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Error estimates for fully discrete BDF finite element approximations of the Allen–Cahn equation

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For a class of compatible profiles of initial data describing bulk phase regions separated by transition zones, we approximate the Cauchy problem of the Allen–Cahn phase field equation by an initial-boundary value problem in a bounded domain with the Dirichlet boundary condition. The initial-boundary value problem is discretized in time by the backward difference formulae (BDF) of order $1 \leqslant q \leqslant 5$ and in space by the Galerkin finite element method of polynomial degree $r-1$, with $r \geqslant 2$. We establish an error estimate of $O(\tau^q \varepsilon^{-q-\frac{1}{2}} + h^r \varepsilon^{-r-\frac{1}{2}} + \mathrm{e}^{-c/\varepsilon})$ with explicit dependence on the small parameter ε describing the thickness of the phase transition layer. The analysis utilizes the maximum-norm stability of BDF and finite element methods with respect to the boundary data, the discrete maximal L^p-regularity of BDF methods for parabolic equations, and the Nevanlinna–Odeh multiplier technique combined with a time-dependent inner product motivated by a spectrum estimate of the linearized Allen–Cahn operator.

Keywords: Allen–Cahn equation; phase transition layer; BDF methods; finite element method; maximum-norm stability; time-dependent norm; multiplier; G-stability; discrete maximal L^p-regularity.

1. Introduction

The Allen–Cahn (AC) equation

$$\begin{cases} u_t - \Delta u + \dfrac{1}{\varepsilon^2} f(u) = 0 & \text{in } \mathbb{R}^d \times (0,T), \\ u(\cdot,0) = u_0 & \text{in } \mathbb{R}^d, \end{cases} \tag{1.1}$$

with $d \in \{2,3\}$, is a model describing phase separation of a binary alloy at a fixed temperature [6], where $f(\upsilon) = \upsilon^3 - \upsilon$ is the derivative of the Ginzburg–Landau energy function $F(\upsilon) = (\upsilon^2-1)^2/4$. The solution of (1.1) is equal to -1 and 1 in the two phases of the alloy, respectively, separated by a phase transition zone of width $O(\varepsilon)$, in which the solution changes rapidly from

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-1 to 1. The Cauchy problem of the AC equation is connected to the mean curvature flow of closed surfaces, see [20], i.e., as the small parameter ε tends to zero, the surface determined by the level set $\Gamma_\varepsilon(t) = \{x \in \mathbb{R}^d : u(x,t) = 0\}$ tends to a surface $\Gamma(t)$ that evolves with velocity $\boldsymbol{v} = H\boldsymbol{\nu}$ (called mean curvature flow), where H and $\boldsymbol{\nu}$ denote the mean curvature and unit normal vector, respectively, on the surface $\Gamma(t)$.

In view of its application as a phase field model and its connection to mean curvature flow, many numerical methods and analyses have been developed for approximating the mean curvature flow through AC related diffusive phase field models as $\varepsilon \to 0$. Error analysis for the AC equation and related phase field models (instead of the limit of the interface $\Gamma_\varepsilon(t)$ as $\varepsilon \to 0$) has also been conducted in many articles. As pointed out in [12, 23], error estimation using a straightforward Gronwall inequality argument would yield a constant factor $\mathrm{e}^{CT/\varepsilon^2}$, which grows exponentially as $\varepsilon \to 0$. Such error estimates are not useful when the width ε of the phase transition zone in the phase field model is small. To overcome this difficulty, Feng and Prohl [23] established an error estimate for the AC equation in a bounded domain with only polynomial dependence on ε^{-1} by utilizing the spectrum estimate of the linearized AC operator in a bounded domain [17], i.e.,

$$\|\nabla v\|^2_{L^2(\Omega)} + \frac{1}{\varepsilon^2}(f'(u(\cdot,t))v, v) \geqslant -\lambda \|v\|^2_{L^2(\Omega)} \quad \forall v \in H^1(\Omega)\ \forall t \in [0,T], \tag{1.2}$$

with λ a positive constant, independent of ε and $t \in [0,T]$, and $u(\cdot,t)$ the solution of the AC equation. This spectral estimate is valid for smooth interfaces away from singularities such as the collapse of an interface.

The spectrum estimate (1.2) was also used to remove the exponential dependence on ε^{-1} in error analyses for other numerical methods and related phase-field equations, including the implicit Euler method for the non-isothermal AC phase field equations [25], stabilized semi-implicit schemes for the AC equation [45], and a posteriori error estimates for the AC equation [9–11, 29]. These articles concern either implicit or semi-implicit Euler methods for the AC equation and error estimates of $O((\tau + h^r)\varepsilon^{-\sigma})$, where σ is some positive number.

Spectrum estimates similar to (1.2) were also used in establishing error estimates for the Ginzburg–Landau equations [8], the Cahn–Hilliard equation and Hele–Shaw flow [9, 22, 24, 44], as well as for phase field models with nonlinear constitutive laws [19].

Since ε is often very small, there is also a vast literature on constructing energy-decaying time-stepping methods for phase field models with large time stepsizes (compared with ε), including stabilized semi-implicit schemes [15, 16, 35, 42], invariant energy quadratization methods [46–48], and the scalar auxiliary variable approach [41] and [3].

In the literature, practical computations are often in a bounded domain, while many of the properties of the AC equation were established for the Cauchy problem (1.1), including the convergence to mean curvature flow and the regularity of the solution for very small ε; see [20] and [38]. These properties were proved when the initial value u_0 is a compatible profile describing bulk phase regions separated by transition zones of width $O(\varepsilon)$, i.e.,

$$u_0(x) = \Theta(\Lambda_0(x)/(\sqrt{2}\varepsilon)) \tag{1.3}$$

with $\Lambda_0(x)$ denoting the signed distance to a closed smooth interface Γ_0 (separating the two phases at initial time) and $\Theta : \mathbb{R} \to [-1,1]$ denoting the unique increasing solution of the boundary value problem

$$\begin{cases} -\Theta''(r)+2f(\Theta(r))=0, \quad r\in\mathbb{R}, \\ \lim_{r\to\pm\infty}\Theta(r)=\pm 1. \end{cases} \tag{1.4}$$

Figure 1 illustrates an example of such initial data, with values changing from -1 to 1 in the phase transition zone (shadow region).

It was shown in [38, §2.4] that, for an initial value $u_0\in L^\infty(\mathbb{R}^d)$, the Cauchy problem has a unique mild solution in $L^\infty(\mathbb{R}^d\times[0,T])$. Moreover, if the initial value u_0 is a compatible profile in the form of (1.3), then the mild solution of the Cauchy problem (1.1) is a classical solution with the following properties ([38, §4 and §5]):

(P1) The following spectrum estimate holds:

$$\|\nabla v\|^2_{L^2(\mathbb{R}^d)}+\frac{1}{\varepsilon^2}(f'(u(\cdot,t))v,v)_{\mathbb{R}^d}\geqslant -\lambda\|v\|^2_{L^2(\mathbb{R}^d)} \quad \forall v\in H^1(\mathbb{R}^d)\ \forall t\in[0,T].$$

(P2) The following regularity estimates hold in any bounded domain Ω:

$$\|\partial_t^k u\|_{L^\infty(0,T;W^{m,\infty}(\Omega))}\leqslant C\varepsilon^{-k-m}, \quad 0\leqslant k\leqslant q+1,\ \ 0\leqslant m\leqslant r,$$
$$\|\partial_t^k u\|_{L^\infty(0,T;H^m(\Omega))}\leqslant C\varepsilon^{-k-m+\frac12}, \quad 0\leqslant k\leqslant q+1,\ \ 0\leqslant m\leqslant r,$$

for the solution u of the AC equation (1.1).

In fact, (P1) was proved in [38, Theorem 5.1 and p. 1585]; (P2) is a consequence of the asymptotic expansion [38, (1.17)] (our t corresponds to h^2t therein), which implies $\|\nabla^m\partial_t^k u\|_{L^\infty(\Omega)}=O(\varepsilon^{-k-m})$. Since the function $\partial_t^{k+1}u$ is concentrated in a phase transition zone of width $O(\varepsilon)$ (this can also be seen from the asymptotic expansion), it follows that $\|\nabla^m\partial_t^k u\|_{H^1(\Omega)}=O(\varepsilon^{-k-m+\frac12})$.

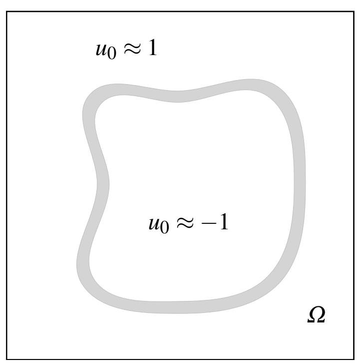

Fig. 1. An initial data that describes bulk phase regions separated by a phase transition zone of width $O(\varepsilon)$.

In view of the discrepancy between theoretical analysis (in the whole space) and practical computation (in a bounded domain), we consider the discretization of the Cauchy problem (1.1) with initial value u_0 a compatible profile of the form (1.3) as follows: we solve an initial-boundary value problem

$$\begin{cases} u_t - \Delta u + \dfrac{1}{\varepsilon^2} f(u) = 0 & \text{in } \ \Omega \times (0,T], \\ u = \phi & \text{on } \ \partial\Omega \times (0,T], \\ u(\cdot,0) = u_0 & \text{in } \ \Omega, \end{cases} \tag{1.5}$$

in a bounded convex polygonal/polyhedral domain $\Omega \subset \mathbb{R}^d$, $d \in \{2,3\}$, with an unknown function ϕ on the boundary $\partial\Omega$, based on the following assumption on the solution of the Cauchy problem (1.1) restricted to Ω:

$$\|\phi - 1\|_{L^\infty(\partial\Omega)} \leqslant C\mathrm{e}^{-c/\varepsilon}. \tag{$\star$}$$

In particular, the solution of the Cauchy problem (1.1) satisfies (1.5) for some function ϕ (i.e., the value of u on $\partial\Omega$) satisfying condition ($\star$) when the domain Ω encloses the phase transition zone with $\mathrm{dist}(\partial\Omega, \Gamma_\varepsilon(t))$ uniformly bounded from below by a positive constant. This is due to the asymptotic expansion [38, (1.17)] and the exponential decay property [38, Theorem 4.2], which imply that the solution tends to 1 exponentially with respect to $\mathrm{dist}(x, \Gamma_\varepsilon(t))/\varepsilon$. Since the solution of (1.5) is exactly the solution of (1.1) restricted to Ω, property (P1) yields

$$\|\nabla v\|_{L^2(\Omega)}^2 + \frac{1}{\varepsilon^2}(f'(u(\cdot,t))v, v) \geqslant -\lambda \|v\|_{L^2(\Omega)}^2 \quad \forall v \in H_0^1(\Omega) \ \forall t \in [0,T], \tag{1.6}$$

since the extension Ev of a $v \in H_0^1(\Omega)$ as a zero function outside Ω is an element of $H^1(\mathbb{R}^d)$.

Let $t_n = n\tau$, $n = 0,1,\dots,N$, be a uniform partition of the time interval $[0,T]$ with stepsize $\tau = T/N$. Let S_h be the Lagrange finite element subspace of $H^1(\Omega)$ consisting of piecewise polynomials of degree $r-1$ associated to a regular and quasi-uniform triangulation of the domain Ω with mesh size h. Let $\mathring{S}_h$ consist of the elements of S_h that vanish on the boundary $\partial\Omega$.

