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A third order accurate, energy stable exponential time differencing multi-step scheme for Landau-Brazovskii model

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ABSTRACT

In this article, we propose and analyze a global-in-time energy stable third-order accurate in time exponential time differencing multi-step (ETD-MS) numerical scheme for the Landau-Brazovskii (LB) equation, which is a generic model to describe weakly first-order order-disorder phase transition for isotropic systems. The ETD-based explicit multi-step temporal discretization is combined with the Fourier collocation spectral approximation in the numerical design, and a third-order stabilizing term is added to ensure energy stability. In turn, a global-in-time energy estimate for the ETD-MS numerical scheme is established. In more details, an a-priori assumption at the previous time steps, combined with an H^2 estimate of the numerical solution at the next time step, is the key point in the analysis. Such a global-in-time energy estimate is the first such result of a third-order stabilized numerical scheme for a gradient flow. Moreover, an $\ell^\infty(0,T;\ell^2)\cap\ell^\infty(0,T;H_h^2)$ error estimate is derived, with the help of careful Fourier eigenvalue analysis. Numerical experiments are conducted to verify the theoretical results, and several structures in block copolymers are effectively simulated for a long time in two- and three-dimensional spaces, which demonstrate the accuracy and high efficiency of the proposed numerical scheme.

1. Introduction

The phase field crystal model has been used to study the microstructural evolution of crystal growth on atomic length and diffusive time scales [1]. The LB equation in [2] is one important phase field crystal model in modern physics, which is a general framework for systems undergoing a phase transition driven by a short-wavelength instability between the disordered liquid and ordered crystalline phases [3]. This model has been applied to a variety of specific physical systems, including block copolymers [4,5] and liquid crystals [3]. Within the mean-field approximation, it has been demonstrated that the LB model can account for many ordered structures such as the lamellar, cylindrical, and spherical phases [4,6].

In fact, the LB model in [7] is an approximate theory of self-consistent field theory in weak segregation. The free energy density functional [2,3,6,8] is given by

$$E(\phi) := \int_\Omega \left(\frac{\xi^2}{2}[(\Delta+1)\phi]^2 + F(\phi) \right) \mathrm{d}\boldsymbol{x}, \tag{1}$$

where $F(\phi) = \frac{1}{4!}\phi^4 - \frac{\gamma}{3!}\phi^3 + \frac{\alpha}{2!}\phi^2$; the order parameter $\phi(\boldsymbol{x},t)$ is the real-valued periodic function, which is the density deviation of a kind of monomer from the disordered phase; ξ, α and $\gamma > 0$ are phenomenological constants [8]. In comparison with the

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typical Swift-Hohenberg model in [9] with double-well bulk energy, the LB energy functional includes a cubic term that can be used to characterize the asymmetry of the order phase [10]. Notice that $E(\phi)$ is invariant under the transformation $\phi \to -\phi$, $\gamma \to -\gamma$. Furthermore, the following mean zero condition of order parameter is imposed on the LB system, to ensure the mass conservation [11]:

$$\overline{\phi} := \frac{1}{|\Omega|}\int_{\Omega} \phi \mathrm{d}\boldsymbol{x} = 0. \tag{2}$$

To find the stationary states of the LB model, the L^2-gradient flow of the free energy reads as

$$\frac{\partial \phi}{\partial t} = -\frac{\delta E}{\delta \phi} = -\xi^2(\Delta+1)^2\phi - f(\phi), \tag{3}$$

where $f(\phi) = F'(\phi) = \alpha\phi - \frac{\gamma}{2!}\phi^2 + \frac{1}{3!}\phi^3$. Inspired by the conservative Allen-Cahn (CAC) equation developed in [12], a nonlocal Lagrange multiplier is added to conserve the total mass of ϕ, thus the total system (CAC-LB) becomes

$$\frac{\partial \phi}{\partial t} = -\xi^2(\Delta+1)^2\phi - f(\phi) + \beta(t), \qquad \beta(t) := \frac{1}{|\Omega|}\int_{\Omega} \left(\xi^2\phi + f(\phi)\right) \mathrm{d}\boldsymbol{x}. \tag{4}$$

The system (4) satisfies two important physical properties: the energy dissipation law in the sense that $\frac{\mathrm{d}}{\mathrm{d}t}E \le 0$, and the mass conservation represented by $\frac{\mathrm{d}}{\mathrm{d}t}\overline{\phi} = 0$. Another efficient method that similarly preserves mass is the projection method [13]. As one typical system of phase field modeling, the LB model has played a key role in explaining how fluctuations affect the properties of order-disorder phase transitions [2,9,10]. Therefore, an accurate, stable and effective numerical method for the LB model is highly desired.

Various unconditionally energy stable schemes for phase field crystal equation have been reported in the existing literature [11,14–18], such as the common semi-implicit scheme [19], the convex splitting approach [20–25] and the stabilization methods [26,27].

High-order numerical schemes have attracted a lot of attention in recent years [28–30]. In particular, the exponential time differencing (ETD) is a very effective method [25,27,31–38] to deal with parabolic equations, which achieves high-order accuracy by explicit treatment of nonlinear terms. Specifically, the ETD method involves exact integration of the linear part, followed by an approximation to the nonlinear terms [39,40], with two popular approaches: the multi-step algorithm [41] and the Runge-Kutta method [42].

Meanwhile, a theoretical justification of energy stability without Lipschitz assumption on the non-linearity turns out to be a very challenging issue. Shen and Yang [43] proved energy stability for both Allen-Cahn and Cahn-Hilliard equations by a nonlinear truncation technique. This idea has been extended in recent works [27,44,45]. An alternate approach is to justify an L^∞ bound of the numerical solution [25,35,46,47]. In particular, for the phase field crystal equation, a local in time bound of the numerical solution has been established in [25], with the help of the convergence estimate with a fixed final time. Instead of such a local-in-time analysis, a global-in-time H^2 estimate has also been derived in [35], which in turn justifies the L^∞ bound. As a result, the explicitly computed nonlinear term could be appropriately bounded, and the energy stability becomes theoretically available.

The goal of this paper is to develop a fully discrete, third order accurate (in time) numerical scheme for the LB system (4), with global-in-time energy stability at any final time. We apply the ETD-based multi-step approximation in time and the Fourier collocation spectral method in space. In more details, a second-order Lagrange approximation is applied to the nonlinear terms, and an artificial stabilizing term $A\tau^3\frac{\partial\phi(t)}{\partial t}$ is added, where A is a positive constant independent of time step τ. In addition, a global-in-time energy stability estimate for the numerical scheme is established, with the help of an H^2 estimate for the numerical solution. Accordingly, the uniform-in-time $\|\cdot\|_\infty$ bound for the numerical solution and A are recovered by a Sobolev embedding from H^2 to L^∞. To derive a uniform bound for the various global operators involved in the algorithm, we perform careful eigenvalue estimates for these operators. Moreover, mass conservative property has also been proved. A careful Fourier eigenvalue analysis results in an $\ell^\infty(0,T;\ell^2)\cap\ell^\infty(0,T;H_h^2)$ error estimate for the proposed scheme. Furthermore, a few numerical experiments are carried out to verify the accuracy, effectiveness and energy stability of the proposed scheme. Specifically, two-dimensional (2D) and 3D periodic crystal structures in block copolymers are effectively obtained in a long-time simulation.

This article is organized as follows. In Section 2, the fully discrete scheme of the LB model is proposed. We review the Fourier collocation spectral spatial approximation and introduce the third order ETD-based scheme; some preliminary estimates are derived and the mass conservation property is proved. Afterward, a global-in-time energy stability analysis is established in Section 3. In Section 4, the third-order convergence analysis for the numerical scheme is presented, in the $\ell^\infty(0,T;\ell^2)\cap\ell^\infty(0,T;H_h^2)$ norm. In addition, a few numerical experiments are performed in Section 5. Finally, some concluding remarks are made in Section 6.

2. The numerical scheme

A fully discrete numerical scheme is proposed for the LB equation in this section. We first review Fourier collocation spectral spatial approximation, and develop a third-order ETD-based scheme with a stabilization term $A\tau^3\frac{\partial\phi(t)}{\partial t}$. Afterward, some preliminary estimates are presented, with the help of Fourier eigenvalue analysis. In addition, the mass conservation analysis is established.

2.1. Review of the fourier collocation spectral approximation

Firstly, a brief introduction to the Bravais lattice and reciprocal lattice is necessary. Each of the d-dimensional periodic system can be described by a Bravis lattice [8], namely, $\mathrm{R} = \sum_{i=1}^{d} p_i \mathbf{a}_i,\ p_i \in \mathbb{Z}$, where the vector $\mathbf{a}_i \in \mathbb{R}^d$ forms the primitive Bravis lattice $\mathbf{A} = (\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_d) \in \mathbb{R}^{d\times d}$. The associated reciprocal lattice becomes $\mathrm{R}^* = \sum_{i=1}^{d} P_i \mathbf{b}_i,\ P_i \in \mathbb{Z}$. The primitive reciprocal lattice vector $\mathbf{b}_i \in \mathbb{R}^d$ satisfies the dual relationship $\mathbf{a}_i \mathbf{b}_j = 2\pi\delta_{i,j}$. Without loss of generality, we will discuss the 2D problem thereafter.

Denote the computational domain as $\Omega = (0, L_x) \times (0, L_y)$, and consider an invertible matrix $\mathbf{B} = 2\pi \cdot diag(L_x^{-1}, L_y^{-1}) \in \mathbb{R}^{2\times 2}$, associated with the 2D primitive reciprocal lattice. Let N be a even number, and $h_x = \frac{L_x}{2N+1}$, $h_y = \frac{L_y}{2N+1}$. All the variables are evaluated at the regular numerical grid (x_i, y_j), with $x_i = ih_x,\ y_j = jh_y,\ 0 \le i,\ j \le 2N$. We set a uniform time step size as $\tau > 0$, and $t_i = i\tau$ for $0 \le i \le \infty$. All the 2D periodic grid functions on $\Omega_{\mathcal{N}}$ are denoted by $\mathcal{M}^{\mathcal{N}}$, and $\mathcal{B}^N$ is the space of trigonometric polynomials in x and y of degree up to N. In this paper, C is a general constant, independent of the mesh size h_x, h_y and time step size τ.

