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Numerical analysis of the Allen-Cahn equation and approximation for mean curvature flows

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Summary. We propose and analyze a semi-discrete (in time) scheme and a fully discrete scheme for the Allen-Cahn equation $u_t - \Delta u + \varepsilon^{-2} f(u) = 0$ arising from phase transition in materials science, where ε is a small parameter known as an "interaction length". The primary goal of this paper is to establish some useful a priori error estimates for the proposed numerical methods, in particular, by focusing on the dependence of the error bounds on ε. Optimal order and quasi-optimal order error bounds are shown for the semi-discrete and fully discrete schemes under different constraints on the mesh size h and the time step size k and different regularity assumptions on the initial datum function u_0. In particular, all our error bounds depend on $\frac{1}{\varepsilon}$ only in some lower polynomial order for small ε. The cruxes of the analysis are to establish stability estimates for the discrete solutions, to use a spectrum estimate result of de Mottoni and Schatzman [18, 19] and Chen [12] and to establish a discrete counterpart of it for a linearized Allen-Cahn operator to handle the nonlinear term. Finally, as a nontrivial byproduct, the error estimates are used to establish convergence and rate of convergence of the zero level set of the fully discrete solution to the motion by mean curvature flow and to the generalized motion by mean curvature flow.

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1 Introduction

In this paper we shall propose and analyze a semi-discrete (in time) method and a fully discrete finite element time stepping method for the Allen-Cahn equation

$$u_t - \Delta u + \frac{1}{\varepsilon^2} f(u) = 0 \quad \text{in } \Omega_T := \Omega \times (0, T), \tag{1}$$

$$\frac{\partial u}{\partial n} = 0 \quad \text{in } \partial\Omega_T := \partial\Omega \times (0, T), \tag{2}$$

$$u = u_0 \quad \text{in } \Omega \times \{0\}, \tag{3}$$

where $\Omega \subset \mathbf{R}^N$ $(N = 2, 3)$ is a bounded domain with $C^{1,1}$ boundary $\partial\Omega$ or a convex polygonal domain. $T > 0$ is a fixed constant, and f is the derivative of a smooth double equal well potential taking its global minimum value 0 at $u = \pm 1$. A typical example of f is

$$f(u) := F'(u) \quad \text{and} \quad F(u) = \frac{1}{4}(u^2 - 1)^2.$$

The existence of two stable states suggests that nonconvex energy is associated with the equation (see the discussion below). In order to achieve broader applicability, in this paper we shall consider more general potentials which satisfy some structural assumptions (see Sect. 2), and our analysis will be carried out based on these assumptions. We like to remark that for the purpose of studying the curvature driven geometric flows associated with the Allen-Cahn equation (see the discussion below), the following double obstacle potential has been extensively considered in the literature (see [14,29–31, 28] and references therein)

$$f(u) := F'(u) = -u + \partial I_{[-1,1]}(u) \text{ and } F(u) = \frac{1}{2}(1 - u^2) + I_{[-1,1]}(u),$$

where $I_{[-1,1]}(u)$ and $\partial I_{[-1,1]}(u)$ stands for the indicator function and its subdifferential.

The equation (1) was originally introduced by Allen-Cahn [4] to describe the motion of antiphase boundaries in crystalline solids. It was proposed as a simple model for the process of phase separation of a binary alloy at a fixed temperature. Here the function u represents the concentration of one of the two metallic components of the alloy. The parameter ε is an "interaction length", which is small compared to the characteristic dimensions on the laboratory scale. The boundary condition (2), the outward normal derivative $\frac{\partial u}{\partial n}$ vanishes on $\partial\Omega$, means that no mass loss occurs across the walls of the container Ω. Note that the equation (1) differs from the original Allen-Cahn equation (see [4]) in the scaling of the time so that t here, called the *fast time*, represents $\frac{t}{\varepsilon^2}$ in the original formulation. For more physical background, derivation, and discussion of the Allen-Cahn equation and related equations, we refer to [4,18,19,10,32,9] and the references therein.

It is well-known that the Allen-Cahn equation (1) is a gradient flow with the Liapunov energy functional

$$(4) \qquad \mathcal{J}_\varepsilon(u) := \int_\Omega \phi_\varepsilon(u)\,\mathrm{d}x \quad \text{and} \quad \phi_\varepsilon(u) = \frac{1}{2}|\nabla u|^2 + \frac{1}{\varepsilon^2}F(u).$$

Here, the energy density $\phi_\varepsilon(u)$ is a nonconvex function. It is also known [1] that the elliptic operator $L_{AC}(u) := -\Delta u + \frac{1}{\varepsilon^2} f(u)$ associated with the Allen-Cahn equation (1) is the representation of the Fréchet derivative $\mathcal{J}_\varepsilon'(u)$ of $\mathcal{J}_\varepsilon(u)$ in the space $L^2(\Omega)$.

Another gradient flow for the same Liapunov energy functional in (4) is the Cahn-Hilliard equation

$$(5) \qquad u_t + \Delta(\Delta u - \frac{1}{\varepsilon^2} f(u)) = 0,$$

which was originally introduced by Cahn-Hilliard [9] to describe the complicated phase separation and coarsening phenomena in a melted alloy that is quenched to a temperature at which only two different concentration phases can exist stably (see [2] and references therein). It is also known [1] that the elliptic operator $L_{CH}(u) := \Delta(\Delta u - \frac{1}{\varepsilon^2} f(u))$ associated with the Cahn-Hilliard equation (5) is the representation of the Fréchet derivative $J_\varepsilon'(u)$ in the space $H^{-1}(\Omega)$. On the other hand, unlike the Allen-Cahn equation, the Cahn-Hilliard equation is known to *conserve* the total mass because $\frac{d}{dt}\int_\Omega u(x,t)dx = 0$ for the solution of the Cahn-Hilliard equation (but not for the solution of the Allen-Cahn equation).

The Allen-Cahn equation (1) has been extensively studied in the past decade mainly due to its connection to some interesting and complicated geometric problems of moving surfaces (curves in 2-dimension) [4,26,11, 21,27,14,18,19,29,13]. It was first formally proved that, as $\varepsilon \searrow 0$, the zero level set of u, denoted by $\Gamma_t^\varepsilon := \{x \in \Omega;\ u(x,t) = 0\}$ approaches to a surface Γ_t which evolves according to the geometric law

$$(6) \qquad V = \kappa,$$

where V is the normal velocity of the surface Γ_t and κ is its mean curvature, see [4,25]. The rigorous justification of this limit was successfully carried out by Evans, Soner and Souganidis [21], who have established a global result: for all time $t \geq 0$, the limit of the zero level set of the solution of the Allen-Cahn equation (1) is contained in the generalized solution of the motion by mean curvature flow established in [16] and [22]. Later, Ilmanen [27] proved that this limit is actually one of the Brakke's motion by mean curvature solution [7], which is a subset of the unique generalized solution of the mean curvature flow established in [16] and [22].

Clearly, the study of the Allen-Cahn equation (1) is of great value for understanding phase transition in materials science and for investigating curvature driven flows in geometry. In particular, when singularities develop in the flows since the solution of the Allen-Cahn equation is known to exist for all the time; hence, little manipulation is needed in order to handle possible singularities. Due to the nonlinearity in the equation, its solution only can be sought numerically. The primary numerical challenge for solving the Allen-Cahn equation results from the presence of the small parameter ε for both applications in front of the nonlinear term in the equation. Recall that the zero level set of the solution of (1) approximates the mean curvature flow only when ε is small. On the other hand, the equation becomes a singularly perturbed heat equation for ε small. To resolve the solution numerically, one has to use small (space) mesh size h and (time) step size k, which must be related to the parameter ε.

In recent years, extensive research has been done on numerical simulations of the curvature driven flows by computing the zero level set of the solution of the Allen-Cahn equation (1) with both the polynomial potential and the double obstacle potential, and on convergence and error analysis of the numerical interfaces to the geometric surfaces/curves driven by their curvatures [6,20,30,31,15,28]. For the double obstacle Allen-Cahn equation, Nochetto and Verdi [31] proposed a fully discrete method which uses the P_1-conforming finite element for space discretization and the backward Euler method for time stepping. It was proved under the mesh constraint $k, h^2 = o(\varepsilon^3)$ that the zero level set of the numerical solution converges past singularities to the true interface, provided the limit interface does not develop an interior (i.e., no fattening occurs). A linear rate of convergence $O(\varepsilon)$ for interface was also established under the more stringent mesh constraint $k, h^2 = O(\varepsilon^4)$. Nochetto and Verdi [30] proposed another fully discrete method in which the P_1-conforming finite element method with mass lumping is used for space discretization and combined with the forward Euler method for time discretization. Under the mesh constraint $k, h^2 = o(\varepsilon^4)$, it was shown that the zero level set of the fully discrete solution converges past singularities to the true interface, provided no fattening occurs. A rate of convergence $O(\varepsilon^2)$ for the interface was derived for smooth flows, provided $k, h^2 = O(\varepsilon^5)$ and exact integration is used for the potential term. Chen *et al* [15] considered the advected Cahn-Allen equation

$$u_t - \Delta u - \mathbf{q} \cdot \nabla u + \frac{1}{\varepsilon^2} f(u) = 0$$

with the polynomial potential. Here, $\mathbf{q}$ is a given bounded continually differentiable vector field with bounded derivative in Ω_T. They proposed a fully discrete scheme which uses a finite difference scheme in space combined with the forward Euler time stepping, and showed that the zero level set of the fully discrete solution approaches the true interface of the motion by mean curvature with advection (i.e., $V = \kappa + \mathbf{q} \cdot \mathbf{n}_\Gamma$), provided $h = O(\varepsilon^p)$ for some $p > 1$ and the time step size k satisfies the Courant-Friedrich-Lewy (CFL) condition. A linear rate of convergence $O(\varepsilon)$ for the interface was also derived for smooth flows. More recently, Kühn [28] considered the advected Cahn-Allen equation with a forcing term (a non-homogeneous term) and proposed a fully discrete method which uses the P_1-conforming finite element for space discretization and the forward Euler method for time stepping. It was proved that the zero level set of the numerical solution converges past singularities to the true interface of the advected mean curvature flows, provided no fattening occurs and $k, h^2 = O(\varepsilon^4)$. A rate of convergence $O(\varepsilon^2)$ for the approximation of the interface was also obtained under the more stringent mesh constraint $k, h^2 = O(\varepsilon^5)$ for smooth flows. We point out that the proofs of all the papers cited above are based on some maximum principle and comparison principle type arguments.

Unlike the numerical works mentioned above, the focus of this paper is not only on approximating the interfaces of the curvature driven flows, but on approximating the solution of the Allen-Cahn equation (1). The primary goal of the paper is to develop some semi-discrete (in time) and fully discrete approximations for the initial-boundary value problem (1)-(3), and to establish useful a priori error bounds, which show growth only in low polynomial order of $\frac{1}{\varepsilon}$, for both schemes under some reasonable constraints on mesh sizes h and k. To our knowledge, such error estimates for the Allen-Cahn equation have not been known in the literature. On the other hand, such error bounds are valuable to have for computing the solution u of the Allen-Cahn equation, which gives the concentration of one of metallic components of a binary alloy. To illustrate that this is not an easy task, we like to point out that if one tries to derive error estimates using a straightforward perturbation argument, one immediately gets error bounds which depend on the factor $\exp(\frac{T}{\varepsilon^2})$ (see (4.10) on page 17 of [6]), which are not useful for small ε, as pointed out in [6].

The subsequent analysis applies to a general class of admissible double equal well potentials and initial data $u_0 \in H^2$ that can be bounded in terms of a negative power $(-\sigma_2)$ of ε; see the general assumptions (GA_1)-(GA_3) in Sect. 2, and Theorems 3-5 for a semi-discretization in time and a fully space-time discretization of (1)-(3).

We exemplify our results of the fully discrete scheme for the case $f(u) = u^3 - u$. The scheme reads as follows:

$$(7) \qquad \Big(\frac{U^{m+1} - U^m}{k}, v_h\Big) + \big(\nabla U^{m+1}, \nabla v_h\big) + \frac{1}{\varepsilon^2}\,(f(U^{m+1}), v_h) = 0$$

for all $v_h \in \mathcal{S}_h$. Here, $k > 0$ denotes the time step, and $\mathcal{S}_h \subset H^1(\Omega)$ is the continuous piecewise linear finite element space. We refer to Sect. 4 for further details on the setup.

