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ROBUST A PRIORI AND A POSTERIORI ERROR ANALYSIS FOR THE APPROXIMATION OF ALLEN–CAHN AND GINZBURG–LANDAU EQUATIONS PAST TOPOLOGICAL CHANGES*

SÖREN BARTELS†, RÜDIGER MÜLLER‡, AND CHRISTOPH ORTNER§

Abstract. A priori and a posteriori error estimates are derived for the numerical approximation of scalar and complex valued phase field models. Particular attention is devoted to the dependence of the estimates on a small parameter and to the validity of the estimates in the presence of topological changes in the solution that represents singular points in the evolution. For typical singularities the estimates depend on the inverse of the parameter in a polynomial as opposed to exponential dependence of estimates resulting from a straightforward error analysis. The estimates naturally lead to adaptive mesh refinement and coarsening algorithms. Numerical experiments illustrate the reliability and efficiency of this approach for the evolution of interfaces and vortices that undergo topological changes.

Key words. Allen–Cahn equation, Ginzburg–Landau equation, mean curvature flow, finite element method, error analysis, adaptive methods

AMS subject classifications. 65M15, 65M50, 65M60

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1. Introduction.

The numerical analysis of phase field models such as the Allen–Cahn equation

$$\begin{aligned} \partial_t u - \Delta u + \varepsilon^{-2} f(u) &= 0 \quad \text{in } (0,T)\times\Omega, \\ \partial_n u &= 0 \quad \text{on } (0,T)\times\partial\Omega, \\ u(0,\cdot) &= u_0, \end{aligned} \tag{1}$$

with $T > 0$, $\Omega \subseteq \mathbb{R}^d$, $d = 2, 3$, $f(u) = u^3 - u$, and $0 < \varepsilon \ll 1$ has recently attracted considerable attention. Based on uniform bounds for the principal eigenvalue of the linearized Allen–Cahn operator about the solution $u(t,\cdot)$, i.e.,

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

where $(\cdot,\cdot)$ denotes the inner product in $L^2(\Omega)$, the seminal work [FP03] derived optimal a priori error estimates for the finite element approximation of (1) which avoid the use of a maximum principle and are robust in ε^{-1}, i.e., depend on ε^{-1} only in a low order polynomial. This is in contrast to a straightforward error analysis

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that leads to exponential dependence of error estimates on ε^{-1}, which is of limited practical value. Unfortunately, uniform bounds for $\lambda_{AC}(t)$ are only available as long as the interface $\Gamma_t := \{x \in \Omega : u(t,x) = 0\}$ is smooth and $u(t,\cdot)$ has the right profile across Γ_t (cf. [AF93, Che94, dMS95]); those bounds break down when topological changes of the interface occur. In this paper we show that minor modifications of the arguments in [FP03] and the subsequent papers [FP04a, FP04b, KNS04, FP05, Bar05a, Bar05b, FW05, FW07, FHL07, KKL07, BM10a] allow us to robustly control the approximation of a large class of evolutions that develop singularities. Our key observation is that topological changes for which $\lambda_{AC}(t) \sim \varepsilon^{-2}$ occur within time intervals of length comparable to ε^2. Therefore, if only finitely many topological changes happen, then we may expect that the bound

$$\int_0^T \lambda_{AC}^+(t)\,\mathrm{d}t \le C_0 + \log(\varepsilon^{-\kappa}), \tag{3}$$

where $x^+ := \max\{x, 0\}$, holds uniformly in ε^{-1}. The logarithmic term reflects transition regions in which λ_{AC} decays from ε^{-2} to an ε independent value. This bound is sufficient for a robust a priori error analysis, whereas a uniform bound $\lambda_{AC}(t) \le C$ for almost every $t \in (0,T)$ would exclude generic singularities, i.e., topological changes of the interface Γ_t.

The numerical experiments reported below confirm that the bound (3) is realistic and may therefore be assumed for a robust a priori error analysis. It may, however, be difficult to prove (3) rigorously in particular when the mathematical model is more involved than the simple model problem (1). Therefore we also investigate a different approach following ideas of [KNS04, Bar05a] for the a posteriori analysis. The latter paper proposes the approximation of the principal eigenvalue of the linearized Allen–Cahn operator about an approximate solution $U(t,\cdot)$, i.e.,

$$-\Lambda_{AC}(t) := \inf_{v \in H^1(\Omega)\setminus\{0\}} \frac{\|\nabla v\|^2_{L^2(\Omega)} + \varepsilon^{-2}(f'(U(t))v, v)}{\|v\|^2_{L^2(\Omega)}}, \tag{4}$$

which is accessible up to approximation errors. By computing $\Lambda_{AC}(t)$, important information about the evolution is extracted from the approximate solution. In particular, we can verify (3) a posteriori, and this allows a rigorous a posteriori error analysis if the corresponding residual $\mathcal{R}_U$ is sufficiently small: The estimates $f' \ge -1$ and $-(f(u) - f(U) - f'(u)e)e \le 3|U||e|^3$ for $e = u - U$ together with the definition of Λ_{AC} lead to the error inequality (assuming here for simplicity that $\|U(t)\|_{L^\infty(\Omega)} \le 1$ for almost every $t \in (0,T)$)

$$\begin{aligned}\frac{d}{dt}&\|e(t)\|^2_{L^2(\Omega)} + \varepsilon^2\|\nabla e(t)\|^2_{L^2(\Omega)}\\ &\le \varepsilon^{-2}\|\mathcal{R}_U(t)\|^2_* + 2(1 + \Lambda_{AC}^+(t))\|e(t)\|^2_{L^2(\Omega)} + 6\varepsilon^{-2}\|e(t)\|^3_{L^3(\Omega)}.\end{aligned}$$

A generalized Gronwall lemma that is based on a continuation argument implies the error estimate

$$\sup_{s\in[0,T]} \|e(s)\|^2 + \varepsilon^2 \int_0^T \|\nabla e(t)\|^2_{L^2(\Omega)}\,\mathrm{d}t \le C_1\eta^2 \exp\left(2\int_0^T (1 + \Lambda_{AC}^+(t))\,\mathrm{d}t\right)$$

provided that

$$\eta^2 := \|e(0)\|^2_{L^2(\Omega)} + \varepsilon^{-2}\int_0^T \|\mathcal{R}_U(t)\|^2_*\,\mathrm{d}t \le C_2\varepsilon^8 \exp\left(2\int_0^T (1 + \Lambda_{AC}^+(t))\,\mathrm{d}t\right)^{-3}$$

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with constants $C_1, C_2 > 0$ that do not depend on ε. The bounds on the residual and the error exhibit only polynomial dependence on ε^{-1}, provided that the integral of $\Lambda^+_{AC}(t)$ over $(0,T)$ grows at most logarithmically in ε^{-1} similar to (3), which can be monitored numerically. From an analytical point of view, our results prove stability with polynomial dependence on ε^{-1} for solutions of (1). We remark that a posteriori error estimates and related adaptive mesh refinement methods are of particular importance for the approximation of phase field models, owing to their strongly localized features.

The observation that the quantity λ_{AC} and the uniform bounds of [dMS95] are important for a robust error analysis for (1) has first been noticed in [EJ95]. It is also formulated in [EJ95] that a rigorous a posteriori analysis should extract the stability properties from the approximate solution. Therefore, we make the philosophy to replace *as much as possible "analytical knowledge" by "computational knowledge"* outlined in [EJ95] precise for the prototypical model problem (1).

We simultaneously derive error estimates for the numerical approximation of the Ginzburg–Landau equation, which is the complex valued version of (1), typically subject to Dirichlet boundary conditions on some part Γ_{D} of $\partial\Omega$. In this case the set $\Gamma_t := \{x \in \Omega : |u(t,x)| = 0\}$ is $(d-2)$-dimensional and points or lines in this set are called vortices. If $d = 2$, then it is known that degree-one vortices are stable, i.e., $\Lambda_{GL}(t) \sim 1$ [LL94, Mir95, Lin97], whereas higher-degree vortices are unstable, i.e., $\Lambda_{GL}(t) \sim \varepsilon^{-2}$ [Bea03], and split into several vortices of degree one. Another critical topological change occurs when two degree-one vortices of different sign annihilate. The results of this paper show that the annihilation of vortices can be reliably simulated while the splitting of higher degree vortices may be critical. This is in agreement with theoretical results that state that unstable higher degree vortices can exist for a positive, ε independent period [BOS07]. We stress, however, that our estimator is capable of detecting automatically such exceptional scenarios. For other aspects in the approximation of Ginzburg–Landau equations we refer the reader to the survey article [DGP92] and the monograph [HT01].

Closely related to the numerical analysis of (1) is the approximation of mean curvature flow, for which (1) is a regularization; cf. [Bra78, Ilm93, Küh98]. We refer the reader to [Wal96, NV97, DD00] and the recent survey article [DDE05] for algorithms and error estimates for various discretizations of the mean curvature flow as well as further references. Here, we consider only lowest order finite element methods for the approximation of the simple model problem (1) but notice that to the best of our knowledge the estimates we derive are the first ones that provide rigorous error control for the approximation of evolving interfaces that undergo topological changes. This underlines one advantage of diffuse interface models in comparison to sharp interface methods which typically require artificial adaptations at such events.

We remark that the approach presented in this paper also applies to more sophisticated models such as the Cahn–Hilliard or Cahn–Larché equations; cf. [GW05, BM10a, BM10b]. Employing the concept of elliptic reconstruction [MN03, LM06], the techniques developed in this paper also lead to optimal and robust error estimates in $L^\infty(0,T;L^2(\Omega))$ as well as to estimates for nonconforming and discontinuous Galerkin methods; details will appear elsewhere [BM11].

The outline of this paper is as follows. We introduce notation, generalized Gronwall lemmas, finite element spaces, and discrete time derivatives in section 2. Section 3 discusses the a posteriori error analysis of (1), while a priori error control is provided in section 4. Various numerical experiments illustrate the theoretical results and are

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reported in section 5.

2. Preliminaries. We specify in this section employed notation and data qualification, define weak solutions of (1), state two generalized Gronwall lemmas, and introduce lowest order finite element spaces as well as discrete time derivatives.

2.1. Notation. Let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, be a bounded, polygonal, or polyhedral Lipschitz domain. The outer unit normal on $\partial\Omega$ is denoted by n, and $\partial_n v$ is the normal derivative of a function v on $\partial\Omega$. Standard notation is used for Sobolev and Lebesgue spaces, and we write $\|\cdot\|$ whenever $\|\cdot\|_{L^2(\Omega)}$ is meant; $(\cdot,\cdot)$ denotes the inner product in $L^2(\Omega;\mathbb{R}^\ell)$, $\ell \in \mathbb{N}$. For a Banach space X its dual is denoted X^* and $\langle\cdot,\cdot\rangle$ is the corresponding duality pairing. We define $\sum_{j=1}^{0} a_j := 0$ for any given sequence (a_j). For a real number $r \geq 0$ we set $B_r := \{x \in \mathbb{R}^\ell : |x| < r\}$. The identity matrix in $\mathbb{R}^{\ell\times\ell}$ is denoted $I_{\ell\times\ell}$.

2.2. Data qualification and weak solution. Throughout this paper we assume that $\ell \in \{1, 2\}$, $0 < \varepsilon \leq 1$, and that f satisfies the following conditions.

Assumption (GA).

(i) There exists a nonnegative function $F \in C^2(\mathbb{R}^\ell)$ such that $f = DF$.

(ii) There exists $C_f \geq 0$ such that $Df(u) \geq -C_f I_{\ell\times\ell}$ in the sense of bilinear forms for all $u \in \mathbb{R}^\ell$.