The exact boundary value ϕ of the solution is unknown, but it is known that the solution differs from 1 only by a small function of $O(\mathrm{e}^{-c/\varepsilon})$ on the boundary $\partial\Omega \times [0,T]$. Therefore, for given starting approximations $u_h^0, u_h^1, \dots, u_h^{q-1} \in S_h$ to the nodal values $u(\cdot,t_j)$, $j = 0,1,\dots,q-1$, we discretize (1.5) in time by the q-step BDF method (with $1 \leqslant q \leqslant 5$), with the finite element method in space: find $u_h^n \in S_h$ such that

$$\begin{cases} \Big(\dfrac{1}{\tau}\displaystyle\sum_{j=0}^{q} \delta_j u_h^{n-j}, v_h\Big) + (\nabla u_h^n, \nabla v_h) + \Big(\dfrac{1}{\varepsilon^2} f(u_h^n), v_h\Big) = 0 & \forall v_h \in \mathring{S}_h, \\ u_h^n = 1 & \text{on } \partial\Omega, \end{cases} \tag{1.7}$$

with an approximate boundary condition on $\partial\Omega$, where δ_j, $j = 0,\dots,q$, are the coefficients of the generating polynomial of the q-step BDF method,

$$\delta(\zeta) = \sum_{j=1}^{q} \frac{1}{j}(1-\zeta)^j = \sum_{j=0}^{q} \delta_j \zeta^j; \tag{1.8}$$

see [27, §V.2] (where $\alpha_i = \delta_{q-i}$). The starting approximations $u_h^1, \dots, u_h^{q-1}$ should be computed by other methods (or with smaller stepsizes and mesh sizes); this will not be analyzed in this article.

For sufficiently accurate given starting approximations, we establish an error estimate of $O(\tau^q \varepsilon^{-q-\frac12} + h^r \varepsilon^{-r-\frac12} + \mathrm{e}^{-c/\varepsilon})$ under the stepsize and mesh conditions $\tau = O(\varepsilon^{1+\frac{5}{q}})$ and $h = O(\varepsilon^{1+\frac{5}{r}})$, with a simple expression on the dependence on ε. Our analysis combines the following three techniques, among which the first yields an L^∞-stability result of the BDF methods, which is of independent interest.

First, to estimate the influence of the boundary error, we introduce $\theta_h^n \in S_h$ to be the solution of the linear equation

$$\begin{cases} \Big(\frac{1}{\tau}\sum_{j=0}^{q}\delta_j\theta_h^{n-j}, v\Big) + (\nabla\theta_h^n, \nabla v) = 0 \quad \forall v \in \mathring{S}_h, \\ \theta_h^n = I_h u(\cdot,t_n) - u_h^n \qquad \text{on } \partial\Omega, \end{cases} \quad n = q,\dots,N, \tag{1.9}$$

with starting values

$$\theta_h^j = R_h u(\cdot,t_j) - u_h^j, \quad j = 0,\dots,q-1,$$

where I_h and R_h denote the Lagrange interpolation and Ritz projection operators onto S_h (see §2.3 for their definition and properties).

We need to estimate $\|\theta_h^n\|_{L^\infty(\Omega)}$ in terms of the boundary values $I_h u(\cdot,t_n) - u_h^n$. However, the maximum principle does not hold for high-order BDF methods (1.9) (see [13]). To overcome this difficulty, we prove L^∞-stability of the BDF methods with respect to the boundary data in Lemma 3.2 (a weaker version of the maximum principle).

Second, the analysis of the q-step BDF method requires testing the error equation by $e_h^n - \eta_q e_h^{n-1}$, with $e_h^n = R_h u(\cdot,t_n) - u_h^n - \theta_h^n \in \mathring{S}_h$, where $\eta_1 = \eta_2 = 0$ and $\eta_q \in (0,1)$ for $q \geqslant 3$. In order to use the spectrum estimate (1.6) with such multipliers η_q, we introduce and utilize the following time-dependent inner product and norm on $H_0^1(\Omega)$:

$$\langle v, w\rangle_t := (\nabla v, \nabla w) + \frac{1}{\varepsilon^2}(f'(u(\cdot,t))v, w) + 2\lambda(v,w) \quad \forall v, w \in H_0^1(\Omega), \tag{1.10}$$

$$\|v\|_t := \sqrt{\langle v, v\rangle_t} \quad \forall v \in H_0^1(\Omega), \tag{1.11}$$

in the error analysis of the BDF methods. The spectral estimate (1.6) implies that

$$\|v\|_t^2 \geqslant \lambda\|v\|^2 \quad \forall v \in H_0^1(\Omega) \ \ \forall t \in [0,T]. \tag{1.12}$$

Time-dependent inner products and norms are used in [36] and [5] to establish stability estimates of BDF methods for evolving surface PDEs and for quasi-linear parabolic equations, respectively. In this article, we use time-dependent inner products to remove the exponential dependency on $1/\varepsilon$ by utilizing (1.12), which is a consequence of property (P1).

Third, existence and uniqueness of numerical solutions as well as error estimates are proved by constructing a modified numerical scheme coinciding with the original numerical scheme when the error of the numerical solution is $o(\varepsilon^2)$ in the L^∞-norm. Then, we derive L^∞ error estimates by using discrete maximal L^p-regularity for sufficiently large p. This shows that the L^∞ error is indeed $o(\varepsilon^2)$ under a certain stepsize condition. These results are proved for general $\varepsilon \in [0,1]$ without smallness assumption on ε; see Remark 5.2.

2. Notation and preliminary results

2.1 BDF methods

For $\varphi \in (0,\pi)$, we denote by Σ_φ the closed sector of half-angle $\varphi, \Sigma_\varphi := \{z \in \mathbb{C} : |\arg(z)| \leqslant \varphi\}$. It is well known that the BDF methods are strongly $A(\alpha_q)$-stable with $\alpha_1 = \alpha_2 = 0.5\pi$, $\alpha_3 \approx 0.4779\pi$, $\alpha_4 \approx 0.4075\pi$, and $\alpha_5 \approx 0.2880\pi$; see [27, §V.2]. The $A(\alpha_q)$-stability means that $\delta(\zeta) \in \Sigma_{\pi-\alpha_q}$ for $\zeta \in \mathbb{C}$ and $|\zeta| = 1$, with $\delta(\zeta)$ defined in (1.8). The order of the q-step BDF method is q, i.e.,

$$\sum_{i=0}^{q}(q-i)^\ell\delta_i = \ell q^{\ell-1}, \quad \ell = 0,1,\dots,q. \tag{2.1}$$

These properties will be used in the analysis of method (1.7).

2.2 Generating function of a sequence

The generating function $\tilde{v}$ of a given bounded sequence of functions $v^n, n = 0, 1, \ldots,$ is defined by

$$\tilde{v}(\zeta) = \sum_{n=0}^{\infty} v^n \zeta^n.$$

The generating function is analytic in the unit disk $D = \{z \in \mathbb{C} : |z| < 1\}$.

2.3 Interpolation and L^2 and Ritz projections

We denote by $(\cdot,\cdot)$ and $\|\cdot\|$ the inner product and norm on $L^2(\Omega)$, respectively. The Lagrangian interpolation operator $I_h : C(\overline{\Omega}) \to S_h$ is defined by requiring $I_h u$ to be equal to u at the nodes of finite elements [14, §3.2–3.3]. This interpolation satisfies

$$\|I_h w - w\| \leqslant Ch^r \|w\|_{H^r(\Omega)} \qquad \forall w \in H^r(\Omega) \text{ for } r \geqslant 2, \tag{2.2}$$

$$\|I_h w - w\|_{L^\infty(\Omega)} \leqslant Ch^k \|w\|_{W^{k,\infty}(\Omega)} \quad \forall w \in C(\overline{\Omega}) \cap W^{k,\infty}(\Omega),\ 0 \leqslant k \leqslant r. \tag{2.3}$$

Let $P_h : L^2(\Omega) \to \mathring{S}_h$ be the L^2-orthogonal projection onto the subspace $\mathring{S}_h$, defined by

$$(P_h w, v_h) = (w, v_h) \quad \forall v_h \in \mathring{S}_h,$$

and $R_h : H^1(\Omega) \to S_h$ be the Ritz projection onto the finite element space, defined by

$$\begin{cases} (\nabla R_h w, \nabla v_h) = (\nabla w, \nabla v_h) & \forall v_h \in \mathring{S}_h, \\ R_h w = I_h w & \text{on } \partial\Omega. \end{cases}$$

It is easy to see that R_h maps $H_0^1(\Omega)$ into $\mathring{S}_h$ (preserving the zero boundary condition).

Both the L^2 and Ritz projections are bounded in $L^\infty(\Omega)$, i.e.,

$$\|P_h w\|_{L^\infty(\Omega)} \leqslant C\|w\|_{L^\infty(\Omega)} \qquad \forall w \in L^\infty(\Omega), \tag{2.4}$$

$$\|R_h w\|_{L^\infty(\Omega)} \leqslant C\ell_h \|w\|_{L^\infty(\Omega)} \qquad \forall w \in H^1(\Omega) \cap L^\infty(\Omega), \tag{2.5}$$

where

$$\ell_h = \begin{cases} \ln(2 + 1/h), & r = 1, \\ 1, & r \geqslant 2. \end{cases} \tag{2.6}$$

For these estimates we refer to [43, Lemma 6.1] and [33,40], and [32, Theorem 5.1], respectively (for both 2D and 3D cases). The L^∞-stability of the Ritz projection implies also the L^∞ error estimate:

$$\|R_h w - w\|_{L^\infty(\Omega)} \leqslant C\ell_h h^\alpha \|w\|_{C^\alpha(\overline{\Omega})} \quad \forall w \in H^1(\Omega) \cap C^\alpha(\overline{\Omega}) \quad \forall \alpha \in [0,1]. \tag{2.7}$$

2.4 Maximum-norm estimates

Let $\Delta_h : \mathring{S}_h \to \mathring{S}_h$ be the discrete Laplacian operator defined by

$$(\Delta_h w_h, v_h) = -(\nabla w_h, \nabla v_h) \quad \forall w_h, v_h \in \mathring{S}_h.$$

Then, for any given $\varphi \in (\frac{\pi}{2}, \pi)$, the following resolvent estimate holds for all complex numbers z in the sector Σ_φ:

$$\|z(z - \Delta_h)^{-1} P_h\|_{L^\infty(\Omega) \to L^\infty(\Omega)} \leqslant C_\varphi. \tag{2.8}$$

This result was proved in [33, Theorem 15] (with a logarithmic factor) and [34, Theorem 3.1].

2.5 Sobolev and Besov spaces

For $1 \leqslant p \leqslant \infty$ and an integer $k \geqslant 0$, we denote by $W^{k,p}(\Omega)$ the conventional Sobolev space of functions defined in Ω; see [1]. For $k \geqslant 1, W_0^{k,p}(\Omega)$ denotes the completion of $C_0^\infty(\Omega)$ in $W^{k,p}(\Omega)$. In particular, $W_0^{1,p}(\Omega)$ consists of functions in $W^{1,p}(\Omega)$ with zero traces on the boundary $\partial\Omega$. The abbreviations $H^k(\Omega) = W^{k,2}(\Omega)$ and $H_0^k(\Omega) = W_0^{k,2}(\Omega)$ will be used as usual.