Suppose there exist constants $\sigma_j \geq 0$, $j = 1, 2, 3$ such that

$$\mathcal{J}_\varepsilon(u_0) := \frac{1}{2} \| \nabla u_0 \|_{L^2}^2 + \frac{1}{\varepsilon^2} \| F(u_0) \|_{L^1} \leq C\varepsilon^{-2\sigma_1} , \tag{8}$$

$$\| \Delta u_0 - \frac{1}{\varepsilon^2} f(u_0) \|_{L^2} \leq C\, \varepsilon^{-\sigma_2} , \tag{9}$$

$$\lim_{s \to 0^+} \|\nabla u_t(s)\|_{L^2} \leq C\varepsilon^{-\sigma_3}. \tag{10}$$

Our main result for the case $f(u) = u^3 - u$ is the following:

Theorem 1 *Let $\{U^m\}_{m=0}^M$ solve (7) on a quasi-uniform time mesh $J_k := \{t_m\}_{m=0}^M$ of size $O(k)$ and a quasi-uniform space mesh $\mathcal{T}_h$ of size $O(h)$. Suppose that u_0 satisfies (8)-(10). Then, under the following mesh and starting value constraints*

$$\begin{aligned}
&1).\quad h|\ln h|^{\frac{3-N}{4-N}} \leq \varepsilon^{\frac{2}{4-N}\max\{\sigma_1+3,\, \sigma_2+2\}}, \qquad (N = 2, 3)\\
&2).\quad k^2 + h^4 \leq \varepsilon^{2\alpha_3},\\
&3).\quad \| U^0 - u_0 \|_{L^2} \leq Ch^2 \| u_0 \|_{H^2},
\end{aligned}$$

where

$$\alpha_3 = \max\{\sigma_1 + 2, \sigma_3\} + \frac{N \max\{\sigma_1 + 1, \sigma_2\} + 8}{4 - N},$$

the solution of (7) satisfies the error estimates

$$\begin{aligned}
\text{(i)}\quad &\max_{0 \leq m \leq M} \| u(t_m) - U^m \|_{L^2} + \Big(k \sum_{m=1}^M k \| d_t(u(t_m) - U^m) \|_{L^2}^2 \Big)^{\frac{1}{2}}\\
&\leq \tilde{C}\,(k + h^2)\, \varepsilon^{\min\{-\sigma_1-2, -\sigma_3\}},\\
\text{(ii)}\quad &\Big(k \sum_{m=1}^M \| \nabla(u(t_m) - U^m) \|_{L^2}^2 \Big)^{\frac{1}{2}} \leq \tilde{C}\,(k + h)\, \varepsilon^{\min\{-\sigma_1-3, -\sigma_3-1\}},\\
\text{(iii)}\quad &\max_{0 \leq m \leq M} \| u(t_m) - U^m \|_{L^\infty} \leq \tilde{C}\,[\, h^{\frac{4-N}{2}}\, |\ln h|^{\frac{3-N}{2}} \varepsilon^{\min\{-\sigma_1-1, -\sigma_2\}}\\
&\qquad + (k + h^2)\, h^{-\frac{N}{2}}\, \varepsilon^{\min\{-\sigma_1-2, -\sigma_3\}}\,],
\end{aligned}$$

for some positive constant $\tilde{C} = \tilde{C}(u_0; C_0, T, \Omega)$.

Remark 1 (a). Both, $L^\infty(J; L^2)$ and $L^2(J; H^1)$ estimates are optimal with respect to h and k, and $L^\infty(J; L^\infty)$ estimate is quasi-optimal.

(b). If the condition (10) is dropped, quasi-optimal error bounds with a loss of $\frac{\beta}{2}$ power for arbitrary $0 < \beta < 2$ will be in place of above optimal error bounds, which can be proved in the same way as Theorem 3 is done.

(c). Theorem 1 is a special case of Theorem 5 with $\alpha_0 = 2, \delta = 1, \gamma_1 = 1$ and $\gamma_2 = 3$.

To establish the above error estimates, the following three ingredients play a crucial role in our analysis.

- To establish stability estimates for the discrete solutions of the semi-discrete (in time) and the fully discrete schemes.
- To handle the (nonlinear) potential term in the error equation using a spectrum analysis result due to de Mottoni and Schatzman [18,19] and Chen [12] for the linearized Allen-Cahn operator

$$\mathcal{L}_{AC} := -\Delta + f'(u)I, \tag{11}$$

  where I denotes the identity operator and u is a solution of the Allen-Cahn equation (1), see Proposition 3 for details.
- To prove a discrete counterpart of the above spectrum estimate under some mesh constraint on h, see Proposition 8 for details.

As a nontrivial byproduct, the above $L^\infty(J; L^\infty)$ error estimate combined with the estimates for the solution and its zero level set of the Allen-Cahn equation established in [11,21,5] immediately gives the following convergence rate estimates for the zero level set of the fully discrete solution to the motion by mean curvature flow and to the generalized motion by mean curvature flow, see Section 5 for details.

Theorem 2 *Let $\{\Gamma_t\}_{t\geq 0}$ denote the generalized motion by mean curvature flow defined in [16,21,22], and let $U_{\varepsilon,h,k}(x,t)$ denote the piecewise linear interpolation (in time) of the fully discrete solution $\{U^m\}$. Define $\Gamma_t^{\varepsilon,h,k} = \{x \in \Omega;\ U_{\varepsilon,h,k}(x,t) = 0\}$, the zero level set of $U_{\varepsilon,h,k}$. Also, let t_* denote the first time the classical evolution by mean curvature has a singularity. Suppose that $\Gamma_0 = \{x \in \overline{\Omega};\ u_0(x) = 0\}$ is a smooth hypersurface compactly contained in Ω. In addition to the mesh constraints of Theorem 1, assume that h and k satisfy the parabolic relation $k = O(h^2)$. Then we have*

(i) *there exists a constant $\varepsilon_0 > 0$ such that for $t < t_*$*

$$\sup_{x\in\Gamma_t^{\varepsilon,h,k}} \{\, \mathrm{dist}(x, \Gamma_t)\,\} \leq C\,\varepsilon^2 |\ln \varepsilon|^2 \quad \forall \varepsilon \in (0, \varepsilon_0), \tag{12}$$

(ii) *suppose* $\{\Gamma_t\}_{t\geq 0}$ *does not develop an interior, then there exists a constant* $\varepsilon_1 > 0$ *such that for* $t \geq 0$

$$\sup_{x\in\Gamma_t^{\varepsilon,h,k}} \{\, \mathrm{dist}(x, \Gamma_t)\,\} \leq C\,\varepsilon \quad \forall \varepsilon \in (0, \varepsilon_1). \tag{13}$$

Remark 2 Note that the estimate (12) is valid before the onset of singularities, but the estimate (13) holds for all times.

Another advantage of our approach for establishing the error estimates is that the idea is also applicable to the Cahn-Hilliard equation (5) since the approach does not rely on the maximum and comparison principles, which are known not to hold for the Cahn-Hilliard equation. On the other hand, a similar spectrum estimate does hold for the Cahn-Hilliard equation [3,12]. Indeed, in the companion papers [23,24], we present a study for the Cahn-Hilliard equation parallel to that for the Allen-Cahn equation carried out in this paper.

The paper is organized as follows: In Sect. 2, we shall derive some a priori estimates for the solution of (1)-(3), special attention is given to dependence of the solution on ε in various norms. In Sect. 3 we consider the backward Euler semi-discrete (in time) scheme for the Allen-Cahn equation and establish some stability estimates for the semi-discrete solution. We then obtain quasi-optimal order and optimal order error bounds, which depend on $\frac{1}{\varepsilon}$ only in a low polynomial order for small ε, under different constraints on the time step size k and different regularity assumptions on the initial datum function u_0, see Theorem 3. The spectrum estimate plays a crucial role in the proof. In Sect. 4 we propose a fully discrete approximation obtained by discretizing the semi-discrete scheme of Sect. 3 in space using the P_1-conforming finite element method. Optimal order error bounds, depending on $\frac{1}{\varepsilon}$ only in a low polynomial order, are shown for the fully discrete method in Theorem 5. The main ideas are to establish some stability estimates for the fully discrete solution, and more importantly to prove a discrete counterpart of the spectrum estimate. Finally, in Sect. 5 we present a nontrivial byproduct of our $L^\infty(J; L^\infty)$ error estimates, namely, to establish $O(\varepsilon)$ order rate convergence of the zero level set of the fully discrete solution to the generalized motion by mean curvature flow for all times $t \geq 0$, provided that the generalized mean curvature flow does not develop interiors (no fattening occurs). This rate of convergence will be strengthened to $O(\varepsilon^2|\ln\varepsilon|^2)$ order for the mean curvature flow before the onset of singularities.

2 Energy estimates for the differential problem

In this section, we present some energy estimates in various function spaces up to $H^1(J; H^2(\Omega))$ in terms of negative powers of ε for the solution u of the Allen-Cahn equation (1) for given $u_0 \in H^2(\Omega)$. Here $J = (0, T)$, and $H^k(\Omega)$ denotes the standard Sobolev space of the functions which and their up to kth order derivatives are L^2-integrable. Throughout this paper, the standard space, norm and inner product notation are adopted. Their definitions can be found in [8,17]. In particular, $(\cdot, \cdot)$ denotes the standard inner product on $L^2(\Omega)$. Also, C and $\widetilde{C}$ are used to denote generic positive constants which are independent of ε and the time and space mesh sizes k and h.

We make the following general assumptions on the derivative f of the potential function F:

General Assumption 1 (GA_1)

1) $f = F'$, for $F \in C^4(\mathbf{R})$, such that $F(\pm 1) = 0$, and $F > 0$ elsewhere.
2) $f'(u)$ satisfies for some $p > 2$ and positive numbers $\tilde{c}_i > 0$, $i = 0, .., 3$,

$$\tilde{c}_1 \,|\, u \,|^{p-2} - \tilde{c}_0 \le f'(u) \le \tilde{c}_2 \,|\, u \,|^{p-2} + \tilde{c}_3 \,.$$

3) There exist $0 < \gamma_1 \le 1$, $\gamma_2 > 0$ and $\delta > 0$ such that for all $|a| \le 2$

$$\big(f(a) - f(b), a - b\big) \ge \gamma_1 \big(f'(a)(a - b), a - b\big) - \gamma_2 \,|\, a - b \,|^{2+\delta} \,.$$

Remark 3 It is trivial to check that $(\mathrm{GA}_1)_2$ implies

$$-(f'(u)v, v) \le \tilde{c}_0 \,\|\, v \,\|_{L^2}^2 \,, \quad \forall\, v \in L^2(\Omega)\,, \tag{14}$$

which will be utilized several times in the paper.

Example 1 The potential function $F(u) = \frac{1}{4}\big(u^2 - 1\big)^2$, consequently, $f(u) = u^3 - u$, is often used in physical and geometrical applications [2,4,5,9,11, 21]. For convenience, we verify $(\mathrm{GA}_1)_1$-$(\mathrm{GA}_1)_3$ for the case in the following. First, $(\mathrm{GA}_1)_1$ holds trivially. Since $f'(u) = 3u^2 - 1$, $(\mathrm{GA}_1)_2$ holds with $\tilde{c}_1 = \tilde{c}_2 = 3$ and $\tilde{c}_0 = \tilde{c}_3 = 1$. A direct calculation gives

$$f(a) - f(b) = (a - b)\big[f'(a) + (a - b)^2 - 3(a - b)a\big]\,. \tag{15}$$

Hence, $(\mathrm{GA}_1)_3$ holds with $\gamma_1 = 1$, $\gamma_2 = 3$, and $\delta = 1$. Also, (14) holds with $\tilde{c}_0 = 1$.