(iii) There exist $\delta > 0$ with $\delta < 2$ if $d = 2$, and $\delta \leq 1$ if $d = 3$ and a nonnegative function $g \in C(\mathbb{R}^\ell)$ such that for all $a, b \in \mathbb{R}^\ell$ we have

$$\big(f(a) - f(b) - Df(b)(a-b)\big)\cdot(a-b) \geq -g(b)|a-b|^{2+\delta}.$$

The closed subset $\Gamma_{\mathrm{D}} \subseteq \partial\Omega$ is assumed to be either empty or of positive surface measure. We define

$$\mathbb{V} := H^1_{\mathrm{D}}(\Omega;\mathbb{R}^\ell) = \{v \in H^1(\Omega;\mathbb{R}^\ell) : v|_{\Gamma_{\mathrm{D}}} = 0\}$$

and denote by $\|\cdot\|_*$ the induced norm on $\mathbb{V}^*$. Assumption (GA) implies that there exists

$$u \in X_{AC/GL} := H^1(0,T;L^2(\Omega;\mathbb{R}^\ell)) \cap L^\infty(0,T;H^1(\Omega;\mathbb{R}^\ell))$$

satisfying

$$\langle\partial_t u(t), v\rangle + (\nabla u(t), \nabla v) = -\varepsilon^{-2}(f(u(t)), v) \tag{5}$$

for almost every $t \in (0,T)$ and every $v \in \mathbb{V}$ as well as

$$u(0) = u_0, \qquad u(t)|_{\Gamma_{\mathrm{D}}} = u_{\mathrm{D}}.$$

The function u is called a weak solution of the Allen–Cahn or Ginzburg–Landau equation for $\ell = 1, 2$, respectively. We suppress the explicit dependence of u upon ε but stress that all appearing constants do not depend on ε^{-1}. We remark that (5) is the L^2 gradient flow of the energy functional

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

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2.3. Generalized Gronwall lemmas. We include generalizations of the discrete and the continuous Gronwall lemma, which allow an additional superlinear term that can be controlled as long as the function or sequence remains sufficiently small. This is precisely what is required to make use of the error inequality stated in the introduction. The proof of the following lemma is adapted from [KNS04]; a similar result can be found in [FW05].

LEMMA 2.1. *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* $A \geq 0$ *satisfy*

$$y_1(t) + \int_0^t y_2(s)\,\mathrm{d}s \leq A + \int_0^t a(s)y_1(s)\,\mathrm{d}s + \int_0^t y_3(s)\,\mathrm{d}s$$

for all $t \in [0,T]$. *Assume that for* $B \geq 0$, $\beta > 0$, *and every* $t \in [0,T]$ *we have*

$$\int_0^t y_3(s)\,\mathrm{d}s \leq B \sup_{s\in[0,t]} y_1^\beta(s) \int_0^t (y_1(s) + y_2(s))\,\mathrm{d}s.$$

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

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

Proof. Set $\theta := 8AE$ if $A > 0$, and let $\theta > 0$ such that $4B(1+T)\theta^\beta E \leq 1$ otherwise. Define

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

Since $y_1(0) \leq A < \theta$ and since Υ is continuous, we have $I_\theta = [0,t_m]$ for some $0 < t_m \leq T$. For every $t \in [0,t_m]$ we have

$$\begin{aligned} y_1(t) + \int_0^t y_2(s)\,\mathrm{d}s &\leq A + \int_0^t a(s)y_1(s)\,\mathrm{d}s + B \sup_{s\in[0,t]} y_1^\beta(s) \int_0^t (y_1(s) + y_2(s))\,\mathrm{d}s \\ &\leq A + \int_0^t a(s)y_1(s)\,\mathrm{d}s + B(1+T)\theta^{1+\beta}. \end{aligned}$$

An application of Gronwall's lemma (cf., e.g., [IT79]), the condition on A, and the choice of θ yield that for all $t \in [0,t_m]$ we have

$$y_1(t) + \int_0^t y_2(s)\,\mathrm{d}s \leq (A + B(1+T)\theta^{1+\beta})E \leq \frac{\theta}{4}.$$

This implies $\Upsilon(t_m) < \theta$, hence $t_m = T$, and thus proves the lemma if $A > 0$. If $A = 0$, we may choose θ arbitrarily small to deduce the assertion. ∎

Remark 2.2. (i) Nonnegativity of a is needed to control $a(s)y_1(s)$ by the term $a(s)\big(y_1(s) + \int_0^s y_2(r)\,\mathrm{d}r\big)$ in the application of the classical Gronwall lemma.

(ii) The factor 8 in the lemma can be replaced by any real number bigger than 4 or by 4 if $a \not\equiv 0$.

A discrete version of this lemma reads as follows; the proof is adapted from [FP03].

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LEMMA 2.3. *Let $\tau > 0$ and suppose that the nonnegative real sequences $(y_k^j)_{j=0}^M$, $k = 1, 2, 3$, $(a^j)_{j=0}^M$, and the real number $A \geq 0$ satisfy*

$$y_1^m + \tau \sum_{j=1}^m y_2^j \leq A + \tau \sum_{j=1}^m a^j y_1^j + \tau \sum_{j=1}^{m-1} y_3^j$$

for all $m = 1, 2, \ldots, M$, that $\sup_{j=1,2,\ldots,M} \tau a^j \leq 1/2$, and $M\tau = T$. Assume that for $B \geq 0$, $\beta > 0$, and every $m = 1, 2, \ldots, M$ we have

$$\tau \sum_{j=1}^{m-1} y_3^m \leq B \sup_{j=1,2,\ldots,m-1} (y_1^j)^\beta \tau \sum_{j=1}^{m-1} (y_1^j + y_2^j).$$

Set $E := \exp\left(2\tau \sum_{j=1}^M a^j\right)$ and assume that $8AE \leq (8B(1+T)E)^{-1/\beta}$. Then

$$\sup_{j=1,2,\ldots,M} y_1^j + \tau \sum_{j=1}^M y_2^j \leq 8A \exp\left(2\tau \sum_{j=1}^M a^j\right).$$

Proof. Set $\theta := 8AE$. We proceed by induction and suppose that for some $L \geq 1$ we have

$$\sup_{j=1,2,\ldots,L-1} y_1^j + \tau \sum_{j=1}^{L-1} y_2^j \leq \theta,$$

which is satisfied for $L = 1$. For all $m = 1, 2, \ldots, L$ we then have

$$\begin{aligned} y_1^m + \tau \sum_{j=1}^m y_2^j &\leq A + \tau \sum_{j=1}^m a^j y_1^j + B \sup_{j=1,2,\ldots,m-1} (y_1^j)^\beta \tau \sum_{j=1}^{m-1} (y_1^j + y_2^j) \\ &\leq A + \tau \sum_{j=0}^m a^j y_1^j + B(1+T)\theta^{1+\beta}. \end{aligned}$$

The implicit version of the discrete Gronwall lemma (cf., e.g., [QV94]), the condition on A, and the definition of θ prove that for all $m = 1, 2, \ldots, L$ we have

$$y_1^m + \tau \sum_{j=1}^m y_2^j \leq 2(A + B(1+T)\theta^{1+\beta})E \leq \frac{\theta}{2}.$$

This completes the inductive argument and proves the lemma. ∎

Remark 2.4. The factor 2 on the right-hand side of the estimate of Lemma 2.3 can be replaced by a factor $1 + o(1)$ provided that $\sup_{j=1,2,\ldots,M} \tau a^j = o(1)$ as $\tau \to 0$. Analogously, the factor 8 may be replaced by $4(1 + o(1))$.

2.4. Finite element spaces. Let $\mathcal{T}$ be a regular triangulation of Ω into triangles or tetrahedra. The lowest order finite element space $\mathcal{S}^1(\mathcal{T})$ consists of all $\mathcal{T}$-elementwise affine, globally continuous functions, and we set

$$\mathbb{V}_h := \mathcal{S}^1(\mathcal{T})^\ell \cap H^1_{\mathrm{D}}(\Omega; \mathbb{R}^\ell).$$

We let $\mathcal{J} : \mathbb{V} \to \mathbb{V}_h$ denote the quasi-interpolation operator of [Clé75] which satisfies for all $v \in \mathbb{V}$

$$\|h_{\mathcal{T}}^{-1}(v - \mathcal{J}v)\| + \|\nabla(v - \mathcal{J}v)\| + \|h_{\mathcal{F}}^{-1/2}(v - \mathcal{J}v)\|_{L^2(\cup\mathcal{F})} \leq C_{C\ell}\|\nabla v\|. \tag{6}$$

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Here, $h_{\mathcal{T}}$ denotes the elementwise constant meshsize, i.e., $h_{\mathcal{T}}|_K = \operatorname{diam}(K)$ for all $K \in \mathcal{T}$, $\mathcal{F}$ is the set of faces (edges if $d = 2$) in $\mathcal{T}$, and $h_{\mathcal{F}}$ is defined through $h_{\mathcal{F}}|_F = \operatorname{diam}(F)$ for all $F \in \mathcal{F}$. For all $F \in \mathcal{F}$ we let n_F denote a unit normal to F and set for $v_h \in \mathbb{V}_h$

$$[\nabla v_h \cdot n_{\mathcal{F}}] := \begin{cases} |(\nabla v_h|_{K_1} - \nabla v_h|_{K_2}) \cdot n_F| & \text{for } F = K_1 \cap K_2 \text{ and } K_1, K_2 \in \mathcal{T}, \\ |(\nabla v_h|_K) \cdot n_F| & \text{for } F = K \cap \overline{\partial\Omega \setminus \Gamma_{\mathrm{D}}} \text{ and } K \in \mathcal{T}, \\ 0 & \text{for } F \subseteq \Gamma_D. \end{cases}$$

The elementwise application of the Laplace operator to an elementwise smooth function ψ is defined through $(\Delta_{\mathcal{T}}\psi)|_K := \Delta\psi|_K$ for all $K \in \mathcal{T}$. We let $\mathcal{P} : \mathbb{V} \to \mathbb{V}_h$ denote the elliptic projection defined for $v \in \mathbb{V}$ through

$$(\mathcal{P}v, V) + (\nabla\mathcal{P}v, \nabla V) = (v, V) + (\nabla v, \nabla V)$$

for all $V \in \mathbb{V}_h$. For quasi-uniform meshes with $0 < h := \|h_{\mathcal{T}}\|_{L^\infty(\Omega)} \le 1/2$, if the Laplace operator is H^2 regular in Ω in the sense that there exists $C_\Delta > 0$ such that $\|D^2 v\| \le C_\Delta \|\Delta v\|$ for all $v \in \mathbb{V} \cap H^2(\Omega; \mathbb{R}^\ell)$, then we have (cf. [Cia02, Whe73])

$$\|\mathcal{P}v - v\| + h\|\nabla(\mathcal{P}v - v)\| + h^{d/2}|\log h|^{(d-3)/2}\|\mathcal{P}v - v\|_{L^\infty(\Omega)} \le C_{\mathcal{P}} h^2 \|v\|_{H^2(\Omega)} \tag{7}$$

for all $v \in \mathbb{V} \cap H^2(\Omega; \mathbb{R}^\ell)$.