For $s \in [0,2]$, we let $\dot{H}^s(\Omega) \subset L^2(\Omega)$ denote the Hilbert space induced by the norm

$$\|\varphi\|_{\dot{H}^s(\Omega)} := \Big(\sum_{j=1}^{\infty} \lambda_j^{2s} |(\varphi, \phi_j)|^2\Big)^{1/2},$$

where ϕ_j and $\lambda_j, j = 1,2,\dots,$ are the $L^2(\Omega)$-orthonormal eigenfunctions and eigenvalues of the Dirichlet Laplacian operator $-\Delta_D$, arranged in nondecreasing order, $\lambda_j \leqslant \lambda_{j+1}$. In particular, $\dot{H}^0(\Omega) = L^2(\Omega)$, $\dot{H}^1(\Omega) = H_0^1(\Omega)$ and $\dot{H}^2(\Omega) = H^2(\Omega) \cap H_0^1(\Omega)$; see [43, chapter 3].

For $s \in (0,2)$, the Besov space

$$B^{s;2,p}(\Omega) = (\dot{H}^{-2}(\Omega), \dot{H}^2(\Omega))_{\frac{s+2}{4},p}$$

is defined as the real interpolation space between two Sobolev spaces; see [1, §7.32]. If $0 \leqslant s_1 < s < s_2 \leqslant 2$ and $(1-\alpha)s_1 + \alpha s_2 = s$, then the following reiteration property holds:

$$B^{s;2,p}(\Omega) = (\dot{H}^{s_1}(\Omega), \dot{H}^{s_2}(\Omega))_{\alpha,p}.$$

If $s_2 > s_1$, then $B^{s_2;2,p}(\Omega) \hookrightarrow B^{s_1;2,q}(\Omega)$ for all $1 \leqslant p,q \leqslant \infty$. In particular, we will use the property $B^{s;2,p}(\Omega) \hookrightarrow L^2(\Omega)$ for $s > 0$ and $1 \leqslant p \leqslant \infty$.

2.6 Some abbreviations

For the solution $u(x,t)$ defined in $\Omega \times [0,T]$, we shall use the abbreviation $u(t) = u(\cdot,t)$. Throughout this article, we denote by C a generic positive constant independent of ε, τ and h (not necessarily the same at different occurrences).

3. Maximum-norm estimate for θ_h^n

In this section, we present an estimate for the solutions θ_h^n of (1.9). The result will be used in the next two sections to prove existence, uniqueness and convergence of the numerical solutions.

We need the following estimate for finite element solutions of an elliptic equation with a complex coefficient.

Lemma 3.1 For $z \in \Sigma_\varphi$ with $\varphi \in (\frac{\pi}{2}, \pi)$, the complex-valued finite element solution $u_h \in S_h$ of the boundary value problem

$$\begin{cases} (zu_h, v_h) + (\nabla u_h, \nabla v_h) = 0 & \forall\, v_h \in \mathring{S}_h, \\ u_h = I_h g & \text{on } \partial\Omega, \end{cases} \tag{3.1}$$

with $g \in C(\partial\Omega \to \mathbb{C})$, satisfies

$$\|u_h\| \leqslant C_\varphi \|g\|_{L^\infty(\partial\Omega)},$$

where the constant C_φ is independent of z and h.

Proof. It is known that the finite element solution $u_{g,h} \in S_h$ of the boundary value problem

$$\begin{cases} (\nabla u_{g,h}, \nabla v_h) = 0 & \forall v_h \in \mathring{S}_h, \\ u_{g,h} = I_h g & \text{on } \partial\Omega, \end{cases} \tag{3.2}$$

satisfies a weak maximum principle (cf. [40] and [32] for 2D and 3D cases, respectively), i.e.,

$$\|u_{g,h}\|_{L^\infty(\Omega)} \leqslant C\|I_h g\|_{L^\infty(\partial\Omega)} \leqslant C\|g\|_{L^\infty(\partial\Omega)}. \tag{3.3}$$

Now, $u_h - u_{g,h} \in \mathring{S}_h$ is the finite element solution of a homogeneous Dirichlet boundary value problem, i.e.,

$$(z(u_h - u_{g,h}), v_h) + (\nabla(u_h - u_{g,h}), \nabla v_h) = -(z u_{g,h}, v_h) \quad \forall v_h \in \mathring{S}_h.$$

This can be equivalently written as

$$(z - \Delta_h)(u_h - u_{g,h}) = -zP_h u_{g,h},$$

where P_h is the L^2 projection operator onto $\mathring{S}_h$, and $\Delta_h : \mathring{S}_h \to \mathring{S}_h$ is the discrete Laplacian operator; see §2.4. Hence, we have

$$\|u_h - u_{g,h}\|_{L^\infty(\Omega)} = \|z(z - \Delta_h)^{-1} P_h u_{g,h}\|_{L^\infty(\Omega)} \leqslant C\|u_{g,h}\|_{L^\infty(\Omega)},$$

where the last inequality is due to (2.8). In view of (3.3), this estimate implies

$$\|u_h\|_{L^\infty(\Omega)} \leqslant C\|u_{g,h}\|_{L^\infty(\Omega)} \leqslant C\|g\|_{L^\infty(\partial\Omega)},$$

which is the desired result. □

Lemma 3.2 The solution of (1.9) satisfies the following estimate:

$$\max_{0\leqslant n\leqslant N} \|\theta_h^n\| \leqslant C\ell_\tau \max_{q\leqslant n\leqslant N} \|u(t_n) - u_h^n\|_{L^\infty(\partial\Omega)} + C\ell_h \max_{0\leqslant n\leqslant q-1} \|u(t_n) - u_h^n\|_{L^\infty(\Omega)},$$

where ℓ_h is defined in (2.6) and $\ell_\tau = \log(2 + 1/\tau)$.

Proof. We decompose the solution of (1.9) into

$$\theta_h^n = \vartheta_h^n + \Theta_h^n,$$

where $\Theta_h^n \in \mathring{S}_h$ and $\vartheta_h^n \in S_h$, $n = q, \dots, N$, are the finite element solutions of the following variational problems:

$$\Big(\frac{1}{\tau}\sum_{j=0}^{q} \delta_j \Theta_h^{n-j}, v_h\Big) + (\nabla\Theta_h^n, \nabla v_h) = 0 \quad \forall v_h \in \mathring{S}_h, \tag{3.4}$$

and

$$\begin{cases} \Big(\dfrac{1}{\tau}\displaystyle\sum_{j=0}^{q} \delta_j \vartheta_h^{n-j}, v_h\Big) + (\nabla\vartheta_h^n, \nabla v_h) = 0 & \forall v_h \in \mathring{S}_h, \\ \vartheta_h^n = g_h^n & \text{on } \partial\Omega, \end{cases} \tag{3.5}$$

respectively, with the starting values

$$\Theta_h^j = R_h u(\cdot, t_j) - u_h^j, \quad \vartheta_h^j = 0 \quad \text{and} \quad g_h^j := 0 \quad \text{for} \quad j = 0, \dots, q-1,$$

and boundary values

$$g_h^n := I_h u(\cdot, t_n) - u_h^n \quad \text{for} \quad n \geqslant q.$$

We note that Θ_h^n account for the starting errors, while ϑ_h^n account for the errors on the boundary $\partial\Omega$.

We express the solution of (3.4) in terms of the starting values (cf. [43, (10.10)])

$$\Theta_h^n = \sum_{m=0}^{q-1} \boldsymbol{\beta}_{n,m}(R_h u(\cdot,t_m) - u_h^m), \quad \text{for } n \geqslant q, \tag{3.6}$$

where $\boldsymbol{\beta}_h^{n,m} = -\sum_{j=q-m}^{q} \delta_j \boldsymbol{\beta}_h^{n-m-j}$ with the operators $\boldsymbol{\beta}_h^n$ determined by the power series expansion

$$(\delta(\zeta) - \tau\Delta_h)^{-1} = \sum_{n=0}^{\infty} \boldsymbol{\beta}_h^n \zeta^n. \tag{3.7}$$

There exists a $\kappa \in (0, \frac{\pi}{2})$ (independent of τ, cf. [28, Lemma B.1]) such that

$$\delta(\mathrm{e}^{z\tau}) \in \Sigma_{\pi-\frac{1}{2}\alpha_q} \qquad \forall z \in \Sigma_{\kappa+\frac{\pi}{2}}, \tag{3.8}$$

$$C_1|z| \leqslant |\delta(\mathrm{e}^{z\tau})| \leqslant C_2|z| \qquad \forall z \in \Sigma_{\kappa+\frac{\pi}{2}}, \tag{3.9}$$

$$|z - \tau^{-1}\delta(\mathrm{e}^{z\tau})| \leqslant C|z|^2\tau \qquad \forall z \in \Sigma_{\kappa+\frac{\pi}{2}}. \tag{3.10}$$

Using Cauchy's integral formula, we have

$$\begin{aligned}\boldsymbol{\beta}_h^n &= \frac{1}{2\pi\mathrm{i}} \int_{|\zeta|=\frac{1}{2}} (\delta(\zeta) - \tau\Delta_h)^{-1} \zeta^{-n-1} \mathrm{d}\zeta \\ &= \frac{1}{2\pi\mathrm{i}} \int_{\Gamma^\tau} \mathrm{e}^{t_n z} (\delta(\mathrm{e}^{-z\tau}) - \tau\Delta_h)^{-1} \mathrm{d}z \quad \text{(by a change of variable } \zeta = \mathrm{e}^{-z\tau}\text{)},\end{aligned}$$

where $\Gamma^\tau = \{\frac{1}{\tau}\ln 2 + \mathrm{i}s : |s| \leqslant \frac{\pi}{\tau}\}$. Since $\mathrm{e}^{t_n z}(\delta(\mathrm{e}^{-z\tau}) - \tau\Delta_D)^{-1}$ is analytic in the region enclosed by Γ^τ, $\Gamma^\tau_{\kappa+\frac{\pi}{2}}$ and $z = \mathbb{R} \pm \mathrm{i}\frac{\pi}{\tau}$, with

$$\begin{aligned}\Gamma^\tau_{\kappa+\frac{\pi}{2}} =& \left\{ z \in \mathbb{C} : \arg(z) = \kappa + \frac{\pi}{2}, \frac{1}{2\tau}\ln 2 \leqslant |z| \leqslant \frac{\pi}{\tau\cos(\kappa)} \right\} \\ & \bigcup \left\{ z \in \mathbb{C} : |\arg(z)| < \kappa + \frac{\pi}{2}, |z| = \frac{1}{2\tau}\ln 2 \right\},\end{aligned}$$

and the integration on the two lines $z = \mathbb{R} \pm \mathrm{i}\frac{\pi}{\tau}$ cancels each other, it follows that the integration contour Γ^τ can be further deformed to $\Gamma^\tau_{\kappa+\frac{\pi}{2}}$. In other words,

$$\boldsymbol{\beta}_h^n = \frac{1}{2\pi\mathrm{i}} \int_{\Gamma^\tau_{\kappa+\frac{\pi}{2}}} \mathrm{e}^{t_n z} (\delta(\mathrm{e}^{-z\tau}) - \tau\Delta_h)^{-1} \mathrm{d}z. \tag{3.11}$$

Now (2.8) and (3.9) imply

$$\|\big(\tau^{-1}\delta(\mathrm{e}^{-z\tau}) - \Delta_h\big)^{-1}\|_{L^\infty(\Omega)\to L^\infty(\Omega)} \leqslant C|\tau^{-1}\delta(\mathrm{e}^{-z\tau})|^{-1} \leqslant C\tau|z|^{-1}. \tag{3.12}$$

Therefore,

$$\begin{aligned}\|\boldsymbol{\beta}_h^n\|_{L^\infty(\Omega)\to L^\infty(\Omega)} &= \left\| \frac{1}{2\pi\mathrm{i}} \int_{\Gamma^\tau_{\kappa+\frac{\pi}{2}}} \mathrm{e}^{t_n z} (\delta(\mathrm{e}^{-z\tau}) - \tau\Delta_h)^{-1} \mathrm{d}z \right\|_{L^\infty(\Omega)\to L^\infty(\Omega)} \\ &\leqslant C \int_{\Gamma^\tau_{\kappa+\frac{\pi}{2}}} |z|^{-1} \mathrm{e}^{-\tau \mathrm{Re}(z)} |\mathrm{d}z| \leqslant C.\end{aligned}$$

This estimate and expression (3.6) imply that

$$\begin{aligned} \|\Theta_h^n\|_{L^\infty(\Omega)} &\leqslant C\sum_{m=0}^{q-1}\|R_hu(t_m)-u_h^m\|_{L^\infty(\Omega)} \\ &\leqslant C\ell_h\sum_{m=0}^{q-1}\|u(t_m)-u_h^m\|_{L^\infty(\Omega)}, \quad \text{for } n\geqslant q, \end{aligned} \tag{3.13}$$

where we have used the L^∞ stability (2.5) in deriving the last inequality.

