Chapter 6
The Allen–Cahn Equation

6.1 Analytical Properties

The *Allen–Cahn equation* is a simple mathematical model for certain phase separation processes. It also serves as a prototypical example for semilinear parabolic partial differential equations. The presence of a small parameter that defines the thickness of interfaces separating different phases makes the analysis challenging. Given $u_0 \in L^2(\Omega)$, $\varepsilon > 0$ and $T > 0$, we seek a function $u : [0, T] \times \Omega \to \mathbb{R}$ that solves

$$\partial_t u - \Delta u = -\varepsilon^{-2} f(u), \quad u(0) = u_0, \quad \partial_n u(t, \cdot)|_{\partial\Omega} = 0,$$

for almost every $t \in [0, T]$ and with $f = F'$ for a nonnegative function $F \in C^1(\mathbb{R})$ satisfying $F(\pm 1) = 0$, cf. Fig. 6.1. Unless otherwise stated, we always consider $F(s) = (s^2 - 1)^2/4$ and $f(s) = s^3 - s$ but other choices are possible as well. We always assume that $|u_0(x)| \leq 1$ for almost every $x \in \Omega$. For this model problem we will discuss aspects of its numerical approximation. For further details on modeling aspects and the analytical properties of the Allen–Cahn and other phase-field equations we refer the reader to the textbook [7] and the articles [1, 2, 4, 6, 10, 11].

The Allen–Cahn equation is the L^2-gradient flow of the functional

$$I_\varepsilon(u) = \frac{1}{2} \int_\Omega |\nabla u|^2 \, \mathrm{d}x + \varepsilon^{-2} \int_\Omega F(u) \, \mathrm{d}x.$$

Solutions tend to decrease the energy and develop interfaces separating regions in which it is nearly constant with values close to the minima of F. We refer to the zero level set of the function u as the interface but note that this does not define a sharp separation of the phases. More precisely, the phases are separated by a region of width ε around the zero level set of u often called the *diffuse interface*.

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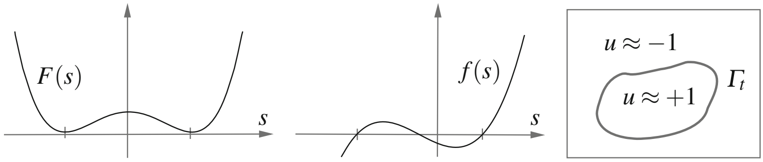

Fig. 6.1 Double well potential $F(s) = (s^2 - 1)^2/4$ and its derivative $f(s) = s^3 - s$ which is monotone outside $[-1, 1]$; solutions develop time-dependent interfaces Γ_t that separate regions in which $u(t, \cdot) \approx \pm 1$

6.1.1 Existence and Regularity

The existence of a unique solution u follows, e.g., from a discretization in time and a subsequent passage to a limit.

Theorem 6.1 (Existence) *For every* $u_0 \in L^2(\Omega)$ *and* $T > 0$ *there exists a weak solution* $u \in H^1([0, T]; H^1(\Omega)') \cap L^2([0, T]; H^1(\Omega))$ *that satisfies* $u(0) = u_0$ *and*

$$\langle \partial_t u, v \rangle + (\nabla u, \nabla v) = -\varepsilon^{-2}(f(u), v)$$

for almost every $t \in [0, T]$ *and every* $v \in H^1(\Omega)$. *If* $u_0 \in H^1(\Omega)$, *then we have* $u \in H^1([0, T]; L^2(\Omega)) \cap L^\infty([0, T]; H^1(\Omega))$ *and*

$$I_\varepsilon(u(T')) + \int_0^{T'} \|\partial_t u\|^2 \, \mathrm{d}t \le I_\varepsilon(u_0)$$

for almost every $T' \in [0, T]$.

Proof The existence of a solution follows from an implicit discretization in time that leads to a sequence of well-posed minimization problems. Straightforward a-priori bounds, together with compact embeddings, then show the existence of a weak limit that solves the weak formulation. If $u_0 \in H^1(\Omega)$, then we may formally choose $v = \partial_t u$ to verify that

$$\|\partial_t u\|^2 + \frac{d}{dt}\frac{1}{2}\|\nabla u\|^2 = -\varepsilon^{-2}\frac{d}{dt}\int_\Omega F(u) \, \mathrm{d}x.$$

An integration over $[0, T]$ implies the asserted bound. This procedure can be rigorously carried out for a time-discretized problem, and then the estimate also holds as the time-step size tends to zero. □

Remarks 6.1 (i) Stationary states for the Allen–Cahn equation are the constant functions $u \equiv \pm 1$ and $u \equiv 0$. The state $u \equiv 0$ is unstable.

(ii) For $\Omega = \mathbb{R}^d$ a stationary solution is given by $u(x) = \tanh(x \cdot a/(\sqrt{2}\varepsilon))$ for all $x \in \mathbb{R}^d$ and an arbitrary vector $a \in \mathbb{R}^d$. This characterizes the profile of typical solutions for Allen–Cahn equations across interfaces.

Since the nonlinearity f is monotone outside the interval $[-1, 1]$, solutions of the Allen–Cahn equation satisfy a maximum principle.

Proposition 6.1 (Maximum principle and uniqueness) *If u is a weak solution of the Allen–Cahn equation and $|u_0(x)| \le 1$ for almost every $x \in \Omega$, then $|u(t,x)| \le 1$ for almost every $(t,x) \in [0,T] \times \Omega$. Solutions with this property are unique.*

Proof Let $\widetilde{u} \in H^1([0,T]; H^1(\Omega)') \cap L^2([0,T]; H^1(\Omega))$ be the function obtained by truncating u at ± 1, i.e.,

$$\widetilde{u}(t,x) = \min\{1, \max\{-1, u(t,x)\}\}$$

for almost every $(t,x) \in [0,T] \times \Omega$. Then $\partial_t \widetilde{u} = \partial_t u$, $\nabla \widetilde{u} = \nabla u$, and $f(\widetilde{u}) = f(u)$ in $\{(t,x) \in [0,T] \times \Omega : |\widetilde{u}(t,x)| < 1\}$ and $\partial_t \widetilde{u} = 0$, $\nabla \widetilde{u} = 0$, and $f(\widetilde{u}) = 0$ otherwise. The function $\widetilde{u}$ is therefore a weak solution of the Allen–Cahn equation. If $u - \widetilde{u} \ne 0$, then either $u \ge \widetilde{u} = 1$ and

$$f(u) - f(\widetilde{u}) \ge f'(\widetilde{u})(u - \widetilde{u}) = f'(1)(u - \widetilde{u}) = 2(u - \widetilde{u})$$

or $u \le \widetilde{u} = -1$ and

$$f(u) - f(\widetilde{u}) \le f'(\widetilde{u})(u - \widetilde{u}) = f'(-1)(u - \widetilde{u}) = 2(u - \widetilde{u}).$$

Altogether we find that almost everywhere in $[0,T] \times \Omega$, we have

$$\big(f(u) - f(\widetilde{u})\big)(u - \widetilde{u}) \ge 2|u - \widetilde{u}|^2.$$

The difference $\delta = u - \widetilde{u}$ satisfies

$$(\partial_t \delta, v) + (\nabla \delta, \nabla v) = -\varepsilon^{-2}(f(u) - f(\widetilde{u}), v),$$

and for $v = \delta$, we obtain

$$\frac{1}{2}\frac{d}{dt}\|\delta\|^2 + \|\nabla \delta\|^2 \le -2\varepsilon^{-2}\|\delta\|^2.$$

With $\delta(0) = 0$, it follows directly that $\delta = 0$ in $[0,T] \times \Omega$. If u_1 and u_2 are solutions with $|u_1|, |u_2| \le 1$ in $[0,T] \times \Omega$, then we have

$$|f(u_1) - f(u_2)| \le c_f |u_1 - u_2|$$

almost everywhere in $[0,T] \times \Omega$ with $c_f = \sup_{s \in [-1,1]} |f'(s)|$. The difference $\delta = u_1 - u_2$ satisfies

$$(\partial_t \delta, v) + (\nabla \delta, \nabla v) = -\varepsilon^{-2}(f(u_1) - f(u_2), v)$$

and the choice of $v = \delta$ leads to

$$\frac{1}{2}\frac{d}{dt}\|\delta\|^2 + \|\nabla\delta\|^2 \leq c_f \varepsilon^{-2}\|\delta\|^2.$$

An application of Gronwall's lemma implies that $u_1 = u_2$. □

As for the linear heat equation, one can show that the solution is regular. The corresponding bounds depend critically however on the small parameter $\varepsilon > 0$.

Theorem 6.2 (Regularity) *If the Laplace operator is H^2 regular in Ω and $u_0 \in H^1(\Omega)$, then $u \in L^\infty([0,T]; H^2(\Omega)) \cap H^2([0,T]; H^1(\Omega)') \cap H^1([0,T]; H^2(\Omega))$ and there exists $\sigma \geq 0$ such that*

$$\sup_{t\in[0,T]} \|u\|_{H^2(\Omega)} + \Big(\int_0^T \|u_{tt}\|^2_{H^1(\Omega)'}\,\mathrm{d}t\Big)^{1/2} + \Big(\int_0^T \|u_t\|^2_{H^2(\Omega)}\,\mathrm{d}t\Big)^{1/2} \leq c\varepsilon^{-\sigma}.$$

If $I_\varepsilon(u_0) \leq c$ and $\|\Delta u_0\| \leq c\varepsilon^{-2}$, then we may choose $\sigma = 2$.

Proof The proof follows with the arguments that are used to prove the corresponding statements for the linear heat equation, cf. [8]. □

6.1.2 Stability Estimates

In the following stability result we assume that an approximate solution satisfies a maximum principle. This is satisfied for certain numerical approximations and the assumption can be weakened to a uniform L^∞-bound. We recall that Gronwall's lemma states that if a nonnegative function $y \in C([0,T])$ satisfies

$$y(T') \leq A + \int_0^{T'} a(t)y(t)\,\mathrm{d}t$$

for all $T' \in [0,T]$ with a nonnegative function $a \in L^1([0,T])$, then we have

$$y(T') \leq A\exp\Big(\int_0^T a\,\mathrm{d}t\Big).$$

Together with a Lipschitz estimate, this will be the main ingredient for the following stability result. Due to its exponential dependence on ε^{-2}, it is of limited practical use.