2.5. Discrete time derivatives. Given a sequence of positive time steps $(\tau_j)_{j=1}^M$ and a sequence $(a^j)_{j=0}^M$, we set for $j = 1, 2, \ldots, M$

$$d_t a^j := \frac{1}{\tau_j}(a^j - a^{j-1}).$$

Notice that $2(d_t a^j)a^j = d_t|a^j|^2 + \tau_j|d_t a^j|^2$ for $j = 1, 2, \ldots, M$. Let $t_m := \sum_{j=1}^m \tau_j$, $m = 0, 1, \ldots, M$, and $T = t_M$. Given a function $w : (0, T) \to L^2(\Omega; \mathbb{R}^\ell)$ with $w \in H^2(0, T; \mathbb{V}^*)$ set $R^j := \partial_t w(t_j) - d_t w(t_j)$ for $j = 1, 2, \ldots, M$. We then have (cf. [Tho97])

$$\sum_{j=1}^M \tau_j \|R^j\|_*^2 \le \frac{\tau^2}{3} \int_0^T \|w_{tt}(s)\|_*^2 \,\mathrm{d}s, \tag{8}$$

where $\tau := \max_{j=1,2,\ldots,M} \tau_j$ and $T := t_M$. Moreover, we have

$$\sum_{j=1}^M \tau_j \|d_t w(t_j)\|_*^2 \le \int_0^T \|\partial_t w(s)\|_*^2 \,\mathrm{d}s. \tag{9}$$

3. Robust a posteriori error analysis. In this section we derive robust a posteriori error estimates for Allen–Cahn ($\ell = 1$) and Ginzburg–Landau ($\ell = 2$) equations following [KNS04, Bar05a]. Given an approximation $\widetilde{U} \in X_{AC/GL}$ with $\widetilde{U}(t)|_{\Gamma_{\mathrm{D}}} = U_{\mathrm{D}}$ for almost every $t \in (0, T)$, we let $e_{\mathrm{D}} \in H^1(\Omega; \mathbb{R}^\ell)$ denote an extension of $u_{\mathrm{D}} - U_{\mathrm{D}}$ if $\Gamma_{\mathrm{D}} \neq \emptyset$ and $e_{\mathrm{D}} \equiv 0$ otherwise, and we set

$$U(t) := \widetilde{U}(t) + e_{\mathrm{D}}.$$

We define the functional $\mathcal{R}_U(t) \in \mathbb{V}^*$ for almost every $t \in (0, T)$ and every $v \in \mathbb{V}$ through

$$\langle \mathcal{R}_U(t), v\rangle := -\varepsilon^{-2}(f(U(t)), v) - \langle \partial_t U(t), v\rangle - (\nabla U(t), \nabla v). \tag{10}$$

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Practical upper bounds for the residual $\mathcal{R}_U(t)$ need to be established for each desired numerical scheme. In section 3.1 we provide such upper bounds for an implicit Euler discretization in time.

A further ingredient in the statement of the a posteriori error estimate is a lower bound $-\bar{\Lambda}(t) \le -\Lambda(t)$ on the principal eigenvalue. In practice, $-\Lambda(t)$ is available up to only approximation errors and at a finite number of time steps, hence we will compute the principal eigenvalue $-\Lambda_h(t)$ in $\mathbb{V}_h$ and, through a posteriori or a priori error estimates, obtain a rigorous lower bound $-\overline{\Lambda}(t)$ (see section 3.2).

THEOREM 3.1. *Let δ, g, and C_f be as in* (GA). *Suppose that $\eta_0, \eta_1 \in L^2(0,T)$ are such that for almost every $t \in (0,T)$ we have*

$$\langle \mathcal{R}_U(t), v\rangle \le \eta_0(t)\|v\| + \eta_1(t)\|\nabla v\|$$

for all $v \in \mathbb{V}$, assume that $\overline{\Lambda} \in L^1(0,T)$ is a function such that for almost every $t \in (0,T)$ we have

$$-\overline{\Lambda}(t) \le -\Lambda(t) := \inf_{v\in\mathbb{V}\setminus\{0\}} \frac{\|\nabla v\|^2 + \varepsilon^{-2}(Df(U(t))v, v)}{\|v\|^2},$$

and set $\mu_\Lambda(t) := 2(1 + C_f + (1-\varepsilon^2)\overline{\Lambda}(t))^+$. Define $\mu_g := \sup_{s\in(0,T)} \|g(U(s))\|_{L^\infty(\Omega)}$. If

$$\begin{aligned}\eta^2 &:= \|e(0)\|^2 + \int_0^T (\eta_0^2(s) + \varepsilon^{-2}\eta_1^2(s))\,\mathrm{d}s \\ &\le \frac{\varepsilon^{8/\delta}}{(2\mu_g C_S(1+T))^{2/\delta}}\left(8\exp\left(\int_0^T \mu_\Lambda(s)\,\mathrm{d}s\right)\right)^{-1-2/\delta}\end{aligned}$$

then

$$\sup_{s\in[0,T]} \|e(s)\|^2 + \varepsilon^2\int_0^T \|\nabla e(s)\|^2\,\mathrm{d}s \le 8\eta^2\exp\left(\int_0^T \mu_\Lambda(s)\,\mathrm{d}s\right).$$

Proof. Subtracting (10) from (5), choosing $v = e$, and using (iii) of (GA), we find

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|e(t)\|^2 + \|\nabla e(t)\|^2 &= \langle \mathcal{R}_U(t), e(t)\rangle - \varepsilon^{-2}(f(u(t)) - f(U(t)), e(t)) \\ &\le \eta_0(t)\|e(t)\| + \eta_1(t)\|\nabla e(t)\| \\ &\quad - \varepsilon^{-2}(Df(U(t))e(t), e(t)) + \varepsilon^{-2}\|g(U(t))\|_{L^\infty(\Omega)}\|e(t)\|^{2+\delta}_{L^{2+\delta}(\Omega)} \\ &\le \frac{1}{4}\eta_0^2(t) + \|e(t)\|^2 + \frac{\varepsilon^{-2}}{2}\eta_1^2(t) + \frac{\varepsilon^2}{2}\|\nabla e(t)\|^2 - (1-\varepsilon^2)\varepsilon^{-2}(Df(U(t))e(t), e(t)) \\ &\quad - (Df(U(t))e(t), e(t)) + \varepsilon^{-2}\mu_g\|e(t)\|^{2+\delta}_{L^{2+\delta}(\Omega)}.\end{aligned}$$

Incorporating the assumed bound for $\overline{\Lambda}(t)$ and (ii) of (GA), we have

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|e(t)\|^2 + \|\nabla e(t)\|^2 &\le \frac{1}{4}\eta_0^2(t) + \|e(t)\|^2 \\ &\quad + \frac{\varepsilon^{-2}}{2}\eta_1^2(t) + \frac{\varepsilon^2}{2}\|\nabla e(t)\|^2 + (1-\varepsilon^2)\overline{\Lambda}(t)\|e(t)\|^2 \\ &\quad + (1-\varepsilon^2)\|\nabla e(t)\|^2 + C_f\|e(t)\|^2 + \varepsilon^{-2}\mu_g\|e(t)\|^{2+\delta}_{L^{2+\delta}(\Omega)} \\ &\le \frac{1}{4}\eta_0^2(t) + \frac{1}{2}\varepsilon^{-2}\eta_1^2(t) + (1 + C_f + (1-\varepsilon^2)\overline{\Lambda}(t))\|e(t)\|^2 \\ &\quad + \left(1 - \frac{\varepsilon^2}{2}\right)\|\nabla e(t)\|^2 + \varepsilon^{-2}\mu_g\|e(t)\|^{2+\delta}_{L^{2+\delta}(\Omega)},\end{aligned}$$

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which leads to

$$\frac{d}{dt}\|e(t)\|^2 + \varepsilon^2\|\nabla e(t)\|^2 \le \eta_0^2(t) + \varepsilon^{-2}\eta_1^2(t) + \mu_\Lambda(t)\|e(t)\|^2 + 2\varepsilon^{-2}\mu_g\|e(t)\|^{2+\delta}_{L^{2+\delta}(\Omega)}.$$

Note that we have defined μ_Λ to be nonnegative, since the coefficient function a in Lemma 2.1 is assumed to be nonnegative.

Hölder's inequality with exponents $2/\delta$ and $2/(2-\delta)$ and Sobolev embedding theorems together with the assumption on δ stated in (iii) of (GA) yield that

$$\|e(t)\|^{2+\delta}_{L^{2+\delta}(\Omega)} \le \|e(t)\|^\delta \|e(t)\|^2_{L^{4/(2-\delta)}(\Omega)} \le C_S\|e(t)\|^\delta(\|e(t)\|^2 + \|\nabla e(t)\|^2). \tag{11}$$

An integration of the last two estimates over $(0,t)$ shows that we are in the situation of Lemma 2.1 with $A = \eta^2$, $B = 2\mu_g\varepsilon^{-4}C_S$, $\beta = \delta/2$, and $E = \exp\big(\int_0^T \mu_\Lambda(s)\,\mathrm{d}s\big)$. This implies the assertion. ∎

Remark 3.2. Using the multiplicative Sobolev inequality $\|e\|^{2+\delta}_{L^{2+\delta}(\Omega)} \le C_{mS}\|\nabla e\|^\delta \|e\|^2$ (cf. [LU68]) one can improve the conditions of the theorem if $d = 2$.

3.1. Residual estimate. We include a brief discussion about estimates for $\mathcal{R}_U$ for a fully implicit, lowest order finite element discretization of (5). For ease of presentation we assume an exact solution of the discrete nonlinear systems of equations; related estimates for semi-implicit discretizations can be found in [KNS04, Bar05a].

PROPOSITION 3.3. *Let $0 = t_0 < t_1 < \cdots < t_M = T$ be a partition of the interval $(0,T)$ with time steps $\tau_j := t_j - t_{j-1}$, $j = 1,2,\dots,M$, and $(\mathcal{T}_j)_{j=0}^M$ a sequence of regular triangulations of Ω. Suppose that $(U^j)_{j=0}^M \subset H^1(\Omega;\mathbb{R}^\ell)$ is such that $U^j \in \mathcal{S}^1(\mathcal{T}_j)^\ell$ and $U^j|_{\Gamma_\mathrm{D}} = U_\mathrm{D}$ for $j = 0,1,\dots,M$, and*

$$\tau_j^{-1}(U^j - \mathcal{I}_{\mathcal{T}_j}U^{j-1}, V) + (\nabla U^j, \nabla V) = -\varepsilon^{-2}(f(U^j), V)$$

for all $V \in \mathbb{V}_h^j := \mathcal{S}^1_\mathrm{D}(\mathcal{T}_j)^\ell$, $j = 1,2,\dots,M$, and where $\mathcal{I}_{\mathcal{T}_j}$ denotes the nodal interpolation operator related to $\mathbb{V}_h^j$. If $U \in X_{AC/GL}$ is obtained by piecewise linear interpolation in time of $(U^j + e_\mathrm{D})_{j=0}^M$, then for all $v \in \mathbb{V}$ we have

$$\langle \mathcal{R}_U(s), v\rangle \le (\eta^j_{t,0} + \eta^j_{c,0})\|v\| + (C_{C\ell}\eta^j_{h,1} + \eta^j_{t,1})\|\nabla v\|,$$

where for $j = 1,2,\dots,M$ and $d_j := \|U^j\|_{L^\infty(\Omega)} + \|U^{j-1}\|_{L^\infty(\Omega)} + \|e_\mathrm{D}\|_{L^\infty(\Omega)}$ we set

$$\begin{aligned}
\eta^j_{h,1} &:= \big\|h_{\mathcal{T}_j}\big(\tau_j^{-1}(U^j - \mathcal{I}_{\mathcal{T}_j}U^{j-1}) - \Delta_{\mathcal{T}_j}U^j + \varepsilon^{-2}f(U^j)\big)\big\| + \|h^{1/2}_{\mathcal{F}_j}[\nabla U^j \cdot n_{\mathcal{F}_j}]\|_{L^2(\cup\mathcal{F}_j)},\\
\eta^j_{t,0} &:= \varepsilon^{-2}\|Df\|_{L^\infty(B_{d_j})}(\|U^{j-1} - U^j\| + \|e_\mathrm{D}\|),\\
\eta^j_{t,1} &:= \|\nabla(U^{j-1} - U^j)\| + \|\nabla e_\mathrm{D}\|,\\
\eta^j_{c,0} &:= \tau_j^{-1}\|\mathcal{I}_{\mathcal{T}_j}U^{j-1} - U^{j-1}\|.
\end{aligned}$$

Proof. For almost every $s \in (t_{j-1}, t_j)$, $j = 1,2,\dots,M$, and all $v \in \mathbb{V}$, we have by definition of $\mathcal{R}_U$ that

$$\begin{aligned}
\langle \mathcal{R}_U(s), v\rangle &= \tau_j^{-1}(U^j - U^{j-1}, v) + (\nabla U(s), \nabla v) + \varepsilon^{-2}(f(U(s)), v)\\
&= \big[\tau_j^{-1}(U^j - \mathcal{I}_{\mathcal{T}_j}U^{j-1}, v) + (\nabla U^j, \nabla v) + \varepsilon^{-2}(f(U^j), v)\big]\\
&\quad + \big[(\nabla(U(s) - U^j), \nabla v) + \varepsilon^{-2}(f(U(s)) - f(U^j), v)\big]\\
&\quad + \tau_j^{-1}(\mathcal{I}_{\mathcal{T}_j}U^{j-1} - U^{j-1}, v)\\
&=: \langle r_h^j, v\rangle + \langle r_t(s), v\rangle + \langle r_c^j, v\rangle.
\end{aligned}$$