In order to trace dependence of the solution on the small parameter $\varepsilon > 0$, we assume that the initial function $u_0 \in H^1(\Omega) \cap H^2(\Omega)$ with $\|\, u_0 \,\|_{L^\infty} \le 1$ satisfies the following conditions:

General Assumption 2 (GA_2)

There exist nonnegative constants σ_1 and σ_2 such that

$$1) \qquad \mathcal{J}_\varepsilon(u_0) = \frac{1}{2} \,\|\, \nabla u_0 \,\|_{L^2}^2 + \frac{1}{\varepsilon^2} \,\|\, F(u_0) \,\|_{L^1} \le C\, \varepsilon^{-2\sigma_1}\,,$$

$$2) \qquad \|\, \Delta u_0 - \frac{1}{\varepsilon^2}\, f(u_0) \,\|_{L^2} \le C\, \varepsilon^{-\sigma_2}\,.$$

Remark 4 In order to show convergence of the zero level set Γ_t^ε of the solution of (1) to the motion by mean curvature flow $\{\Gamma_t\}_{t\geq 0}$, $\sigma_1 = 0$ or $\sigma_1 = \frac{1}{2}$, and $\sigma_2 = 1$ or $\sigma_2 = 2$ are needed, see Sect. 5 and Sect. 1 as well as the references cited there.

Proposition 1 *Suppose that f satisfies (GA$_1$), and u_0 satisfies (GA$_2$). Then, the solution of (1)–(3) satisfies the following estimates:*

$$\text{(i)}\quad \operatorname*{ess\,sup}_{[0,\infty]}\left\{\frac{1}{2}\parallel \nabla u\parallel_{L^2}^2 + \frac{1}{\varepsilon^2}\parallel F(u)\parallel_{L^1}\right\} + \int_0^\infty \parallel u_t(s)\parallel_{L^2}^2\,\mathrm{d}s = \mathcal{J}_\varepsilon(u_0)\,,$$

$$\text{(ii)}\quad \int_0^T \parallel \Delta u(s)\parallel^2\,\mathrm{d}s \leq C\,\varepsilon^{-2(\sigma_1+1)}\,,$$

$$\text{(iii)}\quad \operatorname*{ess\,sup}_{[0,\infty]}\left\{\parallel u_t\parallel_{L^2}^2 + \parallel u\parallel_{H^2}^2\right\} + \int_0^\infty \parallel \nabla u_t(s)\parallel_{L^2}^2\,\mathrm{d}s \leq C\,\varepsilon^{2\min\{-\sigma_1-1,-\sigma_2\}}\,,$$

$$\text{(iv)}\quad \int_0^\infty \Big(\parallel u_{tt}(s)\parallel_{H^{-1}}^2 + \parallel \Delta u_t(s)\parallel_{H^{-1}}^2\,\mathrm{d}s\Big) \leq C\,\varepsilon^{2\min\{-\sigma_1-2,-\sigma_2\}}\,.$$

Here, we denote $H^{-1}(\Omega) = \big(H_0^1(\Omega)\big)^*$.

Proof. (i) This result comes from the basic energy law

$$\frac{d}{dt}\mathcal{J}_\varepsilon(u) = -\parallel u_t\parallel_{L^2}^2,$$

which can be obtained by multiplying (1) by u_t and using the fact $f = F'$.

(ii) Multiplying (1) by $(-\Delta u)$, using Schwarz inequality on the u_t term and integrating by parts on the nonlinear term lead to

$$\parallel \Delta u\parallel_{L^2}^2 \leq \parallel u_t\parallel_{L^2}^2 - \frac{2}{\varepsilon^2}\,(f'(u), |\nabla u|^2). \tag{16}$$

The assertion then follows from (14) and (i).

(iii) We formally differentiate (1) in time,

$$u_{tt} - \Delta u_t + \frac{1}{\varepsilon^2}\,f'(u)u_t = 0\,. \tag{17}$$

Testing the above equation with u_t and applying (14) we get

$$\frac{1}{2}\frac{d}{dt}\parallel u_t\parallel_{L^2}^2 + \parallel \nabla u_t\parallel_{L^2}^2 \leq \frac{\tilde{c}_0}{\varepsilon^2}\parallel u_t\parallel_{L^2}^2\,. \tag{18}$$

The result follows from integrating (18) over $[0, \infty]$ and (16).

(iv) We conclude from (17), assumption $(\mathrm{GA}_1)_2$, and standard embedding results,

$$\begin{aligned}\| u_{tt} \|_{H^{-1}} &\leq \| \nabla u_t \|_{L^2} + \frac{1}{\varepsilon^2} \sup_{\phi \in H^1(\Omega)} \frac{(f'(u)u_t, \phi)}{\| \phi \|_{H^1}} \\ &\leq \| \nabla u_t \|_{L^2} + \frac{C}{\varepsilon^2} \| f'(u) \|_{L^\infty} \| u_t \|_{L^2} \\ &\leq C \left\{ \| \nabla u_t \|_{L^2} + \varepsilon^{-2} \| u_t \|_{L^2} \right\}. \qquad (19)\end{aligned}$$

After squaring the above inequality, using (18) and integrating over $[0, \infty]$, the result then follows.

Proposition 2 *In addition to the assumptions of Proposition 1, suppose that*

$$\lim_{s \to 0^+} \|\nabla u_t(s)\|_{L^2} \leq C\varepsilon^{-\sigma_3} \qquad (20)$$

for some $\sigma_3 \geq 0$*. Then, the solution of (1)-(3) also satisfies the following estimates:*

$$\text{(i)} \;\; \operatorname*{ess\,sup}_{[0,\infty]} \| \nabla u_t \|_{L^2}^2 + \int_0^\infty \| u_{tt}(s) \|_{L^2}^2 \, \mathrm{d}s \leq C\varepsilon^{2\min\{-\sigma_1 - 2, -\sigma_3\}}, \qquad (21)$$

$$\text{(ii)} \;\; \int_0^\infty \| \Delta u_t \|_{L^2}^2 \leq C\varepsilon^{2\min\{-\sigma_1 - 2, -\sigma_3\}}. \qquad (22)$$

Proof. Testing (17) by u_{tt} gives

$$\| u_{tt} \|_{L^2}^2 + \frac{1}{2}\frac{d}{dt} \| \nabla u_t \|_{L^2}^2 + \frac{1}{\varepsilon^2}\Big(f'(u)u_t, u_{tt} \Big) = 0. \qquad (23)$$

The last term on the right hand side of (23) can be bounded as

$$\frac{1}{\varepsilon^2}\Big(f'(u)u_t, u_{tt} \Big) \leq \frac{1}{2} \| u_{tt} \|_{L^2}^2 + \frac{1}{2\varepsilon^4} \|f'(u)\|_{L^\infty} \| u_t \|_{L^2}^2. \qquad (24)$$

Substituting (24) into (23) and integrating over $[0, \infty]$, the proof of (i) is then completed from using the fact that $\|f'(u)\|_{L^\infty} \leq C$ and (i) of Proposition 1. The assertion (ii) follows immediately from (17) and (i).

We conclude this section by citing the following result of [18, 19] and [12] on low bound estimate of the spectrum of the linearized Allen-Cahn operator $\mathcal{L}_{AC}$ in (11). The estimate plays an important role in our error analysis.

Proposition 3 *Suppose that* (GA_1) *holds. Then there exists a positive* ε*-independent constant* C_0 *such that the principle eigenvalue of the linearized Allen-Cahn operator* $\mathcal{L}_{AC}$ *in (11) satisfies for small* $\varepsilon > 0$

$$\lambda_{AC} \equiv \inf_{\substack{\psi \in H^1(\Omega), \\ \psi \neq 0}} \frac{\| \nabla \psi \|_{L^2}^2 + \varepsilon^{-2} \, (f'(u)\psi, \psi)}{\| \psi \|_{L^2}^2} \geq -C_0\,. \qquad (25)$$

3 Error analysis for a semi-discrete (in time) approximation

In this section, we propose and analyze a semi-discrete in time scheme for (1). For this purpose, let $J_k := \{t_m\}_{m=0}^{M}$ denote an (equidistant) partition of the time interval $[0, T]$ with mesh size $k = T/M$. The simplest ansatz is the (implicit) Euler method

$$d_t u^{m+1} - \Delta u^{m+1} + \frac{1}{\varepsilon^2} f(u^{m+1}) = 0 \quad \text{in } \Omega, \tag{26}$$

$$\frac{\partial u^{m+1}}{\partial n} = 0 \quad \text{on } \partial\Omega, \tag{27}$$

$$u^0 = u_0 \quad \text{in } \Omega, \tag{28}$$

where $d_t u^{m+1} := \frac{1}{k}\{u^{m+1} - u^m\}$.

This scheme, or its explicit variant, has been used mostly in the literature [30,31,28]. However, verification of a result for (26)-(28) that corresponds to (i) of Proposition 1 is not immediate, since $(\mathrm{GA}_1)_1$ has no evident discrete analogy. The necessity of this result will be clear in the error analysis for (26)-(28) to be given later in this section. For that we make the final general assumption:

General Assumption 3 (GA_3)

Suppose that there exist $\alpha_0 \geq 0$, $0 < \gamma_3 < 1$, and $\tilde{c}_4 > 0$ such that f satisfies for any $0 < k \leq \varepsilon^{\alpha_0}$ and $\ell \leq M$

(29)
$$\gamma_3 k \sum_{m=1}^{\ell} \|d_t u^m\|_{L^2}^2 + \frac{k}{\varepsilon^2} \sum_{m=0}^{\ell} (f(u^{m+1}), d_t u^{m+1}) + \tilde{c}_4 \mathcal{J}_\varepsilon(u^0) \geq \frac{\tilde{c}_4}{\varepsilon^2} \| F(u^\ell) \|_{L^1}.$$

A direct consequence of (29) are the following stability estimates for the scheme (26)-(28).

Proposition 4 *For $k \leq \varepsilon^{\alpha_0}$, the solution of the scheme (26)-(28) satisfies the following estimates:*

$$\text{(i)} \quad \max_{0 \leq m \leq M} \left\{ \| \nabla u^m \|_{L^2}^2 + \frac{1}{\varepsilon^2} \| F(u^m) \|_{L^1} \right\}$$
$$+ k \sum_{m=1}^{M} \left\{ \| d_t u^m \|_{L^2}^2 + k \| \nabla d_t u^m \|_{L^2}^2 \right\} \leq 2\tilde{c}_4 \, \mathcal{J}_\varepsilon(u^0), \tag{30}$$

$$\text{(31)} \qquad \text{(ii)} \quad k\sum_{m=0}^{M} \| \Delta u^m \|_{L^2}^2 \le 2\tilde{c}_4\Big(\frac{4\tilde{c}_0}{\varepsilon^2}+1\Big)\mathcal{J}_\varepsilon(u_0) \le C\varepsilon^{-2(\sigma_1+1)},$$

$$\text{(iii)} \quad \max_{0\le m\le M}\Big\{\| d_t u^m \|_{L^2}^2 + \| \Delta u^m \|_{L^2}^2\Big\}$$

$$\text{(32)} \qquad +k\sum_{m=0}^{M} k\| d_t^2 u^m \|_{L^2}^2 \le C\varepsilon^{2\min\{-\sigma_1-1,-\sigma_2\}}.$$

Proof. Testing (26) by $d_t u^{m+1}$, the assertion (i) follows immediately from (29).

The proof of (ii) is similar to that of (ii) of Proposition 1. Testing (26) with $(-\Delta u^{m+1})$, and using Schwarz inequality on the $d_t u^{m+1}$ term and integrating by parts on the nonlinear term leads to

$$\text{(33)} \qquad \| \Delta u^{m+1} \|_{L^2}^2 \le \| d_t u^{m+1} \|_{L^2}^2 - \frac{2}{\varepsilon^2}\,(f'(u^{m+1}), |\nabla u^{m+1}|^2).$$

The assertion then follows from (14), (30) and $(\mathrm{GA}_2)_1$.

To show the assertion (iii), we first apply the difference operator d_t to both sides of (26) and get

$$d_t^2 u^{m+1} - \Delta d_t u^{m+1} + \frac{1}{\varepsilon^2}\, d_t f(u^{m+1}) = 0.$$

Testing the above equation with $d_t u^{m+1}$ and using the Mean Value Theorem on $d_t f(u^{m+1})$ leads to

$$\frac{1}{2}d_t\| d_t u^{m+1} \|_{L^2}^2 + \frac{k}{2}\| d_t^2 u^{m+1} \|_{L^2}^2 + \| \nabla d_t u^{m+1} \|_{L^2}^2$$

$$\text{(34)} \qquad = -\frac{2}{\varepsilon^2}\,(f'(\xi), |d_t u^{m+1}|^2) \le \frac{2\tilde{c}_0}{\varepsilon^2}\| d_t u^{m+1} \|_{L^2}^2.$$

Here ξ is a value between u^m and u^{m+1}. Also, we have used (14) to get the last inequality.

