

**ANALYSIS OF A FULLY DISCRETE FINITE ELEMENT
METHOD FOR THE PHASE FIELD MODEL AND
APPROXIMATION OF ITS SHARP INTERFACE LIMITS†**

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ABSTRACT. We propose and analyze a fully discrete finite element scheme for the phase field model describing the solidification process in materials science. The primary goal of this paper is to establish some useful a priori error estimates for the proposed numerical method, in particular, by focusing on the dependence of the error bounds on the parameter ε , known as the measure of the interface thickness. Optimal order error bounds are shown for the fully discrete scheme under some reasonable constraints on the mesh size h and the time step size k . In particular, it is shown that all 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 Chen [15] and to establish a discrete counterpart of it for a linearized phase field operator to handle the nonlinear effect. Finally, as a nontrivial byproduct, the error estimates are used to establish convergence of the solution of the fully discrete scheme to solutions of the sharp interface limits of the phase field model under different scaling in its coefficients. The sharp interface limits include the classical Stefan problem, the generalized Stefan problems with surface tension and surface kinetics, the motion by mean curvature flow, and the Hele-Shaw model.

1. INTRODUCTION

In this paper we shall propose and analyze a fully discrete finite element time-splitting method for the phase field model

$$(1.1) \quad \varepsilon \alpha(\varepsilon)\varphi_t - \varepsilon \Delta \varphi + \frac{1}{\varepsilon} f(\varphi) = s(\varepsilon)u \quad \text{in } \Omega_T := \Omega \times (0, T),$$

$$(1.2) \quad c(\varepsilon)u_t - \Delta u = -\varphi_t \quad \text{in } \Omega_T,$$

$$(1.3) \quad \frac{\partial u}{\partial n} = \frac{\partial \varphi}{\partial n} = 0 \quad \text{in } \partial\Omega_T := \partial\Omega \times (0, T),$$

$$(1.4) \quad \varphi = \varphi_0^\varepsilon, \quad u = u_0^\varepsilon \quad \text{in } \Omega \times \{0\},$$

where $\Omega \subset \mathbf{R}^N$ ($N = 2, 3$) is a bounded domain with the smooth boundary $\partial\Omega$. $T > 0$ is a fixed constant, and f is the derivative of a smooth double equal well

1991 *Mathematics Subject Classification.* 65M60, 65M12, 65M15, 35B25, 35K57, 35Q99, 53A10.

Key words and phrases. Phase field model, Allen-Cahn equation, Cahn-Hilliard equation, Stefan problem, surface tension and kinetics, motion by mean curvature, Hele-Shaw model, phase transition, fully discrete scheme, finite element method.

†To be submitted to *Math. Comp.*

potential taking its global minimum value 0 at $\varphi = \pm 1$. A typical example of f is

$$(1.5) \quad f(\varphi) := F'(\varphi) \quad \text{and} \quad F(\varphi) = \frac{1}{4}(\varphi^2 - 1)^2.$$

The existence of bistable states suggests that nonconvex energy is associated with the model (see the discussion below). We like to remark that nonsmooth potentials have also been considered in the literature for the phase field model, for that we refer to [7, 18] and the references therein. We also note that the super-index ε on the solution $(u^\varepsilon, \varphi^\varepsilon)$ is suppressed for notation brevity.

The phase field model for solidification was introduced by Caginalp [9], Collins and Levine [21], Fix [29] and Langer [32] to treat phenomena such as crystal growth and the fusion and joining of materials, which are not captured by the classical Stefan problem. The model consists of a heat equation (1.2) and a Ginzburg-Landau/Allen-Cahn equation (1.1) (cf. [4, 24]). Note that the original phase field model consists of equations (1.1) and (1.2), with $\alpha(\varepsilon) = O(1)$, $s(\varepsilon) = O(1)$ and $c(\varepsilon) = O(1)$. In the model, u represents the temperature and φ is an order parameter which will vary continuously but somehow describes the phase of the material. φ is scaled so that $\varphi \approx 1$ represents the liquid phase and $\varphi \approx -1$ the solid phase. α, ε, s and c are respectively the relaxation time, a microscopic scale, a surface tension scale, and the specific heat. We emphasize that the parameter ε is usually small compared to the characteristic dimensions on the laboratory scale. The two boundary conditions in (1.3), the outward normal derivatives of u and φ vanish on $\partial\Omega$, imply no gain or loss of heat energy through the walls of the container Ω . For more physical background, derivation, and discussion of the phase field model and related equations, we refer to [2, 5, 6, 9, 21, 28, 29, 31, 32, 35, 37, 41] and the references therein.

It is known [28] that the phase field model can be formulated as a gradient flow with the Liapunov energy functional

$$(1.6) \quad \mathcal{J}_\varepsilon(\varphi, u) := \int_\Omega \phi_\varepsilon(\varphi, u) \, dx,$$

where

$$\phi_\varepsilon(\varphi, u) := \frac{1}{2\alpha(\varepsilon)} |\nabla\varphi|^2 + \frac{1}{\varepsilon^2\alpha(\varepsilon)} F(\varphi) + \frac{c(\varepsilon)s(\varepsilon)}{2\varepsilon\alpha(\varepsilon)} u^2$$

in the Hilbert space $H_0^{-1} \times L^2$, where H_0^{-1} denotes the mean-zero subspace of H^{-1} , the dual of the Sobolev space H^1 . Note that the energy density $\phi_\varepsilon(\varphi, u)$ is not convex in φ .

In addition to the reason that the phase field model for solidification is widely accepted as a good model for treating phenomena which are not covered by the classical Stefan problem, it has also been used as a (computational) model to compute a wide range of sharp interface problems, including the classical and generalized Stefan problems, the motion by mean curvature flow and the Hele-Shaw model by taking advantage of the fact that the solution of the phase field model exists at all times and the singularities of the free boundaries do not pose either numerical or theoretical difficulties. Furthermore, it could provide sufficient information for the possible extensions of these free boundary problems beyond any singularities. Indeed, the connection between the phase field model and the sharp interface problems has been an extensively studied topic in recent years (cf. [2, 3, 7, 10, 11, 17, 16, 24, 39, 40] and the references therein). It was first formally shown by Caginalp [10] that, as

$\varepsilon \searrow 0$, the function u tends to a limit u^0 , which, together with a free boundary $\Gamma := \cup_{0 \leq t \leq T} (\Gamma_t \times \{t\})$, satisfies the following free boundary problem:

$$(1.7) \quad c^0 u_t^0 - \Delta u^0 = 0 \quad \text{in } \Omega_T \setminus \Gamma,$$

$$(1.8) \quad \frac{\partial u^0}{\partial n} = 0 \quad \text{on } \partial\Omega_T,$$

$$(1.9) \quad V = \frac{1}{2} \left[\frac{\partial u^0}{\partial n} \right]_{\Gamma} \quad \text{on } \Gamma,$$

$$(1.10) \quad u^0 = -d^0 (\kappa_{\Gamma} - \alpha^0 V) \quad \text{on } \Gamma,$$

$$(1.11) \quad u^0 = u_0^0 \quad \text{in } \Omega \times \{0\},$$

$$(1.12) \quad \Gamma_0 = \Gamma_{00} \quad \text{when } t = 0,$$

where c^0, α^0, d^0 are non-negative constants independent of ε , V is the normal velocity of the interface Γ (positive when the motion is directed towards the liquid), κ_{Γ} is the sum of the principal curvatures of the interface (in space), n is the unit outward normal to either $\partial\Omega$ or Γ , $\left[\frac{\partial u^0}{\partial n} \right]_{\Gamma} := \frac{\partial u_+^0}{\partial n} - \frac{\partial u_-^0}{\partial n}$ denotes the jump of the normal derivatives of u^0 across Γ . Also $\varphi \rightarrow \pm 1$ uniformly in every compact subset of $\Omega_T \setminus \Gamma$ as $\varepsilon \searrow 0$. Later, the rigorous justification of this limit was successfully carried out by Caginalp and Chen [11], using a similar methodology as in [3], under the assumption that the above free boundary problem has a unique classical solution. Also, Soner [39] proved the weak convergence of solutions of a phase field model with φ -dependent latent heat to the sharp interface limit in a very general setting that is applicable even when the sharp interface problem does not have a classical solution.

We note that when $s(\varepsilon) = 0$ and $\alpha(\varepsilon) = 1$, equation (1.1) decouples from (1.2) and becomes the Allen-Cahn equation [4]

$$\varphi_t - \Delta \varphi + \frac{1}{\varepsilon^2} f(\varphi) = 0.$$

Its connection to the motion by mean curvature flow was established by de Mottoni and Schatzman [22] and to the generalized motion by mean curvature flow by Evans, Soner and Souganidis [24].

When $\alpha(\varepsilon) = c(\varepsilon) = 0$ and $s(\varepsilon) = 1$, equations (1.1) and (1.2) reduce to the Cahn-Hilliard equation [14]

$$\varphi_t + \Delta(\varepsilon \Delta \varphi - \frac{1}{\varepsilon} f(\varphi)) = 0.$$

The convergence of the Cahn-Hilliard equation to the Hele-Shaw model [36] was recently carried out by Alikakos, Bates and Chen [3].

It is clear that the study of the phase field model (1.1)-(1.4) is of great value for understanding solidification processes, in particular, in presence of surface tension and surface kinetics, and for computing a wide range of sharp interface problems by taking advantage of the fact that the solution of the phase field model is known to exist for all time (cf. [23]). As pointed out earlier, this is particularly attractive from the computational point of view. Due to the nonlinearity in the model, its solution only can be sought numerically. The primary numerical challenge for solving the phase field model results from the presence of the ε -dependent coefficients in the equations of the model. Recall that the phase field model approximates the free boundary problem only when ε becomes very small. On the other hand, the

equations of the model become singularly perturbed heat equations for small ε . 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 the past fifteen years, numerical approximations of the phase field model with a *fixed* ε have been developed and analyzed by several authors. Caginalp and Lin [12] and Lin [34] (also see [30]) proposed an explicit finite difference scheme and an implicit Crank-Nicolson scheme for the original phase field model, the convergence and error estimates of the schemes were shown under a restriction which is equivalent to $\alpha(\varepsilon) \leq c(\varepsilon)$. The restriction excludes some physically interesting cases. Chen and Hoffmann [19] proposed a fully discrete finite element method which uses P_1 conforming finite element for space discretization and the backward Euler method for time discretization. An optimal order error estimate in $L^\infty(J; L^2)$ was proved for the fully discrete method. A similar fully discrete finite element method was analyzed later by Yue [43] for the case of nonsmooth initial data. Leyk and Roberts [33] presented a Krylov subspace type (solution) method for solving the algebraic problem resulted from a finite difference discretization of the phase field model. Caginalp and Socolovsky [13] proposed a computational method which consists of smoothing a sharp interface problem within the scaling of the distinguished limits of the phase field model that preserve physically important parameters. The computations from single-needle dendritic to faceted crystals are carried out continuously by adjusting the parameters in the method. Very recently, Provatas, Goldenfeld and Dantzig [38] proposed an adaptive finite element algorithm using dynamic data structures, which enables to simulate system sizes corresponding to experimental conditions. Numerical simulations were presented for two-dimensional, time-dependent dendritic evolution with and without surface tension anisotropy.

We emphasize that the numerical analyses of all papers cited above were developed for the phase field model with a *fixed* ε . No special effort and attention were given to rigorously address issues such as how the mesh sizes h and k depend on ε and how the error bounds depend on ε . In fact, since those error estimate results were derived using a Gronwall inequality type argument at the end of the derivations (cf. [19]), it is not hard to check that all error bounds contain a factor $\exp(\frac{T}{\varepsilon^2})$, which clearly is not very useful when ε is small.

Unlike the numerical works mentioned above, the focus of this paper is on approximating the solution of the phase field model (1.1)-(1.4) for small ε , which is the case for the applications we are interested in. The two primary goals of the paper are: (i) to analyze a fully discrete finite element method for the initial-boundary value problem (1.1)-(1.4), and to establish useful error bounds, which show growth only in low polynomial orders of $\frac{1}{\varepsilon}$, for the proposed scheme under some reasonable constraints on mesh sizes h and k ; (ii) to establish the convergence of the fully discrete finite element solution to the solutions of the sharp interface problems which are the distinguished limits of the phase field model under different scaling in its coefficients. To our knowledge, such error estimates and convergence results for the phase field model have not been known in the literature. On the other hand, such error bounds are valuable to have for computing the solution of the phase field model and the solution of its sharp interface limits.

To avoid some complicated technicalities without compromising the main ideas and results, the analysis of this paper will be carried out for the case of the quartic potential given in (1.5), although the subsequent analysis and results apply to a

general class of admissible double equal well potentials which satisfy some structural assumptions as described in [25, 26, 27]. In the rest of this section, we shall summarize the main results of this paper.

As in [19], the first fully discrete finite element method we propose for the phase field model is the following scheme ($P_{k,h}^A$): find $(\Phi^m, U^m) \in [V_h]^2$ for $m = 1, 2, \dots, M$ such that for all $(\eta_h, v_h) \in [V_h]^2$

$$(1.13) \quad \varepsilon \alpha(\varepsilon)(d_t \Phi^m, \eta_h) + \varepsilon(\nabla \Phi^m, \nabla \eta_h) + \frac{1}{\varepsilon}(f(\Phi^m), \eta_h) = s(\varepsilon)(U^m, \eta_h),$$

$$(1.14) \quad c(\varepsilon)(d_t U^m, v_h) + (\nabla U^m, \nabla v_h) = -(d_t \Phi^m, v_h),$$

with some starting value $(\Phi^0, U^0) \in [V_h]^2$ that approximate $(\varphi_0^\varepsilon, u_0^\varepsilon)$. Here $V_h \subset H^1(\Omega)$ denotes the finite element space of continuous piecewise affine functions, k is the time step and $d_t U^m := \frac{1}{k}(U^m - U^{m-1})$ denotes the backward difference quotient in time.

Clearly, a coupled nonlinear system has to be solved at each time step when using scheme ($P_{k,h}^A$). Computationally, this is not efficient, nor is it convenient. A more practical scheme would be one which computes Φ^m and U^m in succession at each time step; more importantly, this would allow one to use existing computer codes for solving the Allen-Cahn/Ginzburg-Landau equation and for solving the heat equation. To that end, we propose our second fully discrete scheme ($P_{k,h}^B$) which seeks $(\Phi^m, U^m) \in [V_h]^2$ for $m = 1, 2, \dots, M$ satisfying

$$(1.15) \quad \varepsilon \alpha(\varepsilon)(d_t \Phi^m, \eta_h) + \varepsilon(\nabla \Phi^m, \nabla \eta_h) + \frac{1}{\varepsilon}(f(\Phi^m), \eta_h) = s(\varepsilon)(U^{m-1}, \eta_h),$$

$$(1.16) \quad c(\varepsilon)(d_t U^m, v_h) + (\nabla U^m, \nabla v_h) = -(d_t \Phi^m, v_h),$$

for all $(\eta_h, v_h) \in [V_h]^2$, together with some starting value $(\Phi^0, U^0) \in [V_h]^2$.

Remark 1.1. (a). Evidently, scheme ($P_{k,h}^B$) allows independent computations of the iterates Φ^m and U^m at each time step. As expected, the benefit of splitting in scheme ($P_{k,h}^B$) is at an expense of stronger mesh condition on k compared to the fully implicit scheme ($P_{k,h}^A$). See Remarks 3.1, 3.2, and 3.4.

(b). Another way to decouple scheme ($P_{k,h}^A$) is to evaluate the right-hand side of (1.14) in an explicit manner. We found some theoretical indication that an additional term $\frac{\kappa_1}{\varepsilon^{\kappa_2}} d_t^2 \Phi^m$, $\kappa_1, \kappa_2 > 0$ in (1.13) (resp. (1.15)) might help in those scenarios to stabilize the discrete scheme.

We assume there exist nonnegative ε -independent constants σ_j for $j = 1, \dots, 4$ such that

$$(1.17) \quad |\varphi_0^\varepsilon| \leq 1, \quad \text{in } \Omega,$$

$$(1.18) \quad \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) \leq C \varepsilon^{-2\sigma_1},$$

$$(1.19) \quad \|\varepsilon \Delta \varphi_0^\varepsilon - \frac{1}{\varepsilon} f(\varphi_0^\varepsilon) + s(\varepsilon) u_0^\varepsilon\|_{L^2} \leq C \varepsilon^{-\sigma_2},$$

$$(1.20) \quad \|\nabla u_0^\varepsilon\|_{H^\ell} \leq C \varepsilon^{-\sigma_{3+\ell}} \quad \text{for } \ell = 0, 1.$$

The subsequent analysis will be carried out for scheme ($P_{k,h}^B$); a corresponding one for scheme ($P_{k,h}^A$) follows easily using the same arguments. Our first main result is summarized in the following theorem (cf. Theorems 3.1-3.4 below).

Theorem 1.1. *Let $\{(\Phi^m, U^m)\}_{m=0}^M$ solve (1.15)-(1.16) on a regular time mesh $J_k := \{t_m\}_{m=0}^M$ of size $O(k)$ and a quasi-uniform spatial mesh \mathcal{T}_h of size $O(h)$. Suppose (1.17)-(1.20) hold and $\varphi_{tt}, u_{tt} \in L^2(J; L^2)$. Also, assume that the free boundary problem (1.7)-(1.12) has a unique classical solution. Then, if the mesh sizes k and h satisfy some smallness constraints with respect to $\varepsilon > 0$ (see Theorems 3.1-3.4 for explicit formulas), there exists some constant $C_\varepsilon = C_\varepsilon(T, \Omega, \sigma_i, \xi_i; \alpha(\varepsilon), c(\varepsilon), s(\varepsilon); C_0) > 0$ (see Theorems 3.1-3.4 for the explicit form), which grows in a low polynomial order in $\frac{1}{\varepsilon}$ as $\varepsilon \searrow 0$, such that there hold the following error estimates:*

$$\begin{aligned}
\text{(i)} \quad & \max_{0 \leq m \leq M} \sqrt{\varepsilon \alpha(\varepsilon)} \|\varphi(t_m) - \Phi^m\|_{L^2} \leq C_\varepsilon (k + h^2), \\
\text{(ii)} \quad & \max_{0 \leq m \leq M} \sqrt{\varepsilon c(\varepsilon) \alpha(\varepsilon)} \|u(t_m) - U^m\|_{L^2} \leq C_\varepsilon (k + h^2), \\
\text{(iii)} \quad & \left\{ \varepsilon^3 \alpha(\varepsilon) k \sum_{m=1}^M \|\nabla(\varphi(t_m) - \Phi^m)\|_{L^2} \right\}^{\frac{1}{2}} \leq C_\varepsilon (k + h), \\
\text{(iv)} \quad & \left\{ \varepsilon \alpha(\varepsilon) k \sum_{m=1}^M \|\nabla(u(t_m) - U^m)\|_{L^2} \right\}^{\frac{1}{2}} \leq C_\varepsilon (k + h), \\
\text{(v)} \quad & \max_{0 \leq m \leq M} \sqrt{\varepsilon} \|\nabla(\varphi(t_m) - \Phi^m)\|_{L^2} \leq C_\varepsilon (k + h), \\
\text{(vi)} \quad & \max_{0 \leq m \leq M} \|\nabla(u(t_m) - U^m)\|_{L^2} \leq C_\varepsilon (k + h), \\
\text{(vii)} \quad & \left\{ \varepsilon \alpha(\varepsilon) k \sum_{m=1}^M \|d_t(\varphi(t_m) - \Phi^m)\|_{L^2}^2 \right\}^{\frac{1}{2}} \leq C_\varepsilon (k + h^2), \\
\text{(viii)} \quad & \left\{ c(\varepsilon) k \sum_{m=1}^M \|d_t(u(t_m) - U^m)\|_{L^2}^2 \right\}^{\frac{1}{2}} \leq C_\varepsilon (k + h^2), \\
\text{(ix)} \quad & \sqrt{\varepsilon \alpha(\varepsilon)} \max_{0 \leq m \leq M} \|\varphi(t_m) - \Phi^m\|_{L^\infty} \\
& \leq C_\varepsilon \left\{ h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} + [k + h^2] h^{-\frac{N}{2}} \right\} \\
\text{(x)} \quad & \sqrt{\varepsilon c(\varepsilon) \alpha(\varepsilon)} \max_{0 \leq m \leq M} \|u(t_m) - U^m\|_{L^\infty} \\
& \leq C_\varepsilon \left\{ h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} + [k + h^2] h^{-\frac{N}{2}} \right\}.
\end{aligned}$$

Remark 1.2. *We note that the above theorem is a summary of the main results of Theorems 3.1-3.4. To see detailed and precise statements and other related estimates, we refer to Section 3.*

In order to establish the above error estimates, the following three ingredients play a crucial role:

- To establish stability estimates for the solution of the fully discrete method.
- To handle the (nonlinear) potential term in the error equation using a (generalized) spectrum estimate result due to Chen [15] for the linearized phase field operator

$$(1.21) \quad \mathcal{L}_{PF} := \begin{pmatrix} -\varepsilon \Delta - \frac{1}{\varepsilon} f'(\varphi) I & \Theta \\ I & -\Delta \end{pmatrix}$$

with respect to the operator

$$(1.22) \quad \mathcal{N}_{PF} := \begin{pmatrix} \alpha(\varepsilon)\varepsilon & -s(\varepsilon) \\ \Theta & c(\varepsilon) \end{pmatrix},$$

where I and Θ denote the identity and zero operators. Here, φ is the solution of the phase field model (1.1)-(1.4), see Lemma 2.4 for details.

- To establish a discrete counterpart of the above spectrum estimate, we refer to Lemma 3.3 for details.

As a nontrivial byproduct, the above $\ell^\infty(J_k; L^\infty)$ error estimate combined with the convergence result on the phase field model to its sharp interface limiting problems established in [11] immediately allows us to establish the convergence of the fully discrete finite element solution to the solution of the free boundary problem (1.7)-(1.12).

Our second main result is the following convergence theorem.