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Since r_h^j vanishes on $\mathbb{V}_h^j$, we may insert $\mathcal{J}v \in \mathbb{V}_h^j$ in $\langle r_h, v\rangle$. An elementwise integration by parts and (6) lead to

$$\langle r_h^j, v\rangle = \langle r_h^j, v - \mathcal{J}v\rangle \le C_{C\ell}\eta_{h,1}^j \|\nabla v\|.$$

Hölder inequalities, the identity

$$f(U(s)) - f(U^j) = \left(\int_0^1 Df(rU(s) + (1-r)U^j)\,\mathrm{d}r\right)(U(s) - U^j),$$

and linearity of U in s lead to

$$\begin{aligned}\langle r_t(s), v\rangle &\le \|\nabla(U(s) - U^j)\|\|\nabla v\| + \varepsilon^{-2}\|Df\|_{L^\infty(B_{d_j})}\|U(s) - U^j\|\|v\| \\ &\le \eta_{t,0}^j\|v\| + \eta_{t,1}\|\nabla v\|.\end{aligned}$$

An application of Hölder's inequality proves

$$\langle r_c^j, v\rangle \le \tau_j^{-1}\|\mathcal{I}_{\mathcal{T}_j}U^{j-1} - U^{j-1}\|\|v\| = \eta_{c,0}\|v\|.$$

A combination of the estimates proves the lemma. ∎

Remark 3.4. (i) The error indicators η_h, η_t, and η_c control residuals related to spatial discretization, temporal discretization, and coarsening of triangulations.

(ii) If U_D is obtained by nodal interpolation of u_D, an extension $e_\mathrm{D} \in H^1(\Omega;\mathbb{R}^\ell)$ with

$$\|e_\mathrm{D}\|_{L^\infty(\Omega)} \le C\|h_\mathcal{F}^2\partial_\mathcal{F}^2 u_\mathrm{D}\|_{L^\infty(\Gamma_\mathrm{D})}, \quad \|\nabla e_\mathrm{D}\| \le C\|h_\mathcal{F}^{3/2}\partial_\mathcal{F}^2 u_\mathrm{D}\|_{L^2(\Gamma_\mathrm{D})},$$

where $\partial_\mathcal{F}$ denotes the piecewise tangential derivative along Γ_D, has been constructed in [BCD04].

3.2. Eigenvalue approximation. We next investigate the lowest order finite element approximation of the eigenvalue problems refining the results of [Bar05a]. As above we assume an exact solution of nonlinear systems of equations and omit the argument t in the following. We notice that there exist nontrivial functions $w \in \mathbb{V}$ such that for all $v \in \mathbb{V}$ we have

$$(\nabla w, \nabla v) + \varepsilon^{-2}\big(Df(U)w, v\big) = -\Lambda(w, v), \tag{12}$$

and let $P_\Lambda : \mathbb{V} \to \mathbb{V}$ denote the L^2 projection onto the subspace of all $w \in \mathbb{V}$ that satisfy (12). We assume that we are given $(W, \Lambda_h) \in \mathbb{V}_h \times \mathbb{R}$ with $\|W\| = 1$ and such that

$$(\nabla W, \nabla V) + \varepsilon^{-2}(Df(U)W, V) = -\Lambda_h(W, V) \tag{13}$$

for all $V \in \mathbb{V}_h$.

PROPOSITION 3.5 (see [Lar00]). *Let* $(W, \Lambda_h) \in \mathbb{V}_h \times \mathbb{R}$ *satisfy* $\|W\| = 1$ *and* (13) *and assume that*

$$\|W - P_\Lambda W\|^2 \le 1/2. \tag{14}$$

For $k = 1, 2$ *set*

$$\eta_{\Lambda,k} := \|h_\mathcal{T}^k\big(\Delta_\mathcal{T} W - \varepsilon^{-2}Df(U)W - \Lambda W\big)\| + \|h_\mathcal{F}^{k-1/2}[\nabla W \cdot n_\mathcal{F}]\|_{L^2(\cup\mathcal{F})}.$$

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Then

$$-\Lambda_h + \Lambda \le 2C_{C\ell}\eta_{\Lambda,1}(\varepsilon^{-2}\|Df(U)\|_{L^\infty(\Omega)} + (-\Lambda_h)^+)^{1/2}.$$

Proof. We abbreviate $p_\varepsilon := \varepsilon^{-2}Df(U)$ and $w := P_\Lambda W$ and define $\mathcal{R}_{W,\Lambda_h} \in \mathbb{V}^*$ through

$$\langle \mathcal{R}_{W,\Lambda_h}, v\rangle := -\Lambda_h(W,v) - (\nabla W, \nabla v) - \big(p_\varepsilon W, v\big)$$

for all $v \in \mathbb{V}$. Upon choosing $v = W$ in (12) and $v = w$ in the definition of $\mathcal{R}_{W,\Lambda_h}$, we deduce

$$\begin{aligned}(w,W)(\Lambda - \Lambda_h) &= -(\nabla w, \nabla W) - (p_\varepsilon w, W) + (\nabla W, \nabla w) + (p_\varepsilon W, w) + \langle \mathcal{R}_{W,\Lambda_h}, w\rangle \\ &= \langle \mathcal{R}_{W,\Lambda_h}, w\rangle.\end{aligned}$$

Since $\langle \mathcal{R}_{W,\Lambda_h}, V\rangle = 0$ for all $V \in \mathbb{V}_h$, we have

$$\langle \mathcal{R}_{W,\Lambda_h}, w\rangle = \langle \mathcal{R}_{W,\Lambda_h}, w - V\rangle = -\Lambda_h(W, w-V) - (\nabla W, \nabla(w-V)) - (p_\varepsilon W, w - V).$$

A $\mathcal{T}$-elementwise integration by parts, the choice $V = \mathcal{J}w$, and (6) imply

$$\langle \mathcal{R}_{W,\Lambda_h}, w\rangle \le C_{C\ell}\big(\|h_\mathcal{T}(\Delta_\mathcal{T} W - p_\varepsilon W + \Lambda_h W)\| + \|h_\mathcal{F}^{1/2}[\nabla W \cdot n_{\mathcal{E}_h}]\|_{L^2(\cup\mathcal{F})}\big)\|\nabla w\|.$$

Notice that $W \in \mathbb{V}$ so that $-\Lambda \le -\Lambda_h$; since $\|w\| \le \|W\| = 1$, we thus have

$$\|\nabla w\|^2 = -\Lambda(w,w) - (p_\varepsilon w, w) \le (-\Lambda_h)^+ + \|p_\varepsilon\|_{L^\infty(\Omega)}. \tag{15}$$

In view of (14), $\|W\|^2 = 1$, and $(w - W, w) = 0$, we have $(w, W) \ge 1/2$. A combination of the estimates concludes the proof of the lemma. ∎

Remark 3.6. If the Laplace operator is H^2 regular in Ω and (14) holds, then we have

$$-\Lambda_h + \Lambda \le 2C_\mathcal{P} C_\Delta \eta_{\Lambda,2}(\varepsilon^{-2}\|Df(U)\|_{L^\infty(\Omega)} + (-\Lambda_h)^+).$$

The *saturation assumption* (14) is difficult to verify in practice; therefore we include an a priori estimate assuming H^2 regularity of the Laplace operator.

PROPOSITION 3.7. *Suppose that the Laplace operator is H^2 regular in Ω, and let $(W, \Lambda_h) \in \mathbb{V}_h \times \mathbb{R}$ satisfy* (13) *and assume that h is such that*

$$C_\mathcal{P} C_\Delta (C_\mathbb{V} + 2\varepsilon^{-2}\|Df(U)\|_{L^\infty(\Omega)})h^2 \le 1/2,$$

where $C_\mathbb{V} := \inf_{v\in\mathbb{V}:\,\|v\|=1}\|\nabla v\|^2$. Then we have

$$0 \le \Lambda - \Lambda_h \le 4\big(1 + C_\mathbb{V} + (3 + \ell^{1/2})\varepsilon^{-2}\|Df(U)\|_{L^\infty(\Omega)}\big)^2 C_\mathcal{P} C_\Delta h^2.$$

Proof. Let $w \in \mathbb{V}$ satisfy (12) with $\|w\| = 1$. Set $p_\varepsilon := \varepsilon^{-2}Df(U)$ and $q_\varepsilon := p_\varepsilon + \|p_\varepsilon\|_{L^\infty(\Omega)} I_{\ell\times\ell}$. Since W is minimal for

$$V \mapsto (\nabla V, \nabla V) + (p_\varepsilon V, V)$$

among all $V \in \mathbb{V}_h$ with $\|V\| = 1$ we have for all such V that

$$\begin{aligned}0 \le \Lambda - \Lambda_h &\le -\|\nabla w\|^2 - \|q_\varepsilon^{1/2} w\|^2 + \|\nabla V\|^2 + \|q_\varepsilon^{1/2} V\|^2 \\ &\le 2(\nabla V, \nabla(V - w)) + 2(q_\varepsilon V, V - w).\end{aligned} \tag{16}$$

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The bound $-\Lambda \le C_{\mathbb{V}} + \|p_\varepsilon\|_{L^\infty(\Omega)}$ and $-\Delta w + p_\varepsilon w = -\Lambda w$ lead to

$$\|D^2 w\| \le C_\Delta \|\Delta w\| \le C_\Delta (C_{\mathbb{V}} + 2\|p_\varepsilon\|_{L^\infty(\Omega)}) =: C_\Delta \alpha_\varepsilon$$

and $\|\nabla w\| \le \alpha_\varepsilon^{1/2}$. The assumption $C_{\mathcal{P}} C_\Delta \alpha_\varepsilon h^2 \le 1/2$ implies $\big|1 - \|\mathcal{P}w\|\big| \le 1/2$, and we may therefore employ $V = \mathcal{P}w/\|\mathcal{P}w\|$ in (16). Since $\|\nabla \mathcal{P}w\|^2 \le \|\nabla w\|^2 + 1$, we have

$$\begin{aligned}(\nabla V, \nabla(V - w)) &= \frac{1}{\|\mathcal{P}w\|^2}\big((\nabla \mathcal{P}w, \nabla(\mathcal{P}w - w)) + (\nabla \mathcal{P}w, \nabla w)(1 - \|\mathcal{P}w\|)\big)\\ &= \frac{1}{\|\mathcal{P}w\|^2}\big((\mathcal{P}w, \mathcal{P}w - w) + (\nabla \mathcal{P}w, \nabla w)(1 - \|\mathcal{P}w\|)\big)\\ &\le 4(1 + \alpha_\varepsilon) C_{\mathcal{P}} C_\Delta \alpha_\varepsilon h^2.\end{aligned}$$

We notice that

$$\begin{aligned}(q_\varepsilon V, V - w) &= \frac{1}{\|\mathcal{P}w\|^2}\big((q_\varepsilon \mathcal{P}w, \mathcal{P}w - w) + (q_\varepsilon \mathcal{P}w, w)(1 - \|\mathcal{P}w\|)\big)\\ &\le 4\|q_\varepsilon\|_{L^\infty(\Omega)} C_{\mathcal{P}} C_\Delta \alpha_\varepsilon h^2,\end{aligned}$$

combine all estimates, and use $\|q_\varepsilon\|_{L^\infty(\Omega)} \le (1 + \ell^{1/2})\|p_\varepsilon\|_{L^\infty(\Omega)}$ to verify the assertion. ∎

If $f \in C^{1,\alpha}_{loc}(\mathbb{R}^\ell)$, $0 < \alpha \le 1$, it is sufficient to approximate the eigenvalues at a finite number of time steps in order to construct a function $\overline{\Lambda}$ that satisfies the conditions of Theorem 3.1.