The conclusion now follows from summing the inequality (34) over m after multiplying by k, and using (i), (GA_2) and (33).

Next, in Subsection 3.1, we verify validity of assumption (GA_3) for the case $f(u) = u^3 - u$. As will be shown, it is possible, and sometimes even gives better stability, to modify (26) to get a method where $f(u^{m+1})$ is replaced by some $\tilde{f}(u^m, u^{m+1})$. In Subsection 3.2, we give an error analysis for scheme (26)-(28) under the general assumptions (GA_1)-(GA_3).

3.1 Verification of (GA$_3$) for the case $f(u) = u^3 - u$

In this subsection, we verify the general assumption (GA$_3$) for the case $f(u) = u^3 - u$, and therefore obtain the stability estimates (30)-(32) for the scheme (26)-(28) in this case. As can be seen easily, testing the equation (26) with $d_t u^{m+1}$ does not give a positive contribution from the last term on the left hand side to obtain a stability result which is analogous to (i) of Proposition 1 for the solution u^{m+1}. However, it turns out that the stability result holds if k satisfies a constraint as described in (GA$_3$), which will be specified in Proposition 5 below.

To verify (29) for the case $f(u) = u^3 - u$, we first rewrite $f(u^{m+1})$ as follows

$$f(u^{m+1}) = \frac{1}{2}\big(|\, u^{m+1}\,|^2 - 1\big)\big([u^m + u^{m+1}] + k d_t u^{m+1}\big).$$

Then

$$\begin{aligned}
&\frac{1}{2\varepsilon^2}(f(u^{m+1}), d_t u^{m+1}) \\
&\quad = \frac{1}{2\varepsilon^2}\big(|\, u^{m+1}\,|^2 - 1, d_t(|\, u^{m+1}\,|^2 - 1)\big) \\
&\qquad\qquad\qquad + \frac{k}{2\varepsilon^2}\big(|\, u^{m+1}\,|^2 - 1, |\, d_t u^{m+1}\,|^2\big) \\
&\quad \geq \frac{1}{2\varepsilon^2}\Big(|\, u^{m+1}\,|^2 - 1 \pm \big(|\, u^m\,|^2 - 1\big), d_t\big(|\, u^{m+1}\,|^2 - 1\big)\Big) \\
&\qquad\qquad\qquad - \frac{k}{2\varepsilon^2}\|\, d_t u^{m+1}\,\|_{L^2}^2 \\
&\quad \geq \frac{1}{2\varepsilon^2}\, d_t \|\,|\, u^{m+1}\,|^2 - 1\,\|_{L^2}^2 + \frac{k}{2\varepsilon^2}\,\|\, d_t\big(|\, u^{m+1}\,|^2 - 1\big)\,\|_{L^2}^2 \\
&\qquad\qquad\qquad - \frac{k}{2\varepsilon^2}\|\, d_t u^{m+1}\,\|_{L^2}^2 .
\end{aligned} \tag{35}$$

Multiplying (35) by k and summing over m from 0 to M we obtain (29) with $\alpha_0 = 2$, $\gamma_3 = \frac{1}{2}$, and $\tilde{c}_4 = 2$. Moreover, we have

Proposition 5 *For $k \leq \varepsilon^2$, the solution $\{u^m\}_{m=0}^M$ of (26)-(28) satisfies*

$$\begin{aligned}
\max_{0\leq m\leq M}\Big\{\|\, \nabla u^m\,\|_{L^2}^2 + \frac{1}{\varepsilon^2}\|\, F(u^m)\,\|_{L^1}\Big\} + k\sum_{m=1}^{M}\Big\{(1 - \frac{k}{2\varepsilon^2})\,\|\, d_t u^m\,\|_{L^2}^2 \\
+ \frac{k}{2}\,\|\, \nabla d_t u^m\,\|_{L^2}^2 + \frac{k}{2\varepsilon^2}\,\|\, d_t(|\, u^m\,|^2 - 1)\,\|_{L^2}^2\Big\} \leq \mathcal{J}_\varepsilon(u^0)\,.
\end{aligned}$$

Proof. The assertion immediately follows from testing (26) with $d_t u^{m+1}$ and applying (35).

The above derivation also suggests to consider the following variant scheme of (26):

$$(36)\quad d_t u^{m+1} - \Delta u^{m+1} + \frac{1}{4\varepsilon^2}\big\{|\, u^m\,|^2 + |\, u^{m+1}\,|^2 - 2\big\}\big\{u^m + u^{m+1}\big\} = 0\,.$$

It turns out that this new scheme has better stability properties than the scheme (26) does as shown by the next proposition.

Proposition 6 *The solution* $\{u^m\}_{m=0}^M$ *of (36) satisfies for any* $k > 0$

$$\begin{aligned} &k\sum_{m=1}^{M}\Big\{\|\, d_t u^m\,\|_{L^2}^2 + \frac{k}{2}\,\|\,\nabla d_t u^m\,\|_{L^2}^2\Big\} \\ &\quad + \max_{0\le m\le M}\Big\{\frac{1}{2}\,\|\,\nabla u^m\,\|_{L^2}^2 + \frac{1}{\varepsilon^2}\|\, F(u^m)\,\|_{L^1}\Big\} = \mathcal{J}_\varepsilon(u^0)\,. \end{aligned}$$

Proof. After testing (36) by $d_t u^{m+1}$, the only term which needs to be treated specially is

$$\mathcal{A} \equiv \frac{1}{4\varepsilon^2}\big(\{|\, u^m\,|^2 + |\, u^{m+1}\,|^2 - 2\}\{u^m + u^{m+1}\}, d_t u^{m+1}\big)$$

appearing on the left hand side of the equation. We apply a binomial formula twice to reformulate this term as

$$\begin{aligned} \mathcal{A} &= \frac{1}{4\varepsilon^2}\big(\{|\, u^m\,|^2 + |\, u^{m+1}\,|^2 - 2\}, d_t|\, u^{m+1}\,|^2\big) \\ &= \frac{1}{4\varepsilon^2}\Big(\{|\, u^m\,|^2 + |\, u^{m+1}\,|^2 - 2\}, d_t\big[|\, u^{m+1}\,|^2 - 1\big]\Big) \\ &= \frac{1}{4\varepsilon^2}\, d_t\|\,|\, u^{m+1}\,|^2 - 1\,\|_{L^2}^2\,. \end{aligned}$$

The proof then is completed by taking summation over m.

Remark 5 (a). There is an “artificial dissipation effect” in (36) visible from the second term in the proposition. To avoid it, we replace the second term in (36) by $-\frac{1}{2}\Delta\{u^{m+1} + u^m\}$. Then following the proof below for (36), and making use of the binomial formula $(a-b)(a+b) = a^2 - b^2$ we can show that dissipative effect is eliminated.

(b). Note that Proposition 6 holds under no constraint on k.

(c). Despite of the advantage to satisfy the energy law by the scheme (36), we prefer the scheme (26) for its simpler structure. However, it would be interesting to also analyze the scheme (36) and compare the two schemes numerically.

3.2 Error estimates for the scheme (26)-(28)

In this subsection, we present the error analysis for (26)-(28) under the assumptions (GA_1)-(GA_3). As is shown in Subsection 3.1, the stability result of the time-discrete scheme imposes some constraint on the time step size k. In fact, in order to establish convergence of the discrete scheme (26)-(28), this constraint needs to be strengthened according to the following convergence theorem, which is the first of the two main theorems of this section.

Theorem 3 *Let $\{u^m\}_{m=0}^M$ solve (26)-(28) on a quasi-uniform mesh $J_k = \{t_m\}_{m=0}^M$ of mesh size $O(k)$. Suppose (GA_1)-(GA_3) hold. For any fixed $0 < \beta < 2$, let k satisfy the following constraint*

$$k \le \tilde{C} \min\left\{\varepsilon^{\frac{2}{\beta}}, \varepsilon^{\alpha_0}, \varepsilon^{\alpha_1}, \varepsilon^{\alpha_2(\beta)}\right\} \tag{37}$$

where for $N = 2, 3$

$$\alpha_1 = \frac{4\delta \max\{\sigma_1 + 1, \sigma_2\} + 8}{4 + (4 - N)\delta},$$
$$\alpha_2(\beta) = \frac{2\max\{\sigma_1 + 2, \sigma_2\}}{2 - \beta} + \frac{2N\delta \max\{\sigma_1 + 1, \sigma_2\} + 16}{(2 - \beta)(4 - N)\delta}.$$

Then there exists a positive constant $\tilde{C} = \tilde{C}(u_0; \gamma_1, \gamma_2, C_0, T, \Omega)$ such that the solution of (26)-(28) satisfies the following error estimate

$$\max_{0\le m\le M} \| u(t_m) - u^m \|_{L^2} + \Big(k \sum_{m=1}^{M} \Big\{k \| d_t(u(t_m) - u^m) \|_{L^2}^2 + k^\beta \| \nabla(u(t_m) - u^m) \|_{L^2}^2\Big\}\Big)^{\frac{1}{2}} \le \tilde{C}\, k^{\frac{1}{2}(2-\beta)}\, \varepsilon^{\min\{-\sigma_1-2, -\sigma_2\}}.$$

The proof is divided into four steps: the first step deals with consistency error and shows the relevancy of the condition $(GA_1)_3$ imposed on f. Steps two and three use Proposition 3 and stability properties of the implicit Euler-method to avoid exponential blow-up in ε^{-1} of the error constants. In the last step, an inductive argument is used to handle the difficulty caused by the super-quadratic term in $(GA_1)_3$.

Proof. *Step 1:* Let $e^m := u(t_m) - u^m$ denote the error function. Subtracting (26) from (1) and testing the resulting error equation by e^{m+1} we get

$$\frac{1}{2} d_t \| e^{m+1} \|_{L^2}^2 + \frac{k}{2} \| d_t e^{m+1} \|_{L^2}^2 + \| \nabla e^{m+1} \|_{L^2}^2 + \frac{1}{\varepsilon^2}\big(f(u(t_{m+1})) - f(u^{m+1}), e^{m+1}\big) = \big(\mathcal{R}(u_{tt}; m), e^{m+1}\big), \tag{38}$$

where

$$\mathcal{R}(u_{tt}; m) = -\frac{1}{k}\int_{t_m}^{t_{m+1}} (s - t_m) u_{tt}(s)\,\mathrm{d}s\,.$$

From (iv) of Proposition 1

$$\begin{aligned} k\sum_{m=0}^{M} \| \mathcal{R}(u_{tt}; m) \|_{H^{-1}}^2 &\le \frac{1}{k}\sum_{m=0}^{M}\Big[\int_{t_m}^{t_{m+1}} (s - t_m)^2\,\mathrm{d}s\Big] \\ &\quad \times\Big[\int_{t_m}^{t_{m+1}} \| u_{tt}(s) \|_{H^{-1}}^2\,\mathrm{d}s\Big] \\ &\le C\,k^2\,\varepsilon^{2\min\{-\sigma_1-2,-\sigma_2\}}\,. \end{aligned} \tag{39}$$

To control the last term on the left hand side of (38), we use $(\mathrm{GA}_1)_3$ to get

$$\begin{aligned} &\frac{1}{\varepsilon^2}\big(f(u(t_{m+1})) - f(u^{m+1}), e^{m+1}\big) \\ &\quad \ge \frac{\gamma_1}{\varepsilon^2}\big(f'(u(t_{m+1}))e^{m+1}, e^{m+1}\big) - \frac{\gamma_2}{\varepsilon^2}\,\|e^{m+1}\|_{L^{2+\delta}}^{2+\delta}\,. \end{aligned} \tag{40}$$