Theorem 6.3 (Stability) *Let* $u \in H^1([0,T];H^1(\Omega)') \cap L^\infty([0,T];H^1(\Omega))$ *be a weak solution of the Allen–Cahn equation with* $|u| \le 1$ *almost everywhere in* $[0,T]\times\Omega$. *Let* $\widetilde{u} \in H^1([0,T];H^1(\Omega)') \cap L^2([0,T];H^1(\Omega))$ *satisfy* $|\widetilde{u}| \le 1$ *almost everywhere in* $[0,T]\times\Omega$, *and* $\widetilde{u}(0)=\widetilde{u}_0$, *and solve*

$$(\partial_t \widetilde{u}, v) + (\nabla \widetilde{u}, \nabla v) = -\varepsilon^{-2}(f(\widetilde{u}), v) + \langle \widetilde{\mathscr{R}}(t), v\rangle$$

for almost every $t \in [0,T]$, *all* $v \in H^1(\Omega)$, *with a functional* $\widetilde{\mathscr{R}} \in L^2([0,T];H^1(\Omega)')$. *Then we have*

$$\sup_{t\in[0,T]} \|u-\widetilde{u}\|^2 + \int_0^T \|\nabla(u-\widetilde{u})\|^2 \,\mathrm{d}t \le 2\Big(\|u_0-\widetilde{u}_0\|^2 + \int_0^T \|\widetilde{\mathscr{R}}\|^2_{H^1(\Omega)'}\,\mathrm{d}t\Big)\exp\big((1+2c_f\varepsilon^{-2})T\big).$$

Proof With $c_f = \sup_{s\in B_1(0)} |f'(s)|$, we have

$$|f(s_1)-f(s_2)| \le c_f|s_1-s_2|$$

for all $s_1, s_2 \in \mathbb{R}$. The difference $\delta = u - \widetilde{u}$ satisfies

$$(\partial_t\delta, v) + (\nabla\delta,\nabla v) = -\varepsilon^{-2}\big(f(u)-f(\widetilde{u}), v\big) - \langle\widetilde{\mathscr{R}}, v\rangle$$

for almost every $t \in I$ and every $v \in H^1(\Omega)$. For $v=\delta$ we find that

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|\delta\|^2 + \|\nabla\delta\|^2 &\le c_f\varepsilon^{-2}\|\delta\|^2 + \|\widetilde{\mathscr{R}}\|_{H^1(\Omega)'}\|\delta\|_{H^1(\Omega)}\\ &\le c_f\varepsilon^{-2}\|\delta\|^2 + \frac{1}{2}\|\widetilde{\mathscr{R}}\|^2_{H^1(\Omega)'} + \frac{1}{2}(\|\delta\|^2+\|\nabla\delta\|^2)\\ &\le \frac{1}{2}(1+2c_f\varepsilon^{-2})\|\delta\|^2 + \frac{1}{2}\|\widetilde{\mathscr{R}}\|^2_{H^1(\Omega)'} + \frac{1}{2}\|\nabla\delta\|^2.\end{aligned}$$

Absorbing the term $\|\nabla\delta\|^2/2$ on the left-hand side and integrating over $(0,T')$ lead to

$$\|\delta(T')\|^2 + \int_0^{T'}\|\nabla\delta\|^2\,\mathrm{d}t \le \|\delta(0)\|^2 + \int_0^T \|\widetilde{\mathscr{R}}\|^2_{H^1(\Omega)'}\,\mathrm{d}t + (1+2c_f\varepsilon^{-2})\int_0^{T'}\|\delta\|^2\,\mathrm{d}t.$$

Defining $A = \|\delta(0)\|^2 + \int_0^T \|\widetilde{\mathscr{R}}\|^2_{H^1(\Omega)'}\,\mathrm{d}t$, $b = (1 + 2c_f\varepsilon^{-2})$, and setting

$$y(t) = \|\delta(t)\|^2 + \int_0^t \|\nabla\delta\|^2\,\mathrm{d}s,$$

we have $y(T') \le A + a\int_0^{T'} y(t)\,\mathrm{d}t$; Gronwall's lemma implies the estimate of the theorem. □

Remark 6.2 The functional $\widetilde{\mathscr{R}}$ models the error introduced by a discretization of the equation so that we may assume that $\|\widetilde{\mathscr{R}}(t)\|^2_{H^1(\Omega)'} \le c\varepsilon^{-\rho}(h^\alpha + \tau^\beta)$ for a mesh-size $h > 0$ and a time-step size $\tau > 0$, and parameters $\alpha, \beta, \rho > 0$. If $\|u_0 - \widetilde{u}_0\|^2 \le h^\gamma$, then we obtain the error estimate

$$\sup_{t\in[0,T]} \|u - \widetilde{u}\|^2 + \int_0^T \|\nabla(u - \widetilde{u})\|^2\,\mathrm{d}t \le c\varepsilon^{-\rho}(h^\alpha + \tau^\beta + h^\gamma)\exp\big((1 + 2c_f\varepsilon^{-2})T\big).$$

Even for the moderate choice $\varepsilon \approx 10^{-1}$, the exponential factor is of the order 10^{40} and it is impossible to compensate this factor with small mesh- and time-step sizes to obtain a useful error estimate. In practice even smaller values of ε are relevant.

To obtain an error estimate that does not depend exponentially on ε^{-1} and which holds without assuming a maximum principle, refined arguments are necessary. The following generalization of Gronwall's lemma allows us to consider a superlinear term.

Proposition 6.2 (Generalized Gronwall lemma) *Suppose that the nonnegative functions $y_1 \in C([0,T])$, $y_2, y_3 \in L^1([0,T])$, $a \in L^\infty([0,T])$, and the real number $A \ge 0$ satisfy*

$$y_1(T') + \int_0^{T'} y_2(t)\,\mathrm{d}t \le A + \int_0^{T'} a(t)y_1(t)\,\mathrm{d}t + \int_0^{T'} y_3(t)\,\mathrm{d}t$$

for all $T' \in [0,T]$. Assume that for $B \ge 0$, $\beta > 0$, and every $T' \in [0,T]$, we have

$$\int_0^{T'} y_3(t)\,\mathrm{d}t \le B\Big(\sup_{t\in[0,T']} y_1^\beta(t)\Big)\int_0^{T'} (y_1(t) + y_2(t))\,\mathrm{d}t.$$

Set $E = \exp\big(\int_0^T a(t)\,\mathrm{d}t\big)$ and assume that $8AE \le (8B(1+T)E)^{-1/\beta}$. We then have

$$\sup_{t\in[0,T]} y_1(t) + \int_0^T y_2(t)\,\mathrm{d}t \le 8A\exp\Big(\int_0^T a(s)\,\mathrm{d}s\Big).$$

Proof We assume first that $A > 0$, set $\theta = 8AE$, and define

$$I_\theta = \big\{T' \in [0,T] : \Upsilon(T') = \sup_{t\in[0,T']} y_1(t) + \int_0^{T'} y_2(t)\,\mathrm{d}t \le \theta\big\}.$$

Since $y_1(0) \le A < \theta$ and since Υ is continuous and increasing, we have $I_\theta = [0, T_M]$ for some $0 < T_M \le T$. For every $T' \in [0, T_M]$ we have

$$\begin{aligned} y_1(T') + \int_0^{T'} y_2(t)\,\mathrm{d}t &\le A + \int_0^{T'} a(t)y_1(t)\,\mathrm{d}t + B \sup_{t\in[0,T']} y_1^\beta(t) \int_0^{T'} (y_1(t)+y_2(t))\,\mathrm{d}t \\ &\le A + \int_0^{T'} a(t)y_1(t)\,\mathrm{d}t + B(1+T)\theta^{1+\beta}. \end{aligned}$$

An application of the classical Gronwall lemma, the condition on A, and the choice of θ yield that for all $T' \in [0, T_M]$, we have

$$y_1(T') + \int_0^{T'} y_2(t)\,\mathrm{d}t \le (A + B(1+T)\theta^{1+\beta})E \le \frac{\theta}{4}.$$

This implies $\Upsilon(T_M) < \theta$, hence $T_M = T$, and thus proves the lemma if $A > 0$. The argument is illustrated in Fig. 6.2. If $A = 0$, then the above argument holds for every $\theta > 0$ and we deduce that $y_1(t) = y_2(t) = 0$ for all $t \in [0, T]$. □

Remark 6.3 The differential equation underlying the generalized Gronwall lemma has the structure $y' = y^{1+\beta}$. For $\beta > 0$, solutions become unbounded in finite time depending on the initial data, e.g., for $y' = y^2$, we have $y(t) = (t_c - t)^{-1}$ with $t_c = y_0^{-1}$. Therefore, an assumption on A is unavoidable to obtain an estimate on the entire interval $[0, T]$.

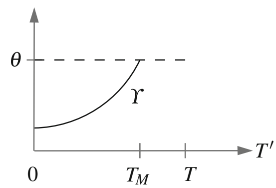

Fig. 6.2 Continuation argument in the proof of the generalized Gronwall lemma

Two elementary properties of the function f are essential for an improved stability result. These define a class of nonlinearities that can be treated with the same arguments.

Lemma 6.1 (Controlled non-monotonicity) *We have* $f'(s) \geq -1$ *and*

$$\big(f(s) - f(r)\big)(s - r) \geq f'(s)(s - r)^2 - 3s(s - r)^3$$

for all $r, s \in \mathbb{R}$.

Proof The lemma follows from the identities $f'(s) = 3s^2 - 1$, $f''(s) = 6s$, and $f'''(s) = 6$ together with a Taylor expansion of f. □

The controlled non-monotonicity of f avoids the use of a Lipschitz estimate. To estimate the resulting term involving f', we employ the smallest eigenvalue of the linearization of the mapping $u \mapsto -\Delta u + f(u(t))$, i.e., of the linear operator $v \mapsto -\Delta v + f'(u(t))v$.

Definition 6.1 For $u \in L^\infty([0, T]; H^1(\Omega))$ let the *principal eigenvalue* λ_{AC}: $[0, T] \to \mathbb{R}$ of the linearized Allen–Cahn operator for $t \in [0, T]$ be defined by

$$\lambda_{AC}(t) = - \inf_{v \in H^1(\Omega)\setminus\{0\}} \frac{\|\nabla v\|^2 + \varepsilon^{-2}\big(f'(u(t))v, v\big)}{\|v\|^2}.$$

Remarks 6.4 (i) As in the theory of ordinary differential equations, the principal eigenvalue contains information about the stability of the evolution.
(ii) If $|u(t)| \leq 1$ in Ω, then we have $-\lambda_{AC}(t) \geq c_P^2 - 1 - c_f \varepsilon^{-2}$ with the Poincaré constant $c_P = \sup_{v \in H^1(\Omega)\setminus\{0\}} \|v\|/\|v\|_{H^1(\Omega)}$ and $c_f = \sup_{s \in [-1,1]} |f'(s)|$. Therefore, $\lambda_{AC}(t) \leq 1 + \varepsilon^{-2}$. The evolution is stable as long as $\lambda_{AC}(t) \leq c$ for an ε-independent constant $c > 0$, and becomes unstable for $\lambda_{AC}(t) \gg 1$.
(iii) For the stable stationary states $u(t) \equiv \pm 1$, the choice of $v \equiv 1$ shows that we have $\lambda_{AC}(t) = -2\varepsilon^{-2} \leq 0$, while for the unstable stationary state $u(t) \equiv 0$ we have $\lambda_{AC}(t) = \varepsilon^{-2}$.
(iv) As long as the curvature of the interface $\Gamma_t = \{x \in \Omega : u(t, x) = 0\}$ is bounded ε-independently, one can show that $\lambda_{AC}(t)$ is bounded ε-independently, cf. [4].