PROPOSITION 3.8. *Suppose that $f \in C^{1,\alpha}_{loc}(\mathbb{R}^\ell)$ for some $0 < \alpha \le 1$, let $t_{j-1} < t < t_j$ be such that $t = t_{j-1} + \varrho(t_j - t_{j-1})$ for some $\varrho \in (0,1)$, and assume that $U(t) = (1-\varrho)U^{j-1} + \varrho U^j$. We then have*

$$-(1-\varrho)\Lambda(t_{j-1}) - \varrho\Lambda(t_j) - \|Df\|_{C^{0,\alpha}(B_{d_j})}\varepsilon^{-2}\|U^{j-1} - U^j\|^\alpha_{L^\infty(\Omega)} \le -\Lambda(t),$$

where $d_j := \|U^{j-1}\|_{L^\infty(\Omega)} + \|U^j\|_{L^\infty(\Omega)}$.

Proof. For all $v \in \mathbb{V}$ with $\|v\| = 1$ we have

$$\begin{aligned}&(1-\varrho)\big((\nabla v, \nabla v) + \varepsilon^{-2}(Df(U^{j-1})v, v)\big) + \varrho\big((\nabla v, \nabla v) + \varepsilon^{-2}(Df(U^j)v, v)\big)\\ &\quad\le (\nabla v, \nabla v) + \varepsilon^{-2}(Df(U(t))v, v) + \varepsilon^{-2}\|(1-\varrho)Df(U^{j-1})\\ &\qquad + \varrho Df(U^j) - Df(U(t))\|_{L^\infty(\Omega)}.\end{aligned}$$

With this estimate the result follows from the definition of $\Lambda(t)$. ∎

4. Robust a priori error analysis. We next provide an a priori error analysis for a fully implicit discretization of (5) modifying slightly the arguments of [FP03]. For ease of presentation we suppose that $\mathcal{T}^j = \mathcal{T}$ for a fixed quasi-uniform triangulation and $\tau_j = \tau$ for a fixed positive number and for $j = 0, 1, \ldots, M$. Moreover, we assume that $u_0 \in H^1(\Omega; \mathbb{R}^\ell)$. Then, let $(U^j)_{j=0}^M \subset \mathcal{S}^1(\mathcal{T})^\ell$ be such that $U^0 = \mathcal{P}u_0$, $U^j|_{\Gamma_{\mathrm{D}}} = U_{\mathrm{D}}$ for all $j = 0, 1, \ldots, M$ and

$$(d_t U^j, V) + (\nabla U^j, \nabla V) = -\varepsilon^{-2}(f(U^j), V) \tag{17}$$

for all $V \in \mathbb{V}_h$ and $j = 1, 2, \ldots, M$. For $j = 0, 1, \ldots, M$ we define

$$E^j := u(t_j) - U^j.$$

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To bound $(E^j)_{j=0}^M$ we make the following regularity assumption and refer the reader to [FP03] for a detailed discussion of these estimates. The validity of a maximum principle is not essential for the error analysis and can be replaced by an upper bound that depends polynomially on ε^{-1}.

Assumption (RA). The Laplace operator is H^2 regular in Ω, we have $f \in C^2(\mathbb{R}^\ell)$, and there are constants $C_\infty, C_u > 0$ and a parameter $\sigma \geq 0$ such that for the solution $u \in X_{AC/GL}$ of (5) we have

$$\sup_{t\in[0,T]} \|u(t)\|_{L^\infty(\Omega)} \leq C_\infty$$

and

$$\sup_{t\in[0,T]} \|u(t)\|_{H^2(\Omega)} + \left(\int_0^T \|u_{tt}\|_*^2 \,\mathrm{d}t\right)^{1/2} + \left(\int_0^T \|u_t\|_{H^2(\Omega)}^2 \,\mathrm{d}t\right)^{1/2} \leq C_u \varepsilon^{-\sigma}.$$

Remark 4.1. For initial data with uniformly bounded energy we may choose $\sigma = 2$; cf. [FP03].

LEMMA 4.2. *Suppose that* (RA) *is satisfied and that*

$$C_{\mathcal{P}} h^{(4-d)/2} |\log h|^{(3-d)/2} C_u \varepsilon^{-\sigma} \leq \min\{C_\infty, \varepsilon^2 C_{f''}^{-1}\}, \qquad C_{f''} C_{S2} C_u \tau \leq \varepsilon^{2+\sigma}, \tag{18}$$

where $C_{f''} := \|D^2 f\|_{L^\infty(B_{3C_\infty})}$ *and* $C_{S2} > 0$ *is such that* $\|v\|_{L^\infty(\Omega)} \leq C_{S2}\|v\|_{H^2(\Omega)}$ *for all* $v \in H^2(\Omega)$. *For* $j = 1, 2, \ldots, M$ *set*

$$-\lambda_h(t_j) := \inf_{v\in\mathbb{V}\setminus\{0\}} \frac{\|\nabla v\|^2 + \varepsilon^{-2}(Df(\mathcal{P}u(t_j))v, v)}{\|v\|^2},$$

and for almost every $t \in (0, T)$ *define*

$$-\lambda(t) := \inf_{v\in\mathbb{V}\setminus\{0\}} \frac{\|\nabla v\|^2 + \varepsilon^{-2}(Df(u(t))v, v)}{\|v\|^2}.$$

(a) *For* $j = 0, 1, \ldots, M$ *we have*

$$\lambda_h(t_j) \leq \lambda(t_j) + 1.$$

(b) *For almost every* $t \in (0, T)$ *we have*

$$|\lambda(t)| \leq C_{\mathbb{V}} + \varepsilon^{-2} C_{f'},$$

where $C_{f'} := \|Df\|_{L^\infty(B_{C_\infty})}$ *and* $C_{\mathbb{V}} := \inf_{v\in\mathbb{V}:\|v\|=1} \|\nabla v\|^2$.

(c) *We have*

$$\left|\int_0^T \lambda^+(t)\,\mathrm{d}t - \tau \sum_{j=1}^M \lambda^+(t_j)\right| \leq 1.$$

Proof. (a) By the mean value theorem we have that

$$Df(\mathcal{P}u(t_j)) - Df(u(t_j)) = D^2 f(\xi)(\mathcal{P}u(t_j) - u(t_j)),$$

with a function ξ such that $|\xi(x)| \leq \|\mathcal{P}u(t_j)\|_{L^\infty(\Omega)} + \|u(t_j)\|_{L^\infty(\Omega)}$ for almost every $x \in \Omega$. Owing to (7) and (18) we have $\|\mathcal{P}u(t_j)\|_{L^\infty(\Omega)} \leq 2C_\infty$ and thus

$$\|Df(\mathcal{P}u(t_j)) - Df(u(t_j))\|_{L^\infty(\Omega)} \leq C_{f''} C_{\mathcal{P}} h^{(4-d)/2} |\log h|^{(3-d)/2} C_u \varepsilon^{-\sigma} \leq \varepsilon^2.$$

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Using this bound in

$$(Df(\mathcal{P}u(t_j))v,v) \geq (Df(u(t_j))v,v) - \|Df(\mathcal{P}u(t_j)) - Df(u(t_j))\|_{L^\infty(\Omega)}(v,v)$$

implies the first assertion.

(b) This bound follows immediately from the definitions of $C_{f'}$ and $C_{\mathbb{V}}$.

(c) For almost every $t \in (0,T)$ let $w(t) \in \mathbb{V}$ with $\|w(t)\| = 1$ satisfy

$$-\lambda(t) = \|\nabla w(t)\|^2 + \varepsilon^{-2}(Df(u(t))w(t), w(t)).$$

Owing to the fact that $w(t)$ is optimal for the right-hand side, we find that

$$\begin{aligned} -\partial_t\lambda(t) &= 2(\nabla w, \nabla w_t) + 2\varepsilon^{-2}(Df(u)w, w_t) + \varepsilon^{-2}(D^2f(u)u_t w, w) \\ &= -2\lambda(t)(w, w_t) + \varepsilon^{-2}(D^2f(u)u_t w, w). \end{aligned}$$

Since $\|w(t)\| = 1$ for all t, we have $2(w, w_t) = \partial_t\|w\|^2 = 0$, from which we can deduce

$$-\partial_t\lambda(t) = \varepsilon^{-2}\big(D^2f(u(t))u_t(t)w(t), w(t)\big),$$

and hence

$$\begin{aligned} \int_0^T |\partial_t\lambda(t)|\,\mathrm{d}t &\leq \varepsilon^{-2}C_{f''}\int_0^T \|u_t(t)\|_{L^\infty(\Omega)}\,\mathrm{d}t \\ &\leq \varepsilon^{-2}C_{f''}C_{S2}T^{1/2}\left(\int_0^T \|u_t\|^2_{H^2(\Omega)}\,\mathrm{d}t\right)^{1/2} \leq \varepsilon^{-2}C_{f''}C_{S2}T^{1/2}C_u\varepsilon^{-\sigma}. \end{aligned}$$

Basic interpolation estimates and (18) lead to the assertion. ∎

We provide an error analysis, assuming for ease of presentation that a discrete maximum principle is satisfied up to a constant factor. It is well known that this is satisfied on weakly acute triangulations in the case of Allen–Cahn or Ginzburg–Landau equations. The assumption can be entirely avoided by arguing as in [FP03].

THEOREM 4.3. *Let δ, C_f, and g be as in* (GA). *Let* (RA) *and* (18) *be satisfied and assume that* $\sup_{j=0,1,\dots,M}\|U^j\|_{L^\infty(\Omega)} \leq 2C_\infty$. *Suppose that there are $C_0 > 0$ and $\kappa \geq 0$ such that*

$$\int_0^T \lambda^+(t)\,\mathrm{d}t \leq C_0 + \log\varepsilon^{-\kappa}. \tag{19}$$

There exist constants $C_1, C_2 > 0$ such that if

$$\tau + h^2 \leq C_1\varepsilon^{2+\sigma+4/\delta+2\kappa+4\kappa/\delta},$$

then

$$\sup_{j=1,2,\dots,M}\|u(t_j) - U^j\| \leq C_2(\tau + h^2)\varepsilon^{-2-\sigma-4\kappa}$$

and

$$\left(\tau\sum_{j=1}^M \|\nabla(u(t_j) - U^j)\|^2\right)^{1/2} \leq C_2(\tau + h)\varepsilon^{-3-\sigma-4\kappa}.$$

Remark 4.4. (i) For smooth initial data with uniformly bounded energy and $F(u) = (|u|^2 - 1)^2/4$, we may choose $\sigma = 2$ and $\delta = 1$ so that the conditions of

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the theorem are satisfied if $\tau + h^2 \le C\varepsilon^{6+4\kappa}$. For smooth evolutions of interfaces or vortices we may choose $\kappa = 0$; cf. [Che94, dMS95, Mir95, Lin97, Bea03].

(ii) The powers $2\kappa(1+1/\delta)$ and -4κ can be replaced by $(1+o(1))\kappa(1+1/\delta)$ and $-2(1+o(1))\kappa$, respectively, provided that $\tau\varepsilon^{-2} = o(1)$; cf. Remark 2.4.

(iii) For the a priori error analysis it is sufficient to require that δ is finite in (iii) of (GA).

Proof. We split the proof into five steps: We select an interpolant of the exact solution, identify a discrete equation satisfied by that approximation, use the techniques discussed in subsection 2.3 to control the distance between the interpolant and the sequence $(U^j)_{j=0}^M$, and finally apply the triangle inequality to prove the asserted bounds.