Step 2: We want to use the following spectrum estimate result (see Proposition 3) to bound from below the first term on the right hand side of (40)

$$\| \nabla\phi \|_{L^2}^2 + \frac{1}{\varepsilon^2}\,(f'(u)\phi, \phi) \ge -C_0 \| \phi \|_{L^2}^2\,, \quad \forall\,\phi \in H^1(\Omega)\,, \tag{41}$$

where $C_0 > 0$ is independent of ε. In the same time, we want to make use of the $H^{-1}(\Omega)$ norm of $\mathcal{R}(u_{tt}; m)$ in order to keep the power of $\frac{1}{\varepsilon}$ as low as possible in the error constant. The latter requires to keep portions of $\| \nabla e^{m+1} \|_{L^2}^2$ on the left hand side of the error equation (38). To the end, we apply (41) with a scaling factor $\gamma_1(1 - \frac{k^\beta}{2})$ on both sides, which together with (40) and (38) gives

$$\begin{aligned} &\frac{1}{2}\,d_t \| e^{m+1} \|_{L^2}^2 + \frac{k}{2} \| d_t e^{m+1} \|_{L^2}^2 + \frac{1}{2}[1 - \gamma_1(1 - \frac{k^\beta}{2})] \| \nabla e^{m+1} \|_{L^2}^2 \\ &\quad \le C_0\gamma_1(1 - \frac{k^\beta}{2}) \| e^{m+1} \|_{L^2}^2 - \frac{\gamma_1 k^\beta}{2\varepsilon^2}\,(f'(u(t_{m+1}))e^{m+1}, e^{m+1}) \\ &\quad + \frac{C}{\varepsilon^2} \| e^{m+1} \|_{L^{2+\delta}}^{2+\delta} + C\,k^{-\beta} \| \mathcal{R}(u_{tt}; m) \|_{H^{-1}}^2\,. \end{aligned} \tag{42}$$

From (14), the second term on the right hand side can be bounded as

$$-\frac{\gamma_1 k^\beta}{2\varepsilon^2}\,(f'(u(t_{m+1}))e^{m+1}, e^{m+1}) \le \tilde{c}_0 \frac{\gamma_1 k^\beta}{2\varepsilon^2} \| e^{m+1} \|_{L^2}^2\,. \tag{43}$$

Then, we obtain from (39) and (43) after summing (42) over m from 0 to $\ell\,(\leq M)$

$$
\begin{aligned}
&\| e^{\ell+1} \|_{L^2}^2 + k \sum_{m=0}^{\ell} \Big(\frac{k}{2} \| d_t e^{m+1} \|_{L^2}^2 + \frac{\gamma_1 k^\beta}{2} \| \nabla e^{m+1} \|_{L^2}^2 \Big) \\
&\qquad \leq \Big(C_0 \gamma_1 + \tilde{c}_0 \gamma_1 k^\beta \varepsilon^{-2} \Big) k \sum_{m=0}^{\ell} \| e^{m+1} \|_{L^2}^2 \\
&\qquad\quad + C\, k^{2-\beta}\, \varepsilon^{2\min\{-\sigma_1-2,-\sigma_2\}} + \frac{Ck}{\varepsilon^2} \sum_{m=0}^{\ell} \| e^{m+1} \|_{L^{2+\delta}}^{2+\delta}. \qquad (44)
\end{aligned}
$$

Step 3: We now need to bound the super-quadratic term at the end of the inequality (44). First, a shift in the super-index leads to

$$
\| e^{m+1} \|_{L^{2+\delta}}^{2+\delta} \leq C \Big(\| e^m \|_{L^{2+\delta}}^{2+\delta} + k^{2+\delta} \| d_t e^{m+1} \|_{L^{2+\delta}}^{2+\delta} \Big). \qquad (45)
$$

For the first term on the right hand side, we interpolate $L^{2+\delta}$ between L^2 and H^2, and use Propositions 1 (iii) and 4 (iii) to get

$$
\begin{aligned}
\| e^m \|_{L^{2+\delta}}^{2+\delta} &\leq C \Big(\| \Delta e^m \|_{L^2}^{\frac{N\delta}{4}} \| e^m \|_{L^2}^{\frac{8+(4-N)\delta}{4}} + \| e^m \|_{L^2}^{2+\delta} \Big) \\
&\leq C \| e^m \|_{L^2}^{\frac{8+(4-N)\delta}{4}} \Big(\| \Delta e^m \|_{L^2}^{\frac{N\delta}{4}} + \| e^m \|_{L^2}^{\frac{N\delta}{4}} \Big) \\
&\leq C\, \varepsilon^{\frac{N\delta}{4} \min\{-\sigma_1-1,-\sigma_2\}} \| e^m \|_{L^2}^{2+\frac{(4-N)\delta}{4}}.
\end{aligned}
$$

Similarly, the second term on the right hand side of (45) can be bounded as

$$
\begin{aligned}
&k^{2+\delta} \| d_t e^{m+1} \|_{L^{2+\delta}}^{2+\delta} \\
&\quad \leq C k^{2+\delta} \Big(\| \Delta d_t e^{m+1} \|_{L^2}^{\frac{N\delta}{4}} \| d_t e^{m+1} \|_{L^2}^{\frac{8+(4-N)\delta}{4}} + \| d_t e^{m+1} \|_{L^2}^{2+\delta} \Big) \\
&\quad \leq C k^{2+\delta} \| d_t e^{m+1} \|_{L^2}^{\frac{8+(4-N)\delta}{4}} \Big(\| \Delta d_t e^{m+1} \|_{L^2}^{\frac{N\delta}{4}} + \| d_t e^{m+1} \|_{L^2}^{\frac{N\delta}{4}} \Big) \\
&\quad \leq C k^{2+\frac{(4-N)\delta}{4}}\, \varepsilon^{\frac{N\delta}{4} \min\{-\sigma_1-1,-\sigma_2\}} \| d_t e^{m+1} \|_{L^2}^{2+\frac{(4-N)\delta}{4}} \\
&\quad \leq C k^{2+\frac{(4-N)\delta}{4}}\, \varepsilon^{\delta \min\{-\sigma_1-1,-\sigma_2\}} \| d_t e^{m+1} \|_{L^2}^{2}. \qquad (46)
\end{aligned}
$$

Now, summing (45) over m from 0 to $\ell\,(\leq M)$ we find that the super-quadratic term at the end of the inequality (44) can be bounded as follows

$$
\begin{aligned}
\frac{k}{\varepsilon^2} \sum_{m=0}^{\ell} \| e^{m+1} \|_{L^{2+\delta}}^{2+\delta} &\leq C k^{2+\frac{(4-N)\delta}{4}}\, \varepsilon^{\delta \min\{-\sigma_1-1,-\sigma_2\}-2}\, k \sum_{m=0}^{\ell} \| d_t e^{m+1} \|_{L^2}^2 \\
&\quad + C\, \varepsilon^{\frac{N\delta}{4} \min\{-\sigma_1-1,-\sigma_2\}-2}\, k \sum_{m=0}^{\ell} \| e^m \|_{L^2}^{2+\frac{(4-N)\delta}{4}}. \qquad (47)
\end{aligned}
$$

The first term on the right hand side of (47) can be absorbed by the corresponding term on the left hand side of (44) if

$$k \le \varepsilon^{\alpha_1} \quad \text{with } \alpha_1 = \frac{4\delta \max\{\sigma_1 + 1, \sigma_2\} + 8}{4 + (4-N)\delta}. \tag{48}$$

The last term in (47) will be bounded by an inductive argument which is given in the next step.

Step 4: We now conclude the proof by the following inductive argumentation. Suppose there exist two positive constants

$$c_1 = c_1(t_\ell, \Omega, u_0, \sigma_i), \quad c_2 = c_2(t_\ell, \Omega, u_0, \sigma_i; C_0),$$

independent of k and ε, such that the following inequality holds

$$\max_{0\le m\le \ell} \| e^m \|_{L^2}^2 + k \sum_{m=1}^{\ell} \Big(\frac{k}{2} \| d_t e^m \|_{L^2}^2 + \frac{\gamma_1 k^\beta}{2} \| \nabla e^m \|_{L^2}^2 \Big)$$
$$\le c_1\, k^{2-\beta}\, \varepsilon^{2\min\{-\sigma_1-2,-\sigma_2\}} \exp\big(c_2 t_\ell\big) \tag{49}$$

for sufficiently small time step k satisfying

$$k \le \min\big\{ \varepsilon^{\alpha_0}, \varepsilon^{\alpha_1}, \varepsilon^{\frac{2}{\beta}} \big\}. \tag{50}$$

Thanks to (iv) of Proposition 1 and (44), we can choose

$$c_1 = 2, \quad c_2 = 2(C_0 + 1)\gamma_1 .$$

Note that the exponent in the last term of (47) is bigger than 2, hence, we can recover (49) at the $(\ell+1)$th time step by using the discrete Gronwall's inequality, provided that k satisfies

$$\varepsilon^{\frac{N\delta}{4}\min\{-\sigma_1-1,-\sigma_2\}-2} \Big[k^{2-\beta}\, \varepsilon^{2\min\{-\sigma_1-2,-\sigma_2\}} \Big]^{1+\frac{(4-N)\delta}{8}}$$
$$\le \frac{c_1}{2}\, k^{2-\beta}\, \varepsilon^{2\min\{-\sigma_1-2,-\sigma_2\}} \exp\big(c_2 t_{\ell+1}\big). \tag{51}$$

This implies that $k \le \tilde{C} \varepsilon^{\alpha_2(\beta)}$ with

$$\alpha_2(\beta) = \frac{2\max\{\sigma_1+2, \sigma_2\}}{2-\beta} + \frac{2N\delta \max\{\sigma_1+1,\sigma_2\} + 16}{(2-\beta)(4-N)\delta}. \tag{52}$$

The proof is complete.

Remark 6 (a). In addition to the spectrum estimate of Proposition 3, the stability estimates of Proposition 4, in particular, the estimate (iii), are also critical to the analysis.

(b). It is clear that the smaller β, the better the error bound is, since the exponent of k is closer to 1.

(c). The proof of Theorem 3 suggests the following numerical stabilization technique for the Allen-Cahn equation (1)

$$d_t u^{m+1} - \left(1 + \frac{k^{\zeta_1}}{\varepsilon^{\zeta_2}}\right)\Delta u^{m+1} + \frac{1}{\varepsilon^2} f(u^{m+1}) = 0 . \tag{53}$$

where $\zeta_i \geq 0$ for $i = 1, 2$. We will not go into further discussion of these methods here.

The error bound given in Theorem 3 is quasi-optimal. The loss of $\frac{\beta}{2}$ power of k is due to the fact that we have to bound the truncation error $\mathcal{R}(u_{tt}; m)$ in (38) in H^{-1} (not L^2) norm because the (weak) regularity assumptions on the initial data u_0 we made in the general assumption (GA_2), see Sect. 2. On the other hand, if the additional regularity assumption (20) on u_0 is assumed, then the error bound of Theorem 3 can be improved to optimal order.