The generalized Gronwall lemma, the controlled non-monotonicity, and the principal eigenvalue λ_{AC} can be used for an improved stability analysis. We first use the non-monotonicity in the equation for the difference $\delta = u - \widetilde{u}$ tested by δ, i.e.,

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|\delta\|^2 + \|\nabla\delta\|^2 &= -\varepsilon^{-2}\big(f(u) - f(\widetilde{u}), u - \widetilde{u}\big) - \langle \widetilde{\mathscr{R}}, \delta\rangle \\ &\leq -\varepsilon^{-2}\big(f'(u)(u - \widetilde{u}), u - \widetilde{u}\big) \\ &\quad + 3\varepsilon^{-2}\|u\|_{L^\infty(\Omega)}\|u - \widetilde{u}\|^3_{L^3(\Omega)} - \langle \widetilde{\mathscr{R}}, \delta\rangle.\end{aligned}$$

The definition of $\lambda_{AC}(t)$ implies that

$$-\lambda_{AC}\|\delta\|^2 \le \|\nabla\delta\|^2 + \varepsilon^{-2}\big(f'(u)\delta, \delta\big)$$

and the combination of the two estimates proves that

$$\frac{1}{2}\frac{d}{dt}\|\delta\|^2 + \|\nabla\delta\|^2 \le \lambda_{AC}\|\delta\|^2 + \|\nabla\delta\|^2 + 3\varepsilon^{-2}\|u\|_{L^\infty(\Omega)}\|\delta\|^3_{L^3(\Omega)} + \langle\widetilde{\mathscr{R}}, \delta\rangle.$$

By slightly refining the argument we may apply the generalized Gronwall lemma to this equation. In the following theorem we employ the principal eigenvalue defined by an approximate solution to the Allen–Cahn equation. This is in the spirit of a posteriori error estimation to obtain a computable bound for the approximation error. It follows the concept that all information about the problem is extracted from the approximate solution.

Theorem 6.4 (Robust stability) *Let $0 < \varepsilon \le 1$ and $u \in H^1([0,T]; H^1(\Omega)') \cap L^2([0,T]; H^1(\Omega))$ be the weak solution of the Allen–Cahn equation. Given a function $\widetilde{u} \in H^1([0,T]; H^1(\Omega)') \cap L^2([0,T]; H^1(\Omega))$ define $\widetilde{\mathscr{R}} \in L^2([0,T]; H^1(\Omega)')$ through*

$$\langle\widetilde{\mathscr{R}}(t), v\rangle = \langle\partial_t\widetilde{u}, v\rangle + (\nabla\widetilde{u}, \nabla v) + \varepsilon^{-2}(f(\widetilde{u}), v)$$

for almost every $t \in [0,T]$ and all $v \in H^1(\Omega)$. Suppose that $\eta_0, \eta_1 \in L^2([0,T])$ are such that for almost every $t \in [0,T]$ and all $v \in H^1(\Omega)$, we have

$$\langle\widetilde{\mathscr{R}}(t), v\rangle \le \eta_0(t)\|v\| + \eta_1(t)\|\nabla v\|.$$

Assume that $\widetilde{\lambda}_{AC} \in L^1([0,T])$ is a function such that for almost every $t \in (0,T)$, we have

$$-\widetilde{\lambda}_{AC}(t) \le \inf_{v \in H^1(\Omega)\setminus\{0\}} \frac{\|\nabla v\|^2 + \varepsilon^{-2}(f'(\widetilde{u}(t))v, v)}{\|v\|^2},$$

and set $\mu_\lambda(t) = 2\big(2 + (1-\varepsilon^2)\widetilde{\lambda}_{AC}(t)\big)^+$. Define

$$\eta_{AC}^2 = \|(u - \widetilde{u})(0)\|^2 + \int_0^T (\eta_0^2 + \varepsilon^{-2}\eta_1^2)\,\mathrm{d}t$$

and assume that

$$\eta_{AC} \le \varepsilon^4\big(6c_S\|\widetilde{u}\|_{L^\infty([0,T];L^\infty(\Omega))}(1+T)\big)^{-1}\Big(8\exp\Big(\int_0^T \mu_\lambda(t)\,\mathrm{d}t\Big)\Big)^{-3/2},$$

then

$$\sup_{s\in[0,T]} \|u-\widetilde{u}\|^2 + \varepsilon^2 \int_0^T \|\nabla(u-\widetilde{u})\|^2 \,\mathrm{d}t \le 8\eta_{\mathrm{AC}}^2 \exp\Big(\int_0^T \mu_\lambda(t)\,\mathrm{d}t\Big).$$

Proof The difference $\delta = u - \widetilde{u}$ satisfies

$$\langle \partial_t \delta, v\rangle + (\nabla\delta, \nabla v) = -\varepsilon^{-2}(f(u) - f(\widetilde{u}), v) - \langle \widetilde{\mathscr{R}}, v\rangle$$

for almost every $t \in [0, T]$ and all $v \in H^1(\Omega)$. Choosing $v = \delta$, using the assumed bound for $\widetilde{\mathscr{R}}$, noting Lemma 6.1, and using Young's inequality we find

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}\|\delta\|^2 + \|\nabla\delta\|^2 &= -\langle\widetilde{\mathscr{R}}, \delta\rangle - \varepsilon^{-2}(f(u) - f(\widetilde{u}), \delta) \\
&\le \eta_0\|\delta\| + \eta_1\|\nabla\delta\| - \varepsilon^{-2}(f'(\widetilde{u})\delta, \delta) + 3\varepsilon^{-2}\|\widetilde{u}\|_{L^\infty(\Omega)}\|\delta\|^3_{L^3(\Omega)} \\
&\le \frac{1}{4}\eta_0^2 + \|\delta\|^2 + \frac{\varepsilon^{-2}}{2}\eta_1^2 + \frac{\varepsilon^2}{2}\|\nabla\delta\|^2 - (1-\varepsilon^2)\varepsilon^{-2}(f'(\widetilde{u})\delta, \delta) \\
&\quad - (f'(\widetilde{u})\delta, \delta) + 3\varepsilon^{-2}\|\widetilde{u}\|_{L^\infty(\Omega)}\|\delta\|^3_{L^3(\Omega)}.
\end{aligned}$$

The assumption on $\widetilde{\lambda}_{\mathrm{AC}}(t)$ shows that

$$-\widetilde{\lambda}_{\mathrm{AC}}(t)\|\delta\|^2 \le \|\nabla\delta\|^2 + \varepsilon^{-2}(f'(\widetilde{u})\delta, \delta).$$

Multiplying this estimate by $1 - \varepsilon^2$ and using $f'(\widetilde{u}) \ge -1$, we derive the bound

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}\|\delta\|^2 + \|\nabla\delta\|^2 &\le \frac{1}{4}\eta_0^2 + \|\delta\|^2 + \frac{\varepsilon^{-2}}{2}\eta_1^2 + \frac{\varepsilon^2}{2}\|\nabla\delta\|^2 + (1-\varepsilon^2)\widetilde{\lambda}_{\mathrm{AC}}\|\delta\|^2 \\
&\quad + (1-\varepsilon^2)\|\nabla\delta\|^2 + \|\delta\|^2 + 3\varepsilon^{-2}\|\widetilde{u}\|_{L^\infty(\Omega)}\|\delta\|^3_{L^3(\Omega)} \\
&\le \frac{1}{4}\eta_0^2 + \frac{1}{2}\varepsilon^{-2}\eta_1^2 + (2 + (1-\varepsilon^2)\widetilde{\lambda}_{\mathrm{AC}})\|\delta\|^2 \\
&\quad + \Big(1 - \frac{\varepsilon^2}{2}\Big)\|\nabla\delta\|^2 + 3\varepsilon^{-2}\|\widetilde{u}\|_{L^\infty(\Omega)}\|\delta\|^3_{L^3(\Omega)},
\end{aligned}$$

which leads to

$$\frac{d}{dt}\|\delta\|^2 + \varepsilon^2\|\nabla\delta\|^2 \le \eta_0^2 + \varepsilon^{-2}\eta_1^2 + \mu_\lambda\|\delta\|^2 + 6\varepsilon^{-2}\|\widetilde{u}\|_{L^\infty(\Omega)}\|\delta\|^3_{L^3(\Omega)}.$$

Hölder's inequality and the Sobolev estimate $\|v\|^2_{L^4(\Omega)} \le c_S\|v\|^2_{H^1(\Omega)}$ for $v \in H^1(\Omega)$ yield that

$$\|\delta\|_{L^3(\Omega)}^3 = \int_\Omega |\delta||\delta|^2 \,\mathrm{d}x \le \|\delta\| \|\delta\|_{L^4(\Omega)}^2 \le c_S \|\delta\| (\|\delta\|^2 + \|\nabla\delta\|^2). \tag{6.1}$$

An integration of the last two estimates over $[0, T']$ shows that we are in the situation of Proposition 6.2 with

$$y_1(t) = \|\delta(t)\|^2,\ y_2(t) = \varepsilon^2 \|\nabla\delta(t)\|^2,\ y_3(t) = 6\varepsilon^{-2} \|\widetilde{u}\|_{L^\infty(\Omega)} \|\delta\|_{L^3(\Omega)}^3,$$

and $A = \eta_{\mathrm{AC}}^2$, $B = 6\varepsilon^{-4} \|\widetilde{u}\|_{L^\infty([0,T];L^\infty(\Omega))} c_S$, $\beta = 1/2$, and $E = \exp\left(\int_0^T \mu_\lambda \,\mathrm{d}t\right)$. The proposition thus implies the assertion. □

Remarks 6.5 (i) The robust stability result can be proved for a class of nonlinearities f satisfying the estimates of Lemma 6.1.
(ii) If the exponential factor is bounded by a polynomial in ε^{-1}, then we have improved the stability result of Theorem 6.3. We discuss this question below.

6.1.3 Mean Curvature Flow

The Allen–Cahn equation is closely related to the *mean curvature flow* that seeks for a given hypersurface $\mathscr{M}_0 \subset \mathbb{R}^d$, a family of hypersurfaces $(\mathscr{M}_t)_{t\in[0,T]}$ such that

$$V = -\frac{d-1}{2} H \quad \text{on } \mathscr{M}_t$$

for every $t \in [0, T]$. Here, V is the normal velocity of points on the surface and H is the mean curvature. For a family of spheres $\big((\partial B_{R(t)}(0)\big)_{t\in[0,T]}$ centered at 0 with positive radii $R : [0, T] \to \mathbb{R}$, we have

$$V(t) = R'(t), \quad H(t) = \frac{1}{(d-1)R(t)}.$$

The family of spheres thus solves the mean curvature flow if

$$R' = -\frac{1}{2R},$$

i.e., if $R(t) = (T_c - t)^{1/2}$, where $T_c = R(0)^2$. This equation has a blowup structure and the solution only exists in the interval $[0, T_c)$, cf. Fig. 6.3. To understand the stability of the evolution, we linearize the right-hand side operator $\psi(R) = 1/(2R)$ of the differential equation at the solution $R(t)$ and obtain

$$-\lambda_{\mathrm{MCF}}(t) = \frac{-1}{2R(t)^2} = \frac{-1}{2(T_c - t)}.$$

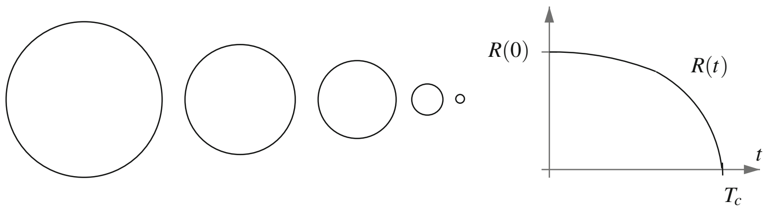

Fig. 6.3 A family of spheres that solve the mean curvature flow within $[0, T_c)$; at $t = T_c$ the surfaces collapse