We denote the index sets

$$\mathcal{P} = \left\{(i,j) \in \mathbb{Z}^2 | 0 \le i, j \le 2N\right\}, \tag{5}$$

$$\mathcal{K} = \left\{\boldsymbol{k} := (k,l)^T \in \mathbb{R}^2 | -N \le k, l \le N\right\}. \tag{6}$$

For $f \in \mathcal{M}^{\mathcal{N}}$, we define an interpolation operator $\mathcal{I}_{\mathcal{N}}$ that reserves the function value on points (x_i, y_j), $(i,j) \in \mathcal{P}$, *i.e.*, $\mathcal{I}_{\mathcal{N}} f(x_i, y_i) = f(x_i, y_j)$.

$$\mathcal{I}_{\mathcal{N}} f(x,y) = \sum_{\boldsymbol{k}\in\mathcal{K}} (\hat{f}_c)_{\boldsymbol{k}} e^{\mathrm{i}\left[(\mathbf{B}\boldsymbol{k})^T (x,y)^T\right]}, \tag{7}$$

$$(\hat{f}_c)_{\boldsymbol{k}} = \frac{1}{(2N+1)^2} \sum_{(i,j)\in\mathcal{P}} f(x_i, y_j) e^{-\mathrm{i}\left[(\mathbf{B}\boldsymbol{k})^T (x_i,y_j)^T\right]}, \tag{8}$$

in which the Fourier collocation coefficients $(\hat{f}_c)_{\boldsymbol{k}}$ could be obtained by discrete Fourier transformation. The discrete differentiation operators in the x-direction is defined as

$$(D_x f)_{i,j} = \sum_{\boldsymbol{k}\in\mathcal{K}} \frac{2k\pi\mathrm{i}}{L_x} (\hat{f}_c)_{\boldsymbol{k}} e^{\mathrm{i}\left[(\mathbf{B}\boldsymbol{k})^T (x_i,y_j)^T\right]}, \quad (D_x^2 f)_{i,j} = \sum_{\boldsymbol{k}\in\mathcal{K}} -\frac{4k^2\pi^2}{L_x^2} (\hat{f}_c)_{\boldsymbol{k}} e^{\mathrm{i}\left[(\mathbf{B}\boldsymbol{k})^T (x_i,y_j)^T\right]}.$$

The differentiation operators $D_y f,\ D_y^2 f$ in the y-direction could be similarly derived. For any $f, g \in \mathcal{M}^{\mathcal{N}}$, $\mathbf{f} = (f^1, f^2)^T$, $\mathbf{g} = (g^1, g^2)^T \in \mathcal{M}^{\mathcal{N}} \times \mathcal{M}^{\mathcal{N}}$, the discrete gradient, divergence and Laplace operators, are introduced as

$$\nabla_{\mathcal{N}} f = \begin{pmatrix} D_x f \\ D_y f \end{pmatrix}, \quad \nabla_{\mathcal{N}} \cdot f = D_x f^1 + D_y f^2, \quad \Delta_{\mathcal{N}} f = D_x^2 f + D_y^2 f.$$

The spectral approximation to the L^2 (denoted as ℓ^2) inner product $(\cdot,\cdot)_{\mathcal{N}}$, norm $\|\cdot\|_{\mathcal{N}}$, norm $\|\cdot\|_\infty$, norm $\|\cdot\|_{L_h^p}$ $(1 \le p < \infty)$, norm $\|\cdot\|_{H_h^m}$ and semi-norm $|\cdot|_{H_h^m}$ $(m \in \mathbb{Z}_+)$, are given by

$$(f,g)_{\mathcal{N}} = h_x h_y \sum_{(i,j)\in\mathcal{P}} f_{ij} g_{ij}, \qquad \|f\|_{\mathcal{N}} = \sqrt{(f,f)_{\mathcal{N}}},$$

$$(\mathbf{f},\mathbf{g})_{\mathcal{N}} = h_x h_y \sum_{(i,j)\in\mathcal{P}} f_{ij}^1 g_{ij}^1 + f_{ij}^2 g_{ij}^2, \qquad \|\mathbf{f}\|_{\mathcal{N}} = \sqrt{(\mathbf{f},\mathbf{f})_{\mathcal{N}}},$$

$$\|f\|_\infty = \max_{0\le i,j\le 2N} |f_{ij}|, \qquad \|f\|_{L_h^p} = \Big(h_x h_y \sum_{(i,j)\in\mathcal{P}} |f_{ij}|^p\Big)^{\frac{1}{p}},$$

$$\|f\|_{H_h^m} = \Big(\sum_{|\alpha|\le m} \|D_\alpha f\|_{\mathcal{N}}^2\Big)^{\frac{1}{2}}, \qquad |f|_{H_h^m} = \Big(\sum_{|\alpha|=m} \|D_\alpha f\|_{\mathcal{N}}^2\Big)^{\frac{1}{2}},$$

where as above $\alpha = (\alpha^1, \alpha^2)$ is a 2-tuple of nonnegative integers with $|\alpha| = \alpha^1 + \alpha^2$, and $D_\alpha = D_x^{\alpha^1} D_y^{\alpha^2}$. The following lemma has been established in existing works.

Lemma 2.1 (*See [31,32,37,48,49]*). *For any functions $f,\ g \in \mathcal{M}^{\mathcal{N}}$, $\mathbf{g} = (g^1, g^2)^T \in \mathcal{M}^{\mathcal{N}} \times \mathcal{M}^{\mathcal{N}}$, we have the following summation by parts formula:*

$$(f, \nabla_{\mathcal{N}} \cdot \mathbf{g})_{\mathcal{N}} = -(\nabla_{\mathcal{N}} f, \mathbf{g})_{\mathcal{N}},\ (f, \Delta_{\mathcal{N}} g)_{\mathcal{N}} = -(\nabla_{\mathcal{N}} f, \nabla_{\mathcal{N}} g)_{\mathcal{N}} = (\Delta_{\mathcal{N}} f, g)_{\mathcal{N}}.$$

The function $\tilde{f} = \mathcal{I}_{\mathcal{N}} f$ is denoted as the continuous periodic expansion of f, and the following approximation property is valid for the interpolation operator $\mathcal{I}_{\mathcal{N}}$.

Lemma 2.2 (*See [49]*). *As long as f and all its derivatives (up to mth order) are continuous and periodic on Ω, the convergence of the derivatives of the projection and interpolation is given by*

$$\|\partial^k f - \partial^k \mathcal{I}_{\mathcal{N}} f\|_{L^2} \le C N^{k-m} \|f\|_{H^m}, \quad 0 \le k \le m,\ m \ge \frac{d}{2}, \tag{9}$$

where d represents the dimension.

In order to preserve the bound in space of H^m, the following lemma is introduced. In fact, the case of $k=0$ was proven in earlier works [50,51], and the case of $k \geq 1$ was analyzed in a recent article [52].

Lemma 2.3 (*See [52]*). *For any $\varphi \in \mathcal{B}^{mN}$ in dimension d, we have*

$$\|\mathcal{I}_{\mathcal{N}}\varphi\|_{H^k} \leq (\sqrt{m})^d \|\varphi\|_{H^k}, \quad k \in \mathbb{Z},\ k \geq 0. \tag{10}$$

The mass conservation identity is discretized as $\overline{f} := \frac{1}{|\Omega_{\mathcal{N}}|}(f,1)_{\mathcal{N}} = 0$, which implies that the Fourier collocation coefficients satisfy $(\hat{f}_c)_{\mathbf{0}} = 0$. The subset of zero-mean grid functions is taken into consideration

$$\mathcal{M}_0^{\mathcal{N}} = \left\{ v \in \mathcal{M}_{\mathcal{N}} \,\middle|\, \overline{v} = 0 \right\} = \left\{ v \in \mathcal{M}_{\mathcal{N}} \,\middle|\, (\hat{f}_c)_{\mathbf{0}} = 0 \right\}.$$

Define the linear operator $L_N = \xi^2(\Delta_{\mathcal{N}} + I)^2 + \kappa I$, with $\kappa > 0$, which is symmetric positive definite on $\mathcal{M}_0^{\mathcal{N}}$. The space-discrete scheme for the equation is to find a function $\widetilde{\phi} : [0,\infty) \to \mathcal{M}_0^{\mathcal{N}}$ such that

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\phi}(t) = -L_N \widetilde{\phi}(t) - f_N(\widetilde{\phi}(t)), & t \in (0,\infty), \\ \widetilde{\phi}(0) = \phi_0, & t = 0, \end{cases} \tag{11}$$

where

$$f_N(v) = g(v) - \beta_N(v), \quad g(v) = f(v) - \kappa v, \quad \beta_N(v) = \frac{1}{|\Omega_{\mathcal{N}}|}(\xi^2 v + f(v), 1)_{\mathcal{N}},$$

and $\phi_0 \in \mathcal{M}_0^{\mathcal{N}}$ is given by the initial data.

2.2. The third-order ETD multi-step numerical scheme

We explicitly approximate the term $f_N(\widetilde{\phi}(t))$ with a second-order Lagrange approximation, leading to a linear system. Meanwhile, a stabilization term $A\tau^3 \frac{\mathrm{d}\widetilde{\phi}(t)}{\mathrm{d}t}$ is introduced, where A is a positive constant independent of τ.

Denote $\phi_h(t_n)$ by ϕ_h^n for $n \geq 0$. The following numerical scheme is proposed.