Theorem 1.2. *Let Ω be a given smooth domain and Γ_{00} be a smooth closed hypersurface in Ω . Suppose that the free boundary problem (1.7)-(1.12) starting from Γ_{00} has a classical solution $(u^0, \Gamma := \cup_{0 \leq t \leq T} (\Gamma_t \times \{t\}))$ such that $\Gamma_t \subset \Omega$ for all $t \in [0, T]$. Let $\{(\varphi_0^\varepsilon, u_0^\varepsilon)\}_{0 < \varepsilon \leq 1}$ be the family of smooth uniformly bounded functions as in Theorem 2.1 and 2.2 of [11]. Let $(\Phi_{\varepsilon, h, k}(x, t), U_{\varepsilon, h, k}(x, t))$ denote the piecewise linear interpolation (in time) of the fully discrete solution $\{(\Phi^m, U^m)\}_{m=0}^M$ of (1.15)-(1.16). Also, let \mathcal{I} and \mathcal{O} stand for the “inside” and “outside” (in Ω_T) of Γ . Then, under the mesh and starting value constraints of Theorem 1.1 we have*

$$\begin{aligned} \text{(i)} \quad & \|U_{\varepsilon, h, k} - u^0\|_{C^0(\overline{\Omega}_T)} \xrightarrow{\varepsilon \searrow 0} 0, \\ \text{(ii)} \quad & \Phi_{\varepsilon, h, k}(x, t) \xrightarrow{\varepsilon \searrow 0} 1 \quad \text{uniformly on compact subset of } \mathcal{O}, \\ \text{(iii)} \quad & \Phi_{\varepsilon, h, k}(x, t) \xrightarrow{\varepsilon \searrow 0} -1 \quad \text{uniformly on compact subset of } \mathcal{I} \end{aligned}$$

in each of six cases of different combinations of c^0 , α^0 and d^0 as described in Theorems 2.1 and 2.2 of [11] (also see Theorem 4.1 below).

Our third main result is the following convergence theorem for the numerical interface.

Theorem 1.3. *Let $\Gamma_t^{\varepsilon, h, k} := \{x \in \Omega; \Phi_{\varepsilon, h, k}(x, t) = 0\}$ denote the zero level set of $\Phi_{\varepsilon, h, k}$. Then under the assumptions of Theorem 1.2, there holds*

$$\sup_{x \in \Gamma_t^{\varepsilon, h, k}} (\text{dist}(x, \Gamma_t)) \xrightarrow{\varepsilon \searrow 0} 0 \quad \text{uniformly on } [0, T].$$

We remark that using a similar approach parallel studies were carried out by the authors in [25] for the Allen-Cahn equation and the related curvature driven flows, and in [26, 27] for the Cahn-Hilliard equation and the Hele-Shaw problem. As pointed out earlier, the former corresponds to $s(\varepsilon) = 0$ and $\alpha(\varepsilon) = 1$ in the phase field model and the latter is obtained when $\alpha(\varepsilon) = c(\varepsilon) = 0$ and $s(\varepsilon) = 1$. The success of the approach, based on a spectrum estimate for the corresponding linearized operators, is due to the fact that it does not rely on the maximum and comparison principles, which are known not to hold for the Cahn-Hilliard equation and the phase field model. On the other hand, the required spectrum estimate does hold in each of the three cases, although the application of the estimate in the

cases of the Cahn-Hilliard equation and the phase field model is rather delicate and complicated.

The paper is organized as follows: In Section 2, we shall derive some a priori estimates for the solution of (1.1)-(1.4). Special attention is given to the dependence of the solution on ε in various norms. In Section 3, we analyze the fully discrete finite element method (1.15)-(1.16) for the phase field model (1.1)-(1.4). The method consists of the (semi-explicit) backward Euler discretization in time and the P_1 conforming finite element discretization in space. Optimal error estimates in energy norm and quasi-optimal error estimate in $\ell^\infty(J_k; L^\infty)$ norm are obtained for the fully discrete solution. It is shown that all the error bounds in Theorem 1.1 (see Theorems 3.1-3.4) depend on $\frac{1}{\varepsilon}$ only in low polynomial orders for small ε . Like in [25, 26, 27], the spectrum estimate (cf. Lemma 2.4) and its discrete counterpart (cf. Lemma 3.3) play a crucial role in the proofs. Finally, Section 4 is devoted to establishing the convergence of the fully discrete solution to the solution of the free boundary problem (1.7)-(1.12) by showing Theorems 1.2 and 1.3. Combining the $\ell^\infty(J_k; L^\infty)$ error estimate and the convergence result of [11], we show that the fully discrete numerical solution converges to the solution (including the free boundary) of the free boundary problem, provided that the latter admits a global (in time) classical solution.

2. ENERGY ESTIMATES FOR THE DIFFERENTIAL PROBLEM

In this section, we derive 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 (φ, u) to the phase field model (1.1)-(1.4) for given $(\varphi_0^\varepsilon, u_0^\varepsilon) \in [H^2(\Omega)]^2$, where $J = (0, T)$. Throughout this paper, the standard space, norm and inner product notation are adopted. Their definitions can be found in [8, 20]. In particular, (\cdot, \cdot) denotes the standard inner product on $L^2(\Omega)$, and $H^k(\Omega)$ denotes the Sobolev space of the functions which and their up to k th order derivatives are L^2 -integrable. Also, C and \tilde{C} are used to denote generic positive constants which are independent of ε and the time and space mesh sizes k and h .

In order to trace dependence of the solution on the small parameter $\varepsilon > 0$, we assume that the initial function φ_0^ε and u_0^ε satisfy the following assumption.

General Assumption (GA)

There exist positive constants σ_j for $j = 1, \dots, 4$, such that (1.17)-(1.20) hold.

We now study dependence of the solution of (1.1)-(1.4) on the given data of the problem, in particular on $\varepsilon > 0$. The first lemma is a corollary of Theorem 3.1 of [11]. It shows boundedness of the first component φ of the solution (φ, u) of the phase field model, provided that the limiting free boundary problem (1.7)-(1.12) has a global (in time) classical solution. This boundedness result enables us to establish improved a priori estimates for the solution of the phase field model. We remark that weaker estimates can be shown without using this boundedness result, hence, without assuming existence of a global (in time) classical solution for the phase field model.

Lemma 2.1. *Let (1.17) hold. Suppose that the free boundary problem (1.7)-(1.12) has a unique global (in time) classical solution. Then there exists a family of smooth initial data functions $\{(\varphi_0^\varepsilon, u_0^\varepsilon)\}_{0 < \varepsilon \leq 1}$ and constants $\varepsilon_0 \in (0, 1]$ and $C_0 > 0$, such that for all $\varepsilon \in (0, \varepsilon_0)$ the solution (φ, u) of the phase field model (1.1)-(1.4) with*

the above initial data u_0^ε satisfies

$$(2.1) \quad \|\varphi\|_{L^\infty(\Omega_T)} \leq \frac{3}{2} C_0.$$

Proof. Using a matched asymptotic expansion technique, it was shown in [11] that there exists a family of smooth approximate solutions $(\varphi_A^\varepsilon, u_A^\varepsilon)$ to the solution (φ, u) of (1.1)-(1.4) satisfying the assumptions of Theorem 3.1 of [11] was constructed in Section 4 of [11]. One condition is $\|\varphi_A^\varepsilon\|_{L^\infty(\Omega_T)} \leq C_0$ for some $C_0 > 0$. It was then proved in Theorem 3.1 of [11] that $(\varphi_A^\varepsilon, u_A^\varepsilon)$ is very “close” to (u, w) in $L^p(\Omega_T)$ for some $p > 2$ (see (3.3) on page 427 of [11]).

Now, (2.1) follows from a regularization argument. The argument goes as follows in three steps: (i) modified f into \bar{f} such that $\bar{f} = f$ in $(-\frac{3}{2}C_0, \frac{3}{2}C_0)$ and \bar{f} is linear for $|\varphi| > 2C_0$; (ii) it is not hard to show that the solution $(\bar{\varphi}, \bar{u})$ of the phase field model with the new nonlinearity \bar{f} satisfies the estimate (2.1) when $\varepsilon \in (0, \varepsilon_0)$ for some small $\varepsilon_0 \in (0, 1]$; (iii) it follows from the uniqueness of the solution of the phase field model that $u \equiv \bar{u}$. \square

Lemma 2.2. *Suppose that $(\varphi_0^\varepsilon, u_0^\varepsilon)$ satisfies (GA), and $f(\varphi) = \varphi^3 - \varphi$. Then, the solution of (1.1)-(1.4) satisfies the following estimates:*

- (i)
$$\operatorname{ess\,sup}_{[0, \infty]} \left\{ \frac{\varepsilon}{2} \|\nabla \varphi\|_{L^2}^2 + \frac{1}{\varepsilon} \|F(\varphi)\|_{L^1} + \frac{s(\varepsilon)c(\varepsilon)}{2} \|u\|_{L^2}^2 \right\} + \int_0^\infty \left[\varepsilon \alpha(\varepsilon) \|\varphi_t(s)\|_{L^2}^2 + \frac{s(\varepsilon)}{2} \|\nabla u(s)\|_{L^2}^2 \right] ds \leq \varepsilon \alpha(\varepsilon) \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon),$$
- (ii)
$$\operatorname{ess\,sup}_{[0, \infty]} \left\{ c(\varepsilon) \|\nabla u\|_{L^2}^2 \right\} + \int_0^\infty \left[\frac{c(\varepsilon)^2}{2} \|u_t(s)\|_{L^2}^2 + \|\Delta u(s)\|_{L^2}^2 \right] ds \leq \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + C [1 + c(\varepsilon)] \varepsilon^{-2\sigma_3},$$
- (iii)
$$\int_0^\infty \|\Delta \varphi(s)\|_{L^2}^2 ds \leq \left[\frac{\alpha(\varepsilon)}{\varepsilon^2} + \varepsilon s(\varepsilon) \alpha(\varepsilon) \right] \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon),$$
- (iv)
$$\operatorname{ess\,sup}_{[0, \infty]} \left\{ \alpha(\varepsilon) \|\varphi_t\|_{L^2}^2 \right\} + \int_0^\infty \|\nabla \varphi_t(s)\|_{L^2}^2 ds \leq \mathcal{B}_1,$$
- (v)
$$\operatorname{ess\,sup}_{[0, \infty]} \|\Delta \varphi\|_{L^2}^2 \leq \mathcal{B}_2,$$
- (vi)
$$\int_0^\infty \|\varphi_{tt}(s)\|_{H^{-1}}^2 ds \leq \mathcal{B}_3,$$
- (vii)
$$\operatorname{ess\,sup}_{[0, \infty]} \left\{ c(\varepsilon) \|u_t\|_{L^2}^2 \right\} + \int_0^\infty \|\nabla u_t\|_{L^2}^2 ds \leq \mathcal{B}_4,$$
- (viii)
$$\operatorname{ess\,sup}_{[0, \infty]} \|\Delta u\|_{L^2}^2 \leq \mathcal{B}_5,$$
- (ix)
$$\int_0^\infty \|u_{tt}\|_{H^{-1}}^2 ds \leq \mathcal{B}_6,$$

where $\mathcal{B}_i \equiv \mathcal{B}_i(\varepsilon; c(\varepsilon), s(\varepsilon), \alpha(\varepsilon))$ for $i = 1, \dots, 4$ are defined as follows:

$$\begin{aligned} \mathcal{B}_1 &:= \left[\frac{2}{\varepsilon^2} + \frac{s(\varepsilon)^2}{c(\varepsilon)^2} \right] \left(\mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + C \varepsilon^{-2\sigma_3} \right) + \frac{C}{\alpha(\varepsilon)} \varepsilon^{-2(\sigma_2+1)}, \\ \mathcal{B}_2 &:= C \left[1 + \frac{\alpha(\varepsilon)s(\varepsilon)^2}{c(\varepsilon)^2} + \frac{s(\varepsilon)^2}{c(\varepsilon)} + \frac{\alpha(\varepsilon)}{\varepsilon} \right] \varepsilon^{2 \min\{-\sigma_2, -\sigma_3\} - 2}, \end{aligned}$$

$$\begin{aligned}
\mathcal{B}_3 &:= \frac{\mathcal{J}_\varepsilon^3(\varphi_0^\varepsilon, u_0^\varepsilon)}{\varepsilon^4} + \frac{\mathcal{B}_1}{\alpha(\varepsilon)^2} + \frac{s(\varepsilon)^2}{\varepsilon^2 \alpha(\varepsilon)^2 c(\varepsilon)^2} \left\{ \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + C(1+c(\varepsilon))\varepsilon^{-2\sigma_3} \right\}, \\
\mathcal{B}_4 &:= \mathcal{B}_3 + \frac{\mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon)}{c(\varepsilon)^2} + \frac{C[1+c(\varepsilon)]}{c(\varepsilon)^2} \varepsilon^{-2\sigma_3} + \frac{1}{2c(\varepsilon)} \left[\varepsilon^{-2\sigma_4} + \frac{\varepsilon^{-2(\sigma_2+1)}}{\alpha(\varepsilon)^2} \right], \\
\mathcal{B}_5 &:= c(\varepsilon)\mathcal{B}_4 + \frac{\mathcal{B}_1}{\alpha(\varepsilon)}, \quad \mathcal{B}_6 := \frac{1}{c(\varepsilon)^2} [\mathcal{B}_4 + \mathcal{B}_3].
\end{aligned}$$

In addition, if

$$(2.2) \quad \lim_{s \rightarrow 0^+} \|\nabla \varphi_t(s)\|_{L^2} \leq C\varepsilon^{-\xi_1}, \quad \lim_{s \rightarrow 0^+} \|\nabla u_t(s)\|_{L^2} \leq C\varepsilon^{-\xi_2},$$

for some $\xi_1, \xi_2 \geq 0$, then there also hold

$$\begin{aligned}
(x) \quad & \int_0^\infty \|\varphi_{tt}(s)\|_{L^2}^2 ds + \operatorname{ess\,sup}_{[0, \infty]} \|\nabla \varphi_t\|_{L^2}^2 + \frac{\varepsilon^2}{\alpha(\varepsilon)} \int_0^\infty \|\Delta \varphi_t(s)\|_{L^2}^2 ds \leq \mathcal{B}_7, \\
(xi) \quad & c(\varepsilon) \int_0^\infty \|u_{tt}(s)\|_{L^2}^2 ds + \operatorname{ess\,sup}_{[0, \infty]} \|\nabla u_t\|_{L^2}^2 \\
& \quad + [1+c(\varepsilon)] \int_0^\infty \|\Delta u_t(s)\|_{L^2}^2 ds \leq \mathcal{B}_8,
\end{aligned}$$

where

$$\begin{aligned}
\mathcal{B}_7 &:= \frac{C}{\varepsilon^4 \alpha(\varepsilon)^2} \left\{ [\alpha(\varepsilon) \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon)]^{\frac{5-N}{2}} \mathcal{B}_2^{\frac{N-1}{2}} \right\} \\
& \quad \times \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + \left[\frac{Cs(\varepsilon)}{\varepsilon \alpha(\varepsilon) c(\varepsilon)} \right]^2 \left\{ \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + C[1+c(\varepsilon)]\varepsilon^{-2\sigma_3} \right\} + \frac{\varepsilon^{-2\xi_1}}{\alpha(\varepsilon)}, \\
\mathcal{B}_8 &:= \frac{1}{c(\varepsilon)} \mathcal{B}_7 + \varepsilon^{-2\xi_2}.
\end{aligned}$$

Proof. (i) The assertion is the immediate consequence of the basic energy law associated with the phase field model

$$\frac{d}{dt} \mathcal{J}_\varepsilon(u(t)) = -\|\phi_t\|_{L^2}^2 - \frac{s(\varepsilon)}{\varepsilon \alpha(\varepsilon)} \|\nabla u\|_{L^2}^2,$$

where $\mathcal{J}_\varepsilon(\cdot, \cdot)$ is defined by (1.6).

(ii) This assertion follows directly from testing equation (1.2) by $-\Delta u$ and using assertion (i).

(iii) Multiplying (1.1) by $-\Delta \varphi$ we get

$$(2.3) \quad \frac{\varepsilon \alpha(\varepsilon)}{2} \frac{d}{dt} \|\nabla \varphi\|_{L^2}^2 + \varepsilon \|\Delta \varphi\|_{L^2}^2 + \left(\frac{1}{\varepsilon} f(\varphi), -\Delta \varphi \right) = s(\varepsilon)(u, -\Delta \varphi).$$

The assertion then follows from combining the above inequality with the following estimates

$$\begin{aligned}
\frac{1}{\varepsilon} (f(\varphi), -\Delta \varphi) &= \frac{1}{\varepsilon} (f'(\varphi), |\nabla \varphi|^2) \geq -\frac{1}{\varepsilon} \|\nabla \varphi\|_{L^2}^2, \\
s(\varepsilon)(u, -\Delta \varphi) &= s(\varepsilon) (\nabla u, \nabla \varphi) \\
&\leq \frac{1}{4\varepsilon} \|\nabla \varphi\|_{L^2}^2 + \varepsilon s(\varepsilon)^2 \|\nabla u\|_{L^2}^2
\end{aligned}$$

(iv) Differentiating (1.1) with respect to time gives

$$(2.4) \quad \varepsilon \alpha(\varepsilon) \varphi_{tt} - \varepsilon \Delta \varphi_t + \frac{1}{\varepsilon} f'(\varphi) \varphi_t = s(\varepsilon) u_t.$$

Now we test (2.4) with φ_t to get

$$\frac{\varepsilon\alpha(\varepsilon)}{2} \frac{d}{dt} \|\varphi_t\|_{L^2}^2 + \varepsilon \|\nabla\varphi_t\|_{L^2}^2 + \frac{1}{\varepsilon} (f'(\varphi), |\varphi_t|^2) = s(\varepsilon)(u_t, \varphi_t).$$

Observing

$$\begin{aligned} \frac{1}{\varepsilon} (f'(\varphi), |\varphi_t|^2) &\geq -\frac{1}{\varepsilon} \|\varphi_t\|_{L^2}^2 \\ s(\varepsilon)(u_t, \varphi_t) &\leq \frac{1}{\varepsilon} \|\varphi_t\|_{L^2}^2 + \varepsilon s(\varepsilon)^2 \|u_t\|_{L^2}^2 \end{aligned}$$

we have

$$\frac{\varepsilon\alpha(\varepsilon)}{2} \frac{d}{dt} \|\varphi_t\|_{L^2}^2 + \varepsilon \|\nabla\varphi_t\|_{L^2}^2 \leq \frac{2}{\varepsilon} \|\varphi_t\|_{L^2}^2 + \varepsilon s(\varepsilon)^2 \|u_t\|_{L^2}^2.$$

Integrating over $[0, T]$ in t gives the assertion.

(v) We proceed as in (iii), (2.3) is replaced by

$$\frac{\varepsilon}{2} \|\Delta\varphi\|_{L^2}^2 + \frac{1}{\varepsilon} \|\nabla\varphi\|_{L^2}^2 \leq \frac{\varepsilon\alpha(\varepsilon)^2}{2} \|\varphi_t\|_{L^2}^2 + s(\varepsilon)^2 \varepsilon \|\nabla u\|_{L^2}^2 + \frac{1}{\varepsilon} \|\nabla\varphi\|_{L^2}^2.$$

Then the assertion follows combining the above estimate with estimates (i), (ii) and (iv).

(vi) We start from (2.4) to obtain

$$\begin{aligned} \|\varphi_{tt}\|_{H^{-1}} &\leq \frac{1}{\alpha(\varepsilon)} \|\nabla\varphi_t\|_{L^2} + \frac{1}{\varepsilon^2\alpha(\varepsilon)} \sup_{\psi \in H^1} \frac{(f'(\varphi)\varphi_t, \psi)}{\|\psi\|_{H^1}} + \frac{s(\varepsilon)}{\varepsilon\alpha(\varepsilon)} \sup_{\psi \in H^1} \frac{(u_t, \psi)}{\|\psi\|_{H^1}} \\ &\leq \frac{1}{\alpha(\varepsilon)} \|\nabla\varphi_t\|_{L^2} + \frac{s(\varepsilon)}{\varepsilon\alpha(\varepsilon)} \|u_t\|_{H^{-1}} + \frac{1}{\varepsilon^2\alpha(\varepsilon)} \sup_{\psi \in H^1} \frac{(f'(\varphi)\varphi_t, \psi)}{\|\psi\|_{H^1}}. \end{aligned}$$

Since $H^1(\Omega) \hookrightarrow L^6(\Omega)$ for $N \leq 3$, the last term above is bounded from above by

$$\frac{C}{\varepsilon^2\alpha(\varepsilon)} \|f'(\varphi)\|_{L^3} \|\varphi_t\|_{L^2} \leq \frac{C}{\varepsilon^2\alpha(\varepsilon)} \left(\tilde{c}_2 \|\nabla\varphi\|_{L^2}^2 + \tilde{c}_3 \right) \|\varphi_t\|_{L^2}.$$

Hence, the assertion follows from (i) and (iv).

(vii) Differentiating (1.2) with respect to time gives

$$(2.5) \quad c(\varepsilon) u_{tt} - \Delta u_t = -\varphi_{tt}.$$

Testing (2.5) with u_t , and integrating the resulting equation with respect to time, the assertion follows from (vi) and (ii).

(viii) The assertion follows directly from equation (1.2), and assertions (vii) and (iv).

(ix) From (2.5), we have

$$\|u_{tt}\|_{H^{-1}} \leq \frac{1}{c(\varepsilon)} \left(\|\nabla u_t\|_{L^2} + \|\varphi_{tt}\|_{H^{-1}} \right).$$

The assertion follows from combining the above inequality and the estimates (vi) and (vii).

(x) We test (2.4) with φ_{tt} and use an interpolation result which bounds the $L^\infty(\Omega)$ -norm by $W^{1,2}(\Omega)$ and $W^{2,2}(\Omega)$ norms to get

$$\begin{aligned} \varepsilon\alpha(\varepsilon)\|\varphi_{tt}\|_{L^2}^2 + \frac{\varepsilon}{2}\frac{d}{dt}\|\nabla\varphi_t\|_{L^2}^2 & \\ & \leq \frac{1}{\varepsilon^3\alpha(\varepsilon)}\|f'(\varphi)\|_{L^\infty}^2\|\varphi_t\|_{L^2}^2 + \frac{s(\varepsilon)^2}{\varepsilon\alpha(\varepsilon)}\|u_t\|_{L^2}^2 \\ & \leq \frac{C}{\varepsilon^3\alpha(\varepsilon)}\left(\|\nabla\varphi\|_{L^2}^{5-N}\|\Delta\varphi\|_{L^2}^{N-1} + \|\varphi\|_{L^2}^2\right)\|\varphi_t\|_{L^2}^2 + \frac{s(\varepsilon)^2}{\varepsilon\alpha(\varepsilon)}\|u_t\|_{L^2}^2. \end{aligned}$$

Integrating in t from 0 to T gives the first part of the assertion. The second part follows from multiplying (2.4) with $-\Delta\varphi_t$ and using the first part estimate and estimates (ii) and (iv).