It remains to estimate $\|\vartheta_h^n\|_{L^2(\Omega)}$. To this end, we multiply (3.5) by ζ^n and sum up the resulting relations for $n=q,q+1,\dots$. With the notation $\tilde\vartheta_h(\zeta)=\sum_{n=q}^\infty \vartheta_h^n\zeta^n$, this yields

$$\begin{cases} (\tau^{-1}\delta(\zeta)\tilde\vartheta_h(\zeta),v_h)+(\nabla\tilde\vartheta_h(\zeta),\nabla v_h)=0 & \forall v_h\in\mathring{S}_h,\\ \tilde\vartheta(\zeta)=\tilde g_h(\zeta) & \text{on } \partial\Omega. \end{cases} \tag{3.14}$$

Let $M_h\big(\tau^{-1}\delta(\zeta)\big)$ denote the operator which maps $\tilde g_h(\zeta)$ to $\tilde\vartheta_h(\zeta)$, defined by (3.14),

$$\tilde\vartheta_h(\zeta)=M_h\big(\tau^{-1}\delta(\zeta)\big)\tilde g_h(\zeta).$$

Then,

$$\vartheta_h^n=\frac{1}{2\pi\mathrm{i}}\int_{|\zeta|=1}\tilde\vartheta_h(\zeta)\zeta^{-n-1}\mathrm{d}\zeta=\frac{1}{2\pi\mathrm{i}}\int_{|\zeta|=1}M_h\big(\tau^{-1}\delta(\zeta)\big)\tilde g_h(\zeta)\zeta^{-n-1}\mathrm{d}\zeta=\sum_{j=0}^n M_{n-j}g_h^j,$$

with

$$M_n=\frac{1}{2\pi\mathrm{i}}\int_{|\zeta|=1}M_h\big(\tau^{-1}\delta(\zeta)\big)\zeta^{-n-1}\mathrm{d}\zeta=\frac{\tau}{2\pi\mathrm{i}}\int_{\Gamma^\tau_{\kappa+\frac{\pi}{2}}}M_h\big(\tau^{-1}\delta(\mathrm{e}^{-\tau z})\big)\mathrm{e}^{t_nz}\mathrm{d}z.$$

Since $\tau^{-1}\delta(\mathrm{e}^{-\tau z})\in\Sigma_{\pi-\alpha_q}$, Lemma 3.1 implies

$$\|M_h\big(\tau^{-1}\delta(\mathrm{e}^{-\tau z})\big)\|_{L^\infty(\partial\Omega)\to L^\infty(\Omega)}\leqslant C.$$

This further implies

$$\begin{aligned} &\|M_n\|_{L^\infty(\partial\Omega)\to L^\infty(\Omega)}\\ &\leqslant\int_{\Gamma^\tau_{\kappa+\frac{\pi}{2}}}C\tau\big\|M_h\big(\tau^{-1}\delta(\mathrm{e}^{-\tau z})\big)\big\|_{L^\infty(\partial\Omega)\to L^\infty(\Omega)}\mathrm{e}^{t_n\mathrm{Re}(z)}|\mathrm{d}z|\\ &\leqslant Cn^{-1}. \end{aligned}$$

Hence, we have

$$\begin{aligned} \|\vartheta_h^n\|_{L^\infty(\Omega)} &=\Big\|\sum_{j=0}^n M_{n-j}g_h^j\Big\|_{L^\infty(\Omega)}\\ &\leqslant\sum_{j=0}^n\|M_{n-j}\|_{L^\infty(\partial\Omega)\to L^\infty(\Omega)}\|g_h^j\|_{L^\infty(\partial\Omega)}\\ &\leqslant C\ell_\tau\max_{0\leqslant j\leqslant n}\|g_h^j\|_{L^\infty(\partial\Omega)}. \end{aligned} \tag{3.15}$$

The desired result of Lemma 3.2 follows from the estimates (3.13) and (3.15). □

Lemma 3.2 and ($\star$) immediately imply the following result.

Proposition 3.1 If $\tau\geqslant c_\star\mathrm{e}^{-\gamma/\varepsilon}$ and $h\geqslant c_\star\mathrm{e}^{-\gamma/\varepsilon}$ for some positive numbers γ and $c_\star$, then the solutions of (1.9) satisfy the following estimate:

$$\max_{0\leqslant n\leqslant N}\|\theta_h^n\|_{L^\infty(\Omega)} \leqslant C\mathrm{e}^{-c/\varepsilon} + C\ell_h \max_{0\leqslant j\leqslant q-1}\|u(t_j)-u_h^j\|_{L^\infty(\Omega)}. \tag{3.16}$$

4. Existence and uniqueness of solutions of a modified equation

Let $\chi:\mathbb{R}\to\mathbb{R}$ be a smooth cut-off function such that

$$\chi(s)=\begin{cases} s & \text{for } |s|\leqslant 1,\\ 0 & \text{for } |s|\geqslant 3,\end{cases} \qquad |\chi(s)|\leqslant 1 \text{ and } |\chi'(s)|\leqslant 1\ \forall s\in\mathbb{R},$$

and define a nonlinear functional $f_\chi(\cdot,t_n):L^2(\Omega)\to L^2(\Omega)$ by

$$f_\chi(\upsilon,t_n)=f(u(t_n))+f'(u(t_n))(\upsilon-u(t_n))+g_\chi(v,t_n)\varepsilon^4\left[\chi\left(\frac{\upsilon-u(t_n)}{\varepsilon^2}\right)\right]^2 \tag{4.1}$$

with

$$g_\chi(\upsilon,t_n)=\int_0^1 f''\left(u(t_n)+\vartheta\varepsilon^2\chi\left(\frac{\upsilon-u(t_n)}{\varepsilon^2}\right)\right)\mathrm{d}\vartheta.$$

Then, we have the following estimates

$$\|g_\chi(\upsilon,t_n)\|_{L^\infty(\Omega)}\leqslant 6(1+\varepsilon^2)\quad \forall\,\upsilon\in L^2(\Omega)$$

and, for $\upsilon_1,\upsilon_2\in L^2(\Omega)$,

$$|f_\chi(\upsilon_1,t_n)-f_\chi(\upsilon_2,t_n)|\leqslant(2+18\varepsilon^4+12\varepsilon^2)|\upsilon_1-\upsilon_2|\quad \text{a.e. in } \Omega. \tag{4.2}$$

Indeed, the former estimate is a consequence of $f''(s)=6s$ and $\|u(t_n)\|_{L^\infty(\Omega)}\leqslant 1$, while the latter follows from

$$\begin{aligned}
&|f_\chi(\upsilon_1,t_n)-f_\chi(\upsilon_2,t_n)|\\
&\leqslant|f'(u(t_n))|\,|\upsilon_1-\upsilon_2|+\Big(\max_{\xi\in\mathbb{R}}|\partial_\xi g_\chi(\xi,t_n)|\varepsilon^4+2\max_{\xi\in\mathbb{R}}|g_\chi(\xi,t_n)|\varepsilon^2\Big)|\upsilon_1-\upsilon_2|\\
&\leqslant 2|\upsilon_1-\upsilon_2|+\Big(\max_{|s|\leqslant|u|+\varepsilon^2}|f'''(s)|\varepsilon^4+2\max_{|s|\leqslant|u|+\varepsilon^2}|f''(s)|\varepsilon^2\Big)|\upsilon_1-\upsilon_2|\\
&\leqslant(2+6\varepsilon^4+12(1+\varepsilon^2)\varepsilon^2)|\upsilon_1-\upsilon_2|;
\end{aligned}$$

note that in the last two inequalities we used the facts that $f'''(s)=6, f''(s)=6s$ and $\|u(t_n)\|_{L^\infty(\Omega)}\leqslant 1$.

If $\|\upsilon-u(t_n)\|_{L^\infty(\Omega)}\leqslant\varepsilon^2$, then $\varepsilon^2\chi\big(\frac{\upsilon-u(t_n)}{\varepsilon^2}\big)=\upsilon-u(t_n)$ and therefore

$$\begin{aligned}
f_\chi(\upsilon,t_n)&=f(u(t_n))+f'(u(t_n))(\upsilon-u(t_n))\\
&\qquad+(\upsilon-u(t_n))^2\int_0^1 f''\big(u(t_n)+\vartheta(\upsilon-u(t_n))\big)\mathrm{d}\vartheta\\
&=f(\upsilon),
\end{aligned}$$

where the last equality is Taylor's formula.

For given $u_h^{n-j}\in S_h,\ j=1,\ldots,q$, we denote by $M:S_h\to S_h$ the map from $\upsilon_h\in S_h$ to $w_h\in S_h$ defined by

$$\begin{cases}\left(\dfrac{1}{\tau}\delta_0 w_h,\phi_h\right)+(\nabla w_h,\nabla\phi_h)+\left(\dfrac{1}{\varepsilon^2}f_\chi(\upsilon_h,t_n),\phi_h\right)=-\left(\dfrac{1}{\tau}\displaystyle\sum_{j=1}^q\delta_j u_h^{n-j},\phi_h\right) & \forall\,\phi_h\in\mathring{S}_h,\\ w_h=1 & \text{on } \partial\Omega.\end{cases}$$

If $Mv_h^{(1)} = w_h^{(1)}$ and $Mv_h^{(2)} = w_h^{(2)}$, then

$$\begin{cases} \frac{\delta_0}{\tau}(w_h^{(1)} - w_h^{(2)}) - \Delta_h(w_h^{(1)} - w_h^{(2)}) = -\frac{1}{\varepsilon^2}P_h\big(f_\chi(v_h^{(1)},t_n) - f_\chi(v_h^{(2)},t_n)\big) & \text{in } \Omega, \\ w_h^{(1)} - w_h^{(2)} = 0 & \text{on } \partial\Omega. \end{cases}$$

Testing this equation by $w_h^{(1)} - w_h^{(2)}$ and using (4.2), we obtain

$$\frac{\delta_0}{\tau}\|w_h^{(1)} - w_h^{(2)}\|^2 + \|\nabla(w_h^{(1)} - w_h^{(2)})\|^2 \leqslant \frac{2+18\varepsilon^4+12\varepsilon^2}{\varepsilon^2}\|v_h^{(1)} - v_h^{(2)}\|\,\|w_h^{(1)} - w_h^{(2)}\|.$$

If $\tau \leqslant \frac{\delta_0}{4(1+9\varepsilon^4+6\varepsilon^2)}\varepsilon^2$, then

$$\|w_h^{(1)} - w_h^{(2)}\| \leqslant \frac{1}{2}\|v_h^{(1)} - v_h^{(2)}\|,$$

which implies that the map M is a contraction on S_h. By the Banach fixed point theorem, M has a unique fixed point. Therefore, we have the following lemma.