We thus see that λ_{MCF} is unbounded at $t = T_c$ when the surfaces collapse. This reflects the occurrence of large unbounded normal velocities. Nevertheless, for every $T' < T_c$, we have

$$\int_0^{T'} \lambda_{\mathrm{MCF}}(t)\,\mathrm{d}t = \frac{-1}{2}\big(\log(T_c - T') - \log T_c\big).$$

Assuming that $\lambda_{\mathrm{MCF}} \approx \lambda_{\mathrm{AC}}$, we will deduce below heuristically that the exponential dependence of the stability estimate in Theorem 6.4 is moderate. To understand the relation between the Allen–Cahn equation and the mean curvature flow let $(\mathcal{M}_t)_{t\in[0,T]}$ be a family of surfaces that solve the mean curvature flow. We assume that for every $t \in [0, T]$, we have $\mathcal{M}_t = \partial\Omega_t$ for a simply connected domain $\Omega_t \subset \mathbb{R}^d$ and let $d_{\mathcal{M}}(t, \cdot)$ be the signed distance function to $\mathcal{M}_t$ that is negative inside Ω_t. Given a trajectory $\phi : [0, T] \to \mathbb{R}^d$ of a point $x_0 = \phi(0) \in \mathcal{M}_0$, i.e., we have $\phi(t) \in \mathcal{M}_t$ for all $t \in [0, T]$, its normal velocity given by

$$V(t, \phi(t)) = n(t, \phi(t)) \cdot \phi'(t).$$

Since $d_{\mathcal{M}}(t, \phi(t)) = 0$ for all $t \in [0, T]$ it follows with $n(t, x) = \nabla d_{\mathcal{M}}(t, x)$ for every $x \in \mathcal{M}_t$ that

$$0 = \partial_t d_{\mathcal{M}}(t, \phi(t)) + \nabla d_{\mathcal{M}}(t, \phi(t)) \cdot \phi'(t),$$

i.e., $V(t, x) = -\partial_t d_{\mathcal{M}}(t, x)$ for every $x \in \mathcal{M}_t$. Noting that $D^2 d_{\mathcal{M}} = D(\nabla d_{\mathcal{M}})$ is the shape operator it follows that for the mean curvature we have $(d-1)H = tr(D^2 d_{\mathcal{M}}) = \Delta d_{\mathcal{M}}$. With $V = -H$ we deduce that $\partial_t d_{\mathcal{M}} - \Delta d_{\mathcal{M}} = 0$ on $\mathcal{M}_t$. The function $\psi(z) = \tanh(z/\sqrt{2})$ satisfies $-\psi''(z) + f(\psi(z)) = 0$, and this implies that for

$$v(t, x) = \psi\Big(\frac{d_{\mathcal{M}}(t, x)}{\varepsilon}\Big)$$

we have

$$v_t - \Delta v + \varepsilon^{-2} f(v) = \varepsilon^{-1}\big(\partial_t d_{\mathscr{M}} - \Delta d_{\mathscr{M}}\big)\,\psi'\big(d_{\mathscr{M}}/\varepsilon\big) - \varepsilon^{-2}\big(\psi''\big(d_{\mathscr{M}}/\varepsilon\big) + f\big(\psi\big(d_{\mathscr{M}}/\varepsilon\big)\big)\big) = \varepsilon^{-1}\big(\partial_t d_{\mathscr{M}} - \Delta d_{\mathscr{M}}\big)\,\psi'\big(d_{\mathscr{M}}/\varepsilon\big).$$

Since $\partial_t d_{\mathscr{M}} - \Delta d_{\mathscr{M}} = 0$ on $\mathscr{M}_t$, we deduce that if $d_{\mathscr{M}}$ is sufficiently smooth, then the function $g = \partial_t d_{\mathscr{M}} - \Delta d_{\mathscr{M}}$ grows linearly in a neighborhood of $\mathscr{M}_t$, i.e., we have $|\partial_t d_{\mathscr{M}} - \Delta d_{\mathscr{M}}| \le c|d_{\mathscr{M}}|$. Noting that the function ψ satisfies $|z\psi'(z)| \le c$, we find that

$$\big|\varepsilon^{-1}(\partial_t d_{\mathscr{M}} - \Delta d_{\mathscr{M}})\psi'\big(d_{\mathscr{M}}/\varepsilon\big)\big| \le c\big|\big(d_{\mathscr{M}}/\varepsilon\big)\psi'\big(d_{\mathscr{M}}/\varepsilon\big)\big| \le c.$$

Therefore, the function $v(t,x) = \psi(d_{\mathscr{M}}(t,x)/\varepsilon)$ solves the dominant terms of the Allen–Cahn equation $\partial_t u - \Delta u = -\varepsilon^{-2} f(u)$ and serves as an approximation of the solution in a neighborhood of width ε of the interface Γ_t. The profile is illustrated in Fig. 6.4. More details can be found in [5].

6.1.4 Topological Changes

The mean curvature flow provides a good approximation of the Allen–Cahn equation in the sense that $v(x,t) = \psi(\mathrm{dist}(x,\mathscr{M}_t)/\varepsilon)$ nearly solves the Allen–Cahn equation; the family $\Gamma_t = \{x \in \Omega : u(x,t) = 0\}$ is a good approximation of a solution for the mean curvature flow. These approximations are valid as long as the interfaces $\mathscr{M}_t$ or Γ_t do not undergo *topological changes*, i.e., as long as $\mathscr{M}_t$ or Γ_t does neither split nor have parts of it disappear. This is closely related to the stability of the solution that is measured by the principal eigenvalue $\lambda_{AC}(t)$. It can be shown and it follows from the discussion of the mean curvature flow above, that λ_{AC} is bounded from above independently of ε as long as the interface Γ_t is smooth and has bounded curvature. When an interface collapses, large, unbounded velocities occur and the eigenvalue

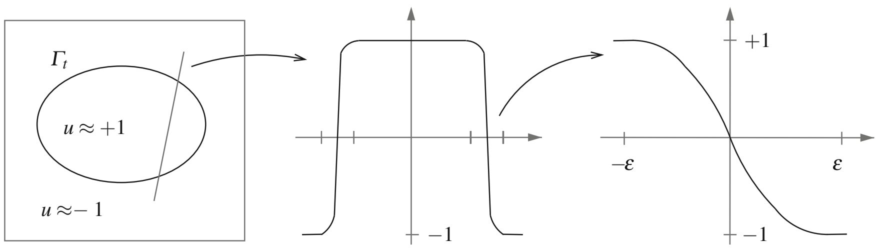

Fig. 6.4 A typical configuration of a solution of the Allen–Cahn equation (*left*) and a solution restricted to a line in the domain (*middle*) together with a magnification of the interface (*right*)

λ_{AC} attains the upper bound $\lambda_{AC} \sim \varepsilon^{-2}$. This however only occurs on a time-interval of length comparable to ε^2, the characteristic time scale for the Allen–Cahn equation. Due to this fact, we have for the temporal integral of the principal eigenvalue that occurs in the stability analysis

$$\int_0^T \lambda_{AC}(t)\,\mathrm{d}t \sim 1 + (\#\text{ topological changes}) \log(\varepsilon^{-1}).$$

The logarithmic contribution results from the transition regions in which λ_{AC} grows like $(T_c - t)^{-1}$ for a topological change at $t = T_c$. Integrating this quantity up to the time $T_c - \varepsilon^2$, where λ_{AC} has nearly reached its maximum, reveals that

$$\int_{T_c-1}^{T_c-\varepsilon^2} \lambda_{AC}(t)\,\mathrm{d}t \sim \frac{1}{2} \int_{T_c-1}^{T_c-\varepsilon^2} (T_c - t)^{-1}\,\mathrm{d}t \sim \log(\varepsilon^{-1}).$$

The logarithmic growth in ε^{-1} of the integrated eigenvalue is precisely what is affordable in the estimate of Theorem 6.4 to avoid an exponential dependence on ε^{-1} and instead obtain an algebraic dependence. A typical behavior of the eigenvalue is depicted in Fig. 6.5.

6.1.5 Mass Conservation

The Allen–Cahn equation describes phase transition processes in which the volume fractions of the phases may change and the only stationary configurations represent

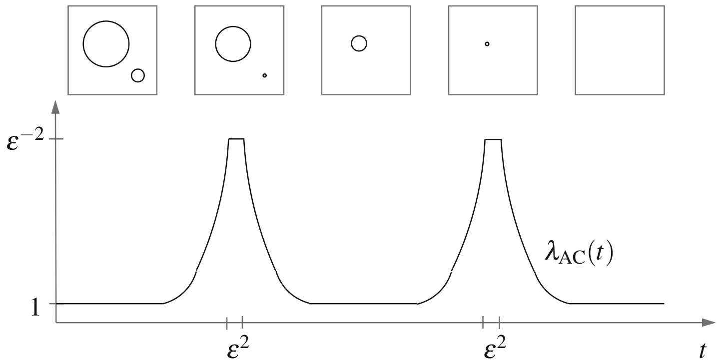

Fig. 6.5 Two topological changes in an evolution defined by the Allen–Cahn equation; the topological changes are accompanied by extreme principal eigenvalues; the eigenvalue increases like $(T_c - t)^{-1}$ before a topological change occurs at T_c

single phases. This corresponds, e.g., to melting processes. In order to model phase separation processes in which the volume fractions are preserved, a constraint has to be incorporated or a fourth order evolution has to be considered. The latter is the H^{-1}-gradient flow of the energy I_ε, where $H^{-1}(\Omega) = X_0'$ is the dual of the space $X_0 = \{v \in H^1(\Omega) : \int_\Omega v \,\mathrm{d}x = 0\}$, i.e.,

$$(\partial_t u, v)_{-1} = -(\nabla u, \nabla v) - \varepsilon^{-2}(f(u), v).$$

Here, the inner product $(v, w)_{-1}$ is for $v, w \in H^{-1}(\Omega)$ defined by

$$(v, w)_{-1} = \int_\Omega \nabla(-\Delta^{-1} v) \cdot \nabla(-\Delta^{-1} w) \,\mathrm{d}x,$$

where $-\Delta^{-1} v$ and $\Delta^{-1} w \in X_0$ are the unique solutions of the Poisson problem

$$-\Delta u = f \text{ in } \Omega, \quad \partial_n u|_{\partial\Omega} = 0$$

with vanishing mean for the right-hand sides $f = v$ and $f = w$, respectively. In the strong form the gradient flow reads

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

together with homogeneous Neumann boundary conditions on $\partial\Omega$ for u and ϕ and initial conditions for u. The variable ϕ is the *chemical potential* and the system is called the *Cahn–Hilliard equation* which can be analyzed with the techniques discussed above. Mass conservation is a consequence of the fact that $\partial_t u$ has vanishing integral mean. Solutions do not obey a maximum principle but satisfy certain L^∞-bounds.

6.2 Error Analysis

In this section we discuss error estimates for numerical approximations of the Allen–Cahn equation obtained with the implicit Euler scheme. The stability result of Theorem 6.4 is already formulated in the spirit of an a posteriori error analysis. We discuss results from [3, 8, 9].

6.2.1 Residual Estimate

We include an estimate for the residual of an approximation obtained with the implicit Euler scheme. The result can be modified to control the error of other approximation schemes.