(xi) After differentiating (1.2) with respect to t , we test the resulting equation with u_{tt} to get

$$c(\varepsilon)\|u_{tt}\|_{L^2}^2 + \frac{1}{2}\frac{d}{dt}\|\nabla u_t\|_{L^2}^2 \leq \frac{1}{c(\varepsilon)}\|\varphi_{tt}\|_{L^2}^2.$$

Then the first part of the assertion follows from (x) and the second part follows from differentiating (1.2) in t and testing the the resulting equation with $-\Delta u_t$. \square

Lemma 2.3. *Under the assumptions of Lemma 2.1 and 2.2, the estimates (vi)-(xi) of Lemma 2.2 are improved to new estimates which have the same forms as previous ones while each \mathcal{B}_j is replaced by $\tilde{\mathcal{B}}_j$ for $j = 3, 4, \dots, 8$, respectively. The numbers $\{\tilde{\mathcal{B}}_j\}_{j=3}^8$ are given by*

$$\begin{aligned} \tilde{\mathcal{B}}_3 & := \frac{\mathcal{B}_1}{\alpha(\varepsilon)^2} + \frac{s(\varepsilon)^2}{\varepsilon^2\alpha(\varepsilon)^2c(\varepsilon)^2}\left\{\mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + C[1+c(\varepsilon)]\varepsilon^{-2\sigma_3}\right\} \\ & \quad + \frac{1}{\varepsilon^4\alpha(\varepsilon)^2}\left\{\mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon)\right\}, \\ \tilde{\mathcal{B}}_4 & := \tilde{\mathcal{B}}_3 + \frac{\mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon)}{c(\varepsilon)^2} + \frac{C[1+c(\varepsilon)]}{c(\varepsilon)^2}\varepsilon^{-2\sigma_3} + \frac{1}{2c(\varepsilon)}\left[\varepsilon^{-2\sigma_4} + \frac{\varepsilon^{-2(\sigma_2+1)}}{\alpha(\varepsilon)^2}\right], \\ \tilde{\mathcal{B}}_5 & := c(\varepsilon)\tilde{\mathcal{B}}_4 + \frac{\mathcal{B}_1}{\alpha(\varepsilon)}, \\ \tilde{\mathcal{B}}_6 & := \frac{1}{c(\varepsilon)^2}\left[\tilde{\mathcal{B}}_4 + \tilde{\mathcal{B}}_3\right], \\ \tilde{\mathcal{B}}_7 & := \frac{C\mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon)}{\varepsilon^4\alpha(\varepsilon)} + \frac{s(\varepsilon)^2}{\varepsilon^2\alpha(\varepsilon)c(\varepsilon)^2}\left\{\mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + C[1+c(\varepsilon)]\varepsilon^{-2\sigma_3}\right\}, \\ \tilde{\mathcal{B}}_8 & := \frac{1}{c(\varepsilon)}\tilde{\mathcal{B}}_7 + \varepsilon^{-2\xi_2}. \end{aligned}$$

Proof. The proofs of the assertions are in the same line as those of (vi)-(xi) of Lemma 2.2; the only difference is that now $|f'(\varphi)|$ is uniformly bounded in ε for $0 < \varepsilon \leq \varepsilon_0$ since φ is uniformly bounded in ε . Hence, there is no need to use Sobolev embedding to control $|f'(\varphi)|$. \square

We conclude this section by citing the following result of [15, 11] on a low bound estimate of the (generalized) spectrum of the linearized phase field operator \mathcal{L}_{CH}

in (1.21) with respect to the operator \mathcal{N}_{CH} in (1.22). The estimate plays a crucial role in our error analysis.

Lemma 2.4. *Suppose that (GA) holds. Let λ_{PF} denote the smallest (generalized) eigenvalue of the eigenvalue problem*

$$\mathcal{L}_{CH} \begin{pmatrix} \psi \\ w \end{pmatrix} = \lambda \mathcal{N}_{CH} \begin{pmatrix} \psi \\ w \end{pmatrix}.$$

Then there exists a positive constant C_0 such that λ_{PF} satisfies

$$(2.6) \quad \lambda_{PF} \geq -C_0.$$

Moreover,

(i) if $\alpha(\varepsilon) \geq c_0$, $s(\varepsilon) \geq 0$, $c(\varepsilon) \geq 0$ for some constant $c_0 > 0$, then

$$(2.7) \quad \inf_{\substack{\psi \in H^1(\Omega) \\ w \in H^2(\Omega)}} \frac{\varepsilon \|\nabla \psi\|_{L^2}^2 + \varepsilon^{-1} (f'(\varphi)\psi, \psi)}{\alpha(\varepsilon) \varepsilon \|\psi\|_{L^2}^2} \geq -C_0;$$

(ii) if $\alpha(\varepsilon) \geq 0$, $s(\varepsilon) \geq c_0$, $\frac{s(\varepsilon)}{c(\varepsilon)} \geq c_0$ for some constant $c_0 > 0$, then

$$(2.8) \quad \lambda_{PF} = \inf_{\substack{\psi \in H^1(\Omega) \\ w \in H^2(\Omega)}} \frac{\varepsilon \|\nabla \psi\|_{L^2}^2 + \varepsilon^{-1} (f'(\varphi)\psi, \psi) + \frac{s(\varepsilon)}{c(\varepsilon)} \|\Delta w - \psi\|_{L^2}^2}{\varepsilon \alpha(\varepsilon) \|\psi\|_{L^2}^2 + s(\varepsilon) \|\nabla w\|_{L^2}^2} \geq -C_0,$$

where φ denotes the first component of the solution vector (φ, u) to the phase field model (1.1)-(1.4).

Remark 2.1. *It is easy to see that (2.8) also holds under the assumptions of (i), and (2.7) is a stronger estimate than (2.8) in this case. If $c(\varepsilon) = 0$, it is assumed that $\psi = \Delta w$, and the term $\frac{s(\varepsilon)}{c(\varepsilon)} \|\Delta w - \psi\|_{L^2}$ is removed in (2.8). The above results were established in [11, 15] for any φ which satisfies some special profile (cf. page 427 of [11]). It was shown that the first component φ of the solution vector (φ, u) to the phase field model (1.1)-(1.4) indeed satisfies the required profile.*

3. ERROR ANALYSIS FOR A FULLY DISCRETE FINITE ELEMENT APPROXIMATION

In this section, we shall establish some stability and convergence properties for scheme $(P_{k,h}^B)$. We remark that a corresponding analysis for scheme $(P_{k,h}^A)$ follows from the same arguments.

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, 20] for further details. Let V_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,

$$V_h := \{v_h \in C(\overline{\Omega}) : v_h|_K \in P_1(K), \forall K \in \mathcal{T}_h\}.$$

For the error analysis, we need to introduce the elliptic projection operator $P_h : H^1(\Omega) \rightarrow V_h$,

$$(3.1) \quad (\nabla[\psi - P_h\psi], \nabla v_h) = 0 \quad \forall v_h \in V_h,$$

$$(3.2) \quad (\psi - P_h\psi, 1) = 0.$$

It is well-known that P_h has the following approximation properties [42, 20, 8]:

$$(3.3) \quad \|\psi - P_h\psi\|_{L^2} + h\|\nabla(\psi - P_h\psi)\|_{L^2} \leq Ch^2\|\psi\|_{H^2} \quad \forall \psi \in H^2(\Omega),$$

$$(3.4) \quad \|\psi - P_h\psi\|_{L^\infty} \leq Ch^{\frac{4-N}{2}}|\ln h|^{\frac{3-N}{2}}\|\psi\|_{H^2} \quad \forall \psi \in H^2(\Omega),$$

$$(3.5) \quad \|(\psi - P_h\psi)_t\|_{L^2(J;L^2)} \leq Ch^2\|\psi_t\|_{L^2(J;H^2)} \quad \forall \psi \in H^1(J;H^2),$$

$$(3.6) \quad \|(\psi - P_h\psi)_t\|_{L^2(J;H^{-1})} \leq Ch^2\|\psi\|_* \quad \forall \psi \in W,$$

where

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

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

We note that a short proof of (3.4) can be found in [25].

To be used in later analysis, we also define the discrete (negative) Laplace operator $-\Delta_h : V_h \cup H^1(\Omega) \rightarrow V_h$ by

$$(3.7) \quad (-\Delta_h\psi, \eta_h) = (\nabla\psi, \nabla\eta_h) \quad \forall \eta_h \in V_h \cap H^1(\Omega).$$

We now state a basic stability result for the discrete scheme $(P_{k,h}^B)$

Lemma 3.1. *Let $f(\varphi) = \varphi^3 - \varphi$, and $c(\varepsilon) \geq c_0 > 0$. The solution $\{(\Phi^m, U^m)\}_{m=0}^M$ of (1.15)-(1.16) satisfies for values $k < \min\{\alpha(\varepsilon)^2\varepsilon^4, \frac{c(\varepsilon)^2}{s(\varepsilon)^2\varepsilon^2}\}$,*

$$\begin{aligned} & \max_{0 \leq m \leq M} \left\{ \varepsilon \|\nabla\Phi^m\|_{L^2}^2 + \frac{1}{\varepsilon} \|F(\Phi^m)\|_{L^1} + s(\varepsilon)c(\varepsilon) \|U^m\|_{L^2}^2 \right\} \\ & + k \sum_{m=0}^M \left\{ \varepsilon \left(\alpha(\varepsilon) - \frac{\sqrt{k}}{\varepsilon^2} \right) \|d_t\Phi^m\|_{L^2}^2 + \frac{s(\varepsilon)}{2} \|\nabla U^m\|_{L^2}^2 + \frac{\varepsilon k}{2} \|\nabla d_t\Phi^m\|_{L^2}^2 \right. \\ & \left. + \frac{k}{2\varepsilon} \|d_t(|\Phi^m|^2 - 1)\|_{L^2}^2 + \frac{ks(\varepsilon)[c(\varepsilon) - \varepsilon s(\varepsilon)\sqrt{k}]}{2} \|d_tU^m\|_{L^2}^2 \right\} \\ & \leq \varepsilon \alpha(\varepsilon) \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon). \end{aligned}$$

Proof. We first rewrite $f(\Phi^m)$ as follows

$$f(\Phi^m) = \frac{1}{2}(|\Phi^m|^2 - 1)([\Phi^m + \Phi^{m-1}] + kd_t\Phi^m).$$

Multiplying the equation by $d_t\Phi^m$ gives

$$(3.8) \quad \begin{aligned} & \frac{1}{2\varepsilon}(f(\Phi^m), d_t\Phi^m) = \frac{1}{2\varepsilon}(|\Phi^m|^2 - 1, d_t(|\Phi^m|^2 - 1)) \\ & + \frac{k}{2\varepsilon}(|\Phi^m|^2 - 1, |d_t\Phi^m|^2) \\ & \geq \frac{1}{2\varepsilon}(|\Phi^m|^2 - 1 \pm (|\Phi^{m-1}|^2 - 1), d_t(|\Phi^m|^2 - 1)) - \frac{k}{2\varepsilon} \|d_t\Phi^m\|_{L^2}^2 \\ & \geq \frac{1}{2\varepsilon} d_t \| |\Phi^m|^2 - 1 \|_{L^2}^2 + \frac{k}{2\varepsilon} \|d_t(|\Phi^m|^2 - 1)\|_{L^2}^2 - \frac{k}{2\varepsilon} \|d_t\Phi^m\|_{L^2}^2. \end{aligned}$$

We now test (1.15) with $d_t\Phi^m$ and (1.16) with $s(\varepsilon)U^m$. Adding the resulting equations leads to

$$\begin{aligned}
(3.9) \quad & \varepsilon\alpha(\varepsilon) \|d_t\Phi^m\|_{L^2}^2 + \frac{\varepsilon}{2} d_t \|\nabla\Phi^m\|_{L^2}^2 + \frac{\varepsilon k}{2} \|\nabla d_t\Phi^m\|_{L^2}^2 \\
& + \frac{1}{2\varepsilon} d_t \|\Phi^m\|^2 - 1\|_{L^2}^2 + \frac{k}{2\varepsilon} \|d_t(\|\Phi^m\|^2 - 1)\|_{L^2}^2 \\
& + \frac{c(\varepsilon)s(\varepsilon)}{2} d_t \|U^m\|_{L^2}^2 + \frac{kc(\varepsilon)s(\varepsilon)}{2} \|d_tU^m\|_{L^2}^2 + s(\varepsilon) \|\nabla U^m\|_{L^2}^2 \\
& \leq \frac{k}{2\varepsilon} \|d_t\Phi^m\|_{L^2}^2 - s(\varepsilon)k (d_tU^m, d_t\Phi^m) \\
& \leq \frac{\sqrt{k}}{\varepsilon} \|d_t\Phi^m\|_{L^2}^2 + \frac{k^{\frac{3}{2}}\varepsilon s(\varepsilon)^2}{2} \|d_tU^m\|_{L^2}^2.
\end{aligned}$$

The assertion follows from summing (3.9) over m from 0 to M . \square

Remark 3.1. *The mesh condition guarantees that all coefficients on the right-hand side of the stability estimate are positive. In case of scheme (1.13)-(1.14) the constraint weakens to $k \leq \alpha(\varepsilon)\varepsilon^2$.*

Lemma 3.2. *Let $f(\varphi) = \varphi^3 - \varphi$. Under the mesh constraint of Lemma 3.1, the solution $\{U^m\}_{m=0}^M$ of (1.15)-(1.16) also satisfies the following stability estimate:*

$$\begin{aligned}
& \max_{1 \leq m \leq M} \left\{ \varepsilon\alpha(\varepsilon) \|d_t\Phi^m\|_{L^2}^2 + s(\varepsilon) \|\nabla U^m\|_{L^2}^2 \right\} + k \sum_{m=1}^M \left\{ \frac{\varepsilon\alpha(\varepsilon)k}{8} \|d_t^2\Phi^m\|_{L^2}^2 \right. \\
& \quad \left. + \varepsilon \|\nabla d_t\Phi^m\|_{L^2}^2 + c(\varepsilon)s(\varepsilon) \|d_tU^m\|_{L^2}^2 + \frac{s(\varepsilon)k}{2} \|\nabla d_tU^m\|_{L^2}^2 \right\} \\
& \leq C \left\{ \frac{\alpha(\varepsilon)[1 + s(\varepsilon)^2\varepsilon^3]}{\varepsilon} \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + s(\varepsilon)\varepsilon^{-2\sigma_3} \right\}.
\end{aligned}$$

Proof. First, take $\eta_h = d_t\Phi^m$ after applying the difference operator d_t to (1.15) and $v_h = s(\varepsilon)d_tU^m$ in (1.16), then add the resulting equations. The assertion immediately follows from taking summation over m , using Lemma 3.1 and the following inequalities

$$\begin{aligned}
& (d_t f(\Phi^m), d_t\Phi^m) = (f'(\xi), |d_t\Phi^m|^2) \geq -\|d_t\Phi^m\|_{L^2}^2, \\
& |s(\varepsilon)k(d_t^2U^m, d_t\Phi^m)| \leq \frac{\varepsilon\alpha(\varepsilon)k}{8} \|d_t^2U^m\|_{L^2}^2 + \frac{8s(\varepsilon)^2k}{\varepsilon\alpha(\varepsilon)} \|d_t\Phi^m\|_{L^2}^2.
\end{aligned}$$

\square

In order to establish error bounds that depend on low order polynomials of $\frac{1}{\varepsilon}$, we need discrete versions of the spectral estimates of Lemma 2.4. To that end, we define

$$(3.10) \quad C_1 = \max_{|\xi| \leq 2C_0} |f''(\xi)|,$$

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

$$\begin{aligned}
(3.11) \quad \operatorname{ess\,sup}_J \|\varphi - P_h\varphi\|_{L^\infty} & \leq C_2 h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \operatorname{ess\,sup}_J \|\varphi\|_{H^2} \\
& \leq C_2 h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \mathcal{B}_2^{\frac{1}{2}}.
\end{aligned}$$

Lemma 3.3. *Suppose that the assumptions of Lemma 2.1-2.4 hold, and C_0 and ε_0 are same as there. Then for $\varepsilon \in (0, \varepsilon_0]$ there hold the following estimates:*

(i) *if $\alpha(\varepsilon) \geq c_0, s(\varepsilon) \geq 0, c(\varepsilon) \geq 0$ for some constant $c_0 > 0$, then*

$$(3.12) \quad \lambda_{PF}^h \equiv \inf_{0 \neq \psi \in H^1(\Omega)} \frac{\varepsilon \|\nabla \psi\|_{L^2}^2 + \frac{1}{\varepsilon} (f'(P_h \varphi) \psi, \psi)}{\varepsilon \alpha(\varepsilon) \|\psi\|_{L^2}^2} \geq -2C_0;$$

(ii) *if $\alpha(\varepsilon) \geq 0, s(\varepsilon) \geq c_0, \frac{s(\varepsilon)}{c(\varepsilon)} \geq c_0$ for some constant $c_0 > 0$, then*

$$(3.13) \quad \lambda_{PF}^h \equiv \inf_{\substack{\psi \in H^1(\Omega) \\ w \in H^2(\Omega)}} \left\{ \frac{\varepsilon \|\nabla \psi\|_{L^2}^2}{\varepsilon \alpha(\varepsilon) \|\psi\|_{L^2}^2 + s(\varepsilon) \|\nabla w\|_{L^2}^2} + \frac{\frac{1}{\varepsilon} (f'(P_h \varphi) \psi, \psi) + \frac{s(\varepsilon)}{c(\varepsilon)} \|\Delta w - \psi\|_{L^2}^2}{\varepsilon \alpha(\varepsilon) \|\psi\|_{L^2}^2 + s(\varepsilon) \|\nabla w\|_{L^2}^2} \right\} \geq -2C_0,$$

provided that k and h satisfy

$$(3.14) \quad h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \leq \left(C_1 C_2 \mathcal{B}_2^{\frac{1}{2}} \right)^{-1} C_0 \alpha(\varepsilon) \varepsilon^2.$$

In the above, φ denotes the first component of the solution vector (φ, u) to the phase field model (1.1)-(1.4).

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

$$\begin{aligned} \operatorname{ess\,sup}_J \|P_h \varphi\|_{L^\infty} &\leq \operatorname{ess\,sup}_J \{ \|\varphi\|_{L^\infty} + \|\varphi - P_h \varphi\|_{L^\infty} \} \\ &\leq \frac{4}{3} \operatorname{ess\,sup}_J \|\varphi\|_{L^\infty} \leq 2C_0. \end{aligned}$$

provided that h satisfies (3.14).

By Mean Value Theorem,

$$(3.15) \quad \begin{aligned} \operatorname{ess\,sup}_J \|f'(P_h \varphi) - f'(\varphi)\|_{L^\infty} &\leq \sup_{|\xi| \leq 2C_0} |f''(\xi)| \operatorname{ess\,sup}_J \|\varphi - P_h \varphi\|_{L^\infty} \\ &\leq C_1 C_2 h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \mathcal{B}_2^{\frac{1}{2}} \\ &\leq C_0 \alpha(\varepsilon) \varepsilon^2. \end{aligned}$$

Using the inequality $a \geq b - |a - b|$ and (3.15), we get

$$(3.16) \quad f'(P_h \varphi) \geq f'(\varphi) - |f'(P_h \varphi) - f'(\varphi)| \geq f'(\varphi) - C_0 \alpha(\varepsilon) \varepsilon^2.$$

Substituting (3.16) into the definition of λ_{PF}^h , in case (i) we get

$$\begin{aligned} \lambda_{PF}^h &\geq \inf_{0 \neq \psi \in H^1(\Omega)} \frac{\varepsilon \|\nabla \psi\|_{L^2}^2 + \frac{1}{\varepsilon} (f'(\varphi) \psi, \psi)}{\varepsilon \alpha(\varepsilon) \|\psi\|_{L^2}^2} - C_0 \\ &\geq -2C_0. \end{aligned}$$

In case (ii) we have

$$\begin{aligned} \lambda_{PF}^h &\geq \inf_{\substack{\psi \in H^1(\Omega) \\ w \in H^2(\Omega)}} \left\{ \frac{\varepsilon \|\nabla \psi\|_{L^2}^2 + \frac{1}{\varepsilon} (f'(\varphi) \psi, \psi) + \frac{s(\varepsilon)}{c(\varepsilon)} \|\Delta w - \psi\|_{L^2}^2}{\varepsilon \alpha(\varepsilon) \|\psi\|_{L^2}^2 + s(\varepsilon) \|\nabla w\|_{L^2}^2} \right. \\ &\quad \left. - \frac{C_0 \alpha(\varepsilon) \varepsilon \|\psi\|_{L^2}^2}{\varepsilon \alpha(\varepsilon) \|\psi\|_{L^2}^2 + s(\varepsilon) \|\nabla w\|_{L^2}^2} \right\} \\ &\geq -2C_0. \end{aligned}$$

The proof is completed. \square

We now are ready to state the first main theorem, which establishes error estimates for the scheme (1.15)-(1.16) in the case (i) as defined in Lemma 2.4.