For $n \geq 2$, find $\phi_h^{n+1}(t) : [t_n, t_{n+1}] \to \mathcal{M}_0^{\mathcal{N}}$ such that for any $t \in [t_n, t_{n+1}]$,

$$\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t} + A\tau^3 \frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t} + L_N \phi_h^{n+1}(t) = -\sum_{i=0}^{2} \ell_i(t-t_n) f_N(\phi_h^{n-i}), \tag{12}$$

where

$$\ell_0(s) = 1 + \frac{3s}{2\tau} + \frac{s^2}{2\tau^2}, \quad \ell_1(s) = -\frac{2s}{\tau} - \frac{s^2}{\tau^2}, \quad \ell_2(s) = \frac{s}{2\tau} + \frac{s^2}{2\tau^2}.$$

The initial step is to find $\phi_h^1(t) :\ [0,t_1] \to \mathcal{M}_0^{\mathcal{N}}$ such that for any $t \in [0,t_1]$,

$$\frac{\mathrm{d}a_h^1(t)}{\mathrm{d}t} + A\tau^3 \frac{\mathrm{d}a_h^1(t)}{\mathrm{d}t} + L_N a_h^1(t) = -f_N(\phi_0), \tag{13}$$

$$\frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} + A\tau^3 \frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} + L_N \phi_h^1(t) = -\frac{t}{\tau} f_N(a_h^1) + \frac{t-\tau}{\tau} f_N(\phi_0), \tag{14}$$

where $\phi_h^0 = a_h^0 = \phi_0$. The second step is to find $\phi_h^2(t) :\ [t_1,t_2] \to \mathcal{M}_0^{\mathcal{N}}$ such that for any $t \in [t_1,t_2]$,

$$\frac{\mathrm{d}\phi_h^2(t)}{\mathrm{d}t} + A\tau^3 \frac{\mathrm{d}\phi_h^2(t)}{\mathrm{d}t} + L_N \phi_h^2(t) = -\frac{t}{\tau} f_N(\phi_h^1) + \frac{t-\tau}{\tau} f_N(\phi_0). \tag{15}$$

Note that $\phi_h^{k+1}(t_k) = \phi_h^k(t_k)$, $k = 0, \ldots, n$.

Integrating (12)–(14) from t_n to t_{n+1}, with an integration factor $\mathrm{e}^{K_N t}$, where $K_N = (1 + A\tau^3)^{-1} L_N$. Then we obtain an explicit expression of ϕ_h^{n+1}, ϕ_h^1 and ϕ_h^2.

ETD-MS3: For $n \geq 2$,

$$\begin{aligned} \phi_h^{n+1} &= \mathrm{e}^{-K_N\tau}\phi_h^n - \tau\mathcal{G}_0(K_N\tau)F_N(\phi_h^n) \\ &\quad - \tau\mathcal{G}_1(K_N\tau)\left[\frac{3}{2}F_N(\phi_h^n) - 2F_N(\phi_h^{n-1}) + \frac{1}{2}F_N(\phi_h^{n-2})\right] \\ &\quad - \tau\mathcal{G}_2(K_N\tau)\left[\frac{1}{2}F_N(\phi_h^n) - F_N(\phi_h^{n-1}) + \frac{1}{2}F_N(\phi_h^{n-2})\right], \end{aligned} \tag{16}$$

$$a_h^1 = \mathrm{e}^{-K_N\tau}\phi_0 - \tau\mathcal{G}_0(K_N\tau)F_N(\phi_0), \tag{17}$$

$$\phi_h^1 = \mathrm{e}^{-K_N\tau}\phi_0 - \tau\mathcal{G}_0(K_N\tau)F_N(\phi_0) - \tau\mathcal{G}_1(K_N\tau)\left[F_N(a_h^1) - F_N(\phi_0)\right], \tag{18}$$

$$\phi_h^2 = \mathrm{e}^{-K_N\tau}\phi_1 - \tau\mathcal{G}_0(K_N\tau)F_N(\phi_1) - \tau\mathcal{G}_1(K_N\tau)\left[F_N(\phi_h^1) - F_N(\phi_0)\right], \tag{19}$$

with

$$\begin{aligned}
\mathcal{G}_0(K_N\tau) &= (K_N\tau)^{-1}(I-\mathrm{e}^{-K_N\tau}),\\
\mathcal{G}_1(K_N\tau) &= (K_N\tau)^{-1}[I-(K_N\tau)^{-1}(I-\mathrm{e}^{-K_N\tau})],\\
\mathcal{G}_2(K_N\tau) &= (K_N\tau)^{-1}[I-2(K_N\tau)^{-1}(I-(K_N\tau)^{-1}(I-\mathrm{e}^{-K_N\tau}))],\\
F_N(v) &= (1+A\tau^3)^{-1}f_N(v).
\end{aligned}$$

Remark 2.1. In this article, a continuous version of Dupont-Douglas type stabilization term $A\tau^3\frac{\partial\phi}{\partial t}$ is introduced to ensure the energy stability while achieving third-order accuracy, where A is a positive constant independent of time step τ. This approach is a general method and can be extended to construct higher order ($k>3$) energy stable schemes [36].

2.3. Some preliminary estimates

To facilitate the global-in-time energy estimate and convergence analysis for the numerical scheme, the following preliminary estimates are derived in this subsection, which will be applied in the later analysis.

The following two lemmas will be extensively applied in the nonlinear analysis.

Lemma 2.4. *For any $v,w\in\mathcal{M}^{\mathcal{N}}$, satisfying*

$$\|v\|_\infty\le m_0,\qquad \|w\|_\infty\le m_0, \tag{20}$$

for some constants $m_0>0$, we have

$$\|f(v)-f(w)\|_{\mathcal{N}}\le(\alpha+\gamma m_0+\frac{1}{2}m_0^2)\|v-w\|_{\mathcal{N}}, \tag{21}$$

$$\|F_N(v)-F_N(w)\|_{\mathcal{N}}\le\frac{2\alpha+\kappa+\xi^2+2\gamma m_0+m_0^2}{1+A\tau^3}\|v-w\|_{\mathcal{N}}. \tag{22}$$

Proof. By the Lagrange mean value theorem, we have

$$\|f(v)-f(w)\|_{\mathcal{N}}=\|f'(\delta_1)(v-w)\|_{\mathcal{N}}\le(\alpha+\gamma m_0+\frac{1}{2}m_0^2)\|v-w\|_{\mathcal{N}}, \tag{23}$$

where $\delta_1\in(v,w)$. In turn, the following inequality is valid for the nonlinear term F_N:

$$\begin{aligned}
\|F_N(v)-F_N(w)\|_{\mathcal{N}}\le&\frac{1}{1+A\tau^3}(\|f(v)-f(w)\|_{\mathcal{N}}+\kappa\|v-w\|_{\mathcal{N}})\\
&+\frac{1}{(1+A\tau^3)|\Omega_{\mathcal{N}}|}\|(f(v)-f(w)+\xi^2(v-w),1)_{\mathcal{N}}\|_{\mathcal{N}}\\
\le&\frac{2}{1+A\tau^3}\|f(v)-f(w)\|_{\mathcal{N}}+\frac{\kappa+\xi^2}{1+A\tau^3}\|v-w\|_{\mathcal{N}}.
\end{aligned} \tag{24}$$

A substitution of (23) into (24) completes the proof. □

Lemma 2.5. *For any periodic grid function f, we have*

$$\|f\|_\infty\le\|\widetilde{f}\|_{L^\infty}\le\widehat{C}_1(|\overline{f}|+\|\Delta_{\mathcal{N}}f\|_{\mathcal{N}}), \tag{25}$$

$$\|\nabla_{\mathcal{N}}(f^3)\|_{\mathcal{N}}\le 9\|\widetilde{f}\|_{L^\infty}^2\cdot\|\nabla_{\mathcal{N}}f\|_{\mathcal{N}}, \tag{26}$$

$$\|\nabla_{\mathcal{N}}(f^2)\|_{\mathcal{N}}\le 4\|\widetilde{f}\|_{L^\infty}\cdot\|\nabla_{\mathcal{N}}f\|_{\mathcal{N}}, \tag{27}$$

$$\|\nabla_{\mathcal{N}}f\|_{\mathcal{N}}\le\widehat{C}_2\|\Delta_{\mathcal{N}}f\|_{\mathcal{N}}, \tag{28}$$

in which the constant $\widehat{C}_1$ and $\widehat{C}_2$ are only dependent on Ω, independent of h_x, h_y, f and κ.

Proof. An application of the Sobolev inequality implies that

$$\|f\|_\infty\le\|\mathcal{I}_{\mathcal{N}}f\|_{L^\infty}\le C(\|\mathcal{I}_{\mathcal{N}}f\|_{L^2}+\|\Delta\mathcal{I}_{\mathcal{N}}f\|_{L^2})=C(\|f\|_{\mathcal{N}}+\|\Delta_{\mathcal{N}}f\|_{\mathcal{N}}). \tag{29}$$

Denote $f=f_{new}+\overline{f}$. Because of the fact that $\overline{f_{new}}=0$, we get

$$\|f\|_{\mathcal{N}}\le C(\|f_{new}\|_{\mathcal{N}}+|\overline{f}|),\quad \|f_{new}\|_{\mathcal{N}}\le C\|\Delta_{\mathcal{N}}f_{new}\|_{\mathcal{N}}\le C\|\Delta_{\mathcal{N}}f\|_{\mathcal{N}}. \tag{30}$$

This finishes the proof of inequality (25). Also notice that $(\widetilde{f})^3\in\mathcal{B}^{3N}$ and $(\widetilde{f})^2\in\mathcal{B}^{2N}$. By Lemma 2.3, we arrive at

$$\|\nabla_{\mathcal{N}}(f^3)\|_{\mathcal{N}}=\|\nabla\mathcal{I}_{\mathcal{N}}((\widetilde{f})^3)\|_{L^2}\le(\sqrt{3})^2\|\nabla((\widetilde{f})^3)\|_{L^2}\le 9\|\widetilde{f}\|_{L^\infty}^2\cdot\|\nabla_{\mathcal{N}}f\|_{\mathcal{N}}, \tag{31}$$

$$\|\nabla_{\mathcal{N}}(f^2)\|_{\mathcal{N}} = \|\nabla \mathcal{I}_{\mathcal{N}}((\widetilde{f})^2)\|_{L^2} \le (\sqrt{2})^2 \|\nabla((\widetilde{f})^2)\|_{L^2} \le 4\|\widetilde{f}\|_{L^\infty} \cdot \|\nabla_{\mathcal{N}} f\|_{\mathcal{N}}. \tag{32}$$

Inequality (28) is obvious, based on the elliptic regularity, combined with the fact that $\|\nabla_{\mathcal{N}} f\|_{\mathcal{N}} = \|\nabla \tilde{f}\|$, $\|\Delta_{\mathcal{N}} f\|_{\mathcal{N}} = \|\Delta \tilde{f}\|$. □

For operators $\mathcal{G}_i(a)$ ($i = 0, 1, 2$) in the numerical scheme (16)–(19), the following result will be applied in the subsequent analysis.