Lemma 4.1 Let $\tau \leqslant \frac{\delta_0}{4(1+9\varepsilon^4+6\varepsilon^2)}\varepsilon^2$. Then, given $u_h^{n-j} \in S_h, j = 1,\dots,q$, the modified equation

$$\begin{cases} \frac{1}{\tau}\sum_{j=0}^{q}\delta_j u_h^{n-j} - \Delta u_h^n + \frac{1}{\varepsilon^2}f_\chi(u_h^n,t_n) = 0 & \text{in } \Omega, \\ u_h^n = 1 & \text{on } \partial\Omega, \end{cases} \tag{4.3}$$

has a unique solution $u_h^n \in S_h$.

Existence and uniqueness of solutions to the original scheme (1.7) are proved in the next section based on Lemma 4.1 and a maximum norm error estimate for the modified equation (4.3).

5. Error estimate

In this section, we prove the following theorem, which is the main result of this article.

Theorem 5.1 Let $\varepsilon \in (0,1]$ and let the initial value u_0 be a compatible profile of the form (1.3), so that properties (P1)–(P2) hold. Let γ and $c_\star$ be any fixed positive constants, and let $1 \leqslant q \leqslant 5$.

Assume that the given starting values $u_h^j, j = 0,\dots,q-1$, are sufficiently accurate, i.e.,

$$\max_{0\leqslant j\leqslant q-1}\|u(t_j) - u_h^j\|_{L^\infty(\Omega)} \leqslant C(\tau^q\varepsilon^{-q} + h^r\varepsilon^{-r}). \tag{5.1}$$

Then, under assumption ($\star$) and the condition

$$c_\star \mathrm{e}^{-\gamma/\varepsilon} \leqslant \tau \leqslant \frac{\delta_0}{4(1+9\varepsilon^4+6\varepsilon^2)}\varepsilon^{1+\frac{5}{q}}, \quad c_\star \mathrm{e}^{-\gamma/\varepsilon} \leqslant h \leqslant \frac{\delta_0}{4(1+9\varepsilon^4+6\varepsilon^2)}\varepsilon^{1+\frac{5}{r}}, \tag{5.2}$$

equation (1.7) has a unique solution $u_h^n \in S_h$ for $n = q,\dots,N$, and u_h^n satisfies the following error estimate:

$$\max_{q\leqslant n\leqslant N}\|u(t_n) - u_h^n\| \leqslant C(\mathrm{e}^{-c/\varepsilon} + \tau^q\varepsilon^{-q-\frac{1}{2}} + h^r\varepsilon^{-r-\frac{1}{2}}). \tag{5.3}$$

Remark 5.1 If $r = q = 5$, then $1+\frac{5}{q} = 1+\frac{5}{r} = 2$, and therefore (5.2) is satisfied when $\tau, h \leqslant \delta_0\varepsilon^2/64$. In particular, our result implies that the five-step BDF method can have an error bound of $O(\varepsilon^{4.5})$ under the stepsize condition $\tau = O(\varepsilon^2)$.

Remark 5.2 To prove Theorem 5.1, we shall show that there exists a constant $\varepsilon_\star > 0$ such that (5.3) holds for $\varepsilon \in (0, \varepsilon_\star]$. If $\varepsilon \in [\varepsilon_\star, 1]$, then the parameter ε in problem (1.5) is not small. In this case, the proof of Theorem 5.1 is standard and the details are omitted. In particular, if $\varepsilon \in [\varepsilon_\star, 1]$, then the numerical scheme (1.7) possesses a unique solution $u_h^n \in S_h$ for $\tau < \delta_0 \varepsilon_\star^2$ (because $\varepsilon^{-2} f'(\xi) = \varepsilon^{-2}(3\xi^2 - 1) \geqslant -\varepsilon_\star^{-2}$). Testing (1.7) by $u_h^n - \eta_q u_h^{n-1}$ and using the Nevanlinna–Odeh multiplier technique immediately yields

$$\max_{q \leqslant n \leqslant N} \|u_h^n\| \leqslant C,$$

which implies

$$\max_{q \leqslant n \leqslant N} \|u(t_n) - u_h^n\| \leqslant C \leqslant (C e^{c/\varepsilon_\star}) e^{-c/\varepsilon} + C\tau^q \varepsilon^{-q-\frac{1}{2}} + Ch^r \varepsilon^{-r-\frac{1}{2}}.$$

Hence, estimate (5.3) is valid for all $\varepsilon \in (0, 1]$.

We will use the following result from Dahlquist's G-stability theory in the proof of Theorem 5.1.

Lemma 5.1 (Dahlquist [18]; see also [7] and [27, §V.6]) Let $\delta(\zeta) = \delta_q \zeta^q + \cdots + \delta_0$ and $\mu(\zeta) = \mu_q \zeta^q + \cdots + \mu_0$ be polynomials of degree at most q (and at least one of them of degree q) that have no common divisor. Let $(\cdot, \cdot)$ be a real inner product. If

$$\operatorname{Re} \frac{\delta(\zeta)}{\mu(\zeta)} > 0 \quad \text{for } |\zeta| < 1,$$

then there exists a positive definite symmetric matrix $G = (g_{ij}) \in \mathbb{R}^{q,q}$ such that for $\upsilon^0, \ldots, \upsilon^q$ in the real inner product space,

$$\Big(\sum_{i=0}^{q} \delta_i \upsilon^{q-i}, \sum_{j=0}^{q} \mu_j \upsilon^{q-j} \Big) \geqslant \sum_{i,j=1}^{q} g_{ij} (\upsilon^i, \upsilon^j) - \sum_{i,j=1}^{q} g_{ij} (\upsilon^{i-1}, \upsilon^{j-1}).$$

In combination with the preceding result for the multiplier $\mu(\zeta) = 1 - \eta_q \zeta$, the following property of BDF methods up to order 5 becomes important.

Lemma 5.2 (Nevanlinna & Odeh [39]) For $q \leqslant 5$, there exists a multiplier $0 \leqslant \eta_q < 1$ such that for $\delta(\zeta) = \sum_{\ell=1}^{q} \frac{1}{\ell}(1-\zeta)^\ell$,

$$\operatorname{Re} \frac{\delta(\zeta)}{1 - \eta_q \zeta} > 0 \quad \text{for } |\zeta| < 1.$$

The smallest possible values of η_q are

$$\eta_1 = \eta_2 = 0, \ \eta_3 = 0.0836, \ \eta_4 = 0.2878, \ \eta_5 = 0.8160.$$

Precise expressions for the optimal multipliers for the BDF methods of orders 3,4, and 5 are given in [2].

5.1 Consistency errors

The consistency error d^n of the semi-discrete BDF method is given by

$$d^n = \frac{1}{\tau} \sum_{j=0}^{q} \delta_j u(t_{n-j}) - \partial_t u(t_n). \tag{5.4}$$

By Taylor expanding about t_{n-q} and using the order conditions (2.1), we have

$$d^n = \frac{1}{q!}\left[\frac{1}{\tau}\sum_{j=0}^{q}\delta_j\int_{t_{n-q}}^{t_{n-j}}(t_{n-j}-s)^q\partial_t^{q+1}u(s)\,ds - q\int_{t_{n-q}}^{t_n}(t_n-s)^{q-1}\partial_t^{q+1}u(s)\,ds\right];$$

thus, under obvious regularity requirements, we obtain the desired optimal order consistency estimate

$$\left(\tau\sum_{n=q}^{N}\|d^n\|^2\right)^{\frac{1}{2}} \leqslant C\tau^q\|\partial_t^{q+1}u(t)\|_{L^2(0,T;L^2(\Omega))} \leqslant C\tau^q\varepsilon^{-q-\frac{1}{2}}; \tag{5.5}$$

we used assumption (P2) in the last inequality.

In addition to d^n, the following consistency error (due to spatial discretization) will also appear in our error estimation:

$$q^n = (R_h - P_h)\frac{1}{\tau}\sum_{j=0}^{q}\delta_j u(t_n).$$

Thanks to the regularity property (P2), we have

$$\|q^n\|_{L^2(\Omega)} \leqslant Ch^r\|\partial_t u(t)\|_{L^2(0,T;H^r(\Omega))} \leqslant Ch^r\varepsilon^{-r-\frac{1}{2}}. \tag{5.6}$$

Similarly, the Ritz projection error $\rho_h^n = u(t_n) - R_h u(t_n)$ satisfies

$$\|\rho_h^n\|_{L^2(\Omega)} \leqslant Ch^r\|u(t)\|_{L^2(0,T;H^r(\Omega))} \leqslant Ch^r\varepsilon^{-r+\frac{1}{2}}. \tag{5.7}$$

5.2 Proof of Theorem 5.1

Let $u_h^n \in S_h$ be the unique solution of the modified equation (4.3). We shall prove that

$$u_h^n \in B_\varepsilon(t_n) := \{\upsilon_h \in S_h : \|\upsilon_h - u(t_n)\|_{L^\infty(\Omega)} \leqslant \varepsilon^2\};$$

therefore, $f_\chi(u_h^n, t_n) = f(u_h^n)$ and thus u_h^n is actually a solution of (1.7). Then, the uniqueness result in Lemma 4.1 implies that (1.7) has a unique solution in $B_\varepsilon(t_n)$.

Lemma 3.2 and assumptions ($\star$) and (5.1) imply

$$\max_{0\leqslant n\leqslant N}\|\theta_h^n\| \leqslant C(\mathrm{e}^{-c/\varepsilon} + \tau^q\varepsilon^{-q-\frac{1}{2}} + h^{-r-\frac{1}{2}}). \tag{5.8}$$

Let $e_h^n := R_h u(t_n) - u_h^n - \theta_h^n, n = q,\dots,N$, denote the error of the numerical solutions, with $e_h^j = 0, j = 0,\dots,q-1$, and $e_h^n \in \mathring{S}_h, n = q,\dots,N$. Then, we have the decomposition

$$u(t_n) - u_h^n = e_h^n + \theta_h^n + \rho_h^n. \tag{5.9}$$

Adding (4.3) and (1.9), and subtracting the result from the consistency equation

$$\left(\frac{1}{\tau}\sum_{j=0}^{q}\delta_j u(t_{n-j}), \upsilon_h\right) + \big(\nabla u(t_n), \nabla\upsilon_h\big) + \left(\frac{1}{\varepsilon^2}f_\chi(u(t_n), t_n), \upsilon_h\right) = \big(d^n, \upsilon_h\big),$$

cf. (5.4), we obtain the error equation

$$\frac{1}{\tau}\sum_{j=0}^{q}\delta_j e_h^{n-j} - \Delta_h e_h^n + \frac{1}{\varepsilon^2}P_h\big[f_\chi(u(t_n), t_n) - f_\chi(u_h^n, t_n)\big] = P_h d^n + q^n,$$

with d^n and q^n defined in §5.1. In view of (4.1) and the error decomposition (5.9), we have

$$\begin{aligned}&\frac{1}{\tau}\sum_{j=0}^{q}\delta_j e_h^{n-j}-\Delta_h e_h^n\\&\quad+P_h\frac{f'(u(t_n))}{\varepsilon^2}(e_h^n+\theta_h^n+\rho_h^n)+P_h\frac{g_\chi(u_h^n,t_n)}{\varepsilon^2}\varepsilon^4\left[\chi\left(\frac{e_h^n+\theta_h^n+\rho_h^n}{\varepsilon^2}\right)\right]^2\\&=P_hd^n+q^n,\quad n=q,\dots,N.\end{aligned}\tag{5.10}$$

An immediate consequence of Lemma 5.2 and Lemma 5.1 is the relation

$$\Big(\sum_{i=0}^{q}\delta_i\upsilon^{q-i},\upsilon^q-\eta_q\upsilon^{q-1}\Big)\geqslant\sum_{i,j=1}^{q}g_{ij}(\upsilon^i,\upsilon^j)-\sum_{i,j=1}^{q}g_{ij}(\upsilon^{i-1},\upsilon^{j-1})\tag{5.11}$$

with a positive definite symmetric matrix $G=(g_{ij})\in\mathbb{R}^{q,q}$; this inequality will play a crucial role in our energy estimates.