Theorem 3.1. *Let $\{(\Phi^m, U^m)\}_{m=0}^M$ solve (1.15)-(1.16) 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 (GA) holds and the free boundary problem (1.7)-(1.12) has a unique classical solution. Also, assume that $\alpha(\varepsilon) \geq c_0$, $s(\varepsilon) \geq 0$, $c(\varepsilon) \geq 0$ for some constant $c_0 > 0$. Then under the following mesh and starting value constraints*

- 1). $k \leq \min\{1, \alpha(\varepsilon)^2\} \times$

$$\min\left\{\varepsilon^4, \frac{c(\varepsilon)^2}{\alpha(\varepsilon)^2 s(\varepsilon)^2 \varepsilon^2}, \varepsilon^{\frac{N+12}{8}} [\alpha(\varepsilon)]^{\frac{N-4}{8}} \left[\mathcal{B}_1 + \frac{\mathcal{B}_2}{\alpha(\varepsilon)}\right]^{-\frac{N}{8}} \left[\mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon)\right]^{\frac{N-4}{8}}\right\},$$
- 2). $h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \leq C_0 \alpha(\varepsilon) \varepsilon^2 \left(C_1(\varepsilon) C_2 \mathcal{B}_2^{\frac{1}{2}}\right)^{-1}$
- 3). $\mu(\varepsilon) k^2 + \pi(\varepsilon) h^4 \leq \varepsilon^{-1} [\alpha(\varepsilon)]^{\frac{N-12}{4-N}} \mathcal{B}_2^{-\frac{N}{4-N}},$
- 4). $\|\Phi^0 - \varphi_0^\varepsilon\|_{L^2} \leq C h^2 \|\varphi_0^\varepsilon\|_{H^2},$
- 5). $\|U^0 - u_0^\varepsilon\|_{L^2} \leq C h^2 \|u_0^\varepsilon\|_{H^2},$

for $N = 2, 3$, the solution of (1.15)-(1.16) satisfies the error estimates

- (i) $\max_{0 \leq m \leq M} \sqrt{\varepsilon \alpha(\varepsilon)} \|\varphi(t_m) - \Phi^m\|_{L^2} \leq C \left[\rho_1(\varepsilon)^{\frac{1}{2}} h^2 + \pi(\varepsilon)^{\frac{1}{2}} h^2 + \mu(\varepsilon)^{\frac{1}{2}} k\right],$
- (ii) $\left\{c(\varepsilon) s(\varepsilon) k \sum_{m=0}^M \|u(t_m) - U^m\|_{L^2}^2\right\}^{\frac{1}{2}} \leq C \left[\rho_2(\varepsilon)^{\frac{1}{2}} h^2 + \pi(\varepsilon)^{\frac{1}{2}} h^2 + \mu(\varepsilon)^{\frac{1}{2}} k\right],$
- (iii) $\max_{0 \leq m \leq M} \left\|k \sum_{j=0}^m \nabla(u(t_m) - U^m)\right\|_{L^2} \leq C \left[\rho_3(\varepsilon)^{\frac{1}{2}} h + \pi(\varepsilon)^{\frac{1}{2}} h^2 + \mu(\varepsilon)^{\frac{1}{2}} k\right],$
- (iv) $\left\{\varepsilon^3 \alpha(\varepsilon) k \sum_{m=1}^M \|\nabla(\varphi(t_m) - \Phi^m)\|_{L^2}^2\right\}^{\frac{1}{2}} \leq C \left[\rho_4(\varepsilon)^{\frac{1}{2}} h + \pi(\varepsilon)^{\frac{1}{2}} h^2 + \mu(\varepsilon)^{\frac{1}{2}} k\right],$
- (v) $\sqrt{\varepsilon \alpha(\varepsilon)} \max_{0 \leq m \leq M} \|\varphi(t_m) - \Phi^m\|_{L^\infty}$

$$\leq C \left\{\rho_1(\varepsilon)^{\frac{1}{2}} h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} + [\pi(\varepsilon)^{\frac{1}{2}} h^2 + \mu(\varepsilon)^{\frac{1}{2}} k] h^{-\frac{N}{2}}\right\},$$

where $\rho_i(\varepsilon)$, $\mu(\varepsilon)$ and $\pi(\varepsilon)$ are defined by

$$\begin{aligned}
\rho_1(\varepsilon) &= \varepsilon \alpha(\varepsilon) \mathcal{B}_2, \\
\rho_2(\varepsilon) &= c(\varepsilon) s(\varepsilon) \left\{ \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + [1 + c(\varepsilon)] \varepsilon^{-2\sigma} \right\}, \\
\rho_3(\varepsilon) &= \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + [1 + c(\varepsilon)] \varepsilon^{-2\sigma}, \\
\rho_4(\varepsilon) &= \varepsilon^3 \alpha(\varepsilon) \left[\frac{\alpha(\varepsilon)}{\varepsilon^2} + \varepsilon s(\varepsilon) c(\varepsilon) \right] \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon), \\
(3.17) \quad \mu(\varepsilon) &= \left\{ \varepsilon \alpha(\varepsilon) [1 + \varepsilon^{-2}] + \frac{s(\varepsilon) [1 + c(\varepsilon)]}{c(\varepsilon)} \right\} \tilde{\mathcal{B}}_3 \\
&\quad + s(\varepsilon) c(\varepsilon) [1 + c(\varepsilon)] \tilde{\mathcal{B}}_6 + \frac{s(\varepsilon)^2 k}{\varepsilon \alpha(\varepsilon)} \left\{ \frac{\mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + [1 + c(\varepsilon)] \varepsilon^{-2\sigma_3}}{c(\varepsilon)^2} \right\}
\end{aligned}$$

$$\begin{aligned}
& + \left. \frac{[1 + s(\varepsilon)^2 \varepsilon^3] \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + s(\varepsilon) \varepsilon^{-2\sigma_3+1}}{c(\varepsilon) s(\varepsilon) \varepsilon} \right\}; \\
(3.18) \quad \pi(\varepsilon) &= \left[\frac{1 + \varepsilon s(\varepsilon)^2}{\varepsilon^2 \alpha(\varepsilon)} + \frac{s(\varepsilon)}{c(\varepsilon)} \right] \left[\frac{\alpha(\varepsilon)}{\varepsilon^2} + \varepsilon s(\varepsilon) \alpha(\varepsilon) \right] \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) \\
& + s(\varepsilon) c(\varepsilon) \left\{ \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + [1 + c(\varepsilon)] \varepsilon^{-2\sigma_3} \right\} \\
& + \varepsilon \alpha(\varepsilon) [1 + \varepsilon^{-2}] \tilde{\mathcal{B}}_3 + s(\varepsilon) c(\varepsilon) \varepsilon^{-2\sigma_4} + \frac{s(\varepsilon)}{c(\varepsilon)} \varepsilon^{-2\sigma_2-2} \\
& + \frac{\mathcal{B}_2^{\frac{3}{2}}}{\varepsilon} \left\{ 1 + \left[\mathcal{B}_2 + \frac{\mathcal{B}_1}{\alpha(\varepsilon)} \right]^{\frac{N}{8}} \mathcal{B}_2^{-\frac{N}{8}} \right\} h^{\frac{4-N}{2}}.
\end{aligned}$$

Proof. The proof is divided into four steps. The first step estimates the consistency error of the scheme; the second and third steps deal with the error due to the nonlinear term $f(\varphi)$ and how to bound it in terms of some low order polynomial in $\frac{1}{\varepsilon}$, with the help of the stability estimates of Lemma 3.1 and 3.2 and the spectral estimates of Lemma 3.3; the final step employs an inductive argument to handle the super-quadratic (cubic) term in $(f(a) - f(b), a - b)$.

Step 1: We decompose the global errors $E_\varphi^m := \varphi(t_m) - \Phi^m$ and $E_u^m := u(t_m) - U^m$ into

$$(3.19) \quad E_\varphi^m := \Theta_\varphi^m + \Upsilon_\varphi^m, \quad E_u^m := \Theta_u^m + \Upsilon_u^m,$$

where

$$\begin{aligned}
\Theta_\varphi^m &:= \varphi(t_m) - P_h \varphi(t_m), & \Upsilon_\varphi^m &= P_h \varphi(t_m) - \Phi^m, \\
\Theta_u^m &:= u(t_m) - P_h u(t_m), & \Upsilon_u^m &= P_h u(t_m) - U^m.
\end{aligned}$$

Then the error equations are given by

$$\begin{aligned}
(3.20) \quad & \varepsilon \alpha(\varepsilon) (d_t \Upsilon_\varphi^m, \eta_h) + \varepsilon (\nabla \Upsilon_\varphi^m, \nabla \eta_h) + \frac{1}{\varepsilon} (f(P_h \varphi(t_m)) - f(\Phi^m), \eta_h) \\
& = -\varepsilon \alpha(\varepsilon) (d_t \Theta_\varphi^m, \eta_h) + s(\varepsilon) (\Theta_u^{m-1} + \Upsilon_u^m, \eta_h) \\
& \quad + k s(\varepsilon) (d_t u(t_m), \eta_h) - s(\varepsilon) k (d_t \Upsilon_u^m, \eta_h) \\
& \quad - \frac{1}{\varepsilon} (f(\varphi(t_m)) - f(P_h \varphi(t_m)), \eta_h) + \varepsilon \alpha(\varepsilon) (\mathcal{R}_\varphi^m, \eta_h).
\end{aligned}$$

$$\begin{aligned}
(3.21) \quad & c(\varepsilon) (d_t \Upsilon_u^m, v_h) + (\nabla \Upsilon_u^m, \nabla v_h) \\
& = -(d_t \Upsilon_\varphi^m + d_t \Theta_\varphi^m, v_h) - c(\varepsilon) (d_t \Theta_u^m, v_h) + (c(\varepsilon) \mathcal{R}_u^m + \mathcal{R}_\varphi^m, v_h),
\end{aligned}$$

for all $(\eta_h, v_h) \in [V_h]^2$. Where

$$(3.22) \quad \mathcal{R}_u^m = -\frac{1}{k} \int_{t_m}^{t_{m+1}} (s - t_m) u_{tt}(s) ds, \quad \mathcal{R}_\varphi^m = -\frac{1}{k} \int_{t_m}^{t_{m+1}} (s - t_m) \varphi_{tt}(s) ds.$$

Using Schwartz inequality, we have for $r = -1, 0$

$$\begin{aligned}
(3.23) \quad & k \sum_{m=0}^{\ell} \|\mathcal{R}_\varphi^m\|_{H^r}^2 \leq \frac{1}{k} \sum_{m=0}^{\ell} \left[\int_{t_m}^{t_{m+1}} (s - t_m)^2 ds \right] \left[\int_{t_m}^{t_{m+1}} \|\varphi_{tt}(s)\|_{H^r}^2 ds \right] \\
& \leq C k^2 \|\varphi_{tt}\|_{L^2(J, H^r)}^2 \leq \begin{cases} C k^2 \tilde{\mathcal{B}}_3, & \text{if } r = -1, \\ C k^2 \tilde{\mathcal{B}}_7, & \text{if } r = 0. \end{cases}
\end{aligned}$$

Similarly,

$$(3.24) \quad k \sum_{m=0}^{\ell} \|\mathcal{R}_u^m\|_{H^r}^2 \leq C k^2 \|u_{tt}\|_{L^2(J, H^r)}^2 \leq \begin{cases} C k^2 \tilde{\mathcal{B}}_6, & \text{if } r = -1, \\ \frac{C k^2}{c(\varepsilon)} \tilde{\mathcal{B}}_8, & \text{if } r = 0. \end{cases}$$

Where $\tilde{\mathcal{B}}_j$ for $j = 3, 6, 7, 8$ are defined in Lemma 2.3.

Step 2: In the sequel, it turns out that the most crucial term to handle is $s(\varepsilon)(\Upsilon_u^m, \eta_h)$ in (3.20). Dealing with it requires a preparatory step: first, replacing the super-index m in (3.21) by j , then summing the resulting equation over $1 \leq j \leq m$ yields

$$(3.25) \quad c(\varepsilon)(\Upsilon_u^m, v_h) + (\nabla G_u^m, \nabla v_h) = -(\Theta_\varphi^m + \Upsilon_\varphi^m, v_h) - c(\varepsilon)(\Theta_u^m, v_h) + c(\varepsilon)(E_u^0, v_h) \\ + (E_\varphi^0, v_h) + \left(k \sum_{j=1}^m \{c(\varepsilon)\mathcal{R}_u^j + \mathcal{R}_\varphi^j\}, v_h \right),$$

where

$$G_u^0 = 0, \quad \text{and} \quad G_u^m = k \sum_{j=1}^m \Upsilon_u^j.$$

Now taking $v_h = s(\varepsilon)\Upsilon_u^m$ in (3.25) and $\eta_h = \Upsilon_\varphi^m$ in (3.20), and taking summation over m from 1 to ℓ ($\leq M$) after adding the resulting equations we obtain

$$(3.26) \quad \frac{\varepsilon\alpha(\varepsilon)}{2} \|\Upsilon_\varphi^\ell\|_{L^2}^2 + \frac{s(\varepsilon)}{2} \|\nabla G_u^\ell\|_{L^2}^2 + k \sum_{m=1}^{\ell} \left\{ \frac{\varepsilon\alpha(\varepsilon)k}{2} \|d_t \Upsilon_\varphi^m\|_{L^2}^2 \right. \\ \left. + \frac{s(\varepsilon)k}{2} \|\nabla \Upsilon_u^m\|_{L^2}^2 + \varepsilon \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 + c(\varepsilon)s(\varepsilon) \|\Upsilon_u^m\|_{L^2}^2 \right. \\ \left. + \frac{1}{\varepsilon} (f(P_h\varphi(t_m)) - f(\Phi^m), \Upsilon_\varphi^m) \right\} \\ = k \sum_{m=1}^{\ell} \left\{ \varepsilon\alpha(\varepsilon)(\mathcal{R}_\varphi^m, \Upsilon_\varphi^m) + \left(s(\varepsilon)k \sum_{j=1}^m [c(\varepsilon)\mathcal{R}_u^j - \mathcal{R}_\varphi^j], \Upsilon_u^m \right) \right. \\ \left. - \varepsilon\alpha(\varepsilon)(d_t \Theta_\varphi^m, \Upsilon_\varphi^m) + s(\varepsilon)(\Theta_u^{m-1}, \Upsilon_\varphi^m) - s(\varepsilon)(\Theta_\varphi^m, \Upsilon_u^m) \right. \\ \left. - s(\varepsilon)c(\varepsilon)(\Theta_u^m, \Upsilon_u^m) + c(\varepsilon)s(\varepsilon)(E_u^0, \Upsilon_u^m) + s(\varepsilon)(E_\varphi^0, \Upsilon_u^m) \right. \\ \left. - s(\varepsilon)k(d_t u(t_m), \Upsilon_\varphi^m) - s(\varepsilon)k(d_t \Upsilon_u^m, \Upsilon_\varphi^m) \right\} \\ - \frac{k}{\varepsilon} \sum_{m=1}^{\ell} (f(\varphi(t_m)) - f(P_h\varphi(t_m)), \Upsilon_\varphi^m).$$

Here we have used the fact that $d_t G_u^m = \Upsilon_u^m$ in the first term on the second line.

We now bound terms on the right-hand side of (3.26) as follows. First, using the following summation by parts formula

$$\sum_{m=1}^{\ell} (d_t f^m, g^m) = \frac{1}{k} [(f^\ell, g^\ell) - (f^0, g^0)] - \sum_{m=1}^{\ell} (f^{m-1}, d_t g^m),$$

we have

$$\begin{aligned}
k \sum_{m=1}^{\ell} \left(s(\varepsilon) k \sum_{j=1}^m [c(\varepsilon) \mathcal{R}_u^j - \mathcal{R}_\varphi^j], \Upsilon_u^m \right) &= s(\varepsilon) k^2 \sum_{m=1}^{\ell} \left(\sum_{j=1}^m [c(\varepsilon) \mathcal{R}_u^j - \mathcal{R}_\varphi^j], d_t G_u^m \right) \\
&= s(\varepsilon) k \left\{ \left(\sum_{j=1}^{\ell} [c(\varepsilon) \mathcal{R}_u^j - \mathcal{R}_\varphi^j], G_u^\ell \right) \right. \\
&\quad \left. - \sum_{m=1}^{\ell} \left([c(\varepsilon) \mathcal{R}_u^m - \mathcal{R}_\varphi^m], G_u^{m-1} \right) \right\},
\end{aligned}$$

where we have used the fact that $G_u^0 = 0$. Hence,

$$\begin{aligned}
(3.27) \quad & \left| k \sum_{m=1}^{\ell} \left(s(\varepsilon) k \sum_{j=1}^m [c(\varepsilon) \mathcal{R}_u^j - \mathcal{R}_\varphi^j], \Upsilon_u^m \right) \right| \\
& \leq s(\varepsilon) k \sum_{m=1}^{\ell} [c(\varepsilon) \|\mathcal{R}_u^m\|_{H^{-1}} + \|\mathcal{R}_\varphi^m\|_{H^{-1}}] [\|G_u^\ell\|_{H^1} + \|G_u^{m-1}\|_{H^1}] \\
& \leq \frac{s(\varepsilon)}{4} \|\nabla G_u^\ell\|_{L^2}^2 + s(\varepsilon) k \sum_{m=1}^{\ell} \|\nabla G_u^m\|_{L^2}^2 + \frac{s(\varepsilon)c(\varepsilon)}{4} k \sum_{m=1}^{\ell} \|\Upsilon_u^m\|_{L^2}^2 \\
& \quad + s(\varepsilon)c(\varepsilon) [1 + c(\varepsilon)] k \sum_{m=1}^{\ell} \|\mathcal{R}_u^m\|_{H^{-1}}^2 + \frac{s(\varepsilon)[1 + c(\varepsilon)]}{c(\varepsilon)} k \sum_{m=1}^{\ell} \|\mathcal{R}_\varphi^m\|_{H^{-1}}^2.
\end{aligned}$$

Second,

$$\begin{aligned}
(3.28) \quad & \left| \varepsilon \alpha(\varepsilon) (\mathcal{R}_\varphi^m, \Upsilon_\varphi^m) \right| \leq \varepsilon \alpha(\varepsilon) \|\mathcal{R}_\varphi^m\|_{H^{-1}} \|\Upsilon_\varphi^m\|_{H^1} \\
& \leq \frac{\varepsilon \alpha(\varepsilon)}{4} \|\Upsilon_\varphi^m\|_{L^2}^2 + \frac{\varepsilon^3 \alpha(\varepsilon)}{4} \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 + C \varepsilon \alpha(\varepsilon) [1 + \varepsilon^{-2}] \|\mathcal{R}_\varphi^m\|_{H^{-1}}^2
\end{aligned}$$

Third,

$$\begin{aligned}
(3.29) \quad & \left| s(\varepsilon) k (d_t u(t_m), \Upsilon_\varphi^m) + s(\varepsilon) k (d_t \Upsilon_u^m, \Upsilon_\varphi^m) \right| \\
& \leq s(\varepsilon) k [\|d_t u(t_m)\|_{L^2} + \|d_t \Upsilon_u^m\|_{L^2}] \|\Upsilon_\varphi^m\|_{L^2} \\
& \leq \frac{s(\varepsilon)^2 k^2}{\varepsilon \alpha(\varepsilon)} [\|d_t u(t_m)\|_{L^2}^2 + \|d_t P_h u(t_m)\|_{L^2}^2 + \|d_t U^m\|_{L^2}^2] \\
& \quad + \frac{\varepsilon \alpha(\varepsilon)}{4} \|\Upsilon_\varphi^m\|_{L^2}^2.
\end{aligned}$$

Fourth,

$$\begin{aligned}
(3.30) \quad & \left| \frac{k}{\varepsilon} (f(\varphi(t_m)) - f(P_h \varphi(t_m)), \Upsilon_\varphi^m) \right| = \left| \frac{k}{\varepsilon} (f'(\xi) \Theta_\varphi^m, \Upsilon_\varphi^m) \right| \\
& \leq \frac{\varepsilon \alpha(\varepsilon)}{4} \|\Upsilon_\varphi^m\|_{L^2}^2 + \frac{C}{\varepsilon^3 \alpha(\varepsilon)} \|\Theta_\varphi^m\|_{L^2}^2,
\end{aligned}$$

where we have used the fact that φ and $P_h \varphi$ are bounded (cf. Lemma 2.1 and the first line of the proof of Lemma 3.3).

Finally, the remaining terms on the right-hand side of (3.26), denoted by S_1 , can be bounded together by

$$(3.31) \quad |S_1| \leq \frac{\varepsilon\alpha(\varepsilon)}{4} \|\Upsilon_\varphi^m\|_{L^2}^2 + \frac{\varepsilon^3\alpha(\varepsilon)}{4} \|\nabla\Upsilon_\varphi^m\|_{L^2}^2 + \frac{c(\varepsilon)s(\varepsilon)}{4} \|\Upsilon_u^m\|_{L^2}^2 \\ + C \left\{ \varepsilon\alpha(\varepsilon)[1 + \varepsilon^{-2}] \|d_t\Theta_\varphi^m\|_{H^{-1}}^2 + \frac{s(\varepsilon)^2}{\varepsilon\alpha(\varepsilon)} \|\Theta_u^{m-1}\|_{L^2}^2 \right. \\ \left. + s(\varepsilon)c(\varepsilon) [\|\Theta_u^m\|_{L^2}^2 + \|E_u^0\|_{L^2}^2] + \frac{s(\varepsilon)}{c(\varepsilon)} [\|\Theta_\varphi^m\|_{L^2}^2 + \|E_\varphi^0\|_{L^2}^2] \right\}.$$

Substituting (3.28)-(3.31) into (3.26), and using Lemmas 2.2, 2.3, 3.1, 3.2 and estimates (3.3)-(3.6) we get

$$(3.32) \quad \frac{\varepsilon\alpha(\varepsilon)}{2} \|\Upsilon_\varphi^\ell\|_{L^2}^2 + \frac{s(\varepsilon)}{4} \|\nabla G_u^\ell\|_{L^2}^2 + k \sum_{m=1}^{\ell} \left\{ \frac{\varepsilon\alpha(\varepsilon)k}{2} \|d_t\Upsilon_\varphi^m\|_{L^2}^2 \right. \\ \left. + \frac{s(\varepsilon)k}{2} \|\nabla\Upsilon_u^m\|_{L^2}^2 + \varepsilon \left[1 - \frac{\varepsilon^2\alpha(\varepsilon)}{2} \right] \|\nabla\Upsilon_\varphi^m\|_{L^2}^2 + \frac{c(\varepsilon)s(\varepsilon)}{2} \|\Upsilon_u^m\|_{L^2}^2 \right. \\ \left. + \frac{1}{\varepsilon} (f(P_h\varphi(t_m)) - f(\Phi^m), \Upsilon_\varphi^m) \right\} \\ \leq k \sum_{m=1}^{\ell} \left\{ \varepsilon\alpha(\varepsilon) \|\Upsilon_\varphi^\ell\|_{L^2}^2 + s(\varepsilon) \|\nabla G_u^m\|_{L^2}^2 + C \left\{ s(\varepsilon)c(\varepsilon) [1 + c(\varepsilon)] \|\mathcal{R}_u^m\|_{H^{-1}}^2 \right. \right. \\ \left. \left. + \left(\varepsilon\alpha(\varepsilon)[1 + \varepsilon^{-2}] + \frac{s(\varepsilon)[1 + c(\varepsilon)]}{c(\varepsilon)} \right) \|\mathcal{R}_\varphi^m\|_{H^{-1}}^2 \right\} \right\} \\ + \frac{C s(\varepsilon)^2 k^3}{\varepsilon\alpha(\varepsilon)} \sum_{m=1}^{\ell} \left[\|d_t u(t_m)\|_{L^2}^2 + \|d_t P_h u(t_m)\|_{L^2}^2 + \|d_t U^m\|_{L^2}^2 \right] \\ + C k \sum_{m=1}^{\ell} \left\{ \frac{1}{\varepsilon^3\alpha(\varepsilon)} \|\Theta_\varphi^m\|_{L^2}^2 + \varepsilon\alpha(\varepsilon)[1 + \varepsilon^{-2}] \|d_t\Theta_\varphi^m\|_{H^{-1}}^2 \right. \\ \left. + \frac{s(\varepsilon)^2}{\varepsilon\alpha(\varepsilon)} \|\Theta_u^{m-1}\|_{L^2}^2 + s(\varepsilon)c(\varepsilon) [\|\Theta_u^m\|_{L^2}^2 + \|E_u^0\|_{L^2}^2] \right. \\ \left. + \frac{s(\varepsilon)}{c(\varepsilon)} [\|\Theta_\varphi^m\|_{L^2}^2 + \|E_\varphi^0\|_{L^2}^2] \right\} \\ \leq k \sum_{m=1}^{\ell} \left[\varepsilon\alpha(\varepsilon) \|\Upsilon_\varphi^\ell\|_{L^2}^2 + s(\varepsilon) \|\nabla G_u^m\|_{L^2}^2 \right] + C [\mu(\varepsilon)k^2 + \pi_1(\varepsilon)h^4],$$

where $\mu(\varepsilon)$ is defined by (3.17) and

$$(3.33) \quad \pi_1(\varepsilon) = \left[\frac{1 + \varepsilon^2 s(\varepsilon)^2}{\varepsilon^3\alpha(\varepsilon)} + \frac{s(\varepsilon)}{c(\varepsilon)} \right] \left[\frac{\alpha(\varepsilon)}{\varepsilon^2} + \varepsilon s(\varepsilon)\alpha(\varepsilon) \right] \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) \\ + s(\varepsilon)c(\varepsilon) \left\{ \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + [1 + \varepsilon^{-2\sigma_3}] \right\} \\ + \varepsilon\alpha(\varepsilon) [1 + \varepsilon^{-2}] \tilde{\mathcal{B}}_3 + s(\varepsilon)c(\varepsilon) \varepsilon^{-2\sigma_4} + \frac{s(\varepsilon)}{c(\varepsilon)} \varepsilon^{-2\sigma_2-2},$$

where $\tilde{\mathcal{B}}_3$ and $\tilde{\mathcal{B}}_6$ are defined in Lemma 2.3.