Proposition 6.3 (Residual bounds) *Let* $0 = t_0 < t_1 < \cdots < t_K \leq T$ *and* $\tau_k = t_k - t_{k-1}$, $k = 1, 2, \ldots, K$, *and* $(\mathcal{T}_k)_{k=0,\ldots,K}$ *a sequence of regular triangulations of* Ω. *Suppose that* $(u_h^k)_{k=0,\ldots,K} \subset H^1(\Omega)$, *for* $k = 1, 2, \ldots, K$ *and all* $v_h \in \mathcal{S}^1(\mathcal{T}_k)$, *satisfies*

$$\tau_k^{-1}(u_h^k - \mathcal{I}_k u_h^{k-1}, v_h) + (\nabla u_h^k, \nabla v_h) = -\varepsilon^{-2}(f(u_h^k), v_h),$$

where $\mathcal{I}_k$ *denotes the nodal interpolation operator related to* $\mathcal{S}^1(\mathcal{T}_k)$. *Let* $u_{h,\tau} \in H^1([0, T]; H^1(\Omega))$ *be the piecewise linear interpolation in time of* $(u_h^k)_{k=0,\ldots,K}$ *and define* $\mathcal{R} \in L^2(I; H^1(\Omega)')$ *for* $t \in [0, T]$ *and* $v \in H^1(\Omega)$ *by*

$$\langle \mathcal{R}(t), v\rangle = (\partial_t u_{h,\tau}, v) + (\nabla u_{h,\tau}, \nabla v) + \varepsilon^{-2}(f(u_{h,\tau}), v).$$

For almost every $t \in [t_{k-1}, t_k]$ *and all* $v \in H^1(\Omega)$ *we have*

$$\langle \mathcal{R}(t), v\rangle \leq (\eta^k_{\text{time}'} + \eta^k_{\text{coarse}})\|v\| + (C_{C\ell}\eta^k_{\text{space}} + \eta^k_{\text{time}})\|\nabla v\|,$$

where $\rho_k = \|u_h^k\|_{L^\infty(\Omega)} + \|u_h^{k-1}\|_{L^\infty(\Omega)}$,

$$\eta^k_{\text{space}} = \Big(\sum_{T\in\mathcal{T}_h^k} h_T^2\|\tau_k^{-1}(u_h^k - \mathcal{I}_k u_h^{k-1}) - \Delta_{\mathcal{T}_k} u_h^k + \varepsilon^{-2} f(u_h^k)\|^2_{L^2(T)}\Big)^{1/2}$$
$$+ \Big(\sum_{S\in\mathcal{S}_h^k\cap\Omega} h_S\|[\![\nabla u_h^k \cdot n_S]\!]\|^2_{L^2(S)}\Big)^{1/2} + \Big(\sum_{S\in\mathcal{S}_h^k\cap\partial\Omega} h_S\|\nabla u_h^k \cdot n\|^2_{L^2(S)}\Big)^{1/2},$$

and

$$\begin{aligned}\eta^k_{\text{time}'} &= \varepsilon^{-2}\|f'\|_{L^\infty(B_{\rho_k})}\|u_h^{k-1} - u_h^k\|,\\ \eta^k_{\text{time}} &= \|\nabla(u_h^{k-1} - u_h^k)\|,\\ \eta^k_{\text{coarse}} &= \tau_k^{-1}\|\mathcal{I}_k u_h^{k-1} - u_h^{k-1}\|.\end{aligned}$$

Proof For almost every $t \in (t_{k-1}, t_k)$, $k = 1, 2, \ldots, K$, and all $v \in H^1(\Omega)$, we have by definition of $\mathcal{R}$ that

$$\begin{aligned}\langle \mathcal{R}(t), v\rangle &= \tau_k^{-1}(u_h^k - u_h^{k-1}, v) + (\nabla u_{h,\tau}(t), \nabla v) + \varepsilon^{-2}(f(u_{h,\tau}(t)), v)\\ &= \tau_k^{-1}(u_h^k - \mathcal{I}_k u_h^{k-1}, v) + (\nabla u_h^k, \nabla v) + \varepsilon^{-2}(f(u_h^k), v)\\ &\quad + (\nabla(u_{h,\tau}(t) - u_h^k), \nabla v) + \varepsilon^{-2}(f(u_{h,\tau}(t)) - f(u_h^k), v)\\ &\quad + \tau_k^{-1}(\mathcal{I}_k u_h^{k-1} - u_h^{k-1}, v)\\ &= I + II + \cdots + VI.\end{aligned}$$

Since the sum of the first three terms vanishes for all $v \in \mathcal{S}^1(\mathcal{T}_k)$, we may insert the Clément interpolant $\mathcal{J}_k v \in \mathcal{S}^1(\mathcal{T}_k)$ of v. An element-wise integration by parts and estimates for the Clément interpolant lead to

$$I + II + III = \langle r_h^k, v - \mathscr{J}_k v\rangle \le C_{C\ell}\eta_{\mathrm{space}}^k \|\nabla v\|.$$

A repeated application of Hölder's inequality, the identity

$$f(u_{h,\tau}(t)) - f(u_h^k) = \Big(\int_0^1 f'(r u_{h,\tau}(t) + (1-r)u_h^k)\,\mathrm{d}r\Big)(u_{h,\tau}(t) - u_h^k),$$

and the linearity of $u_{h,\tau}$ in t lead to

$$\begin{aligned} IV + V &\le \|\nabla(u_{h,\tau}(t) - u_h^k)\|\|\nabla v\| + \varepsilon^{-2}\|f'\|_{L^\infty(B_{\rho_k})}\|u_{h,\tau}(t) - u_h^k\|\|v\| \\ &\le \eta_{\mathrm{time}'}^k\|v\| + \eta_{\mathrm{time}}^k\|\nabla v\|. \end{aligned}$$

A further application of Hölder's inequality proves

$$VI \le \tau_k^{-1}\|\mathscr{J}_k u_h^{k-1} - u_h^{k-1}\|\|v\| = \eta_{\mathrm{coarse}}^k\|v\|.$$

A combination of the estimates leads to the asserted bound. □

In combination with Theorem 6.4 we obtain the following a posteriori error estimate. It bounds the approximation error in terms of computable quantities provided that the error estimator is sufficiently small and depends exponentially only on the temporal average of the principal eigenvalue defined by the numerical approximation.

Theorem 6.5 (A posteriori error estimate) *Assume that we are in the setting of Proposition 6.3 and suppose that $\lambda_{\mathrm{AC}}^h \in L^1([0,T])$ is a function, such that for almost every $t \in (0,T)$, we have*

$$-\lambda_{\mathrm{AC}}^h(t) \le \inf_{v\in H^1(\Omega)\setminus\{0\}} \frac{\|\nabla v\|^2 + \varepsilon^{-2}(f'(u_{h,\tau}(t))v, v)}{\|v\|^2},$$

and set $\mu_\lambda(t) = 2(2 + (1-\varepsilon^2)\lambda_{\mathrm{AC}}^h(t))^+$. Define $\eta_\ell(t) = \eta_\ell^k$ for $t \in (t_{k-1}, t_k)$, $k = 1, 2, \ldots, K$, and $\ell \in \{\mathrm{time}', \mathrm{time}, \mathrm{space}, \mathrm{coarse}\}$ and let

$$\eta_{\mathrm{AC}}^2 = \|(u - u_h^0)(0)\|^2 + \int_0^T (\eta_{\mathrm{time}'}^2 + \eta_{\mathrm{coarse}}^2 + \varepsilon^{-2}\eta_{\mathrm{time}}^2 + \varepsilon^{-2}\eta_{\mathrm{space}}^2)\,\mathrm{d}t.$$

If

$$\eta_{\mathrm{AC}} \le \varepsilon^4\big(6c_S\|u_{h,\tau}\|_{L^\infty([0,T];L^\infty(\Omega))}(1+T)\big)^{-1}\Big(8\exp\Big(\int_0^T \mu_\lambda(t)\,\mathrm{d}t\Big)\Big)^{-3/2},$$

then we have

$$\sup_{s\in[0,T]} \|u - u_{h,\tau}\|^2 + \varepsilon^2 \int_0^T \|\nabla(u - u_{h,\tau})\|^2 \,\mathrm{d}t \le 8\eta^2 \exp\Big(\int_0^T \mu_\lambda(t)\,\mathrm{d}t\Big).$$

Proof The theorem is an immediate consequence of Proposition 6.3 and Theorem 6.4. □

6.2.2 A Priori Error Analysis

To derive a robust a priori error estimate for a semidiscrete in time approximation scheme, we try to follow the arguments used in the stability analysis of Theorem 6.3 with exchanged roles of the exact solution and its numerical approximation. As above we avoid the use of a Lipschitz estimate for the nonlinearity, and instead employ a linearization. The non-monotonicity of the resulting equation is controlled by a cubic term. The linearization allows us to incorporate the principal eigenvalue that is assumed to be well-behaved in the sense that a discrete integral grows only logarithmically in ε^{-1}.

Proposition 6.4 (Discrete stability) *Given $\tau > 0$ let $(U^k)_{k=0,\dots,K} \subset H^1(\Omega)$ be such that*

$$(d_t U^k, v) + (\nabla U^k, \nabla v) = -\varepsilon^{-2}(f(U^k), v)$$

for $k = 1, 2, \dots, K$ and all $v \in H^1(\Omega)$. We then have

$$I_\varepsilon(u^L) + (2 - 2\tau\varepsilon^{-2})\frac{\tau}{2}\sum_{k=1}^{K} \|d_t U^k\|^2 \le I_\varepsilon(u^0)$$

for every $1 \le L \le K$. Moreover, if $\|U^0\|_{L^\infty(\Omega)} \le 1$, then $\|U^k\|_{L^\infty(\Omega)} \le 1$ for $k = 1, 2, \dots, K$.

Proof The mean value theorem shows that for every $x \in \Omega$ there exists a number ξ_x such that

$$f(U^k) d_t U^k = d_t F(U^k) + \frac{\tau}{2} f'(\xi_x)(d_t U^k)^2.$$

Using that $f'(\xi_x) \ge -1$ and choosing $v = d_t U^k$, we deduce that

$$\|d_t U^k\|^2 + \frac{d_t}{2}\|\nabla U^k\|^2 + \frac{\tau}{2}\|\nabla d_t U^k\|^2 + d_t \varepsilon^{-2} \int_\Omega F(U^k)\,\mathrm{d}x - \frac{\tau\varepsilon^{-2}}{2}\|d_t U^k\|^2 \le 0.$$

Multiplication by τ and summation over $k = 1, 2, \ldots, L$ imply the assertion. A truncation argument and the characterization of U^k as the minimum of a functional I_ε^k show that $\|U^k\|_{L^\infty(\Omega)} \leq 1$ provided that U^0 has this property. □

Proposition 6.5 (Consistency) *Assume that the weak solution of the Allen–Cahn equation satisfies* $u \in C([0,T]; H^1(\Omega))$ *and* $u \in H^2([0,T]; H^1(\Omega)')$ *with*

$$\int_0^T \|u_{tt}\|_{H^1(\Omega)'}^2 \,\mathrm{d}t \leq c\varepsilon^{-2\sigma}.$$

For $u^k = u(t_k)$, $k = 0, 1, \ldots, K$, *we have*

$$(d_t u^k, v) + (\nabla u^k, \nabla v) = -\varepsilon^{-2}(f(u^k), v) + \mathscr{C}_\tau(t_k; v)$$

for all $v \in H^1(\Omega)$ *with consistency functionals* $\mathscr{C}_\tau(t_k)$ *satisfying*

$$\tau \sum_{k=1}^K \|\mathscr{C}_\tau(t_k)\|_{H^1(\Omega)'}^2 \leq c\tau^2\varepsilon^{-2\sigma}.$$

We have $\sigma = 2$ *if* $I(u_0) \leq c$.