With the Nevanlinna–Odeh multipliers $\eta_q\in[0,1)$, we take in (5.10) the L^2 inner product with $e_h^n-\eta_q e_h^{n-1}$, and obtain

$$\begin{aligned}&\Big(\frac{1}{\tau}\sum_{j=0}^{q}\delta_j e_h^{n-j},e_h^n-\eta_q e_h^{n-1}\Big)+(\nabla e_h^n,\nabla(e_h^n-\eta_q e_h^{n-1}))\\&\quad+\frac{1}{\varepsilon^2}(f'(u(t_n))(e_h^n+\theta_h^n+\rho_h^n),e_h^n-\eta_q e_h^{n-1})\\&\quad+\left(\frac{g_\chi(u_h^n,t_n)}{\varepsilon^2}\varepsilon^4\left[\chi\left(\frac{e_h^n+\theta_h^n+\rho_h^n}{\varepsilon^2}\right)\right]^2,e_h^n-\eta_q e_h^{n-1}\right)\\&=(d^n+q^n,e_h^n-\eta_q e_h^{n-1}),\quad n=q,\dots,N.\end{aligned}\tag{5.12}$$

Using the inner product defined in (1.10), we rewrite (5.12) in the form

$$\begin{aligned}&\Big(\frac{1}{\tau}\sum_{j=0}^{q}\delta_j e_h^{n-j},e_h^n-\eta_q e_h^{n-1}\Big)+\langle e_h^n,e_h^n-\eta_q e_h^{n-1}\rangle_{t_n}\\&\quad+\frac{1}{\varepsilon^2}(f'(u(t_n))(\theta_h^n+\rho_h^n),e_h^n-\eta_q e_h^{n-1})\\&\quad+\left(\frac{g_\chi(u_h^n,t_n)}{\varepsilon^2}\varepsilon^4\left[\chi\left(\frac{e_h^n+\theta_h^n+\rho_h^n}{\varepsilon^2}\right)\right]^2,e_h^n-\eta_q e_h^{n-1}\right)\\&=2\lambda(e_h^n,e_h^n-\eta_q e_h^{n-1})+(d^n+q^n,e_h^n-\eta_q e_h^{n-1}).\end{aligned}\tag{5.13}$$

The spectral estimate (1.6) (as a result of property (P1)) guarantees that $\langle\cdot,\cdot\rangle_{t_n}$ in (5.13) is a time-dependent inner product. It is this time-dependent inner product that helps us to obtain an error estimate without exponential dependence on $1/\varepsilon$.

The first term on the left-hand side of (5.13) can be taken care of exactly as in [39], [36] and [5]: from (5.11), with the notation $E_h^n:=(e_h^{n-q+1},\dots,e_h^n)^T$ and

$$\|E_h^n\|_G^2=\sum_{i,j=1}^{q}g_{ij}(e_h^{n-q+i},e_h^{n-q+j}),$$

we have

$$\Big(\sum_{j=0}^{q}\delta_j e_h^{n-j},e_h^n-\eta_q e_h^{n-1}\Big)\geqslant\|E_h^n\|_G^2-\|E_h^{n-1}\|_G^2.\tag{5.14}$$

Using the Cauchy–Schwarz and arithmetic–geometric mean inequalities, we can estimate the second term on the left-hand side of (5.13) as follows

$$\langle e_h^n, e_h^n - \eta_q e_h^{n-1}\rangle_{t_n} \geqslant \|e_h^n\|_{t_n}^2 - \frac{1}{2}\eta_q\big(\|e_h^n\|_{t_n}^2 + \|e_h^{n-1}\|_{t_n}^2\big). \tag{5.15}$$

Now, to relate $\|e_h^{n-1}\|_{t_n}^2$ back to $\|e_h^{n-1}\|_{t_{n-1}}^2$, we note that, in view of (1.10) and (1.11),

$$\begin{aligned}\|e_h^{n-1}\|_{t_n}^2 &= \|e_h^{n-1}\|_{t_{n-1}}^2 + \frac{1}{\varepsilon^2}([f'(u(t_n)) - f'(u(t_{n-1}))]e_h^{n-1}, e_h^{n-1})\\ &\leqslant \|e_h^{n-1}\|_{t_{n-1}}^2 + \frac{c\tau}{\varepsilon^2}\|e_h^{n-1}\|^2.\end{aligned}$$

Therefore, from (5.15) we obtain

$$\langle e_h^n, e_h^n - \eta_q e_h^{n-1}\rangle_{t_n} \geqslant \Big(1 - \frac{1}{2}\eta_q\Big)\|e_h^n\|_{t_n}^2 - \frac{1}{2}\eta_q\|e_h^{n-1}\|_{t_{n-1}}^2 - \frac{C\tau}{\varepsilon^2}\|e_h^{n-1}\|^2. \tag{5.16}$$

In view of (5.14) and (5.16), relation (5.13) yields

$$\begin{aligned}&(2\|E_h^n\|_G^2 + \tau\eta_q\|e_h^n\|_{t_n}^2) - (2\|E_h^{n-1}\|_G^2 + \tau\eta_q\|e_h^{n-1}\|_{t_{n-1}}^2) + 2\tau\big(1-\eta_q\big)\|e_h^n\|_{t_n}^2\\ &\leqslant \frac{2\tau}{\varepsilon^2}|(f'(u(t_n))(\theta_h^n + \rho_h^n), e_h^n - \eta_q e_h^{n-1})|\\ &\quad + C\tau\left|\left(\frac{g_\chi(u_h^n, t_n)}{\varepsilon^2}\varepsilon^4\left[\chi\left(\frac{e_h^n + \theta_h^n + \rho_h^n}{\varepsilon^2}\right)\right]^2, e_h^n - \eta_q e_h^{n-1}\right)\right|\\ &\quad + 2\tau|(2\lambda e_h^n, e_h^n - \eta_q e_h^{n-1})| + 2\tau|(d^n + q^n, e_h^n - \eta_q e_h^{n-1})| + 2\tau\frac{C\tau}{\varepsilon^2}\|e_h^{n-1}\|^2\\ &\leqslant \frac{C\tau}{\varepsilon^2}\|\theta_h^n + \rho_h^n\|^2 + C\tau(1+\tau/\varepsilon^2)(\|e_h^n\|^2 + \|e_h^{n-1}\|^2) + C\tau\|d^n + q^n\|^2.\end{aligned}$$

Summing here from $n=q$ to $n=m\leqslant N$, and using (5.8), we obtain (note that $\|E_h^{q-1}\|_G = \|e_h^{q-1}\| = 0$)

$$\begin{aligned}&(2\|E_h^m\|_G^2 + \tau\eta_q\|e_h^m\|_{t_m}^2) + \sum_{n=q}^m 2\tau\big(1-\eta_q\big)\|e_h^n\|_{t_n}^2\\ &\leqslant C(1+\varepsilon^{-2})\mathrm{e}^{-2c/\varepsilon} + C\tau^{2q}\varepsilon^{-2q-1} + Ch^{2r}\varepsilon^{-2r-1} + C\tau(1+\tau/\varepsilon^2)\sum_{n=q}^m\|e_h^n\|^2.\end{aligned}$$

Under condition (5.2), using the consistency error estimates (5.5)–(5.7), this estimate can be further reduced to

$$\begin{aligned}&\|E_h^m\|_G^2 + \tau(1-\eta_q)\sum_{n=q}^m\|e_h^n\|_{t_n}^2\\ &\leqslant C(1+\varepsilon^{-2})\mathrm{e}^{-2c/\varepsilon} + C\tau^{2q}\varepsilon^{-2q-1} + Ch^{2r}\varepsilon^{-2r-1} + C\tau\sum_{n=q}^m\|e_h^n\|^2.\end{aligned}$$

Since $\|E_h^m\|_G^2 \geqslant c_q\|e_h^m\|^2$, with $c_q > 0$ denoting the smallest eigenvalue of the positive definite symmetric matrix G, we thus infer that

$$\begin{aligned}&c_q\|e_h^m\|^2 + (1-\eta_q)\tau\sum_{n=q}^m\|e_h^n\|_{t_n}^2\\ &\leqslant C(1+\varepsilon^{-2})\mathrm{e}^{-2c/\varepsilon} + C\tau^{2q}\varepsilon^{-2q-1} + Ch^{2r}\varepsilon^{-2r-1} + C\tau\sum_{n=q}^m\|e_h^n\|^2.\end{aligned}$$

A straightforward application of the discrete Gronwall inequality yields

$$\max_{0\leqslant n\leqslant N}\|e_h^n\| \leqslant C\varepsilon^{-1}\mathrm{e}^{-c/\varepsilon} + C\tau^q\varepsilon^{-q-\frac{1}{2}} + Ch^r\varepsilon^{-r-\frac{1}{2}}. \tag{5.17}$$

Next, following the notation of [4], we introduce a rescaled norm on $\ell^p(L^2(\Omega))$, denoted by $\|\cdot\|_{L^p(L^2(\Omega))}$: for a sequence $(\upsilon^n)_{n=1}^N$ and a given stepsize τ, we denote

$$\big\|(\upsilon^n)_{n=1}^N\big\|_{L^p(L^2(\Omega))} = \Big(\tau\sum_{n=1}^N \|\upsilon^n\|_{L^2(\Omega)}^p\Big)^{1/p},$$

which coincides with the $L^p(0,T;L^2(\Omega))$ norm of the piecewise constant function taking the values υ^n.