Step 3: It remains to bound the last term on the left-hand side of (3.32). This will be done using the discrete spectrum estimate (3.12). First, using the identity

$$f(a) - f(b) = (a - b)[f'(a) + (a - b)^2 - 3(a - b)a], \quad \forall a, b \in \mathbf{R},$$

we get

$$(3.34) \quad \begin{aligned} & (f(P_h\varphi(t_m)) - f(\Phi^m), \Upsilon_\varphi^m) \\ & \geq (f'(P_h\varphi(t_m)), (\Upsilon_\varphi^m)^2) + \|\Upsilon_\varphi^m\|_{L^4}^4 - C \|\Upsilon_\varphi^m\|_{L^3}^3. \end{aligned}$$

Substituting (3.34) into (3.32) yields

$$(3.35) \quad \begin{aligned} & \frac{\varepsilon\alpha(\varepsilon)}{2} \|\Upsilon_\varphi^\ell\|_{L^2}^2 + \frac{s(\varepsilon)}{4} \|\nabla G_u^\ell\|_{L^2}^2 + k \sum_{m=1}^{\ell} \left\{ \frac{\varepsilon\alpha(\varepsilon)k}{2} \|d_t \Upsilon_\varphi^m\|_{L^2}^2 \right. \\ & + \frac{s(\varepsilon)k}{2} \|\nabla \Upsilon_u^m\|_{L^2}^2 + \frac{c(\varepsilon)s(\varepsilon)}{2} \|\Upsilon_u^m\|_{L^2}^2 + \frac{\alpha(\varepsilon)\varepsilon^3}{2} \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 + \frac{1}{\varepsilon} \|\Upsilon_\varphi^m\|_{L^4}^4 \\ & \left. + [1 - \varepsilon^2\alpha(\varepsilon)] \left[\varepsilon \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 + \frac{1}{\varepsilon} (f'(P_h\varphi(t_m)), (\Upsilon_\varphi^m)^2) \right] \right\} \\ & \leq C [\mu(\varepsilon)k^2 + \pi_1(\varepsilon)h^4] + k \sum_{m=1}^{\ell} \varepsilon\alpha(\varepsilon) \|\Upsilon_\varphi^\ell\|_{L^2}^2 + \frac{Ck}{\varepsilon} \sum_{m=1}^{\ell} \|\Upsilon_\varphi^m\|_{L^3}^3 \\ & \quad + s(\varepsilon)k \sum_{m=1}^{\ell} \|\nabla G_u^m\|_{L^2}^2 + \varepsilon\alpha(\varepsilon)k \sum_{m=1}^{\ell} |(f'(P_h\varphi(t_m)), (\Upsilon_\varphi^m)^2)| \\ & \leq [\mu(\varepsilon)k^2 + \pi_1(\varepsilon)h^4] + Ck \sum_{m=1}^{\ell} \varepsilon\alpha(\varepsilon) \|\Upsilon_\varphi^\ell\|_{L^2}^2 + s(\varepsilon)k \sum_{m=1}^{\ell} \|\nabla G_u^m\|_{L^2}^2 \\ & \quad + \frac{Ck}{\varepsilon} \sum_{m=1}^{\ell} \|\Upsilon_\varphi^m\|_{L^3}^3. \end{aligned}$$

Here we have used the fact that $\|P_h\varphi(t_m)\|_{L^\infty} \leq C$ to get the last inequality.

Then, using the discrete spectrum estimate (3.12), the last term on the left-hand side of (3.35) is bounded from below as follows

$$(3.36) \quad \begin{aligned} & [1 - \varepsilon^2\alpha(\varepsilon)] \left[\varepsilon \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 + \frac{1}{\varepsilon} (f'(P_h\varphi(t_m)), (\Upsilon_\varphi^m)^2) \right] \\ & \geq -2C_0 \varepsilon\alpha(\varepsilon) \|\Upsilon_\varphi^m\|_{L^2}^2, \end{aligned}$$

which can be absorbed into the second term on the right-hand side of (3.35).

Finally, we need to bound the last term on the right-hand side of (3.35). This will be done using a spatial-temporal decomposition technique (cf. [25, 27]).

We make a shift in the super-index and use the triangle inequality to get

$$(3.37) \quad \|E_\varphi^m\|_{L^3}^3 \leq \sum_{K \in \mathcal{T}_h} \left[k^3 \|d_t E_\varphi^m\|_{L^3(K)}^3 + \|E_\varphi^{m-1}\|_{L^3(K)}^3 \right].$$

For each term of the second sum on the right-hand side of (3.37), we interpolate $L^3(K)$ between $L^2(K)$ and $H^2(K)$,

$$(3.38) \quad \begin{aligned} & \|E_\varphi^{m-1}\|_{L^3(K)}^3 \leq C \left(\|\Delta E_\varphi^{m-1}\|_{L^2(K)}^{\frac{N}{4}} \|E_\varphi^{m-1}\|_{L^2(K)}^{\frac{12-N}{4}} + \|E_\varphi^{m-1}\|_{L^2(K)}^3 \right) \\ & \leq C \|E_\varphi^{m-1}\|_{L^2(K)}^{\frac{12-N}{4}} \left(\|\Delta E_\varphi^{m-1}\|_{L^2(K)}^{\frac{N}{4}} + \|E_\varphi^{m-1}\|_{L^2(K)}^{\frac{N}{4}} \right) \\ & \leq C \|E_\varphi^{m-1}\|_{L^2(K)}^{\frac{12-N}{4}} \mathcal{B}_2^{\frac{N}{8}}. \end{aligned}$$

The last step follows from (v) of Lemma 2.2 and Lemma 3.1.

Similarly, we can bound the first sum on the right-hand side of (3.37) as

$$\begin{aligned}
(3.39) \quad k^3 \|d_t E_\varphi^m\|_{L^3(K)}^3 &\leq Ck^3 \left(\|\Delta d_t E_\varphi^m\|_{L^2(K)}^{\frac{N}{4}} \|d_t E_\varphi^m\|_{L^2(K)}^{\frac{12-N}{4}} + \|d_t E_\varphi^m\|_{L^2(K)}^3 \right) \\
&\leq Ck^3 \|d_t E_\varphi^m\|_{L^2(K)}^{\frac{12-N}{4}} \left(\|\Delta d_t E_\varphi^m\|_{L^2(K)}^{\frac{N}{4}} + \|d_t E_\varphi^m\|_{L^2(K)}^{\frac{N}{4}} \right) \\
&\leq C \left[\mathcal{B}_2 + \frac{\mathcal{B}_1}{\alpha(\varepsilon)} \right]^{\frac{N}{8}} k^{\frac{12-N}{4}} \|d_t E_\varphi^m\|_{L^2(K)}^{\frac{12-N}{4}}
\end{aligned}$$

Summing (3.38) and (3.39) over all $K \in \mathcal{T}_h$ and using the convexity of the function $g(s) = s^r$ for $r > 1$ and $s \geq 0$ then leads to

$$(3.40) \quad \|E_\varphi^m\|_{L^3}^3 \leq C \|E_\varphi^{m-1}\|_{L^2}^{\frac{12-N}{4}} \mathcal{B}_2^{\frac{N}{8}} + C \left[\mathcal{B}_2 + \frac{\mathcal{B}_1}{\alpha(\varepsilon)} \right]^{\frac{N}{8}} k^{\frac{12-N}{4}} \|d_t E_\varphi^m\|_{L^2}^{\frac{12-N}{4}}.$$

Because of (3.19) and Lemma 2.2, the above estimate leads to

$$\begin{aligned}
\|\Upsilon_\varphi^m\|_{L^3}^3 &\leq C \left\{ \|\Upsilon_\varphi^{m-1}\|_{L^2}^{\frac{12-N}{4}} \mathcal{B}_2^{\frac{N}{8}} + \left[\mathcal{B}_2 + \frac{\mathcal{B}_1}{\alpha(\varepsilon)} \right]^{\frac{N}{8}} k^{\frac{12-N}{4}} \|d_t \Upsilon_\varphi^m\|_{L^2}^{\frac{12-N}{4}} \right. \\
&\quad \left. + \|\Theta_\varphi^{m-1}\|_{L^2}^{\frac{12-N}{4}} \mathcal{B}_2^{\frac{N}{8}} + \left[\mathcal{B}_2 + \frac{\mathcal{B}_1}{\alpha(\varepsilon)} \right]^{\frac{N}{8}} k^{\frac{12-N}{4}} \|d_t \Theta_\varphi^m\|_{L^2}^{\frac{12-N}{4}} \right. \\
&\quad \left. + \|\Theta_\varphi^m\|_{L^3}^3 \right\} \\
&\leq C \left\{ \|\Theta_\varphi^{m-1}\|_{L^2}^{\frac{12-N}{4}} \mathcal{B}_2^{\frac{N}{8}} + \|\Theta_\varphi^m\|_{L^3}^3 + \|\Upsilon_\varphi^{m-1}\|_{L^2}^{\frac{12-N}{4}} \mathcal{B}_2^{\frac{N}{8}} \right\} \\
&\quad + C \left[\mathcal{B}_2 + \frac{\mathcal{B}_1}{\alpha(\varepsilon)} \right]^{\frac{N}{8}} k^2 (\|\Upsilon_\varphi^m\|_{L^2} + \|\Upsilon_\varphi^{m-1}\|_{L^2})^{\frac{4-N}{4}} \|d_t \Upsilon_\varphi^m\|_{L^2}^2 \Big\} \\
&\quad + C \left[\mathcal{B}_2 + \frac{\mathcal{B}_1}{\alpha(\varepsilon)} \right]^{\frac{N}{8}} \left[\|\Theta_\varphi^m\|_{L^2}^{\frac{12-N}{4}} + \|\Theta_\varphi^{m-1}\|_{L^2}^{\frac{12-N}{4}} \right]
\end{aligned}$$

Summing over m from 1 to ℓ and using (3.3)-(3.6), Lemmas 2.2 and 3.1 we get

$$\begin{aligned}
(3.41) \quad \frac{k}{\varepsilon} \sum_{m=1}^{\ell} \|\Upsilon_\varphi^m\|_{L^3}^3 &\leq C \frac{\mathcal{B}_2^{\frac{3}{2}}}{\varepsilon} \left\{ 1 + \left[\mathcal{B}_2 + \frac{\mathcal{B}_1}{\alpha(\varepsilon)} \right]^{\frac{N}{8}} \mathcal{B}_2^{-\frac{N}{8}} \right\} h^{\frac{12-N}{2}} \\
&\quad + C \frac{\mathcal{B}_2^{\frac{N}{8}} k}{\varepsilon} \sum_{m=1}^{\ell} \|\Upsilon_\varphi^{m-1}\|_{L^2}^{\frac{12-N}{4}} \\
&\quad + \frac{C}{\varepsilon} \left[\mathcal{B}_2 + \frac{\mathcal{B}_1}{\alpha(\varepsilon)} \right]^{\frac{N}{8}} [\alpha(\varepsilon) \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon)]^{\frac{4-N}{8}} k^3 \sum_{m=1}^{\ell} \|d_t \Upsilon_\varphi^m\|_{L^2}^2.
\end{aligned}$$

The last term of (3.41) can be absorbed by the corresponding term on the left-hand side of (3.35) if k satisfies

$$(3.42) \quad \frac{C}{\varepsilon} \left[\mathcal{B}_2 + \frac{\mathcal{B}_1}{\alpha(\varepsilon)} \right]^{\frac{N}{8}} [\alpha(\varepsilon) \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon)]^{\frac{4-N}{8}} k \leq \frac{\varepsilon \alpha(\varepsilon)}{8}.$$

Substituting (3.36) and (3.41) into (3.35) leads to the following inequality

$$\begin{aligned}
& \frac{\varepsilon\alpha(\varepsilon)}{2} \|\Upsilon_\varphi^\ell\|_{L^2}^2 + \frac{s(\varepsilon)}{4} \|\nabla G_u^\ell\|_{L^2}^2 + k \sum_{m=1}^{\ell} \left\{ \frac{\varepsilon\alpha(\varepsilon)k}{8} \|d_t \Upsilon_\varphi^m\|_{L^2}^2 \right. \\
(3.43) \quad & \left. + \frac{s(\varepsilon)k}{2} \|\nabla \Upsilon_u^m\|_{L^2}^2 + \frac{c(\varepsilon)s(\varepsilon)}{2} \|\Upsilon_u^m\|_{L^2}^2 + \frac{\varepsilon^3\alpha(\varepsilon)}{2} \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 + \frac{1}{\varepsilon} \|\Upsilon_\varphi^m\|_{L^4}^4 \right\} \\
& \leq (C + 2C_0) k \sum_{m=1}^{\ell} \left[\varepsilon\alpha(\varepsilon) \|\Upsilon_\varphi^\ell\|_{L^2}^2 + \frac{s(\varepsilon)}{2} \|\nabla G_u^m\|_{L^2}^2 \right] \\
& \quad + C \frac{\mathcal{B}_2^{\frac{N}{8}} k}{\varepsilon} \sum_{m=1}^{\ell} \|\Upsilon_\varphi^{m-1}\|_{L^2}^{\frac{12-N}{4}} + C [\mu(\varepsilon)k^2 + \pi(\varepsilon)h^4],
\end{aligned}$$

where $\mu(\varepsilon)$ and $\pi(\varepsilon)$ is defined by (3.18) and (3.17), respectively. We note that the super-quadratic power in the last term allows to control this error contribution by the subsequent inductive argument.

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

$$c_1 = c_1(T, \Omega, \sigma_i), \quad c_2 = c_2(T, \Omega, \sigma_i; C_0),$$

which are independent of ε , h and k such that there holds inequality

$$\begin{aligned}
& \max_{0 \leq m \leq \ell} \left\{ \frac{\varepsilon\alpha(\varepsilon)}{2} \|\Upsilon_\varphi^\ell\|_{L^2}^2 + \frac{s(\varepsilon)}{4} \|\nabla G_u^\ell\|_{L^2}^2 \right\} + k \sum_{m=1}^{\ell} \left\{ \frac{\varepsilon\alpha(\varepsilon)k}{2} \|d_t \Upsilon_\varphi^m\|_{L^2}^2 \right. \\
(3.44) \quad & \left. + \frac{s(\varepsilon)k}{2} \|\nabla \Upsilon_u^m\|_{L^2}^2 + \frac{c(\varepsilon)s(\varepsilon)}{4} \|\Upsilon_u^m\|_{L^2}^2 + \frac{\alpha(\varepsilon)\varepsilon^3}{2} \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 + \frac{1}{\varepsilon} \|\Upsilon_\varphi^m\|_{L^4}^4 \right\} \\
& \leq c_1 [\mu(\varepsilon)k^2 + \pi(\varepsilon)h^4] \exp(c_2 t_\ell)
\end{aligned}$$

for sufficiently small h and k satisfying mesh conditions 1)-3) stated in the theorem. Because of (3.43), we can choose

$$c_1 = 2, \quad c_2 = C + 2C_0.$$

Since the exponent in the first term on the last line of (3.43) is bigger than 2, hence, we can recover (3.44) at the $(\ell + 1)$ th step by applying the discrete Gronwall's inequality, provided that k satisfies

$$\begin{aligned}
& \frac{\mathcal{B}_2^{\frac{N}{8}}}{\varepsilon} [\mu(\varepsilon)k^2 + \pi(\varepsilon)h^4]^{\frac{12-N}{8}} [\varepsilon\alpha(\varepsilon)]^{\frac{N-12}{8}} \\
& \leq \frac{c_1}{2} [\mu(\varepsilon)k^2 + \pi(\varepsilon)h^4] \exp(c_2 t_{\ell+1}),
\end{aligned}$$

which implies that

$$(3.45) \quad \mu(\varepsilon)k^2 + \pi(\varepsilon)h^4 \leq \varepsilon^{-1} [\alpha(\varepsilon)]^{\frac{N-12}{4-N}} \mathcal{B}_2^{-\frac{N}{4-N}}.$$

Finally, the assertions (i)-(ii) follows from (3.44), (3.3), (3.5), and applying the triangle inequality to $E_u^m = \Theta_u^m + \Upsilon_u^m$ and $E_\varphi^m = \Theta_\varphi^m + \Upsilon_\varphi^m$. The assertion (iv) follows from applying the inverse inequality bounding L^∞ norm in terms of L^2 norm, using (3.44) and (3.4). \square

Remark 3.2. (a). The estimates in (i)-(iv) are optimal in both h and k , and the one in (v) is quasi-optimal.

(b). The proof clearly shows how the three mesh conditions arise. The condition 1) is for the stability of the fully discrete scheme, the condition 2) is required for having the discrete spectrum estimate (see Lemma (3.3), finally the condition 3) is caused by the super-quadratic nonlinearity of f (see Step 3 of the proof).

(c). In case of scheme (1.13)-(1.14), the mesh condition 1) weakens to

$$k \leq \min\{1, \alpha(\varepsilon)\} \times \min\left\{\varepsilon^2, \varepsilon^{\frac{N+12}{8}} [\alpha(\varepsilon)]^{\frac{N-4}{8}} \left[\mathcal{B}_1 + \frac{\mathcal{B}_2}{\alpha(\varepsilon)}\right]^{-\frac{N}{8}} \left[\mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon)\right]^{\frac{N-4}{8}}\right\}.$$

(d). The estimates of this theorem are established under the minimum assumptions that $\varphi_{tt} \in L^2(J; H^{-1})$ and $u_{tt} \in L^2(J; H^{-1})$. If $\varphi_{tt} \in L^2(J; L^2)$ and $u_{tt} \in L^2(J; L^2)$ are assumed, analysis can be simplified a little bit in (3.27) and (3.31), and error bounds on $d_t(u(t_m) - U^m)$, $d_t(\varphi(t_m) - \Phi^m)$ and $\nabla(u(t_m) - U^m)$ can also be obtained (see Theorem 3.2 below).

(e). Superconvergence (in h) is seen for $\nabla(P_h \varphi(t_m) - \Phi^m)$ in the L^2 -norm.

(f). Regarding the choices of the starting values Φ^0 and U^0 , clearly, both L^2 -projections $\Phi^0 = Q_h \varphi_0^\varepsilon$ and $U^0 = Q_h u_0^\varepsilon$, and both elliptic projections $\Phi^0 = P_h \varphi_0^\varepsilon$, $U^0 = P_h u_0^\varepsilon$ are valid choices, on the other hand, the L^2 -projections have the advantage of being cheaper to be computed.