Proof Noting that

$$(d_t u^k, v) + (\nabla u^k, \nabla v) + \varepsilon^{-2}(f(u^k), v) = (d_t u^k - \partial_t u(t_k), v) = \mathscr{C}_\tau(t_k; v)$$

for all $v \in H^1(\Omega)$, arguing as in the case of the linear heat equation, and incorporating Theorem 6.2 proves the asserted bound. □

The following lemma is a generalization of the classical discrete Gronwall lemma which states that if

$$y^{L'} \leq A + \tau \sum_{k=1}^{L'} a_k y^k$$

for $0 \leq L' \leq L$ and if $\tau a_k \leq 1/2$ for $k = 1, 2, \ldots, L$, then we have

$$\sup_{k=0,\ldots,L} y^k \leq 2A \exp\Big(2\tau \sum_{k=1}^L a_k\Big).$$

The condition $a_k\tau \leq 1/2$ is required to absorb the term $a_{L'} y^{L'}$.

Lemma 6.2 (Generalized discrete Gronwall lemma) *Let* $\tau > 0$ *and suppose that the nonnegative real sequences* $(y_\ell^k)_{k=0,\ldots,K}$, $\ell = 1, 2, 3$, $(a_k)_{k=0,\ldots,K}$, *and the real number* $A \geq 0$ *satisfy*

$$y_1^L + \tau \sum_{k=1}^{L} y_2^k \le A + \tau \sum_{k=1}^{L} a_k y_1^k + \tau \sum_{k=1}^{L-1} y_3^k$$

for all $L = 0, 1, \ldots, K$, $\sup_{k=1,\ldots,K} \tau a_k \le 1/2$, *and* $K\tau \le T$. *Assume that for* $B \ge 0$, $\beta > 0$, *and every* $L = 1, 2, \ldots, K$, *we have*

$$\tau \sum_{k=1}^{L-1} y_3^k \le B\big(\sup_{k=1,\ldots,L-1} (y_1^k)^\beta\big)\tau \sum_{k=1}^{L-1} (y_1^k + y_2^k).$$

Set $E = \exp\big(2\tau \sum_{k=1}^K a_k\big)$ *and assume that* $8AE \le (8B(1+T)E)^{-1/\beta}$. *Then*

$$\sup_{k=0,\ldots,K} y_1^k + \tau \sum_{k=1}^{K} y_2^k \le 8A \exp\Big(2\tau \sum_{k=1}^{K} a_k\Big).$$

Proof Set $\theta = 8AE$. We proceed by induction and suppose that

$$\sup_{k=0,\ldots,L-1} y_1^k + \tau \sum_{k=1}^{L-1} y_2^k \le \theta.$$

This is satisfied for $L = 1$. For every $L' = 1, 2, \ldots, L$, we then have due to the assumptions of the lemma that

$$\begin{aligned} y_1^{L'} + \tau \sum_{k=1}^{L'} y_2^k &\le A + \tau \sum_{k=1}^{L'} a_k y_1^k + B\big(\sup_{k=1,2,\ldots,L'-1} (y_1^k)^\beta\big)\tau \sum_{k=1}^{L'-1} (y_1^k + y_2^k) \\ &\le A + \tau \sum_{k=1}^{L'} a_k y_1^k + B(1+T)\theta^{1+\beta}. \end{aligned}$$

The classical discrete Gronwall lemma, the condition on A, and the estimate $\theta^\beta \le (8B(1+T)E)^{-1}$ prove that for all $L' = 1, 2, \ldots, L$, we have

$$y_1^{L'} + \tau\varepsilon^2 \sum_{k=1}^{L'} y_2^k \le 2(A + B(1+T)\theta^{1+\beta})E \le \frac{\theta}{2}.$$

This completes the inductive argument and proves the lemma. □

The a priori bounds and the generalized discrete Gronwall lemma lead to a robust a priori error estimate under an assumption on the principal eigenvalue that is motivated by analytical considerations.

Theorem 6.6 (A priori error estimate) *Assume* $\varepsilon \le 1$, $I_\varepsilon(u_0) \le c_0$, *and that there are* $c_1 > 0$, $\kappa \ge 0$ *with*

$$\tau \sum_{k=1}^{K} \lambda_{\mathrm{AC}}^{+}(t_k) \le c_1 + \log \varepsilon^{-\kappa}.$$

Then there exists a constant $c_2 > 0$ *such that if* $\tau \le c_2 \varepsilon^{7+6\kappa}$, *we have*

$$\sup_{k=1,\dots,K} \|u(t_k) - U^k\|^2 + \tau\varepsilon^2 \sum_{k=1}^{K} \|\nabla(u(t_k) - U^k)\|^2 \le c\tau^2 \varepsilon^{-6-4\kappa}.$$

Proof Denoting $u^k = u(t_k)$ the error $e^k = u^k - U^k$ satisfies the identity

$$(d_t e^k, v) + (\nabla e^k, \nabla v) = -\varepsilon^{-2}(f(u^k) - f(U^k), v) + \mathscr{C}_\tau(t_k, v)$$

for all $v \in H^1(\Omega)$. Lemma 6.1, the definition of $\lambda_{\mathrm{AC}}(t_k)$, and $\|u^k\|_{L^\infty(\Omega)} \le 1$ imply that

$$\begin{aligned}
-\varepsilon^{-2}(f(u^k) - f(U^k), e^k) &\le -\varepsilon^{-2}(f'(u^k)e^k, e^k) + 3\varepsilon^{-2}\|u^k\|_{L^\infty(\Omega)}\|e^k\|_{L^3(\Omega)}^3 \\
&= -(1-\varepsilon^2)\varepsilon^{-2}(f'(u^k)e^k, e^k) - (f'(u^k)e^k, e^k) \\
&\quad + 3\varepsilon^{-2}\|e^k\|_{L^3(\Omega)}^3 \\
&\le (1-\varepsilon^2)\lambda_{\mathrm{AC}}(t_k)\|e^k\|^2 + (1-\varepsilon)\|\nabla e^k\|^2 \\
&\quad + \|e^k\|^2 + 3\varepsilon^{-2}\|e^k\|_{L^3(\Omega)}^3.
\end{aligned}$$

Hence, for the choice of $v = e^k$, we find that

$$\begin{aligned}
\frac{1}{2} d_t\|e^k\|^2 + \frac{\tau}{2}\|d_t e^k\|^2 + \|\nabla e^k\|^2 &= \mathscr{C}_\tau(t_k, e^k) - \varepsilon^{-2}(f(u^k) - f(U^k), e^k) \\
&\le \frac{\varepsilon^{-2}}{2}\|\mathscr{C}_\tau(t_k)\|_{H^1(\Omega)'}^2 + \frac{\varepsilon^2}{2}\|e^k\|^2 + \frac{\varepsilon^2}{2}\|\nabla e^k\|^2 \\
&\quad + (1-\varepsilon^2)\lambda_{\mathrm{AC}}(t_k)\|e^k\|^2 + (1-\varepsilon^2)\|\nabla e^k\|^2 \\
&\quad + \|e^k\|^2 + 3\varepsilon^{-2}\|e^k\|_{L^3(\Omega)}^3.
\end{aligned}$$

Using $(a+b)^3 \le 4(a^3 + b^3)$ and $\tau\|d_t e^k\|_{L^\infty(\Omega)} \le 4$ we find that

$$\|e^k\|_{L^3(\Omega)}^3 \le 4\big(\|e^{k-1}\|_{L^3(\Omega)}^3 + \tau^3\|d_t e^k\|_{L^3(\Omega)}^3\big) \le 4\|e^{k-1}\|_{L^3(\Omega)}^3 + 16\tau^2\|d_t e^k\|^2.$$

If τ is sufficiently small so that $48\tau\varepsilon^{-2} \le 1/2$, then the combination of the last two estimates implies

$$d_t\|e^k\|^2 + \varepsilon^2\|\nabla e^k\|^2 \le \varepsilon^{-2}\|\mathscr{C}_\tau(t_k)\|_{H^1(\Omega)'}^2 + \mu_\lambda^k\|e^k\|^2 + 48\varepsilon^{-2}\|e^{k-1}\|_{L^3(\Omega)}^3, \quad (6.2)$$

where $\mu_\lambda^k = 2(2 + \lambda_{\mathrm{AC}}^+(t_k))$. We set

$$y_1^k = \|e^k\|^2,\ y_2^k = \varepsilon^2\|\nabla e^k\|^2,\ y_3^k = 48\varepsilon^{-2}\|e^k\|_{L^3(\Omega)}^3.$$

Noting that $e^0 = 0$ and

$$\|e^{k-1}\|_{L^3(\Omega)}^3 \le \|e^{k-1}\|\|e^{k-1}\|_{L^4(\Omega)}^2 \le c_S\|e^{k-1}\|(\|e^{k-1}\|^2 + \|\nabla e^{k-1}\|^2), \quad (6.3)$$

we find by summation of (6.2) and (6.3) over $k = 1, 2, \ldots, L$ that we are in the situation of Lemma 6.2 with

$$A = \varepsilon^{-2}\tau\sum_{k=1}^K \|\mathscr{C}_\tau(t_k)\|_{H^1(\Omega)'}^2,\ E = \exp\Big(2\tau\sum_{k=1}^K \mu_\lambda^k\Big),\ B = 48\varepsilon^{-4}c_S,$$

and $\beta = 1/2$. Therefore,

$$\sup_{k=0,\ldots,K}\|e^k\|^2 + \varepsilon^2\tau\sum_{k=1}^K\|\nabla e^k\|^2 \le 8AE,$$

provided that $8AE \le (8B(1+T)E)^{-2}$. Since according to Proposition 6.5 we have $A \le c\tau^2\varepsilon^{-6}$, this is satisfied if $c_B\tau^2\varepsilon^{-6}E \le (8B(1+T)E)^{-2}$. With the assumed bound for the discrete integral of λ_{AC}^+, we deduce that

$$E \le \exp(8T)\exp\Big(4\tau\sum_{k=1}^K\lambda_{AC}^+(t_k)\Big) \le c_E\varepsilon^{-4\kappa}.$$

Therefore, the condition $\tau^2 \le c\varepsilon^{14}\varepsilon^{12\kappa}$ implies the assertion. □

Remarks 6.6 (i) If $u_{tt} \in L^2([0,T]; L^2(\Omega))$, then the bound for A in the proof can be improved and the conditions of the theorem can be weakened.
(ii) An a priori error analysis for a fully discrete approximation follows the same strategy by decomposing the error $u(t_k) - u_h^k$ as $(u(t_k) - Q_h u(t_k)) + (Q_h u(t_k) - u_h^k)$ with the H^1-projection Q_h, cf. [8].