Theorem 4 *In addition to the assumptions of Theorem 3, suppose that u_0 satisfies (20). Then there exists a positive constant $\tilde{C} = \tilde{C}(u_0; \gamma_1, \gamma_2, C_0, T, \Omega)$ such that for*

$$k \leq \tilde{C} \, \min\left\{\varepsilon^{\alpha_0}, \varepsilon^{\alpha_3}\right\} \tag{54}$$

with

$$\alpha_3 = \max\{\sigma_1 + 2, \sigma_3\} + \frac{N\delta \max\{\sigma_1 + 1, \sigma_2\} + 8}{(4 - N)\delta}, \tag{55}$$

the solution of (26)-(28) satisfies the following error estimates

$$\text{(i)} \max_{0 \leq m \leq M} \| u(t_m) - u^m \|_{L^2} + \left(k \sum_{m=1}^{M} \{k \| d_t(u(t_m) - u^m) \|_{L^2}^2\right)^{\frac{1}{2}} \leq \tilde{C}\, k\, \varepsilon^{\min\{-\sigma_1 - 2, -\sigma_3\}},$$

$$\text{(ii)} \left(k \sum_{m=0}^{M} \| \nabla(u(t_m) - u^m) \|_{L^2}^2\right)^{\frac{1}{2}} \leq \begin{cases} \tilde{C}\, k\, \varepsilon^{\min\{-\sigma_1 - 3, -\sigma_3 - 1\}} & \textit{if } \gamma_1 = 1, \\ \tilde{C}\, k\, \varepsilon^{\min\{-\sigma_1 - 2, -\sigma_3\}} & \textit{if } 0 < \gamma_1 < 1. \end{cases}$$

Proof. Since the proof is similar to that of Theorem 3, we only point out the main differences in the following. First, with help of (21), (39) now is replaced by

$$
\begin{aligned}
k \sum_{m=0}^{M} \| \mathcal{R}(u_{tt}; m) \|_{L^2}^2 &\leq \frac{1}{k} \sum_{m=0}^{M} \Big[\int_{t_m}^{t_{m+1}} (s - t_m)^2 \, ds \Big] \Big[\int_{t_m}^{t_{m+1}} \| u_{tt}(s) \|_{L^2}^2 \, ds \Big] \\
&\leq C\, k^2\, \varepsilon^{2 \min\{-\sigma_1 - 2, -\sigma_3\}} . \qquad (56)
\end{aligned}
$$

Next, (42) becomes

$$
\begin{aligned}
&\frac{1}{2} d_t \| e^{m+1} \|_{L^2}^2 + \frac{k}{2} \| d_t e^{m+1} \|_{L^2}^2 + (1 - \gamma_1) \| \nabla e^{m+1} \|_{L^2}^2 \\
&\leq (C_0 \gamma_1 + \frac{1}{2}) \| e^{m+1} \|_{L^2}^2 + \frac{\gamma_2}{\varepsilon^2} \| e^{m+1} \|_{L^{2+\delta}}^{2+\delta} + \frac{1}{2} \| \mathcal{R}(u_{tt}; m) \|_{L^2}^2 . \qquad (57)
\end{aligned}
$$

Hence, (44) is replaced by

$$
\begin{aligned}
&\| e^{\ell+1} \|_{L^2}^2 + k \sum_{m=0}^{\ell} \Big\{ \frac{k}{2} \| d_t e^{m+1} \|_{L^2}^2 + (1 - \gamma_1) \| \nabla e^{m+1} \|_{L^2}^2 \Big\} \\
&\leq (2 C_0 \gamma_1 + 1)\, k \sum_{m=0}^{\ell} \| e^{m+1} \|_{L^2}^2 + C\, k^2\, \varepsilon^{2 \min\{-\sigma_1 - 2, -\sigma_3\}} \\
&\quad + \frac{2\gamma_2}{\varepsilon^2} k \sum_{m=0}^{\ell} \| e^{m+1} \|_{L^{2+\delta}}^{2+\delta} . \qquad (58)
\end{aligned}
$$

By exactly repeating Step 3 and Step 4 of the proof of Theorem 3 we obtain the desired $\| e^m \|_{L^2}$ error bound as in (i). Note that (51) now is replaced by

$$
\begin{aligned}
&\varepsilon^{\frac{N\delta}{4} \min\{-\sigma_1 - 1, -\sigma_2\} - 2} \Big[k^2\, \varepsilon^{2 \min\{-\sigma_1 - 2, -\sigma_3\}} \Big]^{1 + \frac{(4-N)\delta}{8}} \\
&\leq \frac{c_1}{2}\, k^2\, \varepsilon^{2 \min\{-\sigma_1 - 2, -\sigma_3\}} \exp\big(c_2 t_{\ell+1} \big) , \qquad (59)
\end{aligned}
$$

which results in the constraint $k \leq \varepsilon^{\alpha_3}$ with α_3 is given by (55).

Finally, if $0 < \gamma_1 < 1$, the bound for $\| \nabla e^m \|_{L^2}$ comes immediately from (58) and (i). For the case $\gamma_1 = 1$, to get the desired error bound, we need a little bit more manipulations.

Applying the Mean Value Theorem on f in (38) and using (14) to get

$$
\begin{aligned}
&\frac{1}{2} d_t \| e^{m+1} \|_{L^2}^2 + \frac{k}{2} \| d_t e^{m+1} \|_{L^2}^2 + \| \nabla e^{m+1} \|_{L^2}^2 \\
&= -\frac{1}{\varepsilon^2} \big(f'(\xi), |e^{m+1}|^2 \big) + \big(\mathcal{R}(u_{tt}; m), e^{m+1} \big) \\
&\leq \frac{1}{2} \| \mathcal{R}(u_{tt}; m) \|_{L^2}^2 + \Big(\frac{1}{2} + \frac{\tilde{c}_0}{\varepsilon^2} \Big) \| e^{m+1} \|_{L^2}^2 , \qquad (60)
\end{aligned}
$$

where ξ is a value between $u(t_{m+1})$ and u^{m+1}.

Multiplying (60) by k and summing over m, the assertion (ii) then follows from applying (56) and (i).

Remark 7 The estimate (ii) of Theorem 4 illustrates the stabilizing effect of small values $0 < \gamma_1 < 1$ from $(\mathrm{GA}_1)_3$ in the numerical scheme.

4 Error analysis for a fully discrete approximation

Let $\mathcal{T}_h$ be a quasi-uniform "triangulation" of Ω such that $\overline{\Omega} = \bigcup_{K\in\mathcal{T}_h} \overline{K}$ ($K \in \mathcal{T}_h$ are tetrahedrons in the case $N = 3$). Here $h := \max_{K\in\mathcal{T}_h} h_K$ denotes the mesh size of $\mathcal{T}_h$, see [8,17] for further details. Let $\mathcal{S}_h$ be the finite element subspace of $H^1(\Omega)$ associated with $\mathcal{T}_h$ and consisting of continuous and piecewise linear functions on $\mathcal{T}_h$, that is,

$$\mathcal{S}_h := \left\{ v_h \in C(\overline{\Omega}) : \; v_h\big|_K \in P_1(K), \; \forall K \in \mathcal{T}_h \right\}.$$

The fully discrete finite element discretization of (26)-(28) is then defined by seeking $\{U^m\}_{m=0}^M$ in $\mathcal{S}_h$ such that for $m = 1, 2, \cdots, M$,

$$(d_t U^m, v_h) + (\nabla U^m, \nabla v_h) + \frac{1}{\varepsilon^2}\,(f(U^m), v_h) = 0 \;\; \forall v_h \in \mathcal{S}_h \tag{61}$$

with a starting value $U^0 \subset \mathcal{S}_h$ to be specified later (see Remark 9).

The following stability results hold for the discrete solution $\{U^m\}_{m=0}^M$.

Proposition 7 *Suppose* (GA_3) *holds, then the solution* $\{U^m\}_{m=0}^M$ *of (61) satisfies the following estimates:*

$$\begin{aligned}
&\text{(i)} \quad \max_{0\le m\le M} \left\{ \| \nabla U^m \|_{L^2}^2 + \frac{1}{\varepsilon^2} \| F(U^m) \|_{L^1} \right\} \\
&\qquad + k \sum_{m=1}^{M} \left\{ \| d_t U^m \|_{L^2}^2 + k \| \nabla d_t U^m \|_{L^2}^2 \right\} \le 2\, \tilde{c}_4\, \mathcal{J}_\varepsilon(U^0)\,,
\end{aligned} \tag{62}$$

$$\begin{aligned}
&\text{(ii)} \quad \max_{0\le m\le M} \| d_t U^m \|_{L^2}^2 + k \sum_{m=1}^{M} k \| d_t^2 U^m \|_{L^2}^2 \\
&\qquad + k \sum_{m=1}^{M} \| \nabla d_t U^m \|_{L^2}^2 \le C \varepsilon^{2\min\{\sigma_1 - 1, -\sigma_2\}}.
\end{aligned} \tag{63}$$

Proof. The assertion (i) comes immediately from setting $v_h = d_t U^m$ in (61) and using (GA_3). To show (ii), we first apply the difference operator d_t on the both sides of (61), then choose $v_h = d_t U^m$, finally use the Mean Value Theorem and (14) to bound the nonlinear term as follows

$$\frac{1}{\varepsilon^2}\Big(d_t f(U^m), d_t U^m \Big) = \Big(f'(\xi), |d_t U^m|^2 \Big) \ge -\frac{\tilde{c}_0}{\varepsilon^2} \| U^m \|_{L^2}^2.$$

The proof then is complete after taking summation over m and using (i) and (GA_2).

The objective of this section is to establish some optimal order error estimates for the global error $E^m := u(t_m) - U^m$ of the fully discrete scheme (61) under some reasonable constraints on h and k and regularity assumptions on u_0. In particular, we are interested in knowing that under what constraints on k and h the error E^m can be bounded in terms of a low order polynomial of $\frac{1}{\varepsilon}$. The main ideas of obtaining that are: first, to establish a discrete version of the spectrum estimate of Proposition 3; then, to use the four-step strategy used in the proof of Theorem 3 to derive the desired estimates.

To analyze the global error E^m, we need to introduce the L^2 projection operator $Q_h : L^2(\Omega) \to \mathcal{S}_h$

$$(u - Q_h u, v_h) = 0 \quad \forall v_h \in \mathcal{S}_h; \tag{64}$$

and the elliptic projection operator $P_h : H^1(\Omega) \to \mathcal{S}_h$

$$(u - P_h u, v_h) + (\nabla[u - P_h u], \nabla v_h) = 0 \quad \forall v_h \in \mathcal{S}_h. \tag{65}$$

It is well-known that Q_h and P_h have the following approximation properties [33, 17, 8]:

$$\| u - Q_h u \|_{L^2} + h \| \nabla(u - Q_h u) \|_{L^2} \leq Ch \|u\|_{H^1} \; \forall u \in H^1(\Omega), \tag{66}$$

$$\| u - Q_h u \|_{L^2} \leq Ch^2 \|u\|_{H^2} \quad \forall u \in H^2(\Omega); \tag{67}$$

$$\| u - P_h u \|_{L^2} + h \| \nabla(u - P_h u) \|_{L^2} \leq Ch^2 \|u\|_{H^2} \; \forall u \in H^2(\Omega), \tag{68}$$

$$\| u - P_h u \|_{L^\infty} \leq Ch^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \|u\|_{H^2} \quad \forall u \in H^2(\Omega), \tag{69}$$

$$\|(u - P_h u)_t\|_{L^2(J;L^2)} \leq Ch^2 \|u_t\|_{L^2(J;H^2)} \quad \forall u \in H^1(J; H^2), \tag{70}$$

$$\|(u - P_h u)_t\|_{L^2(J;H^{-1})} \leq Ch^2 \|u\|_* \quad \forall u \in W, \tag{71}$$

where

$$W = \{w \, ; \, w \in H^1(J; H^1), \; \| w \|_* < \infty\},$$

$$\| w \|_* = \left(\| w \|^2_{H^1(J;H^1)} + \sum_{i,j=1}^{N} \| \partial_{x_j} \partial_{x_i} w_t \|^2_{L^2(J;H^{-1})} \right)^{\frac{1}{2}}.$$

Remark 8 Since the estimate (69) is not used in the literature very often, for readers' convenience we give a short proof here. Note that the norm on the right hand side is $H^2(\Omega)$ norm, not $W^{2,\infty}(\Omega)$ norm.

Let I_h denote the standard Lagrange interpolation operator on $\mathcal{S}_h$, using the inverse inequality and the stability property of P_h in $H^1(\Omega)$ we get

$$\begin{aligned} \| u - P_h u \|_{L^\infty} &\leq \| u - I_h u \|_{L^\infty} + \| P_h(I_h u - u) \|_{L^\infty} \\ &\leq \| u - I_h u \|_{L^\infty} + Ch^{1-\frac{N}{2}} |\ln h|^{\frac{3-N}{2}} \| I_h u - u \|_{H^1}. \end{aligned}$$

The assertion then follows from the well-known estimates for the interpolation operator I_h (see Theorem 4.4.4 of [8]).

As shown in the proofs of Theorems 3 and 4, in order to establish error bounds that depend on low order polynomials of $\frac{1}{\varepsilon}$, the crucial idea is to utilize the spectrum estimate result of Proposition 3 for the linearized Allen-Cahn operator. In the following we show that the spectrum estimate still holds if the function u, which is the solution of (1)-(3), is replaced by its elliptic projection $P_h u$ provided that the mesh size h is small enough. As expected, this result plays a critical role in our error analysis for the fully discrete finite element discretization.