We rewrite (5.10) as

$$\frac{1}{\tau}\sum_{j=0}^q \delta_j e_h^{n-j} - \Delta_h e_h^n = \upsilon_h^n, \quad n = q,\ldots,N, \tag{5.18}$$

with

$$\begin{aligned}\upsilon_h^n = &-P_h\frac{f'(u(t_n))}{\varepsilon^2}(e_h^n+\theta_h^n+\rho_h^n) - P_h\frac{g_\chi(u_h^n,t_n)}{\varepsilon^2}\varepsilon^4\Big[\chi\Big(\frac{e_h^n+\theta_h^n+\rho_h^n}{\varepsilon^2}\Big)\Big]^2\\ &+P_hd^n + (R_h-P_h)\frac{1}{\tau}\sum_{j=0}^q\delta_j u(t_n).\end{aligned}$$

We apply the discrete maximal L^p-regularity to (5.18) (cf. [30, Theorem 4.2]). This yields

$$\begin{aligned}&\Big\|\Big(\frac{1}{\tau}\sum_{j=0}^q\delta_j e_h^{n-j}\Big)_{n=q}^N\Big\|_{L^p(L^2(\Omega))} + \|(\Delta_h e_h^n)_{n=q}^N\|_{L^p(L^2(\Omega))}\\ &\leqslant C\|(\upsilon_h^n)_{n=q}^N\|_{L^p(L^2(\Omega))}\\ &\leqslant C\Big\|\Big(\frac{f'(u(t_n))}{\varepsilon^2}(e_h^n+\theta_h^n+\rho_h^n)\Big)_{n=q}^N\Big\|_{L^p(L^2(\Omega))}\\ &\quad + C\Big\|\Big(\frac{g_\chi(u_n,t_n)}{\varepsilon^2}\varepsilon^4\Big[\chi\Big(\frac{e_h^n+\theta_h^n+\rho_h^n}{\varepsilon^2}\Big)\Big]^2\Big)_{n=q}^N\Big\|_{L^p(L^2(\Omega))}\\ &\quad + C\|(d^n)_{n=q}^N\|_{L^p(L^2(\Omega))} + C\Big\|\Big((R_h-P_h)\frac{1}{\tau}\sum_{j=0}^q\delta_j u(t_n)\Big)_{n=q}^N\Big\|_{L^p(L^2(\Omega))}\\ &\leqslant C\varepsilon^{-2}\big\|(e_h^n+\theta_h^n+\rho_h^n)_{n=q}^N\big\|_{L^p(L^2(\Omega))} + C\|(d^n)_{n=q}^N\|_{L^p(L^2(\Omega))}\\ &\quad + C\Big\|\Big((R_h-P_h)\frac{1}{\tau}\sum_{j=0}^q\delta_j u(t_n)\Big)_{n=q}^N\Big\|_{L^p(L^2(\Omega))}\\ &\leqslant C\varepsilon^{-3}\mathrm{e}^{-c/\varepsilon} + C\tau^q\varepsilon^{-q-2.5} + Ch^r\varepsilon^{-r-2.5} \quad \forall 1<p<\infty.\end{aligned}$$

In [4, p. 1538] it is shown that (for zero starting values $e_h^0 = \cdots = e_h^{q-1} = 0$)

$$\Big\|\Big(\frac{e_h^n-e_h^{n-1}}{\tau}\Big)_{n=q}^N\Big\|_{L^p(L^2(\Omega))} \leqslant C\Big\|\Big(\frac{1}{\tau}\sum_{j=0}^q\delta_j e_h^{n-j}\Big)_{n=q}^N\Big\|_{L^p(L^2(\Omega))}.$$

Therefore,

$$\begin{aligned}&\Big\|\Big(\frac{e_h^n-e_h^{n-1}}{\tau}\Big)_{n=q}^N\Big\|_{L^p(L^2(\Omega))}+\|(\Delta_h e_h^n)_{n=q}^N\|_{L^p(L^2(\Omega))}\\&\leqslant C(\varepsilon^{-3}\mathrm{e}^{-c/\varepsilon}+\tau^q\varepsilon^{-q-2.5}+h^r\varepsilon^{-r-2.5})\quad\forall 1<p<\infty.\end{aligned}\tag{5.19}$$

Adapting the idea of [31, Section 3.4] here, we denote by $\tilde e_h(t)$, $t\in[0,T]$, the piecewise linear interpolant of the sequence $(e_h^n)_{n=0}^N$ at the temporal nodes $t_n=n\tau$, $n=0,1,\dots,N$. Then,

$$\begin{aligned}&\|\partial_t\tilde e_h\|_{L^p(0,T;L^2(\Omega))}+\|\Delta_h\tilde e_h\|_{L^p(0,T;L^2(\Omega))}\\&\leqslant C\bigg(\Big\|\Big(\frac{e_h^n-e_h^{n-1}}{\tau}\Big)_{n=q}^N\Big\|_{L^p(L^2(\Omega))}+\big\|(\Delta_h e_h^n)_{n=q}^N\big\|_{L^p(L^2(\Omega))}\bigg).\end{aligned}\tag{5.20}$$

Let ϕ be the solution of the boundary value problem

$$\begin{cases}\Delta\phi=\Delta_h\tilde e_h & \text{in } \Omega,\\ \phi=0 & \text{on } \partial\Omega.\end{cases}$$

Then

$$\|\phi\|_{H^2(\Omega)}\leqslant C\|\Delta_h\tilde e_h\|_{L^2(\Omega)}$$

and

$$\|\partial_t\phi\|_{L^2(\Omega)}=\|\Delta^{-1}\Delta_h\partial_t\tilde e_h\|_{L^2(\Omega)}\leqslant C\|\partial_t\tilde e_h\|_{L^2(\Omega)};$$

the last inequality was proved in [26, Lemma 5.1]. Thus

$$\|\partial_t\phi\|_{L^p(0,T;L^2(\Omega))}+\|\phi\|_{L^p(0,T;H^2(\Omega))}\leqslant\|\partial_t\tilde e_h\|_{L^p(0,T;L^2(\Omega))}+\|\Delta_h\tilde e_h\|_{L^p(0,T;L^2(\Omega))}.\tag{5.21}$$

By using the inhomogeneous Sobolev embedding (cf. [37, Proposition 1.2.10])

$$W^{1,p}(0,T;X)\cap L^p(0,T;Y)\hookrightarrow L^\infty(0,T;(X,Y)_{1-1/p,p}),$$

where $(X,Y)_{1-1/p,p}=B^{2-\frac{2}{p};2,p}(\Omega)$ denotes the real interpolation space between the two Banach spaces $X=L^2(\Omega)$ and $Y=\dot H^2(\Omega)$ (cf. [1, §7.32]), we obtain

$$\|\phi\|_{L^\infty(0,T;B^{2-\frac{2}{p};2,p}(\Omega))}\leqslant C\big(\|\partial_t\phi\|_{L^p(0,T;L^2(\Omega))}+\|\phi\|_{L^p(0,T;H^2(\Omega))}\big).\tag{5.22}$$

Since $B^{2-\frac{2}{p};2,p}(\Omega)\hookrightarrow C^\alpha(\overline\Omega)$ for some positive α when $p>4/(4-d)$, in this case we have

$$\|\phi\|_{L^\infty(0,T;C^\alpha(\overline\Omega))}\leqslant\|\phi\|_{L^\infty(0,T;B^{2-\frac{2}{p};2,p}(\Omega))}.\tag{5.23}$$

Since e_h^n is the Ritz projection of $\phi(t_n)$, using the L^∞ estimate of the Ritz projection (cf. (2.7)), we have

$$\|e_h^n-\phi(t_n)\|_{L^\infty(\Omega)}\leqslant C\ell_h h^\alpha\|\phi(t_n)\|_{C^\alpha(\overline\Omega)}\leqslant C\|\phi(t_n)\|_{C^\alpha(\overline\Omega)}.\tag{5.24}$$

Then, estimates (5.19)–(5.24) imply

$$\max_{q\leqslant n\leqslant N}\|e_h^n\|_{L^\infty(\Omega)}\leqslant C\varepsilon^{-3}\mathrm{e}^{-c/\varepsilon}+C\tau^q\varepsilon^{-q-2.5}+Ch^r\varepsilon^{-r-2.5}\quad\forall 1<p<\infty.$$

If (5.2) holds, then

$$\tau^q\varepsilon^{-q-2.5}=o(\varepsilon^2)\quad\text{and}\quad h^r\varepsilon^{-r-2.5}=o(\varepsilon^2).$$

Meanwhile, Proposition 3.1 and (5.1)–(5.2) imply

$$\begin{aligned}\max_{q\leqslant n\leqslant N}\|\theta_h^n\|_{L^\infty(\Omega)} &\leqslant C\mathrm{e}^{-\frac{1}{2}c/\varepsilon}+C\ell_h^2(\tau^q\varepsilon^{-q}+Ch^r\varepsilon^{-r})\\ &\leqslant C\mathrm{e}^{-\frac{1}{2}c/\varepsilon}+C\varepsilon^{\frac{1}{2}}\ell_h^2(\tau^q\varepsilon^{-q-\frac{1}{2}}+Ch^r\varepsilon^{-r-\frac{1}{2}})\\ &\leqslant C\mathrm{e}^{-\frac{1}{2}c/\varepsilon}+C(\tau^q\varepsilon^{-q-\frac{1}{2}}+Ch^r\varepsilon^{-r-\frac{1}{2}})\\ &=o(\varepsilon^2),\end{aligned}$$

$$\max_{q\leqslant n\leqslant N}\|\rho_h^n\|_{L^\infty(\Omega)}\leqslant Ch^r\varepsilon^{-r-\frac{1}{2}}=o(\varepsilon^2),$$

where we have used the estimate $\varepsilon^{\frac{1}{2}}\ell_h^2\leqslant C$, which is a consequence of the mesh condition (5.2). Since $u(t_n)-u_h^n=e_h^n+\theta_h^n+\rho_h^n$, for sufficiently small ε the last three estimates yield

$$\max_{q\leqslant n\leqslant N}\|u(t_n)-u_h^n\|_{L^\infty(\Omega)}\leqslant\varepsilon^2. \tag{5.25}$$

Therefore, $u_h^n\in B_\varepsilon(t_n)$ and $f_\chi(u_h^n,t_n)=f(u_h^n)$. This means that u_h^n is a solution of (1.7). This together with (5.17) imply the result of Theorem 5.1. □

6. Numerical examples

The initial and boundary value problem (1.5) with $\phi=1$ is still an L^2 gradient flow of the Cahn–Hilliard energy, i.e., testing (1.5) by u_t and using integration by parts (with $u_t=0$ on $\partial\Omega$) still yields the energy decay property,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega\left(\frac{1}{2}|\nabla u|^2+\frac{1}{\varepsilon^2}F(u)\right)\mathrm{d}x=-\int_\Omega|u_t|^2\mathrm{d}x\leqslant 0. \tag{6.1}$$

In this article, we considered high-order BDF methods (1.7). It turns out that the condition for the error estimate is less restrictive if a high-order method in time is used. This is a desired property of the numerical method. On the other hand, we cannot prove unconditional (uniform in ε) energy decay of the numerical solutions given by high-order BDF methods. We present results of numerical experiments to illustrate the merit of high-order BDF methods.

We consider the AC equation (1.5) with the initial value

$$u_0(x)=\Theta(\Lambda_0(x)/(\sqrt{2}\varepsilon)), \tag{6.2}$$

where $\Lambda_0(x)$ is the signed distance to an ellipse interface

$$\Gamma_0=\left\{(x_1,x_2)\in\mathbb{R}^2:\frac{x_1^2}{0.36}+\frac{x_2^2}{0.04}=1\right\},$$

and the function $\Theta(r)=\tanh(r)$ satisfies (1.4). This example was considered in [21]. We solve the problem by the proposed method in a domain $\Omega=[-1,1]^2$. The 3-stage (5th-order) Runge–Kutta Radau IIA method is used at the first 4 steps to generate sufficiently accurate starting values for the BDF5 method.