Lemma 2.6 (See [31,35]). *For $a > 0$,*
(i) $\mathcal{G}_i(a)$ is decreasing, for $i = 0, 1, 2$.
(ii) $\mathcal{G}_0(a) \le 1$, $\mathcal{G}_1(a) \le \frac{1}{2}$, $\mathcal{G}_2(a) \le \frac{1}{3}$, $\frac{\mathcal{G}_1(a)}{\mathcal{G}_0(a)} \le 1$, $\frac{\mathcal{G}_2(a)}{\mathcal{G}_0(a)} \le 1$, $\forall a > 0$.

Moreover, the following linear operators are also introduced to facilitate the analysis:

$$G_h = \mathcal{G}_0(K_N\tau), \quad G_0 = (\mathcal{G}_0(K_N\tau))^{-1}, \qquad G_h^{(1)} = \mathcal{G}_1(K_N\tau), \quad G_h^{(2)} = \mathcal{G}_2(K_N\tau),$$
$$G_h^{(3)} = (\mathcal{G}_0(K_N\tau))^{-1}\mathcal{G}_1(K_N\tau), \qquad G_h^{(4)} = (\mathcal{G}_0(K_N\tau))^{-1}\mathcal{G}_2(K_N\tau).$$

In more details, for any grid function f with the following discrete Fourier expansion:

$$f_{i,j} = \sum_{\boldsymbol{k}\in\mathcal{K}} \widehat{f}_{\boldsymbol{k}} e^{i[(\mathbf{B}\boldsymbol{k})^T (x_i,y_j)^T]}, \tag{33}$$

an application of the operators G_h, G_0, $G_h^{(1)}$ and $G_h^{(2)}$ gives

$$(G_h f)_{i,j} = \sum_{\boldsymbol{k}\in\mathcal{K}} \frac{1-e^{-\tau\Lambda_{\boldsymbol{k}}}}{\tau\Lambda_{\boldsymbol{k}}} \widehat{f}_{\boldsymbol{k}} e^{i[(\mathbf{B}\boldsymbol{k})^T (x_i,y_j)^T]}, \tag{34}$$

$$(G_0 f)_{i,j} = \sum_{\boldsymbol{k}\in\mathcal{K}} \frac{\tau\Lambda_{\boldsymbol{k}}}{1-e^{-\tau\Lambda_{\boldsymbol{k}}}} \widehat{f}_{\boldsymbol{k}} e^{i[(\mathbf{B}\boldsymbol{k})^T (x_i,y_j)^T]}, \tag{35}$$

$$(G_h^{(1)} f)_{i,j} = \sum_{\boldsymbol{k}\in\mathcal{K}} \frac{1-\frac{1-e^{-\tau\Lambda_{\boldsymbol{k}}}}{\tau\Lambda_{\boldsymbol{k}}}}{\tau\Lambda_{\boldsymbol{k}}} \widehat{f}_{\boldsymbol{k}} e^{i[(\mathbf{B}\boldsymbol{k})^T (x_i,y_j)^T]}, \tag{36}$$

$$(G_h^{(2)} f)_{i,j} = \sum_{\boldsymbol{k}\in\mathcal{K}} \frac{1-2\frac{1-\frac{1-e^{-\tau\Lambda_{\boldsymbol{k}}}}{\tau\Lambda_{\boldsymbol{k}}}}{\tau\Lambda_{\boldsymbol{k}}}}{\tau\Lambda_{\boldsymbol{k}}} \widehat{f}_{\boldsymbol{k}} e^{i[(\mathbf{B}\boldsymbol{k})^T (x_i,y_j)^T]}, \tag{37}$$

with $\Lambda_{\boldsymbol{k}} = (1 + A\tau^3)^{-1}\left(\xi^2(-1+\lambda_{\boldsymbol{k}})^2 + \kappa\right)$, $\lambda_{\boldsymbol{k}} = |\mathbf{B}\boldsymbol{k}|^2$. The definition of operators $G_h^{(3)}$, and $G_h^{(4)}$ is similar. Meanwhile, since the eigenvalues $\frac{1-e^{-\tau\Lambda_{\boldsymbol{k}}}}{\tau\Lambda_{\boldsymbol{k}}}$ and $\frac{\tau\Lambda_{\boldsymbol{k}}}{1-e^{-\tau\Lambda_{\boldsymbol{k}}}}$ are non-negative, we denote $G_h^{(0)} = (G_h)^{\frac{1}{2}}$ and $G_0^{(0)} = (G_0)^{\frac{1}{2}}$, as

$$(G_h^{(0)} f)_{i,j} = (G_h)^{\frac{1}{2}} f_{i,j} = \sum_{\boldsymbol{k}\in\mathcal{K}} \left(\frac{1-e^{-\tau\Lambda_{\boldsymbol{k}}}}{\tau\Lambda_{\boldsymbol{k}}}\right)^{\frac{1}{2}} \widehat{f}_{\boldsymbol{k}} e^{i[(\mathbf{B}\boldsymbol{k})^T (x_i,y_j)^T]}, \tag{38}$$

$$(G_0^{(0)} f)_{i,j} = (G_0)^{\frac{1}{2}} f_{i,j} = \sum_{\boldsymbol{k}\in\mathcal{K}} \left(\frac{\tau\Lambda_{\boldsymbol{k}}}{1-e^{-\tau\Lambda_{\boldsymbol{k}}}}\right)^{\frac{1}{2}} \widehat{f}_{\boldsymbol{k}} e^{i[(\mathbf{B}\boldsymbol{k})^T (x_i,y_j)^T]}. \tag{39}$$

Obviously, the operator $G_h^{(0)}$ is commutative with any differential operator in the Fourier pseudo-spectral space, and the following summation by parts formula is valid:

$$\left(G_h f, g\right)_{\mathcal{N}} = \left(G_h^{(0)} f, G_h^{(0)} g\right)_{\mathcal{N}}, \quad \left(G_0 f, g\right)_{\mathcal{N}} = \left(G_0^{(0)} f, G_0^{(0)} g\right)_{\mathcal{N}}. \tag{40}$$

The following operator is introduced to facilitate the analysis for the diffusion part:

$$(G_h^{(5)} f)_{i,j} = \sum_{\boldsymbol{k}\in\mathcal{K}} \left(\frac{1-e^{-\tau\Lambda_{\boldsymbol{k}}}}{\tau}\right)^{\frac{1}{2}} \lambda_{\boldsymbol{k}} \widehat{f}_{\boldsymbol{k}} e^{i[(\mathbf{B}\boldsymbol{k})^T (x_i,y_j)^T]}. \tag{41}$$

The following identity could be verified in a straightforward way:

$$\left(G_h K_N f, \Delta_{\mathcal{N}}^2 f\right)_{\mathcal{N}} = \|G_h^{(5)} f\|_{\mathcal{N}}^2. \tag{42}$$

Similarly, we define $G_h^{(6)} = (G_h^{(1)})^{\frac{1}{2}}$, $G_h^{(7)} = (G_h^{(2)})^{\frac{1}{2}}$, $G_h^{(8)} = (G_h^{(3)})^{\frac{1}{2}}$ and $G_h^{(9)} = (G_h^{(4)})^{\frac{1}{2}}$. The following summation by parts formula could be derived in the same manner:

$$\left(G_h^{(1)} f, g\right)_{\mathcal{N}} = \left(G_h^{(6)} G_h^{(8)} f, G_h^{(0)} g\right)_{\mathcal{N}}, \tag{43}$$

$$\left(G_h^{(2)} f, g\right)_{\mathcal{N}} = \left(G_h^{(7)} G_h^{(9)} f, G_h^{(0)} g\right)_{\mathcal{N}}. \tag{44}$$

The following preliminary estimates are needed in the subsequent analysis, and the detailed proof will be provided in Appendices A and B, respectively; a similar analysis has also been reported in a related work [35].

Proposition 2.1. *Assume $\kappa \geq \xi^2$. For any function $f \in \mathcal{M}_0^{\mathcal{N}}$, we have*

$$\|G_h^{(5)} f\|_{\mathcal{N}}^2 \geq \frac{2\xi^2}{3(1+A\tau^3)}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} f\|_{\mathcal{N}}^2 + \frac{\kappa - \frac{7\xi^2}{9}}{1+A\tau^3}\|G_h^{(0)}\Delta_{\mathcal{N}} f\|_{\mathcal{N}}^2, \tag{45}$$

$$\tau(K_N f, f)_{\mathcal{N}} \geq \frac{\kappa}{1+A\tau^3}\|f\|_{\mathcal{N}}^2, \quad \|f\|_{\mathcal{N}}^2 \leq \|G_0^{(0)} f\|_{\mathcal{N}}^2 \leq \|f\|_{\mathcal{N}}^2 + \tau(K_N f, f)_{\mathcal{N}}, \tag{46}$$

$$\|G_h^{(0)} f\|_{\mathcal{N}} \leq \|f\|_{\mathcal{N}}, \qquad \|G_h^{(6)} f\|_{\mathcal{N}} \leq \frac{1}{\sqrt{2}}\|f\|_{\mathcal{N}}, \qquad \|G_h^{(8)} f\|_{\mathcal{N}} \leq \|f\|_{\mathcal{N}}, \tag{47}$$

$$\|G_h^{(7)} f\|_{\mathcal{N}} \leq \frac{1}{\sqrt{3}}\|f\|_{\mathcal{N}}, \quad \|G_h^{(9)} f\|_{\mathcal{N}} \leq \|f\|_{\mathcal{N}}, \quad \|G_h^{(6)} f\|_{\mathcal{N}} \leq \|G_h^{(0)} f\|_{\mathcal{N}}, \tag{48}$$

$$\|G_h^{(7)} f\|_{\mathcal{N}}^2 \leq \|G_h^{(0)} f\|_{\mathcal{N}}^2, \quad \|G_h^{(3)} f\|_{\mathcal{N}} \leq \hat{C}_3\|f\|_{\mathcal{N}}, \quad \|G_h^{(4)} f\|_{\mathcal{N}} \leq \hat{C}_3\|f\|_{\mathcal{N}}, \tag{49}$$

where $\hat{C}_3 = \frac{1}{1-e^{-2}}$.