Let

$$C_1 = \max_{|\xi|\le 2} |f''(\xi)|, \tag{72}$$

and C_2 be the smallest positive ε-independent constant such that

$$\| u - P_h u \|_{L^\infty(J;L^\infty)} \le C_2 h^{\frac{4-N}{2}} \,|\ln h|^{\frac{3-N}{2}}\, \varepsilon^{\min\{-\sigma_1-1,-\sigma_2\}}, \tag{73}$$

where u is the solution of (1)-(3). Note that (iii) of Proposition 1 ensures the existence of C_2.

Proposition 8 *Let the assumptions of Proposition 3 hold and C_0 be same as there. Let u be the solution of (1)-(3) and $P_h u$ be its elliptic projection. Then there holds for small $\varepsilon > 0$*

$$\lambda_{AC}^h \equiv \inf_{\substack{\psi\in H^1(\Omega)\\ \psi\neq 0}} \frac{\| \nabla\psi \|_{L^2}^2 + \varepsilon^{-2}\,(f'(P_h u)\psi, \psi)}{\| \psi \|_{L^2}^2} \ge -2C_0\,, \tag{74}$$

provided that h satisfies the constraint

$$h^{\frac{4-N}{2}}\,|\ln h|^{\frac{3-N}{2}} \le C_0(C_1C_2)^{-1}\, \varepsilon^{\max\{\sigma_1+3,\sigma_2+2\}}. \tag{75}$$

Proof. From the definitions of C_1 and C_2, we immediately have

$$\| P_h u \|_{L^\infty(J;L^\infty)} \le \| u \|_{L^\infty(J;L^\infty)} + \| P_h u - u \|_{L^\infty(J;L^\infty)} \le 2$$

if h satisfies (75).

It then follows from the Mean Value Theorem that

$$\begin{aligned} \| f'(P_h u) - f'(u) \|_{L^\infty(J;L^\infty)} &\le \max_{|\xi|\le 2} |f''(\xi)| \| P_h u - u \|_{L^\infty(J;L^\infty)} \\ &\le C_1C_2 h^{\frac{4-N}{2}}\,|\ln h|^{\frac{3-N}{2}} \varepsilon^{\min\{-\sigma_1-1,-\sigma_2\}} \\ &\le C_0\,\varepsilon^2. \end{aligned} \tag{76}$$

Using the inequality $a \ge b - |a-b|$ and (76) we get

$$\begin{aligned} f'(P_h u) &\ge f'(u) - \| f'(P_h u) - f'(u) \|_{L^\infty(J;L^\infty)} \\ &\ge f'(u) - C_0\varepsilon^2\,. \end{aligned} \tag{77}$$

Finally, the proof is completed by substituting (77) into the definition of λ_{AC}^{h} and applying Proposition 3.

Theorem 5 *Let $\{U^m\}_{m=0}^{M}$ solve (61) on a quasi-uniform time mesh $J_k := \{t_m\}_{m=0}^{M}$ of size $O(k)$ and a quasi-uniform space mesh $\mathcal{T}_h$ of size $O(h)$. Suppose that the assumptions of Theorem 4 hold, and α_3 is same as there. Then, under the following mesh and starting value constraints*

$$1).\quad k \le \varepsilon^{\alpha_0}, \tag{78}$$

$$2).\quad h|\ln h|^{\frac{3-N}{4-N}} \le \varepsilon^{\frac{2}{4-N}\max\{\sigma_1+3,\,\sigma_2+2\}}, \qquad (N=2,3) \tag{79}$$

$$3).\quad k^2+h^4 \le \varepsilon^{2\alpha_3}, \tag{80}$$

$$4).\quad \| U^0 - u_0 \|_{L^2} \le Ch^2 \| u_0 \|_{H^2}, \tag{81}$$

the solution of (61) satisfies the error estimates

$$\text{(i)}\quad \max_{0\le m\le M} \| u(t_m) - U^m \|_{L^2} + \Big(k \sum_{m=1}^{M} k \, \| d_t(u(t_m)-U^m) \|_{L^2}^2 \Big)^{\frac{1}{2}} \le \tilde{C}\,(k+h^2)\,\varepsilon^{\min\{-\sigma_1-2,-\sigma_3\}},$$

$$\text{(ii)}\quad \Big(k \sum_{m=1}^{M} \| \nabla(u(t_m)-U^m) \|_{L^2}^2 \Big)^{\frac{1}{2}} \le \begin{cases} \tilde{C}\,(k+h)\,\varepsilon^{\min\{-\sigma_1-3,-\sigma_3-1\}} & \text{if } \gamma_1 = 1, \\ \tilde{C}\,(k+h)\,\varepsilon^{\min\{-\sigma_1-2,-\sigma_3\}} & \text{if } 0<\gamma_1<1, \end{cases}$$

$$\text{(iii)}\quad \max_{0\le m\le M} \| u(t_m) - U^m \|_{L^\infty} \le \tilde{C} \Big[h^{\frac{4-N}{2}} \,|\ln h|^{\frac{3-N}{2}}\, \varepsilon^{\min\{-\sigma_1-1,-\sigma_2\}} + (k+h^2)\,h^{-\frac{N}{2}}\,\varepsilon^{\min\{-\sigma_1-2,-\sigma_3\}} \Big].$$

for some positive constant $\tilde{C} = \tilde{C}(u_0; \gamma_1, \gamma_2, C_0, T, \Omega)$.

Proof. First, we decompose the global error $E^m := u(t_m) - U^m$ of the fully discrete scheme (61) into $E^m = \Theta^m + \Phi^m$, where

$$\Theta^m := u(t_m) - P_h u(t_m), \qquad \Phi^m := P_h u(t_m) - U^m.$$

Notice that $\Phi^m \in \mathcal{S}_h \subset H^1(\Omega)$.

Next, testing the equation (1) with Φ^m and subtracting (61) with $v_h = \Phi^m$ from the resulting equation we get the error equation

$$(d_t E^m, \Phi^m) + (\nabla E^m, \nabla \Phi^m) + \frac{1}{\varepsilon^2}\,(f(u(t_m)) - f(U^m), \Phi^m) = (\mathcal{R}(u_{tt}; m), \Phi^m). \tag{82}$$

After multiplying by k and taking summation on m from 1 to $\ell(\leq M)$ and using (65) we get

$$\frac{1}{2}\| \Phi^{\ell} \|_{L^2}^2 + k\sum_{m=1}^{\ell} \frac{k}{2}\| d_t\Phi^m \|_{L^2}^2$$

$$+ k\sum_{m=1}^{\ell}\Big\{\| \nabla\Phi^m \|_{L^2}^2 + \frac{1}{\varepsilon^2}\Big(f(P_h u(t_m)) - f(U^m), \Phi^m\Big)\Big\}$$

$$= k\sum_{m=1}^{\ell}\Big\{(\mathcal{R}(u_{tt}; m), \Phi^m) - (d_t\Theta^m, \Phi^m) - (\Theta^m, \Phi^m)$$

$$-\frac{1}{\varepsilon^2}\Big(f(u(t_m)) - f(P_h u(t_m)), \Theta^m\Big)\Big\} + \frac{1}{2}\| \Phi^0 \|_{L^2}^2. \tag{83}$$

With help of (39), (62), (68), (70), and Propositions 1 and 2, the first three terms on the right hand side of (83) can be bounded together as follows

$$k\sum_{m=1}^{\ell}\Big\{(\mathcal{R}_{tt}, \Phi^m) - (d_t\Theta^m, \Phi^m) + (\Theta^m, \Phi^m)\Big\}$$

$$\leq k\sum_{m=1}^{\ell}\Big\{\| \mathcal{R}(u_{tt}; m) \|_{L^2}^2 + \| d_t\Theta^m \|_{L^2}^2 + \| \Theta^m \|_{L^2}^2 + \| \Phi^m \|_{L^2}^2\Big\}$$

$$\leq C(k^2 + h^4)\varepsilon^{2\min\{-\sigma_1-2, -\sigma_3\}} + k\sum_{m=1}^{\ell} \| \Phi^m \|_{L^2}^2. \tag{84}$$

To bound the fourth term on the right hand side of (83), we apply the Mean Value Theorem on f, use (14) and (ii) of Proposition 1 to get

$$k\sum_{m=1}^{\ell} -\frac{1}{\varepsilon^2}\Big(f(u(t_m)) - f(P_h u(t_m)), \Theta^m\Big)$$

$$= \frac{k}{\varepsilon^2}\sum_{m=1}^{\ell} -\Big(f'(\xi), |\Theta^m|^2\Big) \leq \frac{\tilde{c}_0}{\varepsilon^2} k\sum_{m=1}^{\ell} \| \Theta^m \|_{L^2}^2$$

$$\leq C\, h^4 \varepsilon^{-2(\sigma_1+2)}. \tag{85}$$

Next, we need to bound from below the last term on the left hand side of (83), which will be handled in the same way as for a similar term in (38) using $(\mathrm{GA}_1)_3$ and the spectrum estimate of Proposition 8.

$$
\begin{aligned}
k\sum_{m=1}^{\ell}\Big\{\gamma_1 \| \nabla \Phi^m \|_{L^2}^2 + \frac{1}{\varepsilon^2}\Big(f(P_h u(t_m)) - f(U^m), \Phi^m\Big)\Big\} \\
\geq k\sum_{m=1}^{\ell}\Big\{\gamma_1\Big[\| \nabla \Phi^m \|_{L^2}^2 + \frac{1}{\varepsilon^2}\Big(f'(P_h u(t_m))\Phi^m, \Phi^m\Big)\Big] \\
-\frac{\gamma_2}{\varepsilon^2} \| \Phi^m \|_{L^{2+\delta}}^{2+\delta}\Big\} \\
\geq -2\gamma_1 C_0 k \sum_{m=1}^{\ell} \| \Phi^m \|_{L^2}^2 - \frac{\gamma_2}{\varepsilon^2} k \sum_{m=1}^{\ell} \| \Phi^m \|_{L^{2+\delta}}^{2+\delta}.
\end{aligned} \tag{86}
$$

Finally, substituting (84)-(86) into (83) we arrive at

$$
\begin{aligned}
\frac{1}{2} \| \Phi^\ell \|_{L^2}^2 + k\sum_{m=1}^{\ell} \frac{k}{2} \| d_t \Phi^m \|_{L^2}^2 + (1-\gamma_1)\, k \sum_{m=1}^{\ell}\Big\{ \| \nabla \Phi^m \|_{L^2}^2 \\
\leq C(k^2+h^4)\, \varepsilon^{2\min\{-\sigma_1-2,-\sigma_3\}} + 2(1+2\gamma_1 C_0)\, k \sum_{m=0}^{\ell} \| \Phi^m \|_{L^2}^2 \\
+ \frac{\gamma_2}{\varepsilon^2} k \sum_{m=1}^{\ell} \| \Phi^m \|_{L^{2+\delta}}^{2+\delta}.
\end{aligned} \tag{87}
$$

Notice that (87) is the fully discrete counterpart of (58) in the proof of Theorem 4, and to (44) in the proof of Theorem 3. Hence, by repeating Step 3 and Step 4 of the proof of Theorem 3 and using a local interpolation argument of [23, 24] (note that the counterparts of the stability estimates of Proposition 4 are those of Proposition 7), we conclude that

(88)

$$
\max_{0\leq m\leq M} \| \Phi^m \|_{L^2} + \Big(k \sum_{m=1}^{M} \{ k \| d_t \Phi^m \|_{L^2}^2 \Big)^{\frac{1}{2}} \leq \tilde{C}\, (k+h^2)\, \varepsilon^{\min\{-\sigma_1-2,-\sigma_3\}},
$$

(89)

$$
\Big(k \sum_{m=1}^{M} \| \nabla \Phi^m \|_{L^2}^2 \Big)^{\frac{1}{2}} \leq \begin{cases} \tilde{C}\, (k+h^2)\, \varepsilon^{\min\{-\sigma_1-3,-\sigma_3-1\}} & \text{if } \gamma_1 = 1, \\ \tilde{C}\, (k+h^2)\, \varepsilon^{\min\{-\sigma_1-2,-\sigma_3\}} & \text{if } 0 < \gamma_1 < 1, \end{cases}
$$

provided that (cf. (59))

$$
\begin{aligned}
\varepsilon^{\frac{N\delta}{4}\min\{-\sigma_1-1,-\sigma_2\}-2} \Big[(k^2+h^4)\, \varepsilon^{2\min\{-\sigma_1-2,-\sigma_3\}} \Big]^{1+\frac{(4-N)\delta}{8}} \\
\leq \frac{c_1}{2}\, (k^2+h^4)\, \varepsilon^{2\min\{-\sigma_1-2,-\sigma_3\}} \exp\big(c_2 t_{\ell+1}\big).
\end{aligned} \tag{90}
$$

It is easy to check that (90) implies that

$$k^2 + h^4 \leq \varepsilon^{2\alpha_3}, \tag{91}$$

where α_3 is defined by (55).