First, we present the numerical simulation of the zero-level set of the solution in Figure 2 with $\varepsilon=0.04,0.02$ and 0.01. The numerical results show that the zero-level sets obtained with several sufficiently small ε are consistent.

The energy curves of numerical solutions corresponding to various ε are presented in Figure

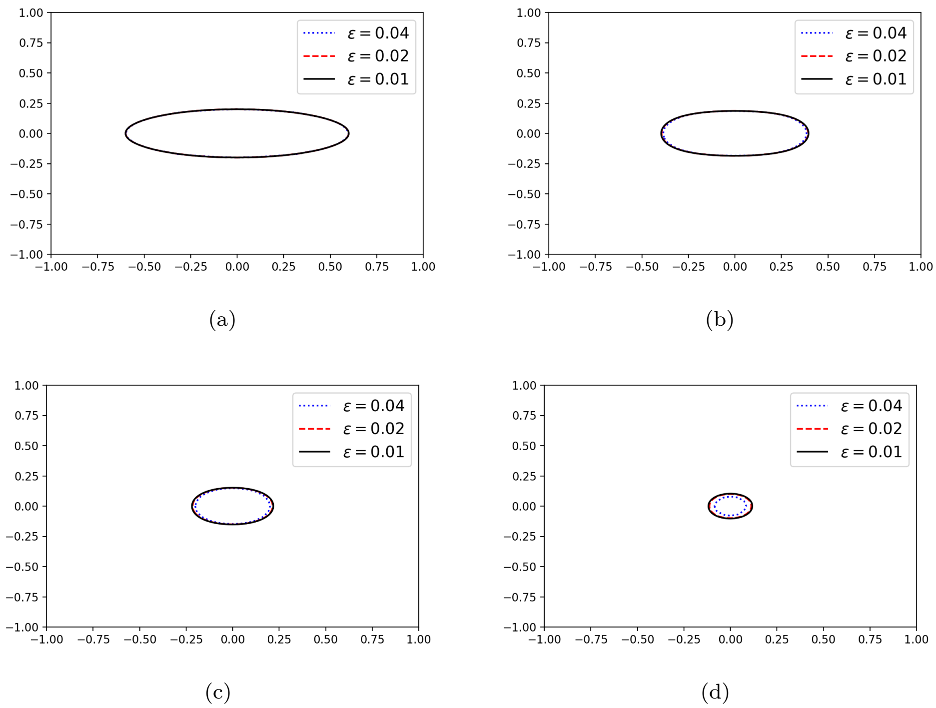

Fig. 2. Snapshots of the zero-level set of u_h^n at time $t = 0, 0.02, 0.04, 0.05$, $\tau = 0.5\varepsilon^2$ and $\varepsilon = 0.04, 0.02, 0.01$.

3, from which we see that the energy decays as time increases. This shows that high-order BDF methods are practically energy stable in numerical simulation for small ε. Since the initial value depends on ε, as shown in (6.2), the initial energy is $O(\varepsilon^{-1})$.

Second, we investigate the temporal convergence rates of numerical solutions with a fix spatial mesh size $h = \varepsilon/\sqrt{2}$. The numerical results at $T = 8\varepsilon^2$, ε and 0.1 are presented in Tables 1–3. These results show that the BDF5 method has much smaller errors than the backward Euler method for all three cases, $T = 8\varepsilon^2$, ε and 0.1. This shows the merit of using high-order BDF methods for the AC equation.

Third, we investigate the spatial convergence rates of numerical solutions with a fixed temporal stepsize. The numerical results at $T = 4\varepsilon^2$, ε and 0.1 are presented in Tables 4–6. These results show that the error decreases as T increases, and high-order finite elements yield higher-order accuracy than low-order finite elements when ε is small. This shows the merit of high-order finite elements for the AC equation. The convergence rates at $T = 0.1$ is not accurate when ε is too small, as the solution is identical to 1 almost everywhere. In this case, the error suddenly

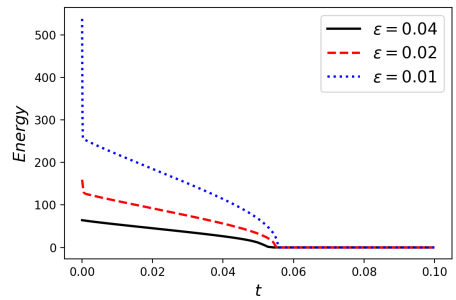

Fig. 3. Energy evolution of numerical solutions, with $\tau = \varepsilon^2$ and $h = \varepsilon/\sqrt{2}$.

Table 1. Time discretization errors $\|u_\tau^N - u_{\tau/2}^N\|_{L^2(\Omega)}$ at $T = 8\varepsilon^2$ with $h = \varepsilon/\sqrt{2}$.

$T = 8\varepsilon^2$	ε \ τ	$2^{-6}\varepsilon^2$	$2^{-7}\varepsilon^2$	$2^{-8}\varepsilon^2$	order
BDF5 Method	0.04	3.365E–10	1.458E–11	5.418E–13	4.8
	0.02	4.854E–11	2.154E–12	8.796E–14	4.6
	0.01	3.865E–11	1.972E–12	8.627E–14	4.5
Backward Euler Method	0.04	9.840E–05	4.914E–05	2.453E–05	1.0
	0.02	1.443E–05	7.181E–06	3.594E–06	1.0
	0.01	2.749E–06	1.379E–06	6.909E–07	1.0

decreases to almost zero when the mesh size reaches a threshold.

7. Conclusion

We have presented an error estimate for fully discrete FEMs with high-order BDF methods for the AC phase field equation with explicit dependence on the parameter ε describing the thickness of the phase transition zone, by utilizing the spectral estimate (1.6) of the linearized AC operator. The error estimation uses the time-dependent inner product (1.10), introduced based on the spectral estimate (1.6), and is presented for the AC equation subject to the Dirichlet boundary condition $u = 1$. The error estimate can be straightforwardly extended to the AC equation with homogeneous Neumann or periodic boundary conditions. The extension to other phase field models, such as the Cahn–Hilliard equation, is possible if the spectral estimate is available. Rigorous analysis for those problems requires further investigation.

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Table 2. Time discretization errors $\|u_\tau^N - u_{\tau/2}^N\|_{L^2(\Omega)}$ at $T = \varepsilon$ with $h = \varepsilon/\sqrt{2}$.

$T = \varepsilon$	ε \ τ	$2^{-6}\varepsilon^2$	$2^{-7}\varepsilon^2$	$2^{-8}\varepsilon^2$	order
BDF5 Method	0.04	5.394E–08	2.692E–09	1.095E–10	4.6
	0.02	4.033E–11	1.783E–12	7.222E–14	4.6
	0.01	2.540E–11	1.259E–12	5.841E–14	4.4
Backward Euler Method	0.04	2.251E–04	1.123E–04	5.596E–05	1.0
	0.02	5.032E–05	2.511E–05	1.254E–05	1.0
	0.01	1.045E–05	5.218E–06	2.607E–06	1.0

Table 3. Time discretization errors $\|u_\tau^N - u_{\tau/2}^N\|_{L^2(\Omega)}$ at $T = 0.1$ with $h = \varepsilon/\sqrt{2}$.

$T = 0.1$	ε \ τ	$2^{-1}\varepsilon^2$	$2^{-2}\varepsilon^2$	$2^{-3}\varepsilon^2$	order
BDF5 Method	0.04	1.717E–09	8.061E–13	4.353E–15	7.5
	0.02	2.641E–13	4.097E–13	2.282E–15	7.5
	0.01	1.224E–13	1.820E–13	2.280E–14	3.0
Backward Euler Method	0.04	2.787E–09	4.994E–09	8.518E–09	–
	0.02	3.748E–09	9.105E–09	2.010E–08	–
	0.01	6.431E–09	2.261E–08	3.283E–08	–

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Table 4. Space discretization errors $\|u_h^N - u_{h/2}^N\|_{L^2(\Omega)}$ at $T = 4\varepsilon^2$, with $\tau = \varepsilon^2/2$.

ε	h	$r=2$	order	$r=3$	order
0.04	$2^{-2}\sqrt{2}\varepsilon$	3.052E–01	–	4.821E–02	–
	$2^{-3}\sqrt{2}\varepsilon$	6.974E–02	2.1	1.032E–02	2.2
	$2^{-4}\sqrt{2}\varepsilon$	1.718E–02	2.0	1.358E–03	2.9
0.02	$2^{2}\sqrt{2}\varepsilon$	1.476E–01	–	3.418E–02	–
	$2^{1}\sqrt{2}\varepsilon$	3.800E–02	1.9	6.968E–03	2.3
	$2^{0}\sqrt{2}\varepsilon$	1.007E–02	1.8	9.489E–04	2.9
0.01	$2^{1}\sqrt{2}\varepsilon$	9.392E–02	–	2.377E–02	–
	$2^{0}\sqrt{2}\varepsilon$	2.488E–02	1.9	4.691E–03	2.3
	$2^{-1}\sqrt{2}\varepsilon$	6.550E–03	1.8	6.877E–04	2.8

Table 5. Space discretization errors $\|u_h^N - u_{h/2}^N\|_{L^2(\Omega)}$ at $T = \varepsilon$, with $\tau = \varepsilon^2$.

ε	h	$r=2$	order	$r=3$	order
0.04	$2^{-2}\sqrt{2}\varepsilon$	2.499E–01	–	1.324E–02	–
	$2^{-3}\sqrt{2}\varepsilon$	6.618E–02	1.9	2.913E–03	2.2
	$2^{-4}\sqrt{2}\varepsilon$	1.813E–02	1.9	2.449E–04	3.5
0.02	$2^{2}\sqrt{2}\varepsilon$	1.072E–01	–	3.390E–02	–
	$2^{1}\sqrt{2}\varepsilon$	4.111E–02	1.4	1.945E–03	4.1
	$2^{0}\sqrt{2}\varepsilon$	1.144E–02	1.8	2.180E–04	3.2
0.01	$2^{1}\sqrt{2}\varepsilon$	7.409E–02	–	1.396E–02	–
	$2^{0}\sqrt{2}\varepsilon$	2.884E–02	1.4	1.492E–03	3.2
	$2^{-1}\sqrt{2}\varepsilon$	8.124E–03	1.8	1.295E–04	3.5

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Table 6. Space discretization errors $\|u_h^N - u_{h/2}^N\|_{L^2(\Omega)}$ at $T = 0.1$, with $\tau = \varepsilon^2$.

ε	h	$r = 2$	order	$r = 3$	order
0.04	$2^{-2}\sqrt{2}\varepsilon$	9.529E–06	–	6.411E–06	–
	$2^{-3}\sqrt{2}\varepsilon$	3.359E–06	1.5	2.073E–06	1.6
	$2^{-4}\sqrt{2}\varepsilon$	9.183E–07	1.9	1.652E–07	3.6
0.02	$2^{2}\sqrt{2}\varepsilon$	8.962E–01	–	8.590E–01	–
	$2^{1}\sqrt{2}\varepsilon$	2.527E–10	29.9	6.285E–10	30.3
	$2^{0}\sqrt{2}\varepsilon$	7.548E–10	−1.6	7.310E–10	−0.2
0.01	$2^{1}\sqrt{2}\varepsilon$	1.118E–00	–	1.020E–00	–
	$2^{0}\sqrt{2}\varepsilon$	1.757E–09	29.2	8.332E–10	30.2
	$2^{-1}\sqrt{2}\varepsilon$	3.348E–09	−0.9	3.082E–09	−1.9

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