6.3 Practical Realization

We discuss in this section alternatives to the implicit Euler scheme and include an estimate for the approximation of the principal eigenvalue that is needed to compute the a posteriori error bound.

6.3.1 Time-Stepping Schemes

The implicit Euler scheme requires the solution of a nonlinear system of equations in every time step and is stable under the condition $\tau \leq 2\varepsilon^2$. We consider various semi-implicit approximation schemes defined by approximating the nonlinear term avoiding some of these limitations.

Algorithm 6.1 (*Semi-implicit approximation*) Given $u_h^0 \in \mathscr{S}^1(\mathscr{T}_h)$, $\tau > 0$, and a continuous function $G : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ let the sequence $(u_h^k)_{k=0,\dots,K}$ be defined by

$$(d_t u_h^k, v_h) + (\nabla u_h^k, \nabla v_h) + \varepsilon^{-2}\big(G(u_h^k, u_h^{k-1}), v_h\big) = 0$$

for all $v_h \in \mathscr{S}^1(\mathscr{T}_h)$.

The function G is assumed to provide a *consistent* approximation of the nonlinear function f in the sense that $G(s, s) = f(s)$.

Examples 6.1 (i) The (fully) implicit Euler scheme corresponds to

$$G^{\mathrm{impl}}(u^k, u^{k-1}) = f(u^k).$$

(ii) The choice of

$$G^{\mathrm{expl}}(u^k, u^{k-1}) = f(u^{k-1})$$

realizes an explicit treatment of the nonlinearity.

(iii) Carrying out one iteration of a Newton scheme in every time step of the implicit Euler scheme with initial guess u_h^{k-1} corresponds to the linearization

$$G^{\mathrm{lin}}(u^k, u^{k-1}) = f(u^{k-1}) + f'(u^{k-1})(u^k - u^{k-1}).$$

(iv) A Crank–Nicolson type treatment of the nonlinear term is

$$G^{\mathrm{cn}}(u^k, u^{k-1}) = \begin{cases} \dfrac{F(u^k) - F(u^{k-1})}{u^k - u^{k-1}} & \text{if } u^k \neq u^{k-1}, \\ f(u^k) & \text{if } u^k = u^{k-1}. \end{cases}$$

We have $G^{\mathrm{cn}}(u^k, u^{k-1}) = (1/4)(u^k + u^{k-1})((u^k)^2 + (u^{k-1})^2 - 2)$.

(v) The decomposition $F = F^{cx} + F^{cv}$ of $F(u^{k-1}) = ((u^k)^2 - 1)^2/4$ into a convex part $F^{cx}(u^{k-1}) = ((u^k)^4 + 1)/4$ and a concave part $F^{cv}(u^{k-1}) = -(1/2)(u^{k-1})^2$ leads with the derivatives f^{cx} and f^{cv} of F^{cx} and F^{cv}, respectively, to the definition

$$G^{\mathrm{cxcv}}(u^k, u^{k-1}) = f^{cx}(u^k) + f^{cv}(u^{k-1}).$$

Remarks 6.7 (i) Only the explicit and linearized treatment of the nonlinear term leads to linear systems of equations in every time step. The convex-concave decomposition leads to monotone systems of equations.
(ii) The best compromise for stability and linearity appears to be the linearized treatment of the nonlinear term.
(iii) The decomposition of F into convex and concave parts corresponds to the general concept to treat monotone terms implicitly and anti-monotone terms explicitly.
(iv) Numerical integration simplifies the nonlinearities, i.e., for all $z, y \in \mathcal{N}_h$, we have

$$\big(G(u_h^k, u_h^{k-1})\varphi_z, \varphi_y\big)_h = G(u_h^k(z), u_h^{k-1}(z))\beta_z\delta_{zy}$$

with $\beta_z = \int_\Omega \varphi_z$, so that the corresponding contribution to the system matrix is given by a diagonal matrix.
(v) The numerical schemes have different numerical dissipation properties.

The stability of the different semi-implicit Euler schemes is a consequence of the following proposition. We omit a discussion of the explicit treatment of the nonlinearity since this is experimentally found to be unstable even for $\tau \sim \varepsilon^2$.

Proposition 6.6 (Semi-implicit Euler schemes) *Given* $u^k, u^{k-1} \in \mathbb{R}$ *and* $\tau > 0$, *we set* $d_t u^k = (u^k - u^{k-1})/\tau$. *We have*

$$\begin{aligned} G^{\mathrm{impl}}(u^k, u^{k-1})d_t u^k &\geq d_t F(u^k) - \frac{\tau}{2}|d_t u^k|^2, \\ G^{\mathrm{cn}}(u^k, u^{k-1})d_t u^k &= d_t F(u^k), \\ G^{\mathrm{cxcv}}(u^k, u^{k-1})d_t u^k &\geq d_t F(u^k), \end{aligned}$$

and if $|u^k|, |u^{k-1}| \leq 1$, *then*

$$G^{\mathrm{lin}}(u^k, u^{k-1})d_t u^k \geq d_t F(u^k) - \frac{7\tau}{2}|d_t u^k|^2.$$

In particular, the implicit Euler scheme is stable if $\tau \leq 2\varepsilon^2$, *the semi-implicit Euler scheme with Crank–Nicolson type treatment of the nonlinear term is unconditionally stable, the semi-implicit Euler scheme with decomposed treatment of the nonlinearity is unconditionally stable, and the semi-implicit Euler scheme with a linearized treatment of the nonlinear term is stable if a discrete maximum principle holds and* $\tau \leq (2/7)\varepsilon^2$, *i.e., under these conditions we have for the solutions of the respective semi-implicit Euler schemes that*

$$I_\varepsilon(u_h^L) \leq I_\varepsilon(u_h^0)$$

for all $L \geq 0$.

Proof A Taylor expansion shows that for some $\xi \in \mathbb{R}$, we have

$$F(u^{k-1}) = F(u^k) + f(u^k)(u^{k-1} - u^k) + \frac{1}{2} f'(\xi)(u^{k-1} - u^k)^2.$$

Since $f'(\xi) \geq -1$ we deduce after division by τ that

$$f(u^k) d_t u^k = d_t F(u^k) + \frac{\tau}{2} f'(\xi)(d_t u^k)^2 \geq d_t F(u^k) - \frac{\tau}{2} |d_t u^k|^2$$

and this implies the bound for G^{impl}. Assuming that $|u^k|, |u^{k-1}| \leq 1$, a similar argument with $f''(s) = 6s$ shows with some $\zeta \in [-1, 1]$ that

$$\begin{aligned}
&\big(f(u^{k-1}) + f'(u^{k-1})(u^k - u^{k-1})\big)(u^k - u^{k-1}) \\
&= f(u^k)(u^k - u^{k-1}) - \frac{1}{2} f''(\zeta)(u^k - u^{k-1})^3 \geq f(u^k)(u^k - u^{k-1}) - 6(u^k - u^{k-1})^2
\end{aligned}$$

and with the previous estimate we deduce that

$$G^{\mathrm{lin}}(u^k, u^{k-1}) d_t u^k \geq d_t F(u^k) - \frac{7\tau}{2} |d_t u^k|^2.$$

If $d_t u^k \neq 0$, then

$$G^{\mathrm{cn}}(u^k, u^{k-1})(u^k - u^{k-1}) = F(u^k) - F(u^{k-1}) = \tau d_t F(u^k),$$

and if $d_t u^k = 0$, then $G^{\mathrm{cn}}(u^k, u^{k-1}) d_t u^k = 0 = \tau d_t F(u^k)$ which implies the asserted identity for G^{cn}. For the convex function F^{cx} and its derivative f^{cx}, we have

$$f^{cx}(u^k)(u^{k-1} - u^k) + F^{cx}(u^k) \leq F^{cx}(u^{k-1}).$$

Analogously, for the convex function $-F^{cv}$ and its derivative $-f^{cv}$, we have

$$-f^{cv}(u^{k-1})(u^k - u^{k-1}) - F^{cv}(u^{k-1}) \leq -F^{cv}(u^k).$$

The combination of the two estimates proves that

$$G^{\mathrm{cxcv}}(u^k, u^{k-1}) d_t u^k = f^{cx}(u^k) d_t u^k + f^{cv}(u^{k-1}) d_t u^k \geq d_t F^{cx}(u^k) + d_t F^{cv}(u^k).$$

The stability of the related schemes now follows from the choice of $v_h = d_t u_h^k$ in the semi-implicit Euler scheme, i.e.,

$$\|d_t u_h^k\|^2 + \frac{d_t}{2} \|\nabla u_h^k\|^2 + \frac{\tau}{2} \|\nabla d_t u_h^k\|^2 + \varepsilon^{-2} \big(G(u_h^k, u_h^{k-1}), d_t u_h^k\big) = 0,$$

together with a summation over $k = 1, 2, \dots, L$, and the corresponding lower bounds for $G(u_h^k, u_h^{k-1})$. □

6.3.2 Computation of the Eigenvalue

The a posteriori error estimate of Theorem 6.5 requires a lower bound for the principal eigenvalue of the linearized Allen–Cahn operator with respect to the approximate solution, i.e., a function λ_{AC}^h such that

$$-\lambda_{\mathrm{AC}}^h(t) \le \inf_{v \in H^1(\Omega)\setminus\{0\}} \frac{\|\nabla v\|^2 + \varepsilon^{-2}(f'(u_{h,\tau}(t))v, v)}{\|v\|^2}.$$

To approximate the infimum on the right-hand side, we replace the space $H^1(\Omega)$ by $\mathscr{S}^1(\mathscr{T}_h)$. We fix a time t in the following and let $-\Lambda \in \mathbb{R}$ be the infimum at time t, i.e., there exists $w \in H^1(\Omega)$ with $\|w\| = 1$ and

$$-\Lambda(w, v) = (\nabla w, \nabla v) + \varepsilon^{-2}(p_h w, v)$$

for all $v \in H^1(\Omega)$ and with $p_h = f'(u_{h,\tau}(t))$.