Step 1. We employ the decomposition

$$E^j = \Theta^j + \Phi^j := \big[u(t_j) - \mathcal{P}u(t_j)\big] + \big[\mathcal{P}u(t_j) - U^j\big].$$

Step 2. Using (5), noting $(\nabla\Theta^j, \nabla V) = -(\Theta^j, V)$, and setting $R^j := \partial_t u(t_j) - d_t u(t_j)$, we have for every $V \in \mathbb{V}_h$

(20)
$$\begin{aligned}(d_t\mathcal{P}u(t_j),V) &+ (\nabla\mathcal{P}u(t_j), \nabla V) - \varepsilon^{-2}(f(\mathcal{P}u(t_j))V)\\ &= -(d_t\Theta^j, V) - (\nabla\Theta^j, \nabla V) - \varepsilon^{-2}(f(\mathcal{P}u(t_j)) - f(u(t_j)), V) - \langle R^j, V\rangle\\ &= -(d_t\Theta^j, V) + (\Theta^j, V) - \varepsilon^{-2}(f(\mathcal{P}u(t_j)) - f(u(t_j)), V) - \langle R^j, V\rangle\\ &=: \langle D^j, V\rangle.\end{aligned}$$

Step 3. Subtracting (17) from (20), choosing $V = \Phi^j$, employing (i) and (ii) of (GA), and incorporating the definition of $\lambda_h(t_j)$ shows that

$$\begin{aligned}\frac{1}{2}d_t\|\Phi^j\|^2 + \frac{\tau}{2}\|d_t\Phi^j\|^2 + \|\nabla\Phi^j\|^2 &= \langle D^j, \Phi^j\rangle + \varepsilon^{-2}(f(\mathcal{P}u(t_j)) - f(U^j), \Phi^j)\\ &\le \|D^j\|_*\|\Phi^j\|_{H^1(\Omega)} + \varepsilon^{-2}(Df(\mathcal{P}u(t_j))\Phi^j, \Phi^j)\\ &\quad + \varepsilon^{-2}\|g(\mathcal{P}u(t_j))\|_{L^\infty(\Omega)}\|\Phi^j\|^{2+\delta}_{L^{2+\delta}(\Omega)}\\ &\le \frac{\varepsilon^{-2}}{2}\|D^j\|_*^2 + \frac{\varepsilon^2}{2}\|\Phi^j\|^2 + \frac{\varepsilon^2}{2}\|\nabla\Phi^j\|^2\\ &\quad + (1-\varepsilon^2)\lambda_h(t_j)\|\Phi^j\|^2 + (1-\varepsilon^2)\|\nabla\Phi^j\|^2 + C_f\|\Phi^j\|^2 + \varepsilon^{-2}C_g\|\Phi^j\|^{2+\delta}_{L^{2+\delta}(\Omega)}.\end{aligned}$$

We have

$$\begin{aligned}\|\Phi^j\|^{2+\delta}_{L^{2+\delta}(\Omega)} &\le C_\delta\big(\|\Phi^{j-1}\|^{2+\delta}_{L^{2+\delta}(\Omega)} + \tau^{2+\delta}\|d_t\Phi^j\|^{2+\delta}_{L^{2+\delta}(\Omega)}\big)\\ &\le C_\delta\|\Phi^{j-1}\|^{2+\delta}_{L^{2+\delta}(\Omega)} + C_\delta\tau^2\|d_t\Phi^j\|^2\\ &\qquad\cdot\left(\sum_{k=j-1,j}(\|\mathcal{P}u(t_k)\|_{L^\infty(\Omega)} + \|U^k\|_{L^\infty(\Omega)})\right)^\delta.\end{aligned}$$

Owing to (18) we have $\|\mathcal{P}u(t_k)\|_{L^\infty(\Omega)} \le 2C_\infty$, $k = j-1, j$. For τ such that

$$8^\delta\varepsilon^{-2}\tau C_\delta C_g C_\infty^\delta \le 1/4$$

the combination of the last two estimates with Lemma 4.2(a) implies

$$d_t\|\Phi^j\|^2 + \frac{\tau}{2}\|d_t\Phi^j\|^2 + \varepsilon^2\|\nabla\Phi^j\|^2 \le \varepsilon^{-2}\|D^j\|_*^2 + \mu_\lambda^j\|\Phi^j\|^2 + 2C_gC_\delta\varepsilon^{-2}\|\Phi^{j-1}\|^{2+\delta}_{L^{2+\delta}(\Omega)},$$

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where $\mu_\lambda^j := 2(C_f + \varepsilon^2 + (1-\varepsilon^2)(\lambda^+(t_j)+1))$, $j = 1, 2, \ldots, M$. We remark that we have estimated λ by λ^+, since Lemma 2.3 requires positive coefficients $(a^j)_{j=0}^M$.

Owing to (b) of Lemma 4.2 and the conditions on τ, we may assume that $2\tau\mu_{\lambda_j} \le 1/2$ for all $j = 1, 2, \ldots, M$. Upon summing over $j = 1, 2, \ldots, M$, noting $\Phi^0 = 0$, and incorporating (11), Lemma 2.3 with $A = \varepsilon^{-2}\tau\sum_{j=1}^M \|D^j\|_*^2$, $E = \exp\left(2\tau\sum_{j=1}^M \mu_\lambda^j\right)$, $B = 2C_gC_\delta\varepsilon^{-2}C_S(1+\varepsilon^{-2})$, and $\beta = \delta/2$ yields that

$$\sup_{j=1,2,\ldots,M} \|\Phi^j\|^2 + \varepsilon^2\tau\sum_{j=1}^M \|\nabla\Phi^j\|^2 \le 8AE$$

provided that with an appropriate constant $C_B > 0$ we have

$$AE \le C_B\varepsilon^{8/\delta}E^{-2/\delta} \le 8^{-1}(8B(1+T)E)^{-2/\delta}. \tag{21}$$

Step 4. Using estimate (c) of Lemma 4.2 and the assumed bound (19), we have

$$E \le \exp\left(4T(C_f+1)\right)\exp\left(4\tau\sum_{j=0}^M \lambda^+(t_j)\right) \le C_E\varepsilon^{-4\kappa}.$$

The estimates (7), (8), and (9) imply that

$$\begin{aligned}\varepsilon^2 A &= \tau\sum_{j=1}^M \|D^j\|_*^2 \\ &\le C_P^2h^4C_u^2 + (1+\varepsilon^{-2}C_{f'})C_{\mathcal{P}}^2h^4TC_u^2\varepsilon^{-2\sigma} + \frac{\tau^2}{3}C_u^2\varepsilon^{-2\sigma} \le C_A(\tau^2+h^4)\varepsilon^{-2(1+\sigma)}.\end{aligned}$$

The conditions of the theorem yield that (21) is satisfied with $C_1^2 = C_A^{-1}C_BC_E^{-1-2/\delta}$.

Step 5. We deduce from (7) that

$$\max_{j=1,2,\ldots,M} \|\Theta^j\|^2 + \tau\sum_{j=1}^M h^2\|\nabla\Theta^j\|^2 \le C_{\mathcal{P}}^2(1+T)h^4C_u\varepsilon^{-2\sigma}.$$

An application of the triangle inequality and a combination of the estimates imply the assertions. ∎

5. Numerical experiments. We illustrate our theoretical findings by some numerical experiments discussing the most relevant effects in a process governed by (5) in two dimensions for the scalar ($\ell = 1$) and the vectorial ($\ell = 2$) cases corresponding to Allen–Cahn and Ginzburg–Landau equations, respectively, with different topological changes. We employed a semi-implicit discretization to approximate (1) and an inverse iteration with a variable shift to compute approximations of the eigenvalue problems.

5.1. Allen–Cahn equations. Our first experiment studies prototypical topological changes of the interface $\Gamma_t := \{x \in \Omega : u(t,x) = 0\}$ in an evolution defined by the Allen–Cahn equation. The initial function u_0 is chosen in such a way that the initial interface Γ_0 consists of two concentric circles centered at the origin; see the left upper plot in Figure 1.

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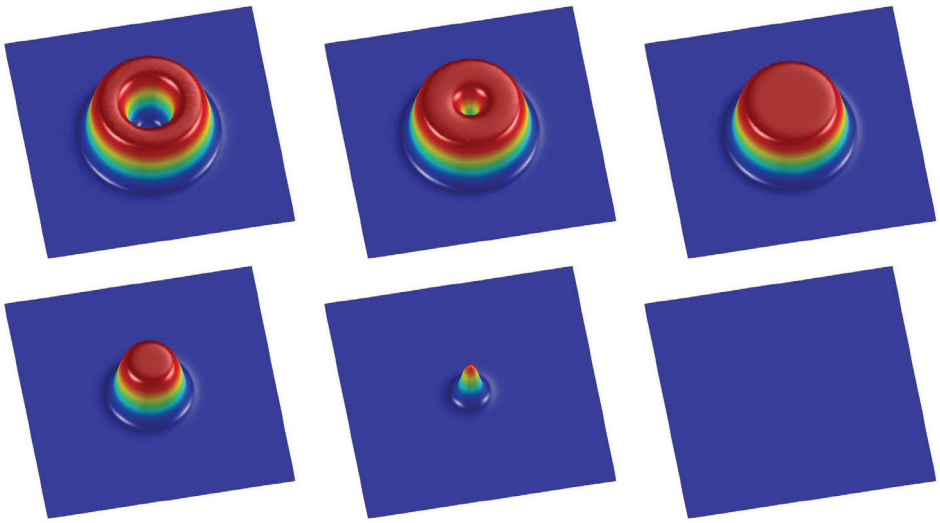

FIG. 1. *Snapshots of the evolution defined by Example* 5.1 *for* $t = 0.0, 0.06, 0.12, 0.29, 0.48, 0.5$, *and* $\varepsilon = 1/16$ *(from left to right and top to bottom). The initial interface consists of two concentric circles and undergoes two topological changes during the evolution.*

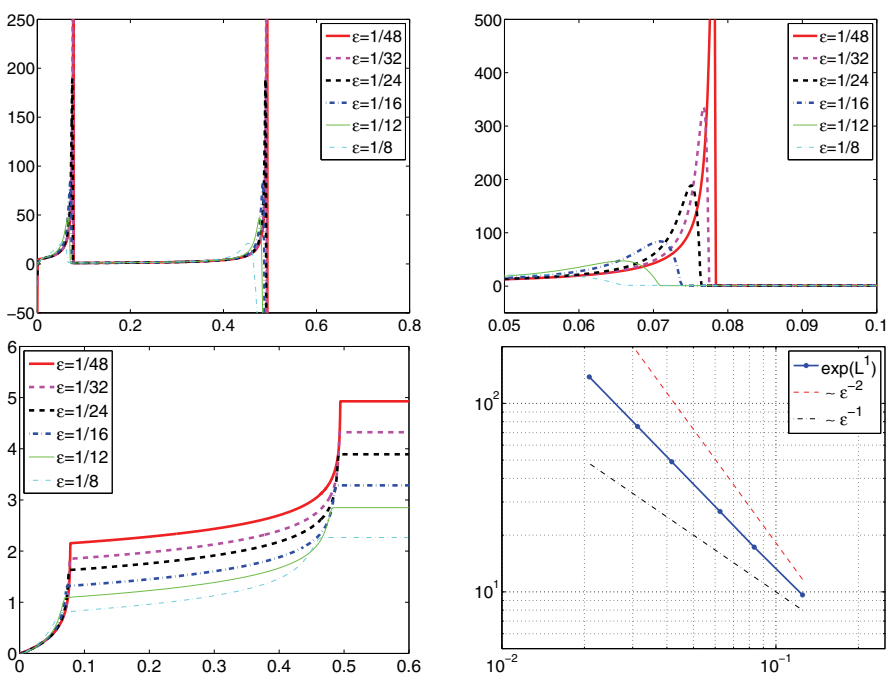

FIG. 2. *Approximated eigenvalue* $\Lambda^+_{AC}(t)$ *in Example* 5.1 *as a function of* $t \in [0, 0.8]$ *(left upper), a detailed plot in the interval* $[0.05, 0.1]$ *(right upper), its integral over* $(0, t)$ *as a function of* $t \in [0, 0.6]$ *(left lower), and the quantity* $\exp\left(\int_0^{0.6} \Lambda^+_{AC}(t)\,\mathrm{d}t\right)$ *in dependence of* ε *(right lower). The eigenvalue grows like* ε^{-2} *at topological changes while its integral only grows logarithmically in* ε^{-1}.

