresponds to the absolute temperature and the critical temperature respectively. Denote by $u_+ > 0$ the positive root of the equation $f(u) = 0$ (see (1.2b)). Under the condition $0 < \theta < \theta_c$ the potential F takes the form of a double-well with two equal minima at u_+ and $-u_+$ which are usually called binodal points. One should note that the condition $0 < \theta < \theta_c$ is of physical importance since it guarantees that that F has a double-well form and phase separation can indeed occur. For $u_s = (1 - \theta/\theta_c)^{\frac{1}{2}}$, the region $(-u_s, u_s)$, where $F''(u) < 0$ is called the spinodal interval. If the quenching is shallow, i.e., the temperature θ is close to the absolute temperature θ_c , then one can expand near $u = 0$ and obtain the usual quartic polynomial approximation of the free energy.

The usual energy conservation takes the form:

$$\frac{d}{dt} \mathcal{E}(u) = - \| |\nabla|^{-1} \partial_t u \|_2^2, \quad \mathcal{E}(u) = \int_{\Omega} \left(\frac{1}{2} \nu |\nabla u|^2 + F(u) \right) dx. \quad (1.3)$$

Note that for $u \in (-1, 1)$, the term $F(u)$ is bounded by an absolute constant, and the only coercive quantity in $\mathcal{E}(u)$ is the gradient term.

Remark 1.1. We note that the usual quartic polynomial approximation of the free energy $F(u)$ is given by (below the series converges for $u \in [-1, 1]$)

$$\begin{aligned} F(u) &= -\frac{\theta_c}{2} u^2 + \theta \sum_{k=0}^{\infty} \frac{u^{2k+2}}{(2k+1)(2k+2)} \\ &\approx F_{\text{quartic}}(u) = \frac{\theta}{2} \cdot \frac{u^4}{6} + \left(\frac{\theta}{2} - \frac{\theta_c}{2} \right) u^2. \end{aligned}$$

The standard double-well potential $\text{const} \cdot (u^2 - 1)^2$ corresponds to the specific choice $\theta/\theta_c = 3/4$. However, this approximation introduces a nontrivial shift of the location of the minimum. Namely for the original free energy $F(u)$, its two equal minima