Proposition 2.2. *For any functions $f, g \in \mathcal{M}_0^{\mathcal{N}}$, we have*

$$\tau\left(G_h K_N f, \Delta_{\mathcal{N}}^2 \mathrm{e}^{-\tau K_N} f\right)_{\mathcal{N}} + \|\Delta_{\mathcal{N}}(g - \mathrm{e}^{-\tau K_N} f)\|_{\mathcal{N}}^2 \geq \tau\|G_h^{(5)} g\|_{\mathcal{N}}^2, \tag{50}$$

$$\tau\left(K_N f, \mathrm{e}^{-\tau K_N} f\right)_{\mathcal{N}} + \|G_0^{(0)}(g - \mathrm{e}^{-\tau K_N} f)\|_{\mathcal{N}}^2 \geq \tau\left(K_N g, g\right)_{\mathcal{N}}. \tag{51}$$

2.4. Mass conservation property of the ETD-MS3

Lemma 2.7. *For the numerical scheme (12)–(15), the mass-conservation property is always valid:*

$$0 = \overline{\phi_0} = \overline{\phi_h^{\,n}} = \overline{\phi_h^{\,n+1}}, \qquad n = 0, 1, 2, \ldots. \tag{52}$$

Proof. It is clear that $\overline{\phi_0} = 0$. The lemma is proved by mathematical induction.

Denote $\widetilde{V}_1(t) = \left(a_h^1(t), 1\right)_{\mathcal{N}}$, $t \in [0, t_1]$. Taking a discrete ℓ^2 inner product with (13) by 1 yields

$$(1 + A\tau^3)\left(\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{V}_1(t) + Q\widetilde{V}_1(t)\right) = (\xi^2 + \kappa)(\phi_0, 1)_{\mathcal{N}}, \tag{53}$$

with $Q = \frac{\xi^2+\kappa}{1+A\tau^3}$. Applying e^{Qt} on both sides of (53) and integrating from 0 to t_1, we obtain

$$\widetilde{V}_1(t_1) - \mathrm{e}^{-Q\tau}\widetilde{V}_1(0) = (I - \mathrm{e}^{Q\tau})(\phi_0, 1)_{\mathcal{N}}. \tag{54}$$

In turn, the identity $\left(a_h^1, 1\right)_{\mathcal{N}} = (\phi_0, 1)_{\mathcal{N}}$ has been derived. For the numerical scheme (14)–(15), it could be analyzed in a similar way as in (53)–(54). Denote $V_1(s_1) = \left(\phi_h^1(s_1), 1\right)_{\mathcal{N}}$, $s_1 \in [0, t_1]$ and $V_2(s_2) = \left(\phi_h^2(s_2), 1\right)_{\mathcal{N}}$, $s_2 \in [t_1, t_2]$, we have

$$V_1(t_1) - \mathrm{e}^{-Q\tau}V_1(0) = (I - \mathrm{e}^{Q\tau})(a_h^1, 1)_{\mathcal{N}}, \tag{55}$$

$$V_2(t_2) - \mathrm{e}^{-Q\tau}V_2(t_1) = (I - \mathrm{e}^{Q\tau})(\phi_h^1, 1)_{\mathcal{N}} + Q\tau\mathcal{G}_0(Q\tau)(\phi_h^1 - \phi_0, 1)_{\mathcal{N}}. \tag{56}$$

The above estimate indicates that $\overline{\phi_0} = \overline{\phi_h^1} = \overline{\phi_h^2}$. Then we are able to assume that $\overline{\phi_h^k} = \overline{\phi_h^{k-1}} = \overline{\phi_h^{k-2}}$, $k = 3, 4, \ldots, n$, and denote $V_{n+1}(s) = \left(\phi_h^{n+1}(s), 1\right)_{\mathcal{N}}$, $s \in [t_n, t_{n+1}]$. Based on the above assumption, taking an inner product with (12) by 1 leads to

$$(1 + A\tau^3)\frac{\mathrm{d}}{\mathrm{d}s}V_{n+1}(s) + QV_{n+1}(s) = (\xi^2 + \kappa)(\phi_h^n, 1)_{\mathcal{N}}. \tag{57}$$

Multiplying both sides of (57) by e^{Qt} and integrating from t_n to t_{n+1}, we get

$$V_{n+1}(t_{n+1}) - \mathrm{e}^{-Q\tau}V_{n+1}(t_n) = (I - \mathrm{e}^{Q\tau})(\phi_h^n, 1)_{\mathcal{N}}, \tag{58}$$

which in turn gives $\left(\phi_h^{n+1}, 1\right)_{\mathcal{N}} = (\phi_h^n, 1)_{\mathcal{N}}$. □

Remark 2.2. In this article, only the 2-D analysis is presented. An extension to the 3-D case is straightforward, and the technical details are skipped for brevity of presentation.

3. Global-in-time energy stability analysis and the uniform-in-time bound for the numerical solution

In this section, we perform a direct analysis for the numerical scheme, and derive a uniform-in-time H^2 estimate. Due to the Sobolev embedding from H^2 to L^∞, we are able to recover a uniform-in-time $\|\cdot\|_\infty$ bound of the numerical solution and a constraint on stability coefficient A. This in turn gives a global-in-time energy stability estimate for the ETD-MS3 scheme (16)–(19).

Note that

$$E_{\mathcal{N}}(v) = (F(v), 1)_{\mathcal{N}} + \frac{\xi^2}{2}\left[\|\Delta_{\mathcal{N}} v\|_{\mathcal{N}}^2 - 2\|\nabla_{\mathcal{N}} v\|_{\mathcal{N}}^2 + \|v\|_{\mathcal{N}}^2\right]. \tag{59}$$

We denote $E_{\mathcal{N}}(\phi_0) := C_0$. The following H_h^2 norm bound for the numerical solution could be derived.

Lemma 3.1. *Assume that $\alpha \geq -\xi^2$. An H_h^2 bound for the solution of numerical scheme (16)–(19) is valid:*

$$\|\Delta_{\mathcal{N}}\phi_h^k\|_{\mathcal{N}} \leq \frac{2}{|\xi|}\left(E_{\mathcal{N}}(\phi_h^k) + \left(9\gamma^4 + 3\xi^4\right)|\Omega_{\mathcal{N}}|\right)^{\frac{1}{2}}, \qquad k = 0, 1, 2, \ldots. \tag{60}$$

Proof. An application of Hölder's and Young's inequalities reveals that

$$\frac{\gamma}{3!}\left((\phi_h^k)^3, 1\right)_{\mathcal{N}} \leq \frac{1}{24\sqrt[3]{18}}\|\phi_h^k\|_{L_h^4}^4 + 9\gamma^4|\Omega_{\mathcal{N}}| \leq \frac{1}{48}\|\phi_h^k\|_{L_h^4}^4 + 9\gamma^4|\Omega_{\mathcal{N}}|, \tag{61}$$

$$\|\nabla_{\mathcal{N}}\phi_h^k\|_{\mathcal{N}}^2 \leq \frac{1}{4}\|\Delta_{\mathcal{N}}\phi_h^k\|_{\mathcal{N}}^2 + \|\phi_h^k\|_{\mathcal{N}}^2, \tag{62}$$

$$\frac{1}{4!}\|\phi_h^k\|_{L_h^4}^4 \geq \xi^2\|\phi_h^k\|_{\mathcal{N}}^2 - 6\xi^4|\Omega_{\mathcal{N}}|. \tag{63}$$

A combination of (59) and (61)–(63) leads to

$$E_{\mathcal{N}}(\phi_h^k) \geq \frac{\alpha}{2}\|\phi_h^k\|_{\mathcal{N}}^2 + \frac{\xi^2}{4}\|\Delta_{\mathcal{N}}\phi_h^k\|_{\mathcal{N}}^2 - \left(9\gamma^4 + 3\xi^4\right)|\Omega_{\mathcal{N}}|. \tag{64}$$

Therefore, it is obvious that

$$\|\Delta_{\mathcal{N}}\phi_h^k\|_{\mathcal{N}}^2 \leq \frac{4}{\xi^2}\left(E_{\mathcal{N}}(\phi_h^k) + \left(9\gamma^4 + 3\xi^4\right)|\Omega_{\mathcal{N}}|\right). \quad \square \tag{65}$$

Recall that $\overline{\phi_h^{n+1}} = \overline{\phi_h^n} = \overline{a_h^1} = \overline{\phi_0} = 0$, $n = 1, 2, \ldots$. Based on Lemmas 2.5 and 3.1, the following bounds for the numerical solution could be derived:

$$\|\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}} \leq \frac{2}{|\xi|}\left(C_0 + \left(9\gamma^4 + 3\xi^4\right)|\Omega_{\mathcal{N}}|\right)^{\frac{1}{2}} := \widetilde{C}_1. \tag{66}$$

$$\|\phi_0\|_\infty \leq \|\widetilde{\phi_0}\|_{L^\infty} \leq \hat{C}_1\left(|\overline{\phi_0}| + \|\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}\right) \leq \hat{C}_1\widetilde{C}_1 := \widetilde{C}_2, \tag{67}$$

$$\|\nabla_{\mathcal{N}}((\phi_0)^3)\|_{\mathcal{N}} \leq 9\|\widetilde{\phi_0}\|_{L^\infty}^2 \cdot \hat{C}_2\|\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}} \leq 9\widetilde{C}_2^2\hat{C}_2\widetilde{C}_1 := \widetilde{C}_3, \tag{68}$$

$$\|\nabla_{\mathcal{N}}((\phi_0)^2)\|_{\mathcal{N}} \leq 4\|\widetilde{\phi_0}\|_{L^\infty} \cdot \hat{C}_2\|\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}} \leq 2\widetilde{C}_2\hat{C}_2\widetilde{C}_1 := \widetilde{C}_4, \tag{69}$$

where $\widetilde{C}_1$, $\widetilde{C}_2$, $\widetilde{C}_3$ and $\widetilde{C}_4$ are global-in-time constants.