Proposition 6.7 (Eigenvalue approximation) *Let $(\Lambda_h, w_h) \in \mathbb{R} \times \mathscr{S}^1(\mathscr{T}_h)$ be such that*

$$-\Lambda_h(w_h, v_h) = (\nabla w_h, \nabla v_h) + \varepsilon^{-2}(p_h w_h, v_h)$$

for all $v_h \in \mathscr{S}^1(\mathscr{T}_h)$. Assume that the Laplace operator with homogeneous Neumann boundary conditions is H^2-regular in Ω in the sense that $\|D^2 v\| \le c_\Delta \|\Delta v\|$ for all $v \in H^2(\Omega)$ with $\partial_n v = 0$ on $\partial\Omega$ and suppose that $\|p_h\|_{L^\infty(\Omega)} \le c_0$. Then there exists $c_1 > 0$ such that if $h \le c_1 \varepsilon$, we have

$$0 \le \Lambda - \Lambda_h \le c\varepsilon^{-4}h^2.$$

Proof In the following we occasionally replace the function p_h by $q_h = p_h + \|p_h\|_{L^\infty(\Omega)}$ which corresponds to a shift of $-\Lambda$ and $-\Lambda_h$ by $\|p_h\|_{L^\infty(\Omega)}$ but allows us to use $q_h \ge 0$. The fact that $\mathscr{S}^1(\mathscr{T}_h) \subset H^1(\Omega)$ implies that we have $-\Lambda \le -\Lambda_h$. Since w_h is minimal for $v_h \mapsto \|\nabla v_h\|^2 + \varepsilon^{-2}(p_h v_h, v_h)$ among functions $v_h \in \mathscr{S}^1(\mathscr{T}_h)$ with $\|v_h\| = 1$ with minimum $-\Lambda_h$ and since $-\Lambda = \|\nabla w\|^2 + \varepsilon^{-2}(p_h w, w)$, we have

$$\begin{aligned} 0 \le \Lambda - \Lambda_h &\le -(\nabla w, \nabla w) - \varepsilon^{-2}(q_h w, w) + \|\nabla v_h\|^2 + \varepsilon^{-2}(q_h v_h, v_h) \\ &\le 2(\nabla v_h, \nabla[v_h - w]) + 2\varepsilon^{-2}(q_h v_h, v_h - w). \end{aligned}$$

We note $-\Lambda \le \varepsilon^{-2}\|p_h\|_{L^\infty(\Omega)}$ and conclude with $-\Delta w = -\Lambda w - \varepsilon^{-2} p_h w$ that

$$\|\nabla w\| \le c\varepsilon^{-1}, \quad \|D^2 w\| \le c\|\Delta w\| \le c\varepsilon^{-2}.$$

We incorporate the H^1-projection $Q_h w \in \mathscr{S}^1(\mathscr{T}_h)$ defined by

$$(\nabla Q_h w, \nabla y_h) + (Q_h w, y_h) = (\nabla w, \nabla y_h) + (w, y_h)$$

for all $y_h \in \mathscr{S}^1(\mathscr{T}_h)$ which satisfies the estimates

$$h\|w - Q_h w\| + \|\nabla(w - Q_h w)\| \le ch^2\|D^2 w\|.$$

We suppose that $h \le c\varepsilon$ is such that

$$\big|1 - \|Q_h w\|\big| \le \|w - Q_h w\| \le ch^2\varepsilon^{-2} \le \frac{1}{2}.$$

Choosing $v_h = Q_h w/\|Q_h w\|$ and noting

$$\|\nabla Q_h w\| + \|Q_h w\| \le \|\nabla w\| + \|w\| \le c\varepsilon^{-1}$$

we find that

$$\begin{aligned}
(\nabla v_h, \nabla[v_h - w]) &= \|Q_h w\|^{-2}\big((\nabla Q_h w, \nabla[Q_h w - w]) + (\nabla Q_h w, \nabla[w - \|Q_h w\| w])\big) \\
&= \|Q_h w\|^{-2}\big((Q_h w, Q_h w - w) + (1 - \|Q_h w\|)(\nabla Q_h w, \nabla w)\big) \\
&\le ch^2\varepsilon^{-2}(1 + \varepsilon^{-2}).
\end{aligned}$$

Analogously, we have

$$\begin{aligned}
(q_h v_h, v_h - w) &= \|Q_h w\|^{-2}\big((Q_h w, Q_h w - w) + (Q_h w, w - \|Q_h w\| w)\big) \\
&= \|Q_h w\|^{-2}\big((Q_h w, Q_h w - w) + (1 - \|Q_h w\|)(Q_h w, w)\big) \\
&\le ch^2\varepsilon^{-2}.
\end{aligned}$$

A combination of the estimates implies the asserted error bound. □

The discrete eigenvalue problem can be recast as the problem of finding a vector $W \in \mathbb{R}^L$ with $W^\top m W = 1$ and

$$(-\Lambda + c_{\text{shift}})mW = (s + \varepsilon^{-2} m_p + c_{\text{shift}} m)W = YW$$

with the mass matrix m, the stiffness matrix s, the weighted mass matrix m_p, and an arbitrary constant c_{shift}. For $c_{\text{shift}} = \varepsilon^{-2}\|p_h\|_{L^\infty(\Omega)} + 1$, we have that the symmetric matrices m and $Y = s + \varepsilon^{-2} m_p + c_{\mathrm{shift}} m$ are positive definite, and we may use the following vector iteration with Rayleigh-quotient approximation to approximate Λ.

Algorithm 6.2 (*Vector iteration*) Given $W_0 \in \mathbb{R}^L$ such that $W_0^\top m W_0 = 1$, compute the sequence Λ^j, $j = 0, 1, 2, \dots$ via $\Lambda^0 = (W^0)^\top Y W^0$ and

$$\widetilde{W}^{j+1} = Y^{-1}(m W^j), \quad W^{j+1} = \frac{\widetilde{W}^{j+1}}{\big((\widetilde{W}^{j+1})^\top m \widetilde{W}^{j+1}\big)^{1/2}}$$

and

$$-\Lambda^{j+1} + c_{\mathrm{shift}} = (W^{j+1})^\top Y W^{j+1}.$$

Stop the iteration if $|\Lambda^{j+1} - \Lambda^j| \le \varepsilon_{\mathrm{stop}}$.

Remark 6.8 The iteration converges to the smallest eigenvalue provided that the initial vector W_0 is not orthogonal to the corresponding eigenspace.

6.3.3 Implementation

The MATLAB code shown in Fig. 6.6 realizes the semi-implicit Euler scheme with linearized treatment of the nonlinear term and computes the principal eigenvalue defined by the approximate solution in every time step. We used the discrete inner product $(\cdot,\cdot)_h$ to simplify the computation of some matrices, i.e., we use the formulations

$$\begin{aligned}(d_t u_h^k, v_h) + (\nabla u_h^k, \nabla v_h) + \varepsilon^{-2}(f'(u_h^{k-1}) u_h^k, v_h)_h \\ = -\varepsilon^{-2}(f(u_h^{k-1}), v_h)_h + \varepsilon^{-2}(f'(u_h^{k-1}) u_h^{k-1}, v_h)_h\end{aligned}$$

and

$$-\lambda_{\mathrm{AC}}^h(t_k)(w_h, v_h) = (\nabla w_h, \nabla v_h) + \varepsilon^{-2}(f'(u_h^k) w_h, v_h)_h$$

for all $v_h \in \mathcal{S}^1(\mathcal{T}_h)$ to find $u_h^k \in \mathcal{S}^1(\mathcal{T}_h)$ and an approximation of the eigenpair $(-\lambda_{\mathrm{AC}}^h(t_k), w_h)$.

```
function ac_linearized_euler(d,red)
[c4n,n4e,Db,Nb] = triang_cube(d);
c4n = 2*(c4n-1/2);
for j = 1:red
    [c4n,n4e,Db,Nb,¬,¬] = red_refine(c4n,n4e,Db,Nb);
end
nC = size(c4n,1);
T = 1;
eps = 2^(-4); tau = (2/3)*eps^2;
K = ceil(T/tau);
u = u_0(c4n,eps);
[s,m,m_lumped] = fe_matrices(c4n,n4e);
w_init = rand(nC,1)-.5;
lambda = zeros(K,1);
for k = 1:K
    b_nonlin = -eps^(-2)*m_lumped*f(u)...
        +eps^(-2)*m_lumped*(df(u).*u);
    m_nonlin = eps^(-2)*m_lumped*diag(df(u));
    b = tau^(-1)*m*u+b_nonlin;
    X = tau^(-1)*m+s+m_nonlin;
    u = X\b;
    c_shift = abs(min(df(u)))+1;
    Y = s+eps^(-2)*m_lumped*spdiags(df(u)+c_shift,0,nC,nC);
    [neg_lambda_shift,w] = vector_iteration(Y,m,w_init);
    lambda(k) = -neg_lambda_shift+eps^(-2)*c_shift;
    figure(1); show_p1(c4n,n4e,Db,Nb,u); axis square;
    figure(2); plot(tau*(1:k),lambda(1:k)); drawnow;
    w_init = w;
end

function val = f(u)
val = u.^3-u;
function val = df(u)
val = 3*u.^2-1;

function val = u_0(x,eps)
dist = sqrt(min((x(:,1)-.3).^2,(x(:,1)+.3).^2)+x(:,2).^2)-.35;
val = -tanh(dist/(sqrt(2)*eps));

function [mu,w] = vector_iteration(Y,m,w)
mu = 0; mu_old = 0;
diff_mu = 1; eps_stop = 1E-01;
while abs(diff_mu) > eps_stop
    w = Y\(m*w);
    w = w/sqrt(w'*m*w);
    mu = w'*Y*w;
    diff_mu = mu-mu_old;
    mu_old = mu;
end
```

Fig. 6.6 Implementation of the linearized implicit Euler scheme with numerical integration for the Allen–Cahn equation and computation of the eigenvalue in each time step

References

1. Alikakos, N.D., Fusco, G.: Slow dynamics for the Cahn-Hilliard equation in higher space dimensions. I. Spectral estimates. Commun. Partial Differ Equ **19**(9–10), 1397–1447 (1994). http://dx.doi.org/10.1080/03605309408821059
2. Barrett, J.W., Blowey, J.F.: An error bound for the finite element approximation of the Cahn-Hilliard equation with logarithmic free energy. Numer. Math. **72**(1), 1–20 (1995). http://dx.doi.org/10.1007/s002110050157
3. Bartels, S., Müller, R., Ortner, C.: Robust a priori and a posteriori error analysis for the approximation of Allen-Cahn and Ginzburg-Landau equations past topological changes. SIAM J. Numer. Anal. **49**(1), 110–134 (2011). http://dx.doi.org/10.1137/090751530
4. Chen, X.: Spectrum for the Allen-Cahn, Cahn-Hilliard, and phase-field equations for generic interfaces. Commun. Partial Differ Equ **19**(7–8), 1371–1395 (1994). http://dx.doi.org/10.1080/03605309408821057
5. Deckelnick, K., Dziuk, G., Elliott, C.M.: Computation of geometric partial differential equations and mean curvature flow. Acta Numer. **14**, 139–232 (2005). http://dx.doi.org/10.1017/S0962492904000224
6. Elliott, C.M., French, D.A.: Numerical studies of the Cahn-Hilliard equation for phase separation. IMA J. Appl. Math. **38**(2), 97–128 (1987). http://dx.doi.org/10.1093/imamat/38.2.97
7. Emmerich, H.: The Diffuse Interface Approach in Materials Science. Lecture Notes in Physics, vol. M 73. Springer, Berlin (2003)
8. Feng, X., Prohl, A.: Numerical analysis of the Allen-Cahn equation and approximation for mean curvature flows. Numer. Math. **94**(1), 33–65 (2003). http://dx.doi.org/10.1007/s00211-002-0413-1
9. Kessler, D., Nochetto, R.H., Schmidt, A.: A posteriori error control for the Allen-Cahn problem: circumventing Gronwall's inequality. M2AN Math. Model. Numer. Anal. **38**(1), 129–142 (2004). http://dx.doi.org/10.1051/m2an:2004006
10. Nochetto, R.H., Verdi, C.: Convergence past singularities for a fully discrete approximation of curvature-driven interfaces. SIAM J. Numer. Anal. **34**(2), 490–512 (1997). http://dx.doi.org/10.1137/S0036142994269526
11. Penrose, O., Fife, P.C.: Thermodynamically consistent models of phase-field type for the kinetics of phase transitions. Phys. D **43**(1), 44–62 (1990). http://dx.doi.org/10.1016/0167-2789(90)90015-H