Theorem 3.2. Under the assumptions and mesh constraints of Theorem 3.1, there exists $h_0 > 0$ and $k_0 > 0$ (or there exists $\varepsilon_1 > 0$) such that the following error estimates hold for $h < h_0$ and $k < k_0$ (or for $\varepsilon < \varepsilon_1$)

$$\begin{aligned} \text{(i)} \quad & \max_{0 \leq m \leq M} \|\Phi^m\|_{L^\infty} \leq 2C_0, \\ \text{(ii)} \quad & \max_{0 \leq m \leq M} \sqrt{\varepsilon c(\varepsilon) \alpha(\varepsilon)} \|u(t_m) - U^m\|_{L^2} \leq C \left[\rho_5(\varepsilon)^{\frac{1}{2}} h^2 + \hat{\pi}(\varepsilon)^{\frac{1}{2}} h^2 + \hat{\mu}(\varepsilon)^{\frac{1}{2}} k \right], \\ \text{(iii)} \quad & \left\{ \varepsilon \alpha(\varepsilon) k \sum_{m=1}^M \|\nabla(u(t_m) - U^m)\|_{L^2}^2 \right\}^{\frac{1}{2}} \leq C \left[\rho_6(\varepsilon)^{\frac{1}{2}} h + \hat{\pi}(\varepsilon)^{\frac{1}{2}} h^2 + \hat{\mu}(\varepsilon)^{\frac{1}{2}} k \right], \\ \text{(iv)} \quad & \sqrt{\varepsilon c(\varepsilon) s(\varepsilon)} \max_{0 \leq m \leq M} \|u(t_m) - U^m\|_{L^\infty} \\ & \leq C \left\{ \rho_5(\varepsilon)^{\frac{1}{2}} h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} + [\hat{\pi}(\varepsilon)^{\frac{1}{2}} h^2 + \hat{\mu}(\varepsilon)^{\frac{1}{2}} k] h^{-\frac{N}{2}} \right\}, \end{aligned}$$

where

$$\begin{aligned} \rho_5(\varepsilon) &= \varepsilon c(\varepsilon) \alpha(\varepsilon) \widetilde{\mathcal{B}}_5, \\ \rho_6(\varepsilon) &= \varepsilon \alpha(\varepsilon) \left\{ \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + [1 + c(\varepsilon)] \varepsilon^{-2\sigma_3} \right\}, \\ \text{(3.46)} \quad \hat{\pi}(\varepsilon) &= \widetilde{\mathcal{B}}_6 + \frac{\pi(\varepsilon)}{\varepsilon^2 \alpha(\varepsilon)} + \frac{s(\varepsilon) [\pi(\varepsilon) + \rho_2(\varepsilon)]}{\varepsilon c(\varepsilon)^2 \alpha(\varepsilon)} + \frac{\pi(\varepsilon) + \rho_1(\varepsilon)}{\varepsilon^4 c(\varepsilon) \alpha(\varepsilon)^2}, \end{aligned}$$

$$\begin{aligned} \text{(3.47)} \quad \hat{\mu}(\varepsilon) &= [1 + c(\varepsilon)] \widetilde{\mathcal{B}}_6 + \frac{\mu(\varepsilon)}{\varepsilon^2 \alpha(\varepsilon)} + \frac{s(\varepsilon)}{\varepsilon c(\varepsilon)^2 \alpha(\varepsilon)} \left[\mu(\varepsilon) \right. \\ & \quad \left. + \frac{\mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + [1 + c(\varepsilon)] \varepsilon^{-2\sigma_3}}{c(\varepsilon)^2} \right] + \frac{\mu(\varepsilon)}{\varepsilon^4 c(\varepsilon) \alpha(\varepsilon)^2}. \end{aligned}$$

In addition, if $\varphi_{tt} \in L^2(J; L^2)$, then we also have

$$(v) \quad \max_{0 \leq m \leq M} \sqrt{\varepsilon} \|\nabla(\varphi(t_m) - \Phi^m)\|_{L^2} \leq C \left[\rho_7(\varepsilon)^{\frac{1}{2}} h + \hat{\pi}(\varepsilon)^{\frac{1}{2}} h^2 + \hat{\mu}(\varepsilon)^{\frac{1}{2}} k \right],$$

$$(vi) \quad \left\{ \varepsilon \alpha(\varepsilon) k \sum_{m=1}^M \|d_t(\varphi(t_m) - \Phi^m)\|_{L^2} \right\}^{\frac{1}{2}} \leq C \left[\rho_8(\varepsilon)^{\frac{1}{2}} h^2 + \hat{\pi}(\varepsilon)^{\frac{1}{2}} h^2 + \hat{\mu}(\varepsilon)^{\frac{1}{2}} k \right],$$

$$(vii) \quad \left\{ \varepsilon k \sum_{m=1}^M k \|d_t \nabla(\varphi(t_m) - \Phi^m)\|_{L^2}^2 \right\}^{\frac{1}{2}} \leq C \left[\rho_9(\varepsilon)^{\frac{1}{2}} h + \hat{\pi}(\varepsilon)^{\frac{1}{2}} h^2 + \hat{\mu}(\varepsilon)^{\frac{1}{2}} k \right],$$

where

$$\rho_7(\varepsilon) = \varepsilon \mathcal{B}_2, \quad \rho_8(\varepsilon) = \frac{\alpha(\varepsilon)^2 \widetilde{\mathcal{B}}_7}{\varepsilon}, \quad \rho_9(\varepsilon) = \frac{\alpha(\varepsilon) k \widetilde{\mathcal{B}}_7}{\varepsilon},$$

$$(3.48) \quad \hat{\pi}(\varepsilon) = \frac{\alpha(\varepsilon)^2}{\varepsilon} \widetilde{\mathcal{B}}_7 + \frac{s(\varepsilon)^2 [\rho_2(\varepsilon) + \pi(\varepsilon)]}{\varepsilon c(\varepsilon) \alpha(\varepsilon)^2} + \frac{\rho_1(\varepsilon) + \pi(\varepsilon)}{\varepsilon^3 \alpha(\varepsilon)},$$

$$(3.49) \quad \hat{\mu}(\varepsilon) = \varepsilon \alpha(\varepsilon) \widetilde{\mathcal{B}}_7 + \frac{\mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + [1 + c(\varepsilon)] \varepsilon^{-2\sigma_3}}{c(\varepsilon)^2} + \frac{\mu(\varepsilon)}{\varepsilon^3 \alpha(\varepsilon)^2} \\ + \frac{s(\varepsilon)^2 \mu(\varepsilon)}{\varepsilon c(\varepsilon) \alpha(\varepsilon)^2}.$$

Furthermore, if $u_{tt} \in L^2(J; L^2)$, then there also hold

$$(viii) \quad \max_{0 \leq m \leq M} \|\nabla(u(t_m) - U^m)\|_{L^2} \leq C \left[\rho_{10}(\varepsilon)^{\frac{1}{2}} h + \hat{\pi}(\varepsilon)^{\frac{1}{2}} h^2 + \hat{\mu}(\varepsilon)^{\frac{1}{2}} k \right],$$

$$(ix) \quad \left\{ c(\varepsilon) k \sum_{m=1}^M \|d_t(u(t_m) - U^m)\|_{L^2} \right\}^{\frac{1}{2}} \leq C \left[\rho_{11}(\varepsilon)^{\frac{1}{2}} h^2 + \hat{\pi}(\varepsilon)^{\frac{1}{2}} h^2 + \hat{\mu}(\varepsilon)^{\frac{1}{2}} k \right],$$

$$(x) \quad \left\{ k \sum_{m=1}^M k \|d_t \nabla(u(t_m) - U^m)\|_{L^2}^2 \right\}^{\frac{1}{2}} \leq C \left[\rho_{12}(\varepsilon)^{\frac{1}{2}} h + \hat{\pi}(\varepsilon)^{\frac{1}{2}} h^2 + \hat{\mu}(\varepsilon)^{\frac{1}{2}} k \right],$$

where

$$\rho_{10}(\varepsilon) = \widetilde{\mathcal{B}}_5, \quad \rho_{11}(\varepsilon) = \frac{c(\varepsilon) \widetilde{\mathcal{B}}_8}{1 + c(\varepsilon)}, \quad \rho_{12}(\varepsilon) = \frac{k \widetilde{\mathcal{B}}_8}{1 + c(\varepsilon)}.$$

Proof. The estimate (iv) of Theorem 3.1 implies that there exist $h_0 > 0$ and $k_0 > 0$ (equivalently, there exists $\varepsilon_1 > 0$), such that

$$(3.50) \quad \max_{0 \leq m \leq M} \|\varphi(t_m) - \Phi^m\|_{L^\infty} \leq \frac{C_0}{2}$$

for $h < h_0$ and $k < k_0$ (or $\varepsilon < \varepsilon_1$). Where $C_0 > 0$ is defined in Lemma 2.1. The assertion (i) then follows immediately from (2.1) and (3.50).

To show the assertions (ii) and (iii), taking $\eta_h = -\Upsilon_u^m$ and $v_h = \varepsilon \alpha(\varepsilon) \Upsilon_u^m$ in (3.20) and (3.21), respectively, and adding the resulting equations yield

$$(3.51) \quad \frac{\varepsilon c(\varepsilon) \alpha(\varepsilon)}{2} \left[d_t \|\Upsilon_u^m\|_{L^2}^2 + k \|d_t \Upsilon_u^m\|_{L^2}^2 \right] + \varepsilon \alpha(\varepsilon) \|\nabla \Upsilon_u^m\|_{L^2}^2 \\ = \varepsilon \alpha(\varepsilon) c(\varepsilon) \left[(\mathcal{R}_u^m, \Upsilon_u^m) - (d_t \Theta_u^m, \Upsilon_u^m) \right] + \varepsilon (\nabla \Upsilon_\varphi^m, \nabla \Upsilon_u^m) \\ - s(\varepsilon) (E_u^{m-1}, \Upsilon_u^m) - s(\varepsilon) k (d_t u(t_m), \Upsilon_u^m) - \frac{1}{\varepsilon} (f(\varphi(t_m)) - f(\Phi^m), \Upsilon_u^m).$$

Each term on the right-hand side of (3.50) can be bounded as follows:

$$(3.52) \quad \begin{aligned} |(\mathcal{R}_u^m, \Upsilon_u^m) - (d_t \Theta_u^m, \Upsilon_u^m)| &\leq [\|\mathcal{R}_u^m\|_{H^{-1}} + \|d_t \Theta_u^m\|_{H^{-1}}] \|\Upsilon_u^m\|_{H^1} \\ &\leq \frac{1}{4c(\varepsilon)} \|\nabla \Upsilon_u^m\|_{L^2}^2 + \frac{1}{4} \|\Upsilon_u^m\|_{L^2}^2 \\ &\quad + C[1 + c(\varepsilon)] [\|\mathcal{R}_u^m\|_{H^{-1}}^2 + \|d_t \Theta_u^m\|_{H^{-1}}^2]. \end{aligned}$$

$$(3.53) \quad \begin{aligned} |\varepsilon(\nabla \Upsilon_\varphi^m, \nabla \Upsilon_u^m) - s(\varepsilon)(E_u^{m-1}, \Upsilon_u^m) - s(\varepsilon)k(d_t u(t_m), \Upsilon_u^m)| \\ \leq \frac{\varepsilon\alpha(\varepsilon)}{4} \|\nabla \Upsilon_u^m\|_{L^2}^2 + \frac{\varepsilon c(\varepsilon)\alpha(\varepsilon)}{4} \|\Upsilon_u^m\|_{L^2}^2 + \frac{4\varepsilon}{\alpha(\varepsilon)} \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 \\ + \frac{Cs(\varepsilon)^2}{\varepsilon c(\varepsilon)\alpha(\varepsilon)} [\|E_u^{m-1}\|_{L^2}^2 + k^2 \|d_t u(t_m)\|_{L^2}^2]. \end{aligned}$$

$$(3.54) \quad \begin{aligned} \left| \frac{1}{\varepsilon} (f(\varphi(t_m)) - f(\Phi^m), \Upsilon_u^m) \right| \\ = \left| \frac{1}{\varepsilon} (f'(\xi^m) E_\varphi^m, \Upsilon_u^m) \right| \leq \frac{\varepsilon c(\varepsilon)\alpha(\varepsilon)}{4} \|\Upsilon_u^m\|_{L^2}^2 + \frac{C}{\varepsilon^3 c(\varepsilon)\alpha(\varepsilon)} \|E_\varphi^m\|_{L^2}^2, \end{aligned}$$

where we have used the Mean Value Theorem on f , and (2.1) and the assertion (i).

Substituting (3.52)-(3.54) into (3.51) and taking sum over m from 1 to ℓ ($\leq M$) gives

$$(3.55) \quad \begin{aligned} &\frac{\varepsilon c(\varepsilon)\alpha(\varepsilon)}{2} \|\Upsilon_u^\ell\|_{L^2}^2 + k \sum_{m=1}^M \left[\frac{\varepsilon c(\varepsilon)\alpha(\varepsilon)k}{2} \|d_t \Upsilon_u^m\|_{L^2}^2 + \frac{\varepsilon\alpha(\varepsilon)}{2} \|\nabla \Upsilon_u^m\|_{L^2}^2 \right] \\ &\leq Ck \sum_{m=1}^M \left\{ [1 + c(\varepsilon)] [\|\mathcal{R}_u^m\|_{H^{-1}}^2 + \|d_t \Theta_u^m\|_{H^{-1}}^2] + \frac{\varepsilon}{\alpha(\varepsilon)} \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 \right. \\ &\quad \left. + \frac{s(\varepsilon)^2}{\varepsilon c(\varepsilon)\alpha(\varepsilon)} [\|E_u^{m-1}\|_{L^2}^2 + k^2 \|d_t u(t_m)\|_{L^2}^2] + \frac{1}{\varepsilon^3 c(\varepsilon)\alpha(\varepsilon)} \|E_\varphi^m\|_{L^2}^2 \right\} \\ &\quad + \varepsilon c(\varepsilon)\alpha(\varepsilon)k \sum_{m=1}^M \|\Upsilon_u^m\|_{L^2}^2 \\ &\leq C [\hat{\pi}(\varepsilon)h^4 + \hat{\mu}(\varepsilon)k^2] + \varepsilon c(\varepsilon)\alpha(\varepsilon)k \sum_{m=1}^M \|\Upsilon_u^m\|_{L^2}^2, \end{aligned}$$

where $\hat{\pi}(\varepsilon)$ and $\hat{\mu}(\varepsilon)$ are defined by (3.46) and (3.47), respectively.

Assertions (ii) and (iii) follow from (3.24), (3.3), (3.5), (3.6), and (i), (ii), (iv) of Theorem 3.1 after applying the Gronwall's inequality to (3.55). The assertion (iv) is obtained by using above estimate, (3.4) and the inverse inequality bounding L^∞ -norm in terms of L^2 -norm.

To show the assertion (v)-(vii), we set $\eta_h = d_t \Upsilon_\varphi^m$ in (3.20) to get

$$(3.56) \quad \begin{aligned} &\frac{\varepsilon\alpha(\varepsilon)}{2} \|d_t \Upsilon_\varphi^m\|_{L^2}^2 + \frac{\varepsilon}{2} d_t \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 + \frac{\varepsilon k}{2} \|d_t \nabla \Upsilon_\varphi^m\|_{L^2}^2 \\ &= \varepsilon\alpha(\varepsilon) [(\mathcal{R}_\varphi^m, d_t \Upsilon_\varphi^m) - (d_t \Theta_\varphi^m, d_t \Upsilon_\varphi^m)] + s(\varepsilon) (\Theta_u^{m-1} + \Upsilon_u^m, d_t \Upsilon_\varphi^m) \\ &\quad + s(\varepsilon)k [(d_t u(t_m), d_t \Upsilon_\varphi^m) + (d_t \Upsilon_u^m, d_t \Upsilon_\varphi^m)] \\ &\quad + \frac{1}{\varepsilon} (f(\varphi(t_m)) - f(\Upsilon_\varphi^m), d_t \Upsilon_\varphi^m). \end{aligned}$$

Its right-hand side, denoted by S_2 , can be bounded together by

$$(3.57) \quad |S_2| \leq \frac{\varepsilon\alpha(\varepsilon)}{4} \|d_t \Upsilon_\varphi^m\|_{L^2}^2 + C \left\{ \varepsilon\alpha(\varepsilon) [\|\mathcal{R}_\varphi^m\|_{L^2}^2 + \|d_t \Theta_\varphi^m\|_{L^2}^2] \right. \\ \left. + \frac{s(\varepsilon)^2}{\varepsilon\alpha(\varepsilon)} [\|E_u^{m-1}\|_{L^2}^2 + \|\Upsilon_u^m\|_{L^2}^2 + k^2 \|d_t u(t_m)\|_{L^2}^2] \right. \\ \left. + \frac{1}{\varepsilon^3\alpha(\varepsilon)} \|E_\varphi^m\|_{L^2}^2 \right\},$$

where we have bounded the last term in the same way as in (3.54).

Substituting (3.57) into (3.56), taking sum over m from 1 to ℓ ($\leq M$) and applying Grownwall's inequality lead to

$$(3.58) \quad \max_{0 \leq m \leq \ell} \frac{\varepsilon}{2} \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 + k \sum_{m=1}^{\ell} \left[\frac{\varepsilon\alpha(\varepsilon)}{4} \|d_t \Upsilon_\varphi^m\|_{L^2}^2 + \frac{\varepsilon k}{2} \|d_t \nabla \Upsilon_\varphi^m\|_{L^2}^2 \right] \\ \leq C [\hat{\pi}(\varepsilon)h^4 + \hat{\mu}(\varepsilon)k^2],$$

where $\hat{\pi}(\varepsilon)$ and $\hat{\mu}(\varepsilon)$ are given by (3.48) and (3.49). Note that we have used (i) and (ii) of Theorem 3.1 and the assertion (ii) above to bound the right-hand side of (3.57).

The assertions (v)-(vii) follows from applying triangle inequality on $E_\varphi^m = \Theta_\varphi^m + \Upsilon_\varphi^m$ and using (3.3), (3.5), (3.44), (3.58) and (3.22).

Finally, we set $v_h = d_t \Upsilon_u^m$ in the error equation (3.21) to get

$$(3.59) \quad \frac{c(\varepsilon)}{2} \|d_t \Upsilon_u^m\|_{L^2}^2 + \frac{1}{2} [d_t \|\nabla \Upsilon_u^m\|_{L^2}^2 + k \|d_t \nabla \Upsilon_u^m\|_{L^2}^2] \\ \leq C \left\{ \frac{1}{c(\varepsilon)} [\|d_t E_\varphi^m\|_{L^2}^2 + \|\mathcal{R}_\varphi^m\|_{L^2}^2] + c(\varepsilon) [\|d_t \Theta_u^m\|_{L^2}^2 + \|\mathcal{R}_u^m\|_{L^2}^2] \right\}.$$

Then, the assertions (viii)-(x) follows immediately from (3.59), (3.5), the assertion (vi) above, (3.23) and (3.24). \square

Remark 3.3. (a). We emphasize that the assertions (i)-(iv) are shown under the regularity assumptions $\varphi_{tt} \in L^2(J; H^{-1})$ and $u_{tt} \in L^2(J; H^{-1})$, the proof of each statement is based on the one which precedes it, hence, the order of the statements are important. On the other hand, it is not hard to see that under the assumptions $\varphi_{tt} \in L^2(J; L^2)$ and $u_{tt} \in L^2(J; L^2)$, the assertions (ii)-(x) can be proved simultaneously, and the proofs of (ii)-(iv) can be shortened a little bit. Finally, it is also not hard to check that a factor $k^{-\frac{1}{2}}$ will appear in the right-hand sides of the assertions (v)-(x) if the assumption (2.2) is removed.

(b). With help of the inverse inequality bounding L^∞ -norm in terms of H^1 -norm, it is easy to see from the above proof that the estimate (v) of Theorem 3.1 and the estimate (iv) of Theorem 3.2 can be improved to the following ones,

$$(3.60) \quad \max_{0 \leq m \leq M} \sqrt{\varepsilon} \|\varphi(t_m) - \Phi^m\|_{L^\infty} \\ \leq C \left\{ \sqrt{\varepsilon} \|\varphi\|_{L^\infty(J; W^{2,\infty})} h^2 + [\hat{\pi}(\varepsilon)^{\frac{1}{2}} h^2 + \hat{\mu}(\varepsilon)^{\frac{1}{2}} k] |\ln h|^{\frac{3-N}{2}} \right\},$$

$$(3.61) \quad \max_{0 \leq m \leq M} \|u(t_m) - U^m\|_{L^\infty} \\ \leq C \left\{ \|u\|_{L^\infty(J; W^{2,\infty})} h^2 + [\hat{\pi}(\varepsilon)^{\frac{1}{2}} h^2 + \hat{\mu}(\varepsilon)^{\frac{1}{2}} k] |\ln h|^{\frac{3-N}{2}} \right\},$$

provided that $\varphi \in L^\infty(J; W^{2,\infty})$ and $u \in L^\infty(J; W^{2,\infty})$.

So far we have derived error bounds for the fully discrete scheme (1.15)-(1.16) in the case (i) defined in Lemmas 2.4 and 3.3, that is, $\alpha(\varepsilon) \geq c_0$, $s(\varepsilon) \geq 0$ and $c(\varepsilon) \geq 0$ for some constant $c_0 > 0$. In the remaining part of this section, we will extend the above error estimate results to the case (ii) which corresponds to $\alpha(\varepsilon) \geq 0$, $c(\varepsilon) \geq c_0$ and $\frac{s(\varepsilon)}{c(\varepsilon)} \geq c_0$ for some constant $c_0 > 0$. As expected, the analysis for the case (ii) is more delicate and complicated than that of the case (i) since the (weaker) spectral estimate (3.13), instead of the stronger estimate (3.12), has to be used to avoid exponential growth of the error bounds in $\frac{1}{\varepsilon}$, which requires the use of some nonstandard test functions in the error analysis to be given next. To reduce some technicalities, we will only present the derivation of error bounds for the case $\varphi_{tt} \in L^2(J; L^2)$ and $u_{tt} \in L^2(J; L^2)$, and leave the derivation for the case $\varphi_{tt} \in L^2(J; H^{-1})$ and $u_{tt} \in L^2(J; H^{-1})$ to interested readers.