Mathematical induction is employed to recover the $\|\cdot\|_\infty$ bound of the numerical solution and establish the global-in-time energy stability for the ETD-MS3 scheme (16)–(19).

3.1. The estimate for the first two time steps

In this subsection, we aim to obtain a rough H_h^2 estimate for a_h^1, ϕ_h^1 and ϕ_h^2, and recover their uniform-in-time $\|\cdot\|_\infty$ bound. Meanwhile, an energy stability analysis has to be established for the numerical solution at the first two time steps.

3.1.1. The estimate for a^1 at the first time step

First, we aim to obtain a rough estimate for a_h^1. Notice that $\phi_h^0 = a_h^0 = \phi_0$.

Lemma 3.2. *Assume that $|\alpha| \leq \xi^2$, $\kappa \geq \xi^2$. Under the following $O(1)$ constraint for the time step size*

$$\tau \leq \min\left\{\frac{3}{2}\widetilde{C}_3^{-2}, \frac{1}{6\gamma^2}\widetilde{C}_4^{-2}, \frac{1}{32}\hat{C}_2^{-2}\right\}, \tag{70}$$

the bounds are available at time step t_1:

$$\|\Delta_{\mathcal{N}}a_h^1\|_{\mathcal{N}} \leq \widetilde{C}_5, \quad \|a_h^1\|_\infty \leq \widetilde{C}_6, \tag{71}$$

where $\widetilde{C}_5 = \left(\widetilde{C}_1^2 + \frac{1}{\xi^2} + \widetilde{C}_1^2\xi^2\right)^{\frac{1}{2}}$, $\widetilde{C}_6 = \hat{C}_1\widetilde{C}_5$, and $\widetilde{C}_i$ $(i = 1, \ldots, 4)$, are defined in (66)–(69).

These constants are global-in-time and depend only on ξ, γ, the Sobolev inequality constants, the initial data, and the domain size.

Proof. We denote $a_h^{1,*} = e^{-K_N\tau}\phi_0$. The numerical scheme (17) is rewritten as the following two-substage system, so that the theoretical analysis could be carried out in a more convenient way:

$$\frac{a_h^{1,*} - \phi_0}{\tau} = -K_N\mathcal{G}_0(K_N\tau)\phi_0, \tag{72}$$

$$\frac{a_h^1 - a_h^{1,*}}{\tau} = -\mathcal{G}_0(K_N\tau)F_N(\phi_0). \tag{73}$$

Taking a discrete ℓ^2 inner product with (72) by $\Delta_{\mathcal{N}}^2(a_h^{1,*} + \phi_0)$ gives

$$\left(a_h^{1,*} - \phi_0, \Delta_{\mathcal{N}}^2(a_h^{1,*} + \phi_0)\right)_{\mathcal{N}} + \tau\left(K_N G_h\phi_0, \Delta_{\mathcal{N}}^2(a_h^{1,*} + \phi_0)\right)_{\mathcal{N}} = 0. \tag{74}$$

An application of summation by parts, combined with (42), results in

$$\|\Delta_{\mathcal{N}} a_h^{1,*}\|_{\mathcal{N}}^2 - \|\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2 + \tau\left(K_N G_h\phi_0, \Delta_{\mathcal{N}}^2 a_h^{1,*}\right)_{\mathcal{N}} + \tau\|G_h^{(5)}\phi_0\|_{\mathcal{N}}^2 = 0. \tag{75}$$

Taking a discrete ℓ^2 inner product with (73) by $2\Delta_{\mathcal{N}}^2 a_h^1$ leads to

$$\left(a_h^1 - a_h^{1,*}, 2\Delta_{\mathcal{N}}^2 a_h^1\right)_{\mathcal{N}} = -2\tau\left(G_h F_N(\phi_0), \Delta_{\mathcal{N}}^2 a_h^1\right)_{\mathcal{N}}. \tag{76}$$

Again, an application of summation by parts implies that

$$\left(a_h^1 - a_h^{1,*}, 2\Delta_{\mathcal{N}}^2 a_h^1\right)_{\mathcal{N}} = \|\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}}^2 - \|\Delta_{\mathcal{N}} a_h^{1,*}\|_{\mathcal{N}}^2 + \|\Delta_{\mathcal{N}}(a_h^1 - a_h^{1,*})\|_{\mathcal{N}}^2. \tag{77}$$

Meanwhile, an application of inequality (50) in Proposition 2.2 reveals that

$$\tau\left(K_N G_h\phi_0, \Delta_{\mathcal{N}}^2 a_h^{1,*}\right)_{\mathcal{N}} + \|\Delta_{\mathcal{N}}(a_h^1 - a_h^{1,*})\|_{\mathcal{N}}^2 \geq \tau\|G_h^{(5)} a_h^1\|_{\mathcal{N}}^2. \tag{78}$$

For any $v, w \in \mathcal{M}_0^{\mathcal{N}}$, it is clear that

$$\left(G_h\beta_N(v), \Delta_{\mathcal{N}}^2 w\right)_{\mathcal{N}} = 0. \tag{79}$$

Subsequently, a combination of (75)–(79) leads to

$$\begin{aligned}
&\|\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}}^2 - \|\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2 + \tau\|G_h^{(5)} a_h^1\|_{\mathcal{N}}^2 + \tau\|G_h^{(5)}\phi_0\|_{\mathcal{N}}^2 \\
\leq& -2\tau\left(G_h F_N(\phi_0), \Delta_{\mathcal{N}}^2 a_h^1\right)_{\mathcal{N}} \\
=& \frac{\tau}{1+A\tau^3}[-\frac{1}{3}\left(G_h(\phi_0)^3, \Delta_{\mathcal{N}}^2 a_h^1\right)_{\mathcal{N}} + \gamma\left(G_h(\phi_0)^2, \Delta_{\mathcal{N}}^2 a_h^1\right)_{\mathcal{N}} \\
&- 2(\alpha-\kappa)\left(G_h\phi_0, \Delta_{\mathcal{N}}^2 a_h^1\right)_{\mathcal{N}}].
\end{aligned} \tag{80}$$

Regarding the first two terms on the right hand side of (80), we obtain

$$\begin{aligned}
-\frac{1}{3}\left(G_h(\phi_0)^3, \Delta_{\mathcal{N}}^2 a_h^1\right)_{\mathcal{N}} =& \frac{1}{3}\left(G_h^{(0)}\nabla_{\mathcal{N}}((\phi_0)^3), G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} a_h^1\right)_{\mathcal{N}} \\
\leq& \frac{1}{3}\|G_h^{(0)}\nabla_{\mathcal{N}}((\phi_0)^3)\|_{\mathcal{N}}\cdot\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}} \\
\leq& \frac{1}{3}\|\nabla_{\mathcal{N}}((\phi_0)^3)\|_{\mathcal{N}}\cdot\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}} \\
\leq& \frac{\widetilde{C}_3}{3}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}} \leq \frac{2}{3\xi^2}\widetilde{C}_3^2 + \frac{\xi^2}{24}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}}^2,
\end{aligned} \tag{81}$$

$$\begin{aligned}
\gamma\left(G_h(\phi_0)^2, \Delta_{\mathcal{N}}^2 a_h^1\right)_{\mathcal{N}} \leq& \gamma\|G_h^{(0)}\nabla_{\mathcal{N}}((\phi_0)^2)\|_{\mathcal{N}}\cdot\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}} \\
\leq& \gamma\|\nabla_{\mathcal{N}}((\phi_0)^2)\|_{\mathcal{N}}\cdot\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}} \\
\leq& \widetilde{C}_4\gamma\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}} \leq \frac{6\gamma^2}{\xi^2}\widetilde{C}_4^2 + \frac{\xi^2}{24}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}}^2,
\end{aligned} \tag{82}$$

in which Lemma 2.1, as well as the inequality (40), the first inequality in (47) and the estimates (68)–(69) have been applied in the derivation. The last term of (80) is split into two parts, and they could be analyzed as follows, with the help of inequality (28) in Lemma 2.5:

$$\begin{aligned}
2(\xi^2-\alpha)\left(G_h\phi_0, \Delta_{\mathcal{N}}^2 a_h^1\right)_{\mathcal{N}} \leq& 2(\xi^2-\alpha)\|\nabla_{\mathcal{N}}\phi_0\|_{\mathcal{N}}\cdot\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}} \\
\leq& 2(\xi^2-\alpha)\widehat{C}_2\|\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}\cdot\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}} \\
\leq& 4\xi^2\widehat{C}_2\widetilde{C}_1\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}} \\
\leq& 32\xi^2\widehat{C}_2^2\widetilde{C}_1^2 + \frac{\xi^2}{8}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}}^2,
\end{aligned} \tag{83}$$

$$\begin{aligned}
2(\kappa-\xi^2)\left(G_h\phi_0, \Delta_{\mathcal{N}}^2 a_h^1\right)_{\mathcal{N}} =& 2(\kappa-\xi^2)\left(G_h^{(0)}\Delta_{\mathcal{N}}\phi_0, G_h^{(0)}\Delta_{\mathcal{N}} a_h^1\right)_{\mathcal{N}} \\
=& (\kappa-\xi^2)\Big(\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2 + \|G_h^{(0)}\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}}^2 \\
&- \|G_h^{(0)}\Delta_{\mathcal{N}}(a_h^1-\phi_0)\|_{\mathcal{N}}^2\Big).
\end{aligned} \tag{84}$$

