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# Robustness of error estimates for phase field models at a class of topological changes

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## Highlights

- Characterization of stability for phase field evolutions at singularities.
- Accuracy of numerical methods when particles vanish.
- Description of phase boundaries when topological changes occur.

## Abstract

A priori and a posteriori error estimates for the numerical approximation of phase field models with a polynomial dependence on the inverse of the interface width as long as no topological changes occur have recently been derived. Numerical experiments show that they remain robust when topological changes of the interface take place. Based on an asymptotic expansion a lower bound for the principal eigenvalue of the linearized Allen–Cahn operator near a generic singularity is derived which explains this experimental observation.


*Keywords:* Allen–Cahn equation; Numerical approximation spectral estimate; Singularities; Scaling; Stability

## 1. Introduction

Phase field equations provide a flexible mathematical tool to describe the evolution of interfaces or surfaces in various processes such as crystal growth, multiphase flows, or crack propagation. In contrast to sharp interface models their numerical implementation can be realized with standard methods and they are capable of describing topological changes effectively. The simplest example is the Allen–Cahn equation

$$\partial_t u - \Delta u = -\varepsilon^{-2} f(u)$$

in which $\varepsilon > 0$ is a small parameter that describes the thickness of the diffuse interface that separates regions in which $u \approx \pm 1$ and $f$ is the derivative of a double well potential, e.g., $f(u) = 2(u^3 - u)$. Fig. 1 displays snapshots of a simple but generic evolution leading to a generic topological change, i.e., a circular interface shrinks and disappears

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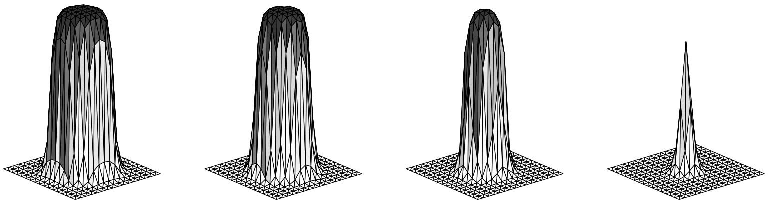

Fig. 1. Numerical experiment leading to a topological change. The circular interface that separates regions in which $u \approx \pm 1$ shrinks and collapses in finite time.

in finite time. Although the mathematical modeling of such events is unclear the agreement with experiments is quite remarkable. The topological change corresponds to a singularity in the evolution and the approximation properties of numerical methods may be critically affected. It is the aim of this article to provide a theoretical justification for the reliability of standard numerical methods at topological changes in a simple model situation.

Spectral estimates have recently been employed to derive error estimates of the form

$$\sup_{t\in[T_0,T_1]} \|u - u_h\| \le c_1 \varepsilon^{-\sigma}(h^\alpha + \tau^\beta) \exp\left(c_2 \int_{T_0}^{T_1} -\lambda_{AC}^-(t)\,dt\right) \tag{1.1}$$

for the numerical approximation of phase field models such as the Allen–Cahn equation cf. [1–4]. The negative part $\lambda_{AC}^- = \min\{\lambda_{AC}, 0\}$ of the principal eigenvalue $\lambda_{AC}$ of the linearized Allen–Cahn operator

$$-\Delta + \varepsilon^{-2} f'(u(t))\,\mathrm{id}$$

about the exact solution at time $t$ enters such estimates exponentially and thus logarithmic bounds for this quantity lead to useful estimates, cf. [4]. For the smooth evolution of developed interfaces it is known that the eigenvalue remains uniformly bounded from below [5–7] while for topological changes its modulus attains the square of the inverse of the interface thickness. Numerical experiments in [4] indicate that the modulus of the principal eigenvalue grows like $1/|t|,\ t < 0$, prior to a topological change at $t = 0$, before it attains the maximal absolute value proportional to $\varepsilon^{-2}$. Hence, an integration of it in time leads to a logarithmic bound which implies the robustness of the error estimate. It is the aim of this paper to provide theoretical support for such a scaling behavior.

For the mean curvature flow

$$V = -H$$

with a circle of radius $\sqrt{2}$ at $t = -1$ as initial data, the evolution is defined through $\dot{R} = -1/R$, i.e., $R(t) = \sqrt{2}|t|^{1/2}$ for $-1 \le t < 0$. The linearization of $H$ in the class of circles is given by

$$H'(t) = -\frac{1}{R(t)^2} = -\frac{1}{2}|t|^{-1}$$

which shows that the linearization of the sharp interface model obeys the scaling property observed for the related phase field model. Since the Allen–Cahn problem approximates the mean curvature flow as the interface thickness tends to zero [8,9] we expect that a similar bound holds for the principal eigenvalue of the linearized Allen–Cahn operator. We adopt the techniques of [6] to give a proof of this statement under the following assumption.

**Assumption A.** The solution $\phi_\varepsilon$ of the Allen–Cahn problem in $B_2 \times (-T, 0)$ with $B_2 := B_2(0) \subset \mathbb{R}^2$, i.e., the function $\phi_\varepsilon$ that satisfies

$$\partial_t \phi_\varepsilon - \Delta\phi_\varepsilon = -\varepsilon^{-2} f(\phi_\varepsilon),$$

with $f(u) := 2(u^2 - 1)u$ and $0 < \varepsilon < 1$, is for $t \le -\varepsilon^2 \log(\varepsilon^{-1})$ given by

$$\phi_\varepsilon(r,t) = \tanh\big((r - \sqrt{2}|t|^{1/2})/\varepsilon\big) + \varepsilon^2 q_\varepsilon(r,t) \tag{1.2}$$

with a function $q_\varepsilon$ that satisfies

$$|q_\varepsilon(r,t)| \le c_0 |t|^{-1}. \tag{1.3}$$