Theorem 3.3. *Let $\{(\Phi^m, U^m)\}_{m=0}^M$ solve (1.15)-(1.16) 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 (GA) and (2.2) hold, and the free boundary problem (1.7)-(1.12) has a unique classical solution. Also, assume that $\alpha(\varepsilon) \geq 0$, $c(\varepsilon) \geq c_0$ and $\frac{s(\varepsilon)}{c(\varepsilon)} \geq c_0$ for some constant $c_0 > 0$. Then under the following mesh and starting value constraints*

- 1). $k \leq \min\{1, \alpha(\varepsilon)^2\} \times$
 $\min\left\{\varepsilon^4, \frac{c(\varepsilon)^2}{\alpha(\varepsilon)s(\varepsilon)^2\varepsilon^2}, \varepsilon^{\frac{N+12}{8}} [\alpha(\varepsilon)]^{\frac{N-4}{8}} \left[\mathcal{B}_1 + \frac{\mathcal{B}_2}{\alpha(\varepsilon)}\right]^{-\frac{N}{8}} \left[\mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon)\right]^{\frac{N-4}{8}}\right\},$
- 2). $h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \leq C_0 \alpha(\varepsilon) \varepsilon^2 \left(C_1(\varepsilon) C_2 \mathcal{B}_2^{\frac{1}{2}}\right)^{-1}$
- 3). $\zeta(\varepsilon) k^2 + \eta(\varepsilon) h^4 \leq \varepsilon^{-1} [\alpha(\varepsilon)]^{\frac{N-12}{4-N}} \mathcal{B}_2^{-\frac{N}{4-N}},$
- 4). $\|\Phi^0 - \varphi_0^\varepsilon\|_{L^2} \leq C h^2 \|\varphi_0^\varepsilon\|_{H^2},$
- 5). $\|U^0 - u_0^\varepsilon\|_{L^2} \leq C h^2 \|u_0^\varepsilon\|_{H^2},$

for $N = 2, 3$, the solution of (1.15)-(1.16) satisfies the error estimates

- (i) $\max_{0 \leq m \leq M} \sqrt{\varepsilon \alpha(\varepsilon)} \|\varphi(t_m) - \Phi^m\|_{L^2} \leq C \left[\rho_1(\varepsilon)^{\frac{1}{2}} h^2 + \eta(\varepsilon)^{\frac{1}{2}} h^2 + \zeta(\varepsilon)^{\frac{1}{2}} k\right],$
- (ii) $\left\{c(\varepsilon) s(\varepsilon) k \sum_{m=0}^M \|u(t_m) - U^m\|_{L^2}^2\right\}^{\frac{1}{2}} \leq C \left[\rho_2(\varepsilon)^{\frac{1}{2}} h^2 + \eta(\varepsilon)^{\frac{1}{2}} h^2 + \zeta(\varepsilon)^{\frac{1}{2}} k\right],$
- (iii) $\max_{0 \leq m \leq M} \left\|k \sum_{j=0}^m \nabla(u(t_m) - U^m)\right\|_{L^2} \leq C \left[\rho_3(\varepsilon)^{\frac{1}{2}} h + \eta(\varepsilon)^{\frac{1}{2}} h^2 + \zeta(\varepsilon)^{\frac{1}{2}} k\right],$
- (iv) $\left\{\varepsilon^3 \alpha(\varepsilon) k \sum_{m=1}^M \|\nabla(\varphi(t_m) - \Phi^m)\|_{L^2}^2\right\}^{\frac{1}{2}} \leq C \left[\rho_4(\varepsilon)^{\frac{1}{2}} h + \eta(\varepsilon)^{\frac{1}{2}} h^2 + \zeta(\varepsilon)^{\frac{1}{2}} k\right],$
- (v) $\sqrt{\varepsilon \alpha(\varepsilon)} \max_{0 \leq m \leq M} \|\varphi(t_m) - \Phi^m\|_{L^\infty}$
 $\leq C \left\{\rho_1(\varepsilon)^{\frac{1}{2}} h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} + [\eta(\varepsilon)^{\frac{1}{2}} h^2 + \zeta(\varepsilon)^{\frac{1}{2}} k] h^{-\frac{N}{2}}\right\},$

where $\rho_i(\varepsilon)$ are same as in Theorem 3.1, $\zeta(\varepsilon)$ and $\eta(\varepsilon)$ are defined by

$$(3.62) \quad \zeta(\varepsilon) = \left[\varepsilon \alpha(\varepsilon) + \frac{s(\varepsilon)}{\varepsilon^2 c(\varepsilon) \alpha(\varepsilon)} \right] \tilde{\mathcal{B}}_7 + \frac{s(\varepsilon)^2 k}{\varepsilon \alpha(\varepsilon)} \left\{ \frac{\mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + [1 + c(\varepsilon)] \varepsilon^{-2\sigma_3}}{c(\varepsilon)^2} \right. \\ \left. + \frac{[1 + s(\varepsilon)^2 \varepsilon^3] \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + s(\varepsilon) \varepsilon^{-2\sigma_3+1}}{c(\varepsilon) s(\varepsilon) \varepsilon} \right\} + \frac{s(\varepsilon)}{\varepsilon^2 \alpha(\varepsilon)} \tilde{\mathcal{B}}_8;$$

$$(3.63) \quad \eta(\varepsilon) = \left[\frac{2\varepsilon^2 s(\varepsilon)^2 + c(\varepsilon)^2}{\varepsilon^3 c(\varepsilon)^2 \alpha(\varepsilon)} + \frac{s(\varepsilon)}{\varepsilon^2 c(\varepsilon) \alpha(\varepsilon)} \right] \left[\frac{\alpha(\varepsilon)}{\varepsilon^2} + \varepsilon s(\varepsilon) \alpha(\varepsilon) \right] \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) \\ + \frac{s(\varepsilon) [2\varepsilon s(\varepsilon) + c(\varepsilon) \alpha(\varepsilon)]}{\varepsilon^2 \alpha(\varepsilon)} \left\{ \varepsilon^{-2\sigma_4} + \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + [1 + c(\varepsilon)] \varepsilon^{-2\sigma_3} \right\} \\ + \frac{s(\varepsilon)^2 \{ \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + C [1 + c(\varepsilon)] \varepsilon^{-2\sigma_3} \}}{\varepsilon \alpha(\varepsilon)} + \frac{\alpha(\varepsilon)^2 \tilde{\mathcal{B}}_7}{\varepsilon} \\ + \frac{s(\varepsilon) [2\varepsilon s(\varepsilon) + c(\varepsilon)] \varepsilon^{-2(\sigma_2+1)}}{\varepsilon^2 c(\varepsilon)^2 \alpha(\varepsilon)} \\ + \frac{\mathcal{B}_2^{\frac{3}{2}}}{\varepsilon} \left\{ 1 + \left[\mathcal{B}_2 + \frac{\mathcal{B}_1}{\alpha(\varepsilon)} \right]^{\frac{N}{8}} \mathcal{B}_2^{-\frac{N}{8}} \right\} h^{\frac{4-N}{2}}.$$

Proof. Since the proof is in the same line as that of Theorem 3.1, in the following we will only give the details that are significantly different from those in the proof of Theorem 3.1.

Step 1: Same as *Step 1* of the proof of Theorem 3.1.

Step 2: Set $v_h = \Upsilon_\varphi^m$ in (3.25) and substitute it into the right-hand side of (3.20) with $\eta_h = \Upsilon_\varphi^m$, we get

$$(3.64) \quad \frac{\varepsilon \alpha(\varepsilon)}{2} \left[d_t \|\Upsilon_\varphi^m\|_{L^2}^2 + k \|d_t \Upsilon_\varphi^m\|_{L^2}^2 \right] + \varepsilon \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 \\ + \frac{1}{\varepsilon} (f(P_h \varphi(t_m)) - f(\Phi^m), \Upsilon_\varphi^m) + \frac{s(\varepsilon)}{c(\varepsilon)} \left[\|\Upsilon_\varphi^m\|_{L^2}^2 + (\nabla G_u^m, \nabla \Upsilon_\varphi^m) \right] \\ = -\varepsilon \alpha(\varepsilon) (d_t \Theta_\varphi^m, \Upsilon_\varphi^m) + s(\varepsilon) (\Theta_u^{m-1}, \Upsilon_\varphi^m) - \frac{s(\varepsilon)}{c(\varepsilon)} (\Theta_\varphi^m, \Upsilon_\varphi^m) \\ - s(\varepsilon) (\Theta_u^m, \Upsilon_\varphi^m) + s(\varepsilon) (E_u^0, \Upsilon_\varphi^m) + \frac{s(\varepsilon)}{c(\varepsilon)} (E_\varphi^0, \Upsilon_\varphi^m) \\ + \varepsilon \alpha(\varepsilon) (\mathcal{R}_\varphi^m, \Upsilon_\varphi^m) + \frac{s(\varepsilon)}{c(\varepsilon)} \left(k \sum_{j=0}^m [c(\varepsilon) \mathcal{R}_u^j + \mathcal{R}_\varphi^j], \Upsilon_\varphi^m \right) \\ - \frac{1}{\varepsilon} (f(\varphi(t_m)) - f(P_h \varphi(t_m)), \Upsilon_\varphi^m) \\ + k s(\varepsilon) (d_t u(t_m), \Upsilon_\varphi^m) - k s(\varepsilon) (d_t \Upsilon_u^m, \Upsilon_\varphi^m).$$

In order to control the last term on the left-hand side of (3.64), we choose $v_h = -\frac{s(\varepsilon)}{c(\varepsilon)}\Delta_h G_u^m$ in (3.25) and obtain

$$\begin{aligned}
(3.65) \quad & s(\varepsilon) (\Upsilon_u^m, -\Delta_h G_u^m) + \frac{s(\varepsilon)}{c(\varepsilon)} \left[\|\Delta_h G_u^m\|_{L^2}^2 - (\Upsilon_\varphi^m, \Delta_h G_u^m) \right] \\
&= \frac{s(\varepsilon)}{c(\varepsilon)} (\Theta_\varphi^m, \Delta_h G_u^m) + s(\varepsilon) \left[(\Theta_u^m, \Delta_h G_u^m) - (E_u^0, \Delta_h G_u^m) \right] \\
&\quad - \frac{s(\varepsilon)}{c(\varepsilon)} (E_\varphi^0, \Delta_h G_u^m) + \frac{s(\varepsilon)}{c(\varepsilon)} \left(k \sum_{j=1}^m [c(\varepsilon)\mathcal{R}_u^j + \mathcal{R}_\varphi^j], \Delta_h G_u^m \right).
\end{aligned}$$

Notice that $\Upsilon_u^m = d_t G_u^m$, hence the first term can be written as

$$s(\varepsilon) (\Upsilon_u^m, -\Delta_h G_u^m) = \frac{s(\varepsilon)}{2} \left[d_t \|\nabla G_u^m\|_{L^2}^2 + k \|\nabla d_t G_u^m\|_{L^2}^2 \right].$$

Adding (3.64) and (3.65), and combining with (3.30) and (3.34) result in

$$\begin{aligned}
& \frac{\varepsilon\alpha(\varepsilon)}{2} d_t \|\Upsilon_\varphi^m\|_{L^2}^2 + \frac{s(\varepsilon)}{2} d_t \|\nabla G_u^m\|_{L^2}^2 + \frac{\varepsilon\alpha(\varepsilon)k}{2} \|d_t \Upsilon_\varphi^m\|_{L^2}^2 \\
& \quad + \frac{s(\varepsilon)k}{2} \|\nabla \Upsilon_u^m\|_{L^2}^2 + \frac{1}{\varepsilon} \|\Upsilon_\varphi^m\|_{L^4}^4 + \varepsilon \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 \\
& \quad + \frac{1}{\varepsilon} (f'(P_h \varphi(t_m)), (\Upsilon_\varphi^m)^2) + \frac{s(\varepsilon)}{c(\varepsilon)} \|\Upsilon_\varphi^m - \Delta_h G_u^m\|_{L^2}^2 \\
& \leq \varepsilon\alpha(\varepsilon) [(d_t \Theta_\varphi^m, \Upsilon_\varphi^m) + (\mathcal{R}_\varphi^m, \Upsilon_\varphi^m)] + s(\varepsilon) (\Theta_u^{m-1}, \Upsilon_\varphi^m) \\
(3.66) \quad & + s(\varepsilon) [(E_u^0, \Upsilon_\varphi^m) - (\Theta_u^m, \Upsilon_\varphi^m)] + \frac{s(\varepsilon)}{c(\varepsilon)} [(E_\varphi^0, \Upsilon_\varphi^m) - (\Theta_\varphi^m, \Upsilon_\varphi^m)] \\
& \quad + \frac{s(\varepsilon)}{c(\varepsilon)} \left[\left(k \sum_{j=0}^m [c(\varepsilon)\mathcal{R}_u^j + \mathcal{R}_\varphi^j], \Upsilon_\varphi^m - \Delta_h G_u^m \right) + (\Theta_\varphi^m, \Delta_h G_u^m \pm \Upsilon_\varphi^m) \right] \\
& \quad + s(\varepsilon) \left[(\Theta_u^m, \Delta_h G_u^m \pm \Upsilon_\varphi^m) - (E_u^0, \Delta_h G_u^m \pm \Upsilon_\varphi^m) \right] \\
& \quad - \frac{s(\varepsilon)}{c(\varepsilon)} (E_\varphi^0, \Delta_h G_u^m \pm \Upsilon_\varphi^m) + ks(\varepsilon)(d_t u(t_m), \Upsilon_\varphi^m) \\
& \quad - s(\varepsilon)k(d_t \Upsilon_u^m, \Upsilon_\varphi^m) + \frac{\varepsilon\alpha(\varepsilon)}{4} \|\Upsilon_\varphi^m\|_{L^2}^2 + \frac{C}{\varepsilon^3\alpha(\varepsilon)} \|\Theta_\varphi^m\|_{L^2}^2 + \frac{C}{\varepsilon} \|\Upsilon_\varphi^m\|_{L^3}^3.
\end{aligned}$$

Using Young's inequality, the right-hand side of (3.66), denoted by S_3^m , can be bounded by (after taking summation over m)

$$\begin{aligned}
(3.67) \quad & \left| k \sum_{m=1}^{\ell} S_3^m \right| \leq C [\eta_1(\varepsilon)h^4 + \zeta(\varepsilon)k^2] + k \sum_{m=1}^{\ell} \left\{ \frac{\varepsilon^2\alpha(\varepsilon)s(\varepsilon)}{2c(\varepsilon)} \|\Upsilon_\varphi^m - \Delta_h G_u^m\|_{L^2}^2 \right. \\
& \quad \left. + \frac{\varepsilon\alpha(\varepsilon)}{2} \|\Upsilon_\varphi^m\|_{L^2}^2 + \frac{C}{\varepsilon} \|\Upsilon_\varphi^m\|_{L^3}^3 \right\},
\end{aligned}$$

where $\zeta(\varepsilon)$ is defined by (3.62) and $\eta_1(\varepsilon)$ has the form

$$(3.68) \quad \eta_1(\varepsilon) = \left[\frac{2\varepsilon^2 s(\varepsilon)^2 + c(\varepsilon)^2}{\varepsilon^3 c(\varepsilon)^2 \alpha(\varepsilon)} + \frac{s(\varepsilon)}{\varepsilon^2 c(\varepsilon) \alpha(\varepsilon)} \right] \left[\frac{\alpha(\varepsilon)}{\varepsilon^2} + \varepsilon s(\varepsilon) \alpha(\varepsilon) \right] \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) \\ + \frac{s(\varepsilon)[2\varepsilon s(\varepsilon) + c(\varepsilon)\alpha(\varepsilon)]}{\varepsilon^2 \alpha(\varepsilon)} \left\{ \varepsilon^{-2\sigma_4} + \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + [1 + c(\varepsilon)] \varepsilon^{-2\sigma_3} \right\} \\ + \frac{s(\varepsilon)^2 \{ \mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon) + C [1 + c(\varepsilon)] \varepsilon^{-2\sigma_3} \}}{\varepsilon \alpha(\varepsilon)} + \frac{\alpha(\varepsilon)^2 \tilde{\mathcal{B}}_7}{\varepsilon} \\ + \frac{s(\varepsilon)[2\varepsilon s(\varepsilon) + c(\varepsilon)] \varepsilon^{-2(\sigma_2+1)}}{\varepsilon^2 c(\varepsilon)^2 \alpha(\varepsilon)}.$$

Substituting (3.67) into (3.66) after taking summation over m leads to

$$(3.69) \quad \frac{\varepsilon \alpha(\varepsilon)}{2} \|\Upsilon_\varphi^\ell\|_{L^2}^2 + \frac{s(\varepsilon)}{2} \|\nabla G_u^\ell\|_{L^2}^2 + k \sum_{m=1}^{\ell} \left\{ \frac{\varepsilon \alpha(\varepsilon) k}{2} \|d_t \Upsilon_\varphi^m\|_{L^2}^2 \right. \\ \left. + \frac{s(\varepsilon) k}{2} \|\nabla \Upsilon_u^m\|_{L^2}^2 + \frac{1}{\varepsilon} \|\Upsilon_\varphi^m\|_{L^4}^4 + \varepsilon \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 \right. \\ \left. + \frac{1}{\varepsilon} (f'(P_h \varphi(t_m)), (\Upsilon_\varphi^m)^2) + \frac{s(\varepsilon)}{c(\varepsilon)} \left[1 - \frac{\varepsilon^2 \alpha(\varepsilon)}{2} \right] \|\Upsilon_\varphi^m - \Delta_h G_u^m\|_{L^2}^2 \right\} \\ \leq C [\eta_1(\varepsilon) h^4 + \zeta(\varepsilon) k^2] + k \sum_{m=0}^{\ell} \left\{ \frac{\varepsilon \alpha(\varepsilon)}{2} \|\Upsilon_\varphi^m\|_{L^2}^2 + \frac{C}{\varepsilon} \|\Upsilon_\varphi^m\|_{L^3}^3 \right\}.$$

Step 3: Two terms in (3.69) remain to be bounded, namely, the first term on the third line and the last term on the right-hand side. In the following, we will bound the first one from below using the discrete spectrum estimate (3.13), and bound the second from above using a spatial-temporal decomposition technique used in *Step 3* of the proof of Theorem 3.1.

First, notice that Δ_h , not Δ , appears in (3.69); in order to use (3.13), we need a preparatory step. Let $\mathcal{F}_\lambda[\cdot]$ denote the convolution operator with a mollifier as defined in [1], it is well-known that for any $v \in H^r(\Omega)$ ($r \geq 0$), $\mathcal{F}_\lambda[v] \in C_0^\infty(\mathbf{R}^N)$ converges to v in H^r -norm as $\lambda \searrow 0$; in particular, for any $\delta > 0$ exists a $\lambda(\delta) > 0$ such that for $0 < \lambda < \lambda(\delta)$

$$\|v - \mathcal{F}_\lambda[v]\|_{H^r} \leq \delta \|v\|_{H^r} \quad \forall v \in H^r \quad (r \geq 0).$$

Now using the identity

$$(3.70) \quad \|\Upsilon_\varphi^m - \Delta_h G_u^m\|_{L^2}^2 \\ = \|\Upsilon_\varphi^m - \Delta \mathcal{F}_\lambda[G_u^m]\|_{L^2}^2 + (\Delta \mathcal{F}_\lambda[G_u^m] - \Delta_h G_u^m, \Upsilon_\varphi^m - \Delta_h G_u^m) \\ + (\Delta \mathcal{F}_\lambda[G_u^m] - \Delta_h G_u^m, \Upsilon_\varphi^m - \Delta \mathcal{F}_\lambda[G_u^m])$$

we conclude that there exists $\lambda(\varepsilon) > 0$ such that for $\lambda < \lambda(\varepsilon)$

$$(3.71) \quad \|\Upsilon_\varphi^m - \Delta_h G_u^m\|_{L^2}^2 \geq \|\Upsilon_\varphi^m - \Delta \mathcal{F}_\lambda[G_u^m]\|_{L^2}^2 \\ - \frac{\varepsilon^2 \alpha(\varepsilon) s(\varepsilon)}{4c(\varepsilon)} \|\Upsilon_\varphi^m - \Delta_h G_u^m\|_{L^2}^2 - \frac{s(\varepsilon)}{2} \|\nabla G_u^m\|_{L^2}^2 - \frac{\varepsilon^3 \alpha(\varepsilon)}{4} \|\nabla \Upsilon_\varphi^m\|_{L^2}^2.$$

To see (3.71), we deal with the last two terms in (3.70) separately. Taking into account that $\Upsilon_\varphi^m - \Delta_h G_u^m \in V_h$, we first conclude that for an appropriately chosen

$$\tilde{\delta}_1 = \tilde{\delta}_1(\delta) > 0,$$

$$\begin{aligned} (\Delta \mathcal{F}_\lambda[G_u^m] - \Delta_h G_u^m, \Upsilon_\varphi^m - \Delta_h G_u^m) &= (\nabla[\mathcal{F}_\lambda[G_u^m] - G_u^m], \nabla[\Upsilon_\varphi^m - \Delta_h G_u^m]) \\ &\leq \tilde{\delta}_1 \|\nabla G_u^m\|_{L^2} \|\nabla[\Upsilon_\varphi^m - \Delta_h G_u^m]\|_{L^2}. \end{aligned}$$

For the second term, we proceed independently for every $K \in \mathcal{T}_h$, and benefit from the fact $(\Delta G_u^m)|_K = 0$. In the following, we choose $\tilde{\delta}_2 = \tilde{\delta}_2(\delta) > 0$ appropriately such that

$$\begin{aligned} &\sum_{K \in \mathcal{T}_h} (\Delta \mathcal{F}_\lambda[G_u^m] - \Delta_h G_u^m, \Upsilon_\varphi^m - \Delta \mathcal{F}_\lambda[G_u^m])_K \\ &= \sum_{K \in \mathcal{T}_h} \left[(\Delta \mathcal{F}_\lambda[G_u^m] - \Delta_h G_u^m, \Upsilon_\varphi^m)_K + (\Delta \mathcal{F}_\lambda[G_u^m] - \Delta_h G_u^m, \Delta[G_u^m - \mathcal{F}_\lambda[G_u^m]])_K \right] \\ &\leq (\nabla[G_u^m - \mathcal{F}_\lambda[G_u^m]], \nabla \Upsilon_\varphi^m) + \tilde{\delta}_2 \sum_{K \in \mathcal{T}_h} \|\Delta \mathcal{F}_\lambda[G_u^m] - \Delta_h G_u^m\|_{L^2(K)} \|G_u^m\|_{H^2(K)} \\ &\leq 2\delta \|\nabla G_u^m\|_{L^2} \|\nabla \Upsilon_\varphi^m\|_{L^2}. \end{aligned}$$

In above, we have used the following fact, which is valid for all $\varphi_h \in V_h$,

$$\begin{aligned} \sum_{K \in \mathcal{T}_h} \|\Delta_h \varphi_h\|_{L^2(K)}^2 &= - \sum_{K \in \mathcal{T}_h} (\nabla \Delta_h \varphi_h, \nabla \varphi_h)_K \\ &\leq C \sum_{K \in \mathcal{T}_h} h_K^{-1} \|\Delta_h \varphi_h\|_{L^2(K)} \|\nabla \varphi_h\|_{L^2(K)}, \end{aligned}$$

hence, $\|\Delta_h \varphi_h\|_{L^2} \leq \min_{K \in \mathcal{T}_h} h_K^{-1} \|\nabla \varphi_h\|_{L^2}$. In addition, we also have utilized the following estimate

$$\|\Delta \mathcal{F}_\lambda[G_u^m]\|_{L^2(K)} \leq (1 + \tilde{\delta}_2) \|G_u^m\|_{H^2(K)} \leq \delta \|G_u^m\|_{H^1(K)},$$

thanks to an inverse inequality. These arguments establish (3.71).