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Example 5.1 (concentric circles). Let $\Omega := (-2,2)^2$, $\Gamma_{\mathrm{D}} := \emptyset$, set $r_1 := 4/10$ and $r_2 := 1$, and define $d_j(x) := |x| - r_j$ for $x \in \Omega$ and $j = 1,2$. For given $\varepsilon > 0$ and $x \in \Omega$ let

$$u_0(x) := -\tanh\big(d(x)/(\sqrt{2}\varepsilon)\big), \qquad d(x) := \max\{-d_1(x), d_2(x)\}.$$

Snapshots of the evolution defined by the initial data of Example 5.1 for $\varepsilon = 1/16$ are shown in Figure 1. The approximations were obtained on uniform triangulations of meshsize $h = \varepsilon/10$ and with the uniform time-step size $\tau = \varepsilon^3/16$; we convinced ourselves that these discretization parameters lead to accurate approximations. We see that the interface Γ_t undergoes two topological changes. The first one occurs at $t \approx 0.08$ when the radius of the inner circle decreases to zero. Subsequently, the radius of the outer circle decreases until at $t \approx 0.5$ the particle has entirely disappeared. For $\varepsilon = 1/8, 1/12, 1/16, 1/24, 1/32, 1/48$, we plotted in Figure 2 the numerically computed eigenvalue $\Lambda_{AC}(t)$ as a function of t (left and right upper plots) and its integral over $(0,t)$ (left lower plot), i.e., the functions

$$t \mapsto \Lambda_{AC}^+(t), \qquad t \mapsto \int_0^t \Lambda_{AC}^+(s)\,\mathrm{d}s.$$

The results show that a uniform bound for $\Lambda_{AC}^+(t)$ breaks down when topological changes occur, and at these events we have $\Lambda_{AC}(t) \sim \varepsilon^{-2}$. In contrast, the integrated eigenvalue grows only slowly in ε^{-1}. In fact, whenever we decrease ε by a factor $1/2$, the integrated eigenvalue increases by a constant rate. This corresponds exactly to a logarithmic growth of the form

$$\int_0^T \Lambda_{AC}^+(t)\,\mathrm{d}t \sim C_0 + \log(\varepsilon^{-\kappa}). \tag{22}$$

The number C_0 counts how many topological changes have occurred and the logarithmic plot of $\exp\big(\int_0^T \Lambda_{AC}^+(t)\,\mathrm{d}t\big)$ in the right lower plot of Figure 2 indicates that we may choose $\kappa \le 2$. The numerical results thus show that robust a posteriori error estimation within our theoretical results is possible in this example. Our upper bounds for the error are also useful for adaptive mesh refinement and coarsening, and we tried the following algorithm, which uses a fixed time-step size, for the initial data of Example 5.1.

Adaptive algorithm. Given a tolerance $\varrho > 0$ carry out for $j = 1, 2, \ldots, M$, the following steps:

(a) **Coarsen** elements in $\mathcal{T}_C \subseteq \mathcal{T}_{j-1}$ to obtain triangulation $\mathcal{T}_{j,0}$ with $\eta_{c,0}^j \le \varrho/10$. Set $k := 0$.

(b) **Compute** $U^{j,k} \in \mathbb{V}_h^{j,k}$ such that for all $V \in \mathbb{V}_h^{j,k}$ we have

$$\tau^{-1}(U^{j,k} - \mathcal{I}_{\mathcal{T}_{j,k}} U^{j-1}, V) + (\nabla U^{j,k}, \nabla V) = -\varepsilon^{-2}(f(U^{j,k}), V).$$

(c) **Refine** elements $K \in \mathcal{T}_{j,k}$ for which $\eta_{h,1}^{j,k}(K) \ge (1/2)\max_{K' \in \mathcal{T}_{j,k}} \eta_{h,1}^{j,k}(K')$, set $k := k+1$, and go to (b) if $\eta_{h,1}^{j,k} \ge \varrho$.

(d) **Update** $U^j := U^{j,k}$, set $j := j+1$, and go to (a).

In Figure 3 we display the adaptively generated triangulations obtained with the adaptive algorithm in Example 5.1 for $\varepsilon = 1/16$ and $\varrho = \varepsilon$. The algorithm automatically refines the grid locally in a neighborhood of the interface and coarsens

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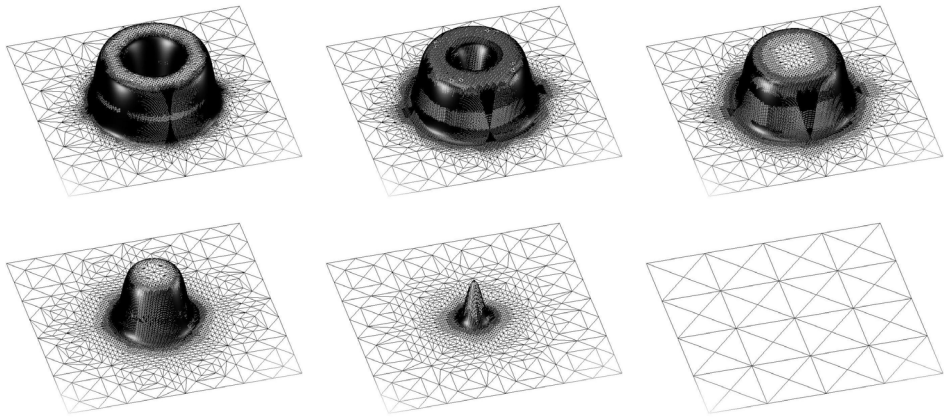

FIG. 3. *Adaptively refined and coarsened triangulations obtained with the adaptive algorithm in Example* 5.1 *with* $\varepsilon = 1/16$ *and* $\varrho = \varepsilon$.

the triangulation when the interface has advanced. We also observe that no strong refinement is carried out in a small neighborhood of the interface Γ_t, where the exact solution is almost linear.

Our second numerical experiment in the context of Allen–Cahn equations addresses a different topological effect, namely the pinching of an interface. Since in two dimensions this phenomenon is sensitively dependent on the choice of initial data, it appears artificial but still fits well into our framework. Moreover, the example is interesting since it does not lead to the uniform a priori bounds for $\lambda_{AC}(t)$ in $(0, T_S)$ in [Che94, dMS95] for any positive number $T_S > 0$. To enforce a pinching effect in two dimensions we choose initial data that depend on ε. We remark that pinching is an important and generic topological effect in three dimensions; cf. [DDE05].

Example 5.2 (dumbbell). Set $\Omega := (-2, 2)^2$, $\Gamma_{\mathrm{D}} := \emptyset$, define $m_1 = -m_3 := (0, 2)$, $m_2 := 0$, and, for a given $\varepsilon > 0$, let $r_1 = r_3 := 2 - 3\varepsilon/2$, $r_2 := 1$, and set $d_j(x) := |x - m_j| - r_j$ for $x \in \Omega$. For $x \in \Omega$ let

$$u_0(x) := -\tanh\big(d(x)/(\sqrt{2}\varepsilon)\big), \qquad d(x) := \max\{-d_1(x), -d_2(x), d_3(x)\}.$$

In Figure 4 we display snapshots of the evolution defined by Example 5.2. Within a short time interval, the initially connected interface Γ_0 splits into two curves. Then, the two components of the interface develop circular shapes and eventually the diameters of the two particles decrease to zero until they collapse at $t \approx 0.13$. The topological changes are accompanied by a strong increase of the eigenvalue $\Lambda_{AC}(t)$. From the left upper plot in Figure 5, where we plotted the function $t \mapsto \Lambda_{AC}(t)$ for various choices of ε, we see that $\Lambda_{AC}(t) \sim \varepsilon^{-2}$ at those events. We magnified the initial behavior of $\Lambda_{AC}(t)$ by using a logarithmic scaling for both axes in the right upper plot of Figure 5. The curves explain the logarithmic scaling behavior (22), illustrated in the left lower plot of Figure 5, which is also valid in this example: Before a time of order ε^2, the eigenvalue $\Lambda_{AC}(t)$ grows until it reaches its value which is proportional to ε^{-2}. After that, the eigenvalue decays like t^{-1} until it reaches an ε independent value. The integral over the first time interval is bounded uniformly while an integration over the second subinterval leads to a logarithmic contribution. Finally, the quantities $\exp\big(\int_0^T \Lambda_{AC}^+(t)\,\mathrm{d}t\big)$ shown in the right lower plot of Figure 5

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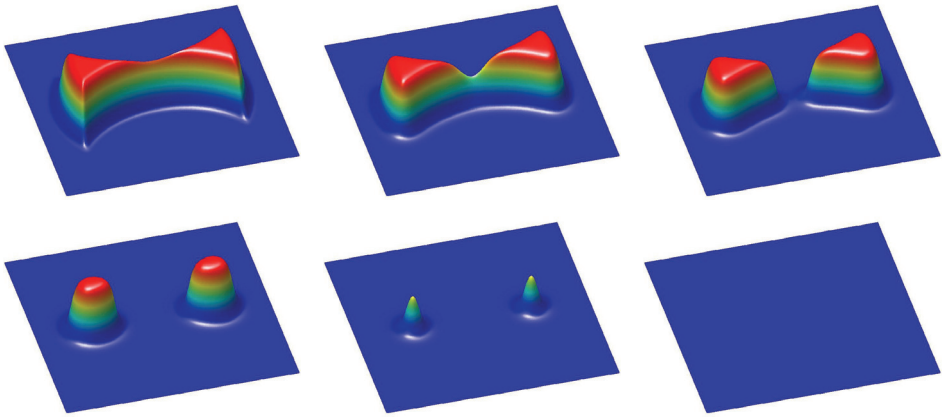

FIG. 4. *Snapshots of the evolution defined by Example* 5.2 *for* $t = 0.0, 0.012, 0.024, 0.073, 0.122, 0.146$ *and* $\varepsilon = 1/16$ *(from left to right and top to bottom). The dumbbell shape of the initial interface defined in Example* 5.2 *immediately splits into two interfaces that develop circular shapes and eventually collapse.*

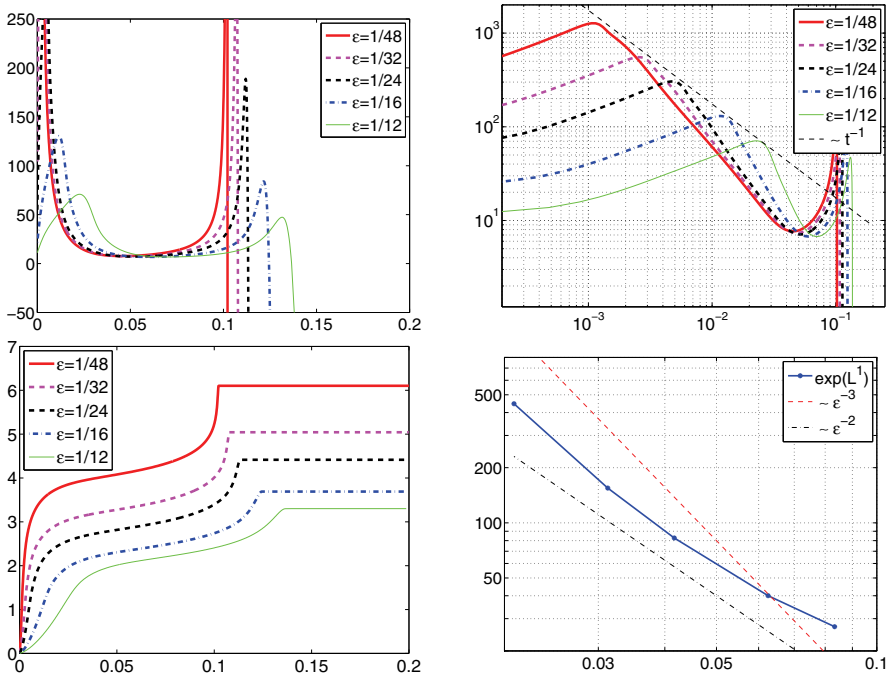

FIG. 5. *Approximated eigenvalue* $\Lambda^+_{AC}(t)$ *in Example* 5.2 *as a function of* $t \in [0, 0.2]$ *(left upper), the same plot with a logarithmic scaling used for both axes (right upper), its integral over* $(0, t)$ *as a function of* $t \in [0, 0.2]$ *(left lower), and the quantity* $\exp\left(\int_0^{0.2} \Lambda^+_{AC}(t)\,\mathrm{d}t\right)$ *as a function of* ε *(right lower). The eigenvalue grows like* ε^{-2} *at topological changes while its integral only grows logarithmically in* ε^{-1}.