A substitution of (81)–(84) into (80) implies that

$$\begin{aligned}
&\|\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}}^2 - \|\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2 + \tau\|G_h^{(5)} a_h^1\|_{\mathcal{N}}^2 + \tau\|G_h^{(5)}\phi_0\|_{\mathcal{N}}^2 \\
\leq& \frac{\tau}{1+A\tau^3}\Bigg[\frac{2}{3\xi^2}\widetilde{C}_3^2 + \frac{6\gamma^2}{\xi^2}\widetilde{C}_4^2 + 32\xi^2\widehat{C}_2^2\widetilde{C}_1^2 + \frac{5\xi^2}{24}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}}^2 \\
&+(\kappa-\xi^2)\left(\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2 + \|G_h^{(0)}\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}}^2 - \|G_h^{(0)}\Delta_{\mathcal{N}}(a_h^1-\phi_0)\|_{\mathcal{N}}^2\right)\Bigg].
\end{aligned} \tag{85}$$

In addition, by inequality (45) in Proposition 2.1, we obtain

$$\begin{aligned}&\tau\|G_h^{(5)}a_h^1\|_{\mathcal{N}}^2+\tau\|G_h^{(5)}\phi_0\|_{\mathcal{N}}^2\\ \geq&\frac{\tau}{1+A\tau^3}\left[\frac{2}{3}\xi^2\left(\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}a_h^1\|_{\mathcal{N}}^2+\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2\right)\right.\\ &\left.+(\kappa-\frac{7\xi^2}{9})\left(\|G_h^{(0)}\Delta_{\mathcal{N}}a_h^1\|_{\mathcal{N}}^2+\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2\right)\right].\end{aligned} \tag{86}$$

A combination of (85) and (86) yields

$$\begin{aligned}&\|\Delta_{\mathcal{N}}a_h^1\|_{\mathcal{N}}^2-\|\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2+\left[\frac{2\xi^2}{3}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2+(\kappa-\xi^2)\|G_h^{(0)}\Delta_{\mathcal{N}}(a_h^1-\phi_0)\|_{\mathcal{N}}^2\right.\\ &\left.+\frac{11\xi^2}{24}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}a_h^1\|_{\mathcal{N}}^2+\frac{2\xi^2}{9}\left(\|G_h^{(0)}\Delta_{\mathcal{N}}a_h^1\|_{\mathcal{N}}^2+\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2\right)\right]\frac{\tau}{1+A\tau^3}\\ \leq&\tau\left(\frac{2}{3\xi^2}\widetilde{C}_3^2+\frac{6\gamma^2}{\xi^2}\widetilde{C}_4^2+32\xi^2\widehat{C}_2^2\widetilde{C}_1^2\right).\end{aligned} \tag{87}$$

As a consequence, the following bound becomes available for $\|\Delta_{\mathcal{N}}a_h^1\|_{\mathcal{N}}^2$:

$$\|\Delta_{\mathcal{N}}a_h^1\|_{\mathcal{N}}^2\leq\widetilde{C}_1^2+\left(\frac{2}{3}\widetilde{C}_3^2+6\gamma^2\widetilde{C}_4^2\right)\frac{\tau}{\xi^2}+32\xi^2\widehat{C}_2^2\widetilde{C}_1^2\tau. \tag{88}$$

Under the following $O(1)$ constraint for the time step size

$$\tau\leq\min\left\{\frac{3}{2}\widetilde{C}_3^{-2},\frac{1}{6\gamma^2}\widetilde{C}_4^{-2},\frac{1}{32}\widehat{C}_2^{-2}\right\}, \tag{89}$$

a rough estimate could be derived for $\|\Delta_{\mathcal{N}}a_h^1\|_{\mathcal{N}}$:

$$\|\Delta_{\mathcal{N}}a_h^1\|_{\mathcal{N}}\leq\widetilde{C}_5:=\left(\widetilde{C}_1^2+\frac{1}{\xi^2}+\widetilde{C}_1^2\xi^2\right)^{\frac{1}{2}}. \tag{90}$$

In turn, an application of estimate (25) in Lemma 2.5 implies that

$$\|a_h^1\|_\infty\leq\widehat{C}_1(|\overline{a_h^1}|+\|\Delta_{\mathcal{N}}a_h^1\|_{\mathcal{N}})\leq\widehat{C}_1\widetilde{C}_5:=\widetilde{C}_6.\quad\square \tag{91}$$

Therefore, the energy estimate becomes available for the numerical solution (13).

Lemma 3.3. *Assume that* $A\geq\frac{1}{2\lambda_1^3}$, *where* $\lambda_1=\frac{3}{2C_L^{(0)}}$, *and* $C_L^{(0)}=\alpha+\gamma\widetilde{C}_6+\frac{1}{2}\widetilde{C}_6^2+\kappa$. *The time step size is taken to satisfy an* $O(1)$ *constraint (70). The numerical scheme (13) satisfies the energy-dissipation property*

$$E_{\mathcal{N}}(a_h^1)\leq E_{\mathcal{N}}(\phi_0)=C_0. \tag{92}$$

Proof. Taking a discrete ℓ^2 inner product with (13) by $\frac{\mathrm{d}a_h^1(t)}{\mathrm{d}t}$, and integrating form 0 to t_1, we obtain

$$\begin{aligned}&(1+A\tau^3)\left\|\frac{\mathrm{d}a_h^1(t)}{\mathrm{d}t}\right\|_{L^2(t_1,t_2;\ell^2)}^2+E_{\mathcal{N}}(a_h^1)-E_{\mathcal{N}}(\phi_h^0)\\ =&\int_0^{t_1}\left(g(a_h^1(t))-g(\phi_0),\frac{\mathrm{d}a_h^1(t)}{\mathrm{d}t}\right)_{\mathcal{N}}\mathrm{d}t-\int_0^{t_1}\left(\beta_N(\phi_0),\frac{\mathrm{d}a_h^1(t)}{\mathrm{d}t}\right)_{\mathcal{N}}\mathrm{d}t.\end{aligned} \tag{93}$$

By Lemma 2.7, the following identity is valid:

$$\int_0^{t_1}\left(1,\frac{\mathrm{d}a_h^1(t)}{\mathrm{d}t}\right)_{\mathcal{N}}\mathrm{d}t=(1,a_h^1(t)-\phi_0)_{\mathcal{N}}=0. \tag{94}$$

Apply Hölder's inequality, Young's inequality, and Lemma 2.4, we derive the following estimate:

$$\begin{aligned}&\int_0^{t_1}\left(g(a_h^1(t))-g(\phi_0),\frac{\mathrm{d}a_h^1(t)}{\mathrm{d}t}\right)_{\mathcal{N}}\mathrm{d}t\\ \leq&\int_0^{t_1}\|g(a_h^1(t))-g(\phi_0)\|_{\mathcal{N}}\left\|\frac{\mathrm{d}a_h^1(t)}{\mathrm{d}t}\right\|_{\mathcal{N}}\mathrm{d}t\\ \leq&C_L^{(0)}\tau\left\|\frac{\mathrm{d}a_h^1(t)}{\mathrm{d}t}\right\|_{L^2(0,t_1;\ell^2)}^2\leq\frac{2\lambda_1C_L^{(0)}}{3}\left\|\frac{\mathrm{d}a_h^1(t)}{\mathrm{d}t}\right\|_{L^2(0,t_1;\ell^2)}^2+\frac{C_L^{(0)}}{3\lambda_1^2}\tau^3\left\|\frac{\mathrm{d}a_h^1(t)}{\mathrm{d}t}\right\|_{L^2(0,t_1;\ell^2)}^2,\end{aligned} \tag{95}$$

Since $A \geq \frac{1}{2\lambda_1^3}$ and $\lambda_1 = \frac{3}{2C_L^{(0)}}$, a combination (93)–(95) gives

$$E_{\mathcal{N}}(a_h^1) \leq E_{\mathcal{N}}(a_h^1) + \left(1 - \frac{2\lambda_1 C_L^{(0)}}{3}\right) \left\| \frac{\mathrm{d}a_h^1(t)}{\mathrm{d}t} \right\|^2_{L^2(t_1,t_2;\ell^2)} + \left(A - \frac{C_L^{(0)}}{3\lambda_1^2}\right)\tau^3 \left\| \frac{\mathrm{d}a_h^1(t)}{\mathrm{d}t} \right\|^2_{L^2(t_1,t_2;\ell^2)} \leq E_{\mathcal{N}}(\phi_0). \quad \square \tag{96}$$

In addition, with the energy stability (92) theoretically justified, a similar analysis could be derived as in (66)–(69), and we are able to obtain a much sharper bound for a_h^1:

$$\|\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}} \leq \widetilde{C}_1, \tag{97}$$

$$\|a_h^1\|_\infty \leq \|\widetilde{a_h^1}\|_{L^\infty} \leq \hat{C}_1(|\overline{a_h^1}| + \|\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}}) \leq \hat{C}_1\widetilde{C}_1 = \widetilde{C}_2, \tag{98}$$

$$\|\nabla_{\mathcal{N}}((a_h^1)^3)\|_{\mathcal{N}} \leq 9\|\widetilde{a_h^1}\|^2_{L^\infty} \cdot \hat{C}_2\|\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}} \leq 9\widetilde{C}_2^2\hat{C}_2\widetilde{C}_1 = \widetilde{C}_3, \tag{99}$$

$$\|\nabla_{\mathcal{N}}((a_h^1)^2)\|_{\mathcal{N}} \leq 4\|\widetilde{a_h^1}\|_{L^\infty} \cdot \hat{C}_2\|\Delta_{\mathcal{N}} a_h^1\|_{\mathcal{N}} \leq 4\widetilde{C}_2\hat{C}_2\widetilde{C}_1 = \widetilde{C}_4. \tag{100}$$

3.1.2. The estimate for ϕ^1 at the first time step

We aim to obtain the estimates for ϕ_h^1, and establish energy estimate at the first time step.