Next, it follows from (3.13) that there exists $\lambda_0 > 0$ such that for $\lambda < \lambda_0$,

$$\begin{aligned} &[1 - \varepsilon^2 \alpha(\varepsilon)] \left\{ \varepsilon \|\Upsilon_\varphi^m\|_{L^2}^2 + \frac{1}{\varepsilon} (f(P_h \varphi(t_m)), (\Upsilon_\varphi^m)^2) \right. \\ &\quad \left. + \frac{s(\varepsilon)}{c(\varepsilon)} \|\Upsilon_\varphi^m - \Delta \mathcal{F}_\lambda[G_u^m]\|_{L^2}^2 \right\} \\ (3.72) \quad &\geq -2C_0 \left\{ \varepsilon \alpha(\varepsilon) \|\Upsilon_\varphi^m\|_{L^2}^2 + s(\varepsilon) \|\nabla \mathcal{F}_\lambda[G_u^m]\|_{L^2}^2 \right\} \\ &\geq -4C_0 \left\{ \varepsilon \alpha(\varepsilon) \|\Upsilon_\varphi^m\|_{L^2}^2 + s(\varepsilon) \|\nabla G_u^m\|_{L^2}^2 \right\}. \end{aligned}$$

Substituting (3.71) and (3.72) into (3.69) gives

$$\begin{aligned}
(3.73) \quad & \frac{\varepsilon\alpha(\varepsilon)}{2} \|\Upsilon_\varphi^\ell\|_{L^2}^2 + \frac{s(\varepsilon)}{2} \|\nabla G_u^\ell\|_{L^2}^2 + k \sum_{m=1}^{\ell} \left\{ \frac{\varepsilon\alpha(\varepsilon)k}{2} \|d_t \Upsilon_\varphi^m\|_{L^2}^2 \right. \\
& + \frac{s(\varepsilon)k}{2} \|\nabla \Upsilon_u^m\|_{L^2}^2 + \frac{1}{\varepsilon} \|\Upsilon_\varphi^m\|_{L^4}^4 + \frac{\varepsilon^3\alpha(\varepsilon)}{4} \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 \\
& \left. + \frac{\varepsilon^2\alpha(\varepsilon)s(\varepsilon)}{4c(\varepsilon)} \|\Upsilon_\varphi^m - \Delta_h G_u^m\|_{L^2}^2 \right\} \\
& \leq C [\eta_1(\varepsilon)h^4 + \zeta(\varepsilon)k^2] + k \sum_{m=0}^{\ell} \left\{ \frac{\varepsilon\alpha(\varepsilon)[C + 8C_0]}{2} \|\Upsilon_\varphi^m\|_{L^2}^2 \right. \\
& \left. + \frac{s(\varepsilon)[1 + 8C_0]}{2} \|\nabla G_u^m\|_{L^2}^2 + \frac{C}{\varepsilon} \|\Upsilon_\varphi^m\|_{L^3}^3 \right\},
\end{aligned}$$

where $\eta(\varepsilon)$ and $\zeta(\varepsilon)$ are defined by (3.62) and (3.63), respectively.

Repeating the spatial-temporal decomposition argument of *Step 3* of the proof of Theorem 3.1, we can bound the last term of (3.73) by (3.41), moreover, if k satisfies the constraint (3.42), we then get from (3.73) and (3.41) that

$$\begin{aligned}
(3.74) \quad & \frac{\varepsilon\alpha(\varepsilon)}{2} \|\Upsilon_\varphi^\ell\|_{L^2}^2 + \frac{s(\varepsilon)}{2} \|\nabla G_u^\ell\|_{L^2}^2 + k \sum_{m=1}^{\ell} \left\{ \frac{\varepsilon\alpha(\varepsilon)k}{2} \|d_t \Upsilon_\varphi^m\|_{L^2}^2 \right. \\
& + \frac{s(\varepsilon)k}{2} \|\nabla \Upsilon_u^m\|_{L^2}^2 + \frac{1}{\varepsilon} \|\Upsilon_\varphi^m\|_{L^4}^4 + \frac{\varepsilon^3\alpha(\varepsilon)}{4} \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 \\
& \left. + \frac{\varepsilon^2\alpha(\varepsilon)s(\varepsilon)}{4c(\varepsilon)} \|\Upsilon_\varphi^m - \Delta_h G_u^m\|_{L^2}^2 \right\} \\
& \leq C [\eta(\varepsilon)h^4 + \zeta(\varepsilon)k^2] + (C + 8C_0) \left\{ \varepsilon\alpha(\varepsilon)k \sum_{m=0}^{\ell} \|\Upsilon_\varphi^m\|_{L^2}^2 \right. \\
& \left. + s(\varepsilon)k \sum_{m=0}^{\ell} \|\nabla G_u^m\|_{L^2}^2 \right\} + \frac{CB_2^{\frac{N}{8}}}{\varepsilon} k \sum_{m=0}^{\ell} \|\Upsilon_\varphi^{m-1}\|_{L^2}^{\frac{12-N}{4}}.
\end{aligned}$$

Again, the super-quadratic power in the last term allows to control this error contribution by an inductive argument.

Step 4: Same as *Step 4* of the proof of Theorem 3.1. Here we only point out that this time the inductive argument leads to

$$\begin{aligned}
(3.75) \quad & \max_{0 \leq m \leq \ell} \left\{ \frac{\varepsilon\alpha(\varepsilon)}{2} \|\Upsilon_\varphi^m\|_{L^2}^2 + \frac{s(\varepsilon)}{2} \|\nabla G_u^\ell\|_{L^2}^2 \right\} + k \sum_{m=1}^{\ell} \left\{ \frac{\varepsilon\alpha(\varepsilon)k}{2} \|d_t \Upsilon_\varphi^m\|_{L^2}^2 \right. \\
& + \frac{s(\varepsilon)k}{2} \|\nabla \Upsilon_u^m\|_{L^2}^2 + \frac{1}{\varepsilon} \|\Upsilon_\varphi^m\|_{L^4}^4 + \frac{\varepsilon^3\alpha(\varepsilon)}{4} \|\nabla \Upsilon_\varphi^m\|_{L^2}^2 \\
& \left. + \frac{\varepsilon^2\alpha(\varepsilon)s(\varepsilon)}{4c(\varepsilon)} \|\Upsilon_\varphi^m - \Delta_h G_u^m\|_{L^2}^2 \right\} \\
& \leq C [\eta(\varepsilon)h^4 + \zeta(\varepsilon)k^2],
\end{aligned}$$

provided that

$$(3.76) \quad \eta(\varepsilon)h^4 + \zeta(\varepsilon)k^2 \leq \varepsilon^{-1} [\alpha(\varepsilon)]^{\frac{N-12}{4-N}} B_2^{-\frac{N}{4-N}}.$$

□

Remark 3.4. *Again, we note that in case of scheme (1.13)-(1.14), the mesh condition 1) weakens to*

$$k \leq \min\{1, \alpha(\varepsilon)\} \times \min\left\{\varepsilon^2, \varepsilon^{\frac{N+12}{8}} [\alpha(\varepsilon)]^{\frac{N-4}{8}} \left[\mathcal{B}_1 + \frac{\mathcal{B}_2}{\alpha(\varepsilon)}\right]^{-\frac{N}{8}} \left[\mathcal{J}_\varepsilon(\varphi_0^\varepsilon, u_0^\varepsilon)\right]^{\frac{N-4}{8}}\right\}.$$

Theorem 3.4. *Under the assumptions and mesh constraints of Theorem 3.3, the estimates (i)-(x) of Theorem 3.2 hold with $\hat{\mu}(\varepsilon)$, $\hat{\pi}(\varepsilon)$, $\hat{\hat{\mu}}(\varepsilon)$ and $\hat{\hat{\pi}}(\varepsilon)$ being replaced by $\hat{\zeta}(\varepsilon)$, $\hat{\eta}(\varepsilon)$, $\hat{\hat{\zeta}}(\varepsilon)$ and $\hat{\hat{\eta}}(\varepsilon)$, respectively. Where $\hat{\zeta}(\varepsilon)$, $\hat{\eta}(\varepsilon)$, $\hat{\hat{\zeta}}(\varepsilon)$ and $\hat{\hat{\eta}}(\varepsilon)$ have the same forms as those for $\hat{\mu}(\varepsilon)$, $\hat{\pi}(\varepsilon)$, $\hat{\hat{\mu}}(\varepsilon)$ and $\hat{\hat{\pi}}(\varepsilon)$ with $\zeta(\varepsilon)$ and $\eta(\varepsilon)$ being in the place of $\mu(\varepsilon)$ and $\pi(\varepsilon)$, respectively in the formulas.*

Proof. Since the proof is a repeat of the proof of Theorem 3.2, so we omit it. \square

We conclude this section by a short proof for Theorem 1.1.

Proof of Theorem 1.1. The assertions are given by (i), (ii), (iv) and (v) of Theorem 3.1, and (ii)-(iv) of Theorem 3.2 for the case (i), and given by (i), (ii), (iv) and (v) of Theorem 3.3, and (ii)-(iv) of Theorem 3.4 for the case (ii). \square

4. CONVERGENCE OF FULLY DISCRETE SOLUTIONS TO THE SOLUTIONS OF THE FREE BOUNDARY PROBLEMS

In this section we shall present a nontrivial byproduct of the error estimates of the previous section. That is, we shall show convergence of the tuple $\{(\Phi^m, U^m)\}_{m=0}^M$ which solves the fully discrete mixed finite element scheme (1.13)-(1.14) to the solution of the free boundary problem (1.7)-(1.12), provided that the latter has a global (in time) classical solution. Specifically, it is proved that the fully discrete solution U^m , as $h, k \searrow 0$, converges to the solution u^0 of the phase field model uniformly in $\bar{\Omega}_T$, and the fully discrete solution Φ^m converges to ± 1 uniformly on every compact subset of $\bar{\Omega}_T \setminus \Gamma$. Hence, the zero level set of Φ^m converges to the free boundary Γ . Our main ideas are to make full use of the convergence result that the free boundary problem is the distinguished limit, as $\varepsilon \searrow 0$, of the phase field model proved by Caginalp and Chen in [11], and to exploit the ‘‘closeness’’ between the solution (φ, u) of the phase field model and its fully discrete approximation $\{(\Phi^m, U^m)\}_{m=0}^M$, which was obtained in the previous section. We note that as in [11], our numerical convergence is also established under the assumption that the free boundary problem has a global (in time) classical solution; we refer to [11] and references therein for further expositions on this assumption and related theoretical works on the phase field model. We also remark that our convergence result covers all six types of free boundary problems corresponding to six different sets of choices of c^0, d^0 and α^0 in (1.7)-(1.12). Recall that the six types of free boundary problems include the classical Stefan problem, generalized Stefan problems with surface tension and surface kinetics, the Hele-Shaw problem, and the motion by mean curvature flow.

Let $(\varphi^\varepsilon, u^\varepsilon)$ denote the solution of the phase field model (1.1)-(1.4). Note that we put back the super index ε on the solution in this section. Define $(\Phi_{\varepsilon, h, k}(x, t), U_{\varepsilon, h, k}(x, t))$ to be the piecewise linear interpolation (in time) of the fully discrete

solution (Φ^m, U^m) , that is,

$$(4.1) \quad \Phi_{\varepsilon, h, k}(\cdot, t) := \frac{t - t_m}{k} \Phi^{m+1}(\cdot) + \frac{t_{m+1} - t}{k} \Phi^m(\cdot),$$

$$(4.2) \quad U_{\varepsilon, h, k}(\cdot, t) := \frac{t - t_m}{k} U^{m+1}(\cdot) + \frac{t_{m+1} - t}{k} U^m(\cdot)$$

for $t_m \leq t \leq t_{m+1}$ and $0 \leq m \leq M - 1$. Note that $\Phi_{\varepsilon, h, k}$ and $U_{\varepsilon, h, k}$ are continuous piecewise linear functions in space and time.

Let $\Gamma_{00} \subset \Omega$ be a smooth closed hypersurface and let $(u^0, \Gamma := \cup_{0 \leq t \leq T} (\Gamma_t \times \{t\}))$ be a smooth solution of the free boundary problem (1.7)-(1.12) starting from Γ_{00} such that $\Gamma \subset \Omega \times [0, T]$. Let $d(x, t)$ denote the signed distance function to Γ_t such that $d(x, t) < 0$ in \mathcal{I}_t , the inside of Γ_t , and $d(x, t) > 0$ in $\mathcal{O}_t := \Omega \setminus (\Gamma_t \cup \mathcal{I}_t)$, the outside of Γ_t . We also define the inside \mathcal{I} and the outside \mathcal{O} of Γ as follows

$$\begin{aligned} \mathcal{I} &:= \{(x, t) \in \Omega \times [0, T]; d(x, t) < 0\}, \\ \mathcal{O} &:= \{(x, t) \in \Omega \times [0, T]; d(x, t) > 0\}. \end{aligned}$$

In addition, let $\Gamma_t^{\varepsilon, h, k}$ denote the zero level set of $\Phi_{\varepsilon, h, k}$ at time t , that is,

$$(4.3) \quad \Gamma_t^{\varepsilon, h, k} := \{x \in \Omega; \Phi_{\varepsilon, h, k}(x, t) = 0\}.$$

As mentioned earlier, our proof of convergence is based on making full use of the convergence result of [11], which shows that the free boundary problem is the distinguished limit, as $\varepsilon \searrow 0$, of the phase field model. For the readers' convenience, we recall the convergence result in the following theorem, and refer to Theorems 2.1 and 2.2 of [11] for more details.

Theorem 4.1. *Let Ω be a given smooth domain and Γ_{00} be a smooth closed hypersurface in Ω . Suppose that the free boundary problem (1.7)-(1.12) starting from Γ_{00} has a smooth solution $(u^0, \Gamma := \cup_{0 \leq t \leq T} (\Gamma_t \times \{t\}))$ such that $\Gamma \subset \Omega \times [0, T]$. Then there exists a family of smooth functions $\{(\varphi_0^\varepsilon, u_0^\varepsilon)\}_{0 < \varepsilon \leq 1}$ which are uniformly bounded in $\varepsilon \in (0, 1]$ and $(x, t) \in \overline{\Omega}_T$, such that if $(\varphi^\varepsilon, u^\varepsilon)$ solves the phase field model (1.1)-(1.4), then*

$$(4.4) \quad (i) \quad \|u^\varepsilon - u^0\|_{C^0(\overline{\Omega}_T)} \xrightarrow{\varepsilon \searrow 0} 0,$$

$$(4.5) \quad (ii) \quad \varphi^\varepsilon \xrightarrow{\varepsilon \searrow 0} 1 \quad \text{uniformly on compact subsets of } \mathcal{O},$$

$$(4.6) \quad (iii) \quad \varphi^\varepsilon \xrightarrow{\varepsilon \searrow 0} -1 \quad \text{uniformly on compact subsets of } \mathcal{I}$$

hold in each of the following six cases:

- (1) α^0, c^0 and d_0 are positive constants in (1.7)-(1.12); $\alpha(\varepsilon) = \alpha^0, c(\varepsilon) = c^0$ and $s(\varepsilon) = \frac{m}{2d_0}$ in (1.1)-(1.4), where

$$m = \int_{-1}^1 \sqrt{2F(s)} \, ds,$$

which only depends on the choice of the potential function F .

- (2) $d^0 = 0, \alpha^0$ and c^0 are positive constants; $\alpha(\varepsilon) = \alpha^0, c(\varepsilon) = c^0$ and $s(\varepsilon) = \varepsilon^{-\frac{1}{2}}$.
(3) $c^0 = 0, \alpha^0$ and d^0 are positive constants; $c(\varepsilon) = \varepsilon^\ell$ for any $\ell \geq 1, \alpha(\varepsilon) = \alpha^0$ and $s(\varepsilon) = \frac{m}{2d_0}$.
(4) c^0 and α^0 are positive constants; $\alpha(\varepsilon) = \alpha^0, c(\varepsilon) = c^0, s(\varepsilon) = \varepsilon^\ell$ for any $\ell \geq 1$. In this case, the equilibrium condition (1.10) is replaced by $\kappa_\Gamma = \alpha^0 V$.

- (5) $\alpha^0 = 0$, d^0 and c^0 are positive constants; and $\alpha(\varepsilon) = \varepsilon^\ell$ for any $\ell \geq 1$,
 $c(\varepsilon) = c^0$ and $s(\varepsilon) = \frac{m}{2d_0}$.
- (6) $c^0 = \alpha^0 = 0$, d^0 is positive constant; $c(\varepsilon) = \varepsilon^\ell$, $\alpha(\varepsilon) = \varepsilon^j$ for any $\ell, j \geq 1$,
and $s(\varepsilon) = \frac{m}{2d_0}$.

Remark 4.1. *The above convergence result was proved in [11] when φ satisfies the Dirichlet boundary condition. However, it was remarked in (4) of Remark 2.3 (see page 424 of [11]) that the conclusion still holds when φ satisfies the homogeneous Neumann boundary condition.*

We also remark that the free boundary problem in case (2) is the classical Stefan problem. The free boundary condition (1.10) in case (5) reduces to the well-known Gibbs-Thomson condition. The free boundary problem in case (4) is the motion by mean curvature flow [22, 24], and the one in case (6) is known as the Hele-Shaw/Mullins-Sekerka problem [3, 36]. The remaining cases (1) and (3) are the generalized Stefan problems with surface tension and surface kinetics.

We are now ready to show Theorem 1.2.

Proof of Theorem 1.2. The triangle inequality implies that

$$\|U_{\varepsilon,h,k} - u^0\|_{C^0(\overline{\Omega}_T)} \leq \|U_{\varepsilon,h,k} - u^\varepsilon\|_{C^0(\overline{\Omega}_T)} + \|u^\varepsilon - u^0\|_{C^0(\overline{\Omega}_T)}.$$

The assertion (i) then follows immediately from (i) of Theorem 4.1 and the L^∞ error estimate given in Theorem 1.1.

To show assertion (ii), let A be any compact subset of \mathcal{O} , for any $(x, t) \in A$, using the triangle inequality we have

$$(4.7) \quad \begin{aligned} |\Phi_{\varepsilon,h,k}(x, t) - 1| &\leq |\Phi_{\varepsilon,h,k}(x, t) - \varphi^\varepsilon(x, t)| + |\varphi^\varepsilon(x, t) - 1| \\ &\leq \|\Phi_{\varepsilon,h,k} - \varphi^\varepsilon\|_{L^\infty(\Omega_T)} + |\varphi^\varepsilon(x, t) - 1|. \end{aligned}$$

Under the assumptions of Theorem 1.2, the first term on the right-hand side of (4.7) is bounded by $C(h^\alpha + k^\beta)$ for some $\alpha, \beta > 0$, hence, it converges to zero uniformly on A (and on Ω) as $h \searrow 0$. From (ii) of Theorem 4.1 we know that the second term on the right-hand side of (4.7) also converges to zero uniformly on A . Note that $h \searrow 0$ as $\varepsilon \searrow 0$. Therefore,

$$\Phi_{\varepsilon,h,k} \xrightarrow{\varepsilon \searrow 0} 1 \quad \text{uniformly on } A.$$

This then completes the proof of the assertion (ii).

The proof of assertion (iii) is almost a repetition of the above proof. The only change is to replace \mathcal{O} by \mathcal{I} and 1 by -1 in the above proof. So we omit it. \square

Another consequence of Theorem 1.1 is the following convergence result of the zero level set $\Gamma_t^{\varepsilon,h,k}$ of $\Phi_{\varepsilon,h,k}$ to the true free boundary Γ_t as described in Theorem 1.3. The proof of Theorem 1.3 is almost the same as that of Theorem 1.3 of [27].

For the reader's convenience, we give a sketch of the proof in the following.

Proof of Theorem 1.3. For any $\delta \in (0, 1)$, define the (open) tubular neighborhood \mathcal{N}_δ of width 2δ of Γ as

$$(4.8) \quad \mathcal{N}_\delta := \{ (x, t) \in \Omega_T; d(x, t) < \delta \}.$$

Let A and B denote the complements of \mathcal{N}_δ in \mathcal{O} and \mathcal{I} , respectively, that is

$$A = \mathcal{O} \setminus \mathcal{N}_\delta, \quad B = \mathcal{I} \setminus \mathcal{N}_\delta.$$

Note that A is a compact subset of \mathcal{O} and B is a compact subset of \mathcal{I} . Hence, from (ii) and (iii) of Theorem 1.2 we know that there exists $\widehat{\varepsilon}_0 > 0$, which only depends on δ , such that for all $\varepsilon \in (0, \widehat{\varepsilon}_0)$

$$(4.9) \quad |\Phi_{\varepsilon,h,k}(x,t) - 1| \leq \delta \quad \forall (x,t) \in A,$$

$$(4.10) \quad |\Phi_{\varepsilon,h,k}(x,t) + 1| \leq \delta \quad \forall (x,t) \in B.$$

Now for any $t \in [0, T]$ and $x \in \Gamma_t^{\varepsilon,h,k}$, since $\Phi_{\varepsilon,h,k}(x,t) = 0$, we have

$$(4.11) \quad |\Phi_{\varepsilon,h,k}(x,t) - 1| = 1,$$

$$(4.12) \quad |\Phi_{\varepsilon,h,k}(x,t) + 1| = 1.$$

Evidently, (4.9) and (4.11) imply that $(x,t) \notin A$, and (4.10) and (4.12) says that $(x,t) \notin B$. Hence (x,t) must reside in the tubular neighborhood \mathcal{N}_δ . Since t is an arbitrary number in $[0, T]$ and x is an arbitrary point on $\Gamma_t^{\varepsilon,h,k}$, therefore, for all $\varepsilon \in (0, \widehat{\varepsilon}_0)$

$$\sup_{x \in \Gamma_t^{\varepsilon,h,k}} (\text{dist}(x, \Gamma_t)) \leq \delta \quad \text{uniformly on } [0, T].$$

The proof is complete. \square

Remark 4.2. *Unlike in [25, 27], Theorem 1.3 does not provide any information about the rate of convergence of the numerical free boundary $\Gamma_t^{\varepsilon,h,k}$ to the true free boundary Γ_t . This is because no rate of convergence for the zero level set of φ^ε to Γ_t was obtained in [11]. In fact, to our knowledge, such a rate of convergence estimate is not known in the literature. On the other hand, if a rate of convergence can be proved for the zero level set of φ^ε to the true free boundary Γ_t , it is easy to show that our numerical free boundary $\Gamma_t^{\varepsilon,h,k}$ should enjoy at least the same rate of convergence to the true free boundary Γ_t .*

Acknowledgment: The first author would like to thank Xinfu Chen for answering his questions about the spectrum estimates in Lemma 2.4. The second author gratefully acknowledges financial support by the DFG.

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