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show that we may choose $\kappa = 3$ in the bound (22) in Example 5.2. In particular, we deduce that robust a posteriori error control is possible.

5.2. Ginzburg–Landau equations. The topological changes for the vector valued version ($\ell = 2$) of (5) are different from the scalar situation ($\ell = 1$). In addition to the fact that the interface Γ_t is $d - \ell$ dimensional, the interaction of nonconnected components of Γ_t is the dominant effect. This is reflected by the quantitative observation that the function $1 - |u(t,x)|$ decays algebraically to 0 away from Γ_t in the Ginzburg–Landau case while it decays exponentially away from a typical Allen–Cahn interface. In the two examples of this subsection we investigate the applicability of our error estimate for the annihilation of two degree-one vortices and the splitting of a degree-two vortex.

Example 5.3 (annihilation). Set $\Omega := (-1,1) \times (-1/2, 1/2)$, $\Gamma_{\mathrm{D}} := \partial\Omega$, and given $\varepsilon > 0$ let $d_\varepsilon := \min\{4/10, \varepsilon + 3/10\}$. For $x = (x_1, x_2) \in \Omega$ set

$$u_0(x) := f_0(|(x_1 \pm d_\varepsilon, x_2)|) \frac{(\mp(x_1 \pm d_\varepsilon), x_2)}{|(x_1 \pm d_\varepsilon, x_2)|} \quad \text{for } \mp x_1 > 0,$$

where $f_0(r) = \min\{r/(2\varepsilon) - r^3/(16\varepsilon), 1\}$ for $r \geq 0$. Set $u_{\mathrm{D}} := u_0|_{\partial\Omega}$.

Figure 6 shows the approximate solution for Example 5.3 with $\varepsilon = 1/16$. We observe that the two vortices located at $(\pm d_\varepsilon, 0)$ attract each other and annihilate at $t \approx 1.25$. The principal eigenvalue of the linearized Ginzburg–Landau operator about the numerical approximation $U(t)$ has a peak when the annihilation takes place, as can be seen in the left plot of Figure 7. Nevertheless, the integrated positive part of the principal eigenvalue Λ_{GL}^+ remains bounded as ε decreases, as can be observed in the right plot of Figure 7. Hence we may choose $\kappa = 0$ in this example and deduce that our error estimator is robust and that the conditions for the a priori error estimate of Theorem 4.3 are satisfied here. We remark that the dependence of d_ε on ε is important in this example in order to observe relevant effects within a uniformly bounded time interval.

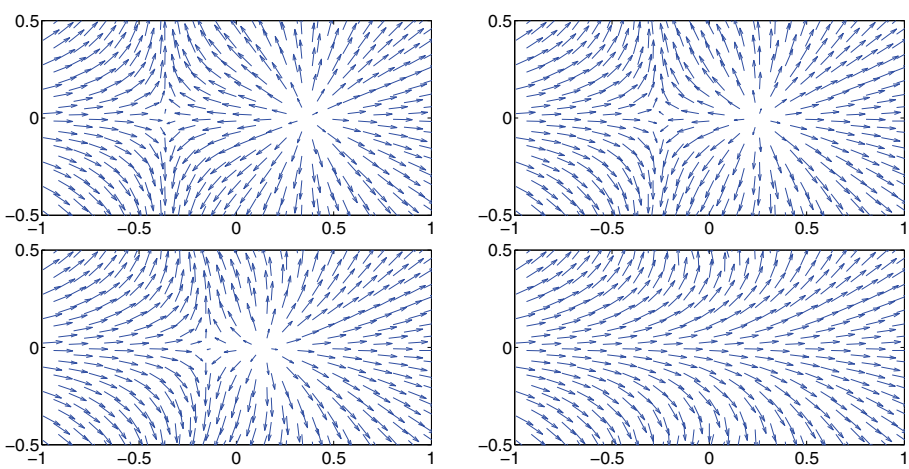

FIG. 6. *Snapshots of the evolution defined by Example* 5.3 *for* $t = 0.01, 0.94, 1.24, 1.41$ *and* $\varepsilon = 1/16$ *(from left to right and top to bottom). The two opposite sign degree-one vortices initially located at* $(\pm d_\varepsilon, 0)$ *attract each other and eventually annihilate.*

In the second example for Ginzburg–Landau evolutions we consider a degree-two vortex located at the origin. It is well known that such a vortex is unstable and splits

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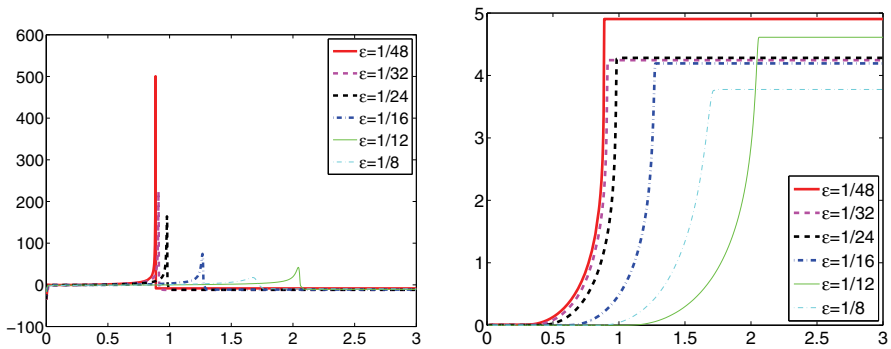

FIG. 7. *Approximated eigenvalue $\Lambda_{GL}(t)$ in Example 5.3 as a function of $t \in [0,3]$ (left) and the integral over $(0,t)$ of its positive part as a function of $t \in [0,3]$ (right). The eigenvalue grows like ε^{-2} when the vortices annihilate while its integral remains uniformly bounded.*

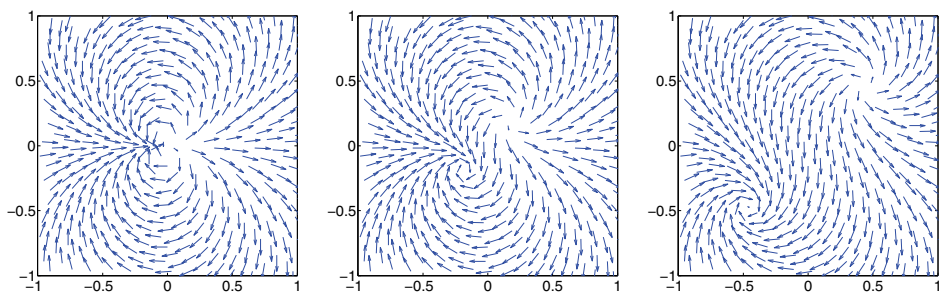

FIG. 8. *Snapshots of the evolution defined by Example 5.4 for $t = 0.01, 0.22, 0.71$, and $\varepsilon = 1/16$ (from left to right and top to bottom). The initial degree-two vortex immediately splits into two degree-one vortices that repel each other.*

into two degree-one vortices that repel each other. We use the identification $\mathbb{C} \simeq \mathbb{R}^2$ to define u_0.

Example 5.4 (splitting). Set $\Omega := (-1,1)^2$, $\Gamma_{\mathrm{D}} := \partial\Omega$, and given $\varepsilon > 0$ and $x = (x_1, x_2) \in \Omega$ let

$$u_0(x) := \frac{x^2}{|x|^2 + \varepsilon^2} = \frac{(x_1^2 - x_2^2, 2x_1x_2)}{x_1^2 + x_2^2 + \varepsilon^2}.$$

Set $u_{\mathrm{D}} := u_0|_{\partial\Omega}$.

The vector fields shown in Figure 8 illustrate the evolution defined by the initial data of Example 5.4. The initial degree-two vortex immediately splits into two degree-one vortices that move into opposite directions until their locations achieve equilibrium positions at $t \approx 0.7$. As can be seen in Figure 9, during this splitting the principal eigenvalue $\Lambda_{GL}(t)$ of the linearized Ginzburg–Landau operator about the numerical approximation $U(t)$ behaves like ε^{-2}. As opposed to the previous examples, it decreases below an ε independent value within only a time interval whose length is comparable to ε. Therefore, the integral of $\Lambda_{GL}^+(t)$ over $(0, 0.7)$ grows like ε^{-1} leading to an exponential growth of the quantity $\exp\big(\int_0^{0.7} \Lambda_{GL}^+(t)\,\mathrm{d}t\big)$, which is also observed in the right lower plot of Figure 9. Hence, our error estimate is not robust in this example. The observations are in agreement with the theoretical predictions of [BOS07], which prove that higher degree vortices can exist for an ε independent

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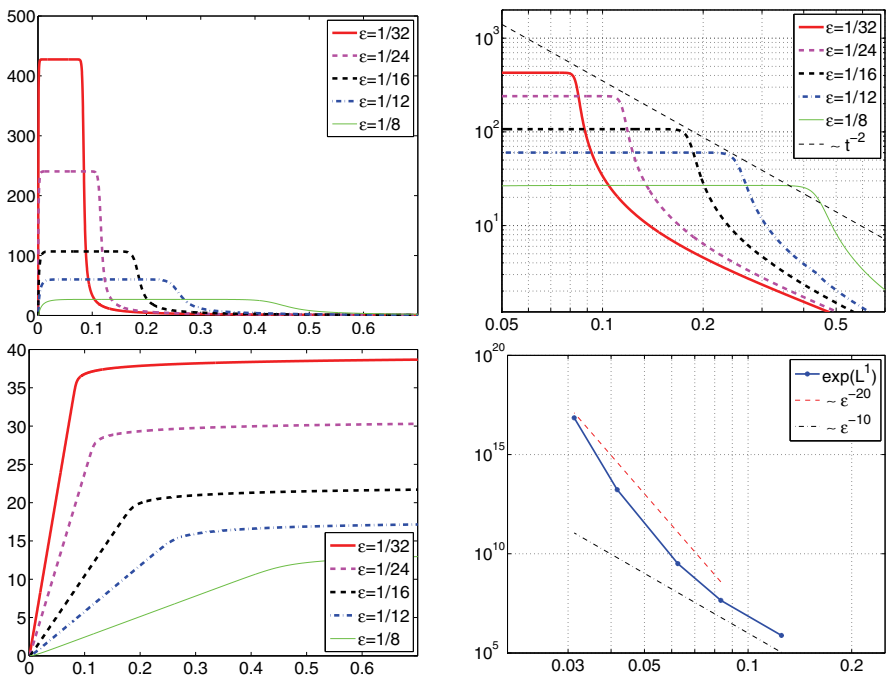

FIG. 9. *Approximated eigenvalue* $\Lambda_{GL}(t)$ *in Example* 5.4 *as a function of* $t \in [0, 0.7]$ *in the upper row. The integral over* $(0, t)$ *of its positive part as a function of* $t \in [0, 0.7]$ *(left lower) and the quantity* $\exp\left(\int_0^{0.7} \Lambda_{GL}^+(t)\,\mathrm{d}t\right)$ *as a function of* ε *(right lower). The eigenvalue grows like* ε^{-2} *when the degree-two vortex splits but reduces to an* ε *independent value after only a time proportional to* ε. *The integrated eigenvalue grows exponentially.*

period, in particular, longer than a time comparable to ε^2. We believe that this example is exceptional since the critical behavior is enforced by the choice of initial data and would not occur within an evolution for initial data that do not contain higher degree vortices.

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