Finally, the assertions (i) and (ii) follow from combining estimates (88)-(89) and (68) with help of the triangle inequality, and the assertion (iii) follows from applying the inverse inequality bounding L^∞ norm in terms of L^2 norm, using (88) and the estimate (69).

Remark 9 (a). Both $L^\infty(J; L^2)$ and $L^2(J; H^1)$ norm estimates are optimal with respect to k and h, and $L^\infty(J; L^\infty)$ estimate is quasi-optimal. We obtain practically useful error bounds that grow at rates of low order polynomials of $\frac{1}{\varepsilon}$.

(b). The proof clearly shows how the three mesh conditions arise. The condition 1) is for the stability of the time discretization (see Sect. 3), the condition 2) is to ensure the discrete spectrum estimate (see Proposition 8), finally, the condition 3) is caused by the super-quadratic nonlinearity of f (see $(\mathrm{GA}_1)_3$). Also notice that only "smallness" of k and h with respect to ε is required but no restriction is imposed on the ratio between k and h in the $L^\infty(J; L^2)$ and $L^2(J; H^1)$ norm estimates.

(c). It is well-known [33] that the finite element solutions of all linear and some nonlinear parabolic problems exhibit a superconvergence property (in h) when compared with the elliptic projections of the solutions of underlying problems. It is worth pointing out that this superconvergence property also holds for the Allen-Cahn equation as showed by the inequality (89).

(d). Regarding the choices of the starting value U^0, although both $U^0 = Q_h u_0$ and $U^0 = P_h u_0$ satisfy the requirement (81) in view of (67) and (68), the L^2 projection $Q_h u_0$ has the advantage of being cheaper to be computed compared to the elliptic projection $P_h u_0$.

(e). If the weaker regularity assumption $u_{tt} \in L^2(J; H^{-1})$ is only assumed, then quasi-optimal order error bounds, with a loss of $\frac{\beta}{2}$ power for arbitrary $0 < \beta < 2$, can be carried out by following the proof of Theorem 3. Notice that the estimate (71) must be used in the place of the estimate (70) in the proof.

(f). A nonconforming finite element scheme to solve (61) might be competitive to deal with interfaces more accurately. In this case, the error bound is complicated by additional terms which reflect inconsistency of the method.

Finally, we have

Proof of Theorem 1 The assertions follow immediately from setting $\alpha_0 = 2$, $\delta = 1$, $\gamma_1 = 1$ and $\gamma_2 = 3$ in Theorem 5.

5 Rate of convergence of the zero level set to the motion by mean curvature flows

In this section we present a nontrivial byproduct of the $L^\infty(J; L^\infty)$ error estimate obtained in the previous section for the fully discrete finite element solution. We show that the zero level set of the fully discrete solution converges to the classical motion by mean curvature flow with a rate of convergence $O(\varepsilon^2|\ln \varepsilon|^2)$ before the onset of singularities, and to the generalized motion by mean curvature flow of [16,22,21] for all times $t \geq 0$ with a rate of convergence $O(\varepsilon)$ provided that the mean curvature flow does not develop an interior. Our main ideas are to make full use of the convergence results of the zero level set of the solution of the Allen-Cahn equation to the the classical motion by mean curvature flow established in [11,5] and to the generalized motion by mean curvature flow showed in [21], and to exploit the "close" relationship between the solution u of the Allen-Cahn equation and its fully discrete finite element approximation $\{U^m\}$. We remark that similar convergence results have been obtained earlier by Nochetto and Verdi in [30,31] for the *double obstacle* Allen-Cahn equation based on constructing fully discrete barriers via a parabolic projection.

Throughout this section, $f(u) = u^3 - u$, and u_ε is used to denote the solution of the Allen-Cahn problem (1)-(3). Let $U_{\varepsilon,h,k}(x,t)$ denote the piecewise linear interpolation (in time) of the fully discrete solution $\{U^m\}$, that is,

$$U_{\varepsilon,h,k}(\cdot,t) := \frac{t-t_m}{k} U^{m+1}(\cdot) + \frac{t_{m+1}-t}{k} U^m(\cdot)$$

for $t_m \leq t \leq t_{m+1}$ and $0 \leq m \leq M-1$. Note that $U_{\varepsilon,h,k}(x,t)$ is a continuous piecewise linear function in space and time.

Let $\{\Gamma_t\}_{t\geq 0}$ denote the generalized motion by mean curvature flow defined in [16,21,22], that is, Γ_t is the zero level set of the solution w of the following nonlinear partial differential equation

$$w_t = \Delta w - \frac{D^2 w Dw \cdot Dw}{|Dw|^2}, \tag{92}$$

$$w(\cdot,0) = w_0(\cdot), \tag{93}$$

with w_0 satisfying $\Gamma_0 = \{x \in \mathbf{R}^N;\ w_0(x) = 0\}$. Here Dw and D^2w denote the gradient and the Hessian of w.

It is explained in [22] that each level set of w evolves according to mean curvature flow, at least in regions where u is smooth and $Dw \neq 0$. Hence, the generalized motion by mean curvature flow $\{\Gamma_t\}_{t\geq 0}$ coincides with the classical smooth differential geometrical flow, as long as the latter exists. In addition, (92)-(93) has a unique continuous solution [22], therefore, $\{\Gamma_t\}_{t\geq 0}$ extends the classical motion past singularities: we refer to [16,22,21] and the references therein for detailed expositions, and to Sect. 2 of [11] and reference therein for further discussions on the classical motion by mean curvature flow.

Define the *inside* I_t and *outside* O_t of Γ_t as follows

$$I_t := \{x \in \mathbf{R}^N;\ w(x,t) > 0\}, \quad O_t := \{x \in \mathbf{R}^N;\ w(x,t) < 0\},$$

and let $d(x,t)$ denote the *signed distance function* to Γ_t that is positive in I_t and negative in O_t.

We are now ready to give a proof of Theorem 2.

Proof of Theorem 2 From Theorem 6.1 of [5] and Theorem 7 of [11] we know that there exist $\widehat{\varepsilon}_0 > 0$ and $\widehat{C}_0 > 0$ such that for all $t < t_*$ and $\varepsilon \in (0, \widehat{\varepsilon}_0)$

$$u_\varepsilon(x,t) \geq 1 - \varepsilon \quad \forall x \in \{x \in \overline{\Omega};\ d(x,t) \geq \widehat{C}_0 \varepsilon^2 |\ln \varepsilon|^2\}, \tag{94}$$

$$u_\varepsilon(x,t) \leq -1 + \varepsilon \quad \forall x \in \{x \in \overline{\Omega};\ d(x,t) \leq -\widehat{C}_0 \varepsilon^2 |\ln \varepsilon|^2\}. \tag{95}$$

Now for any fixed $x \in \Gamma_t^{\varepsilon,h,k}$, since $U_{\varepsilon,h,k}(x,t) = 0$, we have from the estimate (iii) of Theorem 1 that

$$\begin{aligned} |u_\varepsilon(x,t)| &= |u_\varepsilon(x,t) - U_{\varepsilon,h,k}(x,t)| \\ &\leq \tilde{C}\, [\, h^{\frac{4-N}{2}}\, |\ln h|^{\frac{3-N}{2}}\, \varepsilon^{\min\{-\sigma_1 - 1, -\sigma_2\}} \\ &\qquad + h^{2-\frac{N}{2}}\, \varepsilon^{\min\{-\sigma_1 - 2, -\sigma_3\}}\,], \end{aligned} \tag{96}$$

here we have used the assumption $k = O(h^2)$.

Under the mesh conditions of Theorem 1, there exists $\widehat{\widehat{\varepsilon}}_0 > 0$ such that the right hand side of (96) can be strictly bounded from above by $1-\varepsilon$, hence

$$-1 + \varepsilon < u_\varepsilon(x,t) < 1 - \varepsilon, \quad \forall \varepsilon \in (0, \widehat{\widehat{\varepsilon}}_0). \tag{97}$$

Choose $\varepsilon_0 = \min\{\widehat{\varepsilon}_0, \widehat{\widehat{\varepsilon}}_0\}$, it follows from (94), (95) and (97) that x must reside in the tabular neighborhood of Γ_t of width $O(\varepsilon^2|\ln \varepsilon|^2)$ when $\varepsilon \leq \varepsilon_0$, that is,

$$x \in \mathcal{N}_{\varepsilon^2|\ln \varepsilon|^2} := \{x \in \overline{\Omega};\ |d(x,t)| \leq \varepsilon^2 |\ln \varepsilon|^2\}. \tag{98}$$

This completes the proof of (12).

The proof of (13) is almost same, the only change is that the estimates (94) and (95) now is replaced by the following estimates which were established in Theorem 4.1 of [21]: there exist $\widehat{\varepsilon}_1 > 0$ and $\widehat{C}_1 > 0$ such that for all $t \geq 0$ and $\varepsilon \in (0, \widehat{\varepsilon}_1)$

$$u_\varepsilon(x,t) \geq 1 - \varepsilon \quad \forall x \in \{x \in \overline{\Omega};\ d(x,t) \geq \widehat{C}_1 \varepsilon\}, \tag{99}$$

$$u_\varepsilon(x,t) \leq -1 + \varepsilon \quad \forall x \in \{x \in \overline{\Omega};\ d(x,t) \leq -\widehat{C}_1 \varepsilon\}. \tag{100}$$

Note that (99)-(100) are weaker than (95)-(96), however, the former holds for *all times* $t \geq 0$, the latter holds only before the onset of singularities. The remaining part of the proof is exactly same as that of (12), so we omit it. The proof of Theorem 2 is complete.

We conclude this section and the paper with some further remarks.

Remark 10 (a). When $N = 2$, $\sigma_1 = 0$, $\sigma_2 = 1$ and $\sigma_3 = 2$, the exact mesh constraints of Theorem 2 are $k, h^2 = O(\varepsilon^7)$, which is more stringent than the mesh requirements of [30,31]. On the other hand, as expected, the results here are stronger than those of [30,31]. Of course, we should note that different potential functions are treated in [30,31] and here. [30,31] dealt with the double obstacle potential, while the quartic potential is considered in this section.

(b). Clearly, the proof *only* requires that the numerical solution $U_{\varepsilon,h,k}$ satisfies the inequality

$$|u_\varepsilon(x,t) - U_{\varepsilon,h,k}(x,t)| < 1 - \varepsilon \quad \forall x \in \Gamma^{\varepsilon,h,k}. \tag{101}$$

That is, the difference between u_ε and $U_{\varepsilon,h,k}$ is just a little bit less than one. We emphasize that the difference does not have to be very small. This then opens a door for the possibility of establishing the convergence results of Theorem 2 under some weaker mesh constraints than those imposed here.

(c). The smoothness requirement on Γ_0 is not necessary, from [11,5] we know that $C^{3,\alpha}$ is enough.

(d). If the condition that Γ_0 is compactly contained in $\overline{\Omega}$ is dropped, then (12) holds only for $t \le \min\{t_*, t^{\rm touch}\}$ since the estimates (94)-(95) only hold up to $\min\{t_*, t^{\rm touch}\}$ (see [11]), where $t^{\rm touch}$ is the time at which $\Gamma_{t^{\rm touch}}$ touches the boundary $\partial\Omega$ of the domain Ω. Similarly, we expect and conjecture that (13) only holds for $t \le t^{\rm touch}$ if the condition on Γ_0 is dropped.

(e). Since our analysis is based on making full use of the analytical results of [5,11,21], and exploiting the “closeness” of u_ε and $U_{\varepsilon,h,k}$, it allows us to establish the convergence results of Theorem 2 without repeating the complicated techniques, such as constructing barrier functions, of [5,11,21] at the discrete level as done in [30,31,28]. Moreover, this approach allows us to treat every point $x \in \Gamma_t$ indiscriminately and in the same way regardless whether x is a regular or singular point.

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