Lemma 3.4. *Assume that $|\alpha| \leq \xi^2$, $\kappa \geq \xi^2$. Under the following $O(1)$ constraint for the time step size*

$$\tau \leq \left\{ \frac{3}{4}\widetilde{C}_3^{-2}, \frac{1}{12\gamma^2}\widetilde{C}_4^{-2}, \frac{1}{64}\hat{C}_2^{-2}, \frac{1}{9\kappa} \right\}, \tag{101}$$

the bound at time step t_1 is valid:

$$\|\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}} \leq \widetilde{C}_7, \quad \|\phi_h^1\|_\infty \leq \widetilde{C}_8, \tag{102}$$

where $\widetilde{C}_7 = \left(2\widetilde{C}_1^2 + \frac{1}{\xi^2} + \widetilde{C}_1^2\xi^2\right)^{\frac{1}{2}}$, $\widetilde{C}_8 = \hat{C}_1\widetilde{C}_7$, and $\widetilde{C}_i$ $(i = 1, \dots, 4)$, are defined in (66)–(69).

These constants are global-in-time and depend only on ξ, γ, the Sobolev inequality constants, the initial data, and the domain size.

Proof. The proof of this rough estimate is similar to that of Lemma 3.2. The numerical scheme (18) is rewritten as the following two-substage system.

$$\frac{a_h^{1,*} - \phi_0}{\tau} = -K_N\mathcal{G}_0(K_N\tau)\phi_0, \tag{103}$$

$$\frac{\phi_h^1 - a_h^{1,*}}{\tau} = -\mathcal{G}_0(K_N\tau)F_N(\phi_0) - \mathcal{G}_1(K_N\tau)\left[F_N(a_h^1) - F_N(\phi_0)\right]. \tag{104}$$

The Eqs. (103) is the same as (72), so that equality (75) is still valid. Taking a discrete ℓ^2 inner product with (104) by $2\Delta_{\mathcal{N}}^2\phi_h^1$, and performing a similar analysis as in (77)–(80), leads to

$$\begin{aligned} &\|\Delta_{\mathcal{N}}\phi_h^1\|^2_{\mathcal{N}} - \|\Delta_{\mathcal{N}}\phi_0\|^2_{\mathcal{N}} + \tau\|G_h^{(5)}\phi_h^1\|^2_{\mathcal{N}} + \tau\|G_h^{(5)}\phi_0\|^2_{\mathcal{N}} \\ &\leq -2\tau\left(G_hF_N(\phi_0), \Delta_{\mathcal{N}}^2\phi_h^1\right)_{\mathcal{N}} - 2\tau\left(G_h^{(1)}\left[F_N(a_h^1) - F_N(\phi_0)\right], \Delta_{\mathcal{N}}^2\phi_h^1\right)_{\mathcal{N}}. \end{aligned} \tag{105}$$

The first term on the right hand side of (105) could be analyzed in the same way as in (79)–(84).

Regarding the second term on the right hand side of (105), we begin with the following decomposition, based on (79):

$$\begin{aligned} &-2\tau\left(G_h^{(1)}\left[F_N(a_h^1) - F_N(\phi_0)\right], \Delta_{\mathcal{N}}^2\phi_h^1\right)_{\mathcal{N}} \\ &= \frac{\tau}{1 + A\tau^3}[-\frac{1}{3}\left(G_h^{(1)}(a_h^1)^3, \Delta_{\mathcal{N}}^2\phi_h^1\right)_{\mathcal{N}} + \frac{1}{3}\left(G_h^{(1)}(\phi_0)^3, \Delta_{\mathcal{N}}^2\phi_h^1\right)_{\mathcal{N}} \\ &+ \gamma\left(G_h^{(1)}(a_h^1)^2, \Delta_{\mathcal{N}}^2\phi_h^1\right)_{\mathcal{N}} + \gamma\left(G_h^{(1)}(\phi_0)^2, \Delta_{\mathcal{N}}^2\phi_h^1\right)_{\mathcal{N}} - 2(\alpha - \kappa)\left(G_h(a_h^1 - \phi_0), \Delta_{\mathcal{N}}^2\phi_h^1\right)_{\mathcal{N}}]. \end{aligned} \tag{106}$$

The four nonlinear inner product terms could be analyzed in a similar way as in (81)–(82), combined with the help of Eq. (43) and the last two inequalities in (47):

$$\begin{aligned} -\frac{1}{3}\left(G_h^{(1)}(a_h^1)^3, \Delta_{\mathcal{N}}^2\phi_h^1\right)_{\mathcal{N}} &\leq \frac{1}{3}\|G_h^{(6)}G_h^{(8)}\nabla_{\mathcal{N}}((a_h^1)^3)\|_{\mathcal{N}}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}} \\ &\leq \frac{1}{3\sqrt{2}}\|G_h^{(8)}\nabla_{\mathcal{N}}((a_h^1)^3)\|_{\mathcal{N}}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}} \\ &\leq \frac{1}{3\sqrt{2}}\|\nabla_{\mathcal{N}}((a_h^1)^3)\|_{\mathcal{N}}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}} \end{aligned}$$

$$\le \frac{1}{3\sqrt{2}}\widetilde{C}_3\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}} \le \frac{1}{3\xi^2}\widetilde{C}_3^2 + \frac{\xi^2}{24}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}^2, \tag{107}$$

$$\frac{1}{3}\left(G_h^{(1)}(\phi_0)^3, \Delta_{\mathcal{N}}^2\phi_h^1\right)_{\mathcal{N}} \le \frac{1}{3\xi^2}\widetilde{C}_3^2 + \frac{\xi^2}{24}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}^2, \tag{108}$$

$$\begin{aligned}\gamma\left(G_h^{(1)}(a_h^1)^2, \Delta_{\mathcal{N}}^2\phi_h^1\right)_{\mathcal{N}} &\le \frac{\gamma}{\sqrt{2}}\|\nabla_{\mathcal{N}}((a_h^1)^2)\|_{\mathcal{N}}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}\\ &\le \frac{\gamma}{\sqrt{2}}\widetilde{C}_4\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}} \le \frac{3}{\xi^2}\gamma^2\widetilde{C}_4^2 + \frac{\xi^2}{24}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}^2,\end{aligned} \tag{109}$$

$$\gamma\left(G_h^{(1)}(\phi_0)^2, \Delta_{\mathcal{N}}^2\phi_h^1\right)_{\mathcal{N}} \le \frac{3}{\xi^2}\gamma^2\widetilde{C}_4^2 + \frac{\xi^2}{24}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}^2. \tag{110}$$

Again, the linear diffusion inner product on the right hand side of (106) is split into two parts, which are analyzed as follows:

$$\begin{aligned}&2(\xi^2-\alpha)\left(G_h^{(1)}(a_h^1-\phi_0), \Delta_{\mathcal{N}}^2\phi_h^1\right)_{\mathcal{N}}\\ \le&4\xi^2\|G_h^{(6)}G_h^{(8)}\nabla_{\mathcal{N}}(a_h^1-\phi_0)\|_{\mathcal{N}}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}\\ \le&2\sqrt{2}\xi^2\|\nabla_{\mathcal{N}}(a_h^1-\phi_0)\|_{\mathcal{N}}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}\\ \le&2\sqrt{2}\xi^2\widehat{C}_2\|\Delta_{\mathcal{N}}(a_h^1-\phi_0)\|_{\mathcal{N}}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}\\ \le&4\sqrt{2}\xi^2\widehat{C}_2\widetilde{C}_1\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}} \le 32\xi^2\widehat{C}_2^2\widetilde{C}_1^2 + \frac{\xi^2}{4}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}},\end{aligned} \tag{111}$$

$$\begin{aligned}&2(\kappa-\xi^2)\left(G_h^{(1)}(a_h^1-\phi_0), \Delta_{\mathcal{N}}^2\phi_h^1\right)_{\mathcal{N}}\\ \le&2(\kappa-\xi^2)\|G_h^{(6)}\Delta_{\mathcal{N}}(a_h^1-\phi_0)\|_{\mathcal{N}}\|G_h^{(6)}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}\\ \le&2(\kappa-\xi^2)\|G_h^{(0)}\Delta_{\mathcal{N}}(a_h^1-\phi_0)\|_{\mathcal{N}}\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}\\ \le&2(\kappa-\xi^2)\|\Delta_{\mathcal{N}}(a_h^1-\phi_0)\|_{\mathcal{N}}\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}\\ \le&4(\kappa-\xi^2)\widetilde{C}_1\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}} \le 8(\kappa-\xi^2)\widetilde{C}_1^2 + \frac{\kappa-\xi^2}{2}\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}^2,\end{aligned} \tag{112}$$

in which $|\alpha| \le \xi^2$ and the last inequality in (48) have been applied. Furthermore, to obtain a bound for the second term on the right hand side of (112), we apply the Cauchy inequality.

$$\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}^2 \le 2\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2 + 2\|G_h^{(0)}\Delta_{\mathcal{N}}(\phi_h^1-\phi_0)\|_{\mathcal{N}}^2 \le 2\widetilde{C}_1^2 + 2\|G_h^{(0)}\Delta_{\mathcal{N}}(\phi_h^1-\phi_0)\|_{\mathcal{N}}^2. \tag{113}$$

Combining (105)–(113) and repeating (81)–(84), we obtain

$$\begin{aligned}&\|\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}^2 - \|\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2 + \tau\|G_h^{(5)}\phi_h^1\|_{\mathcal{N}}^2 + \tau\|G_h^{(5)}\phi_0\|_{\mathcal{N}}^2\\ \le&\frac{\tau}{1+A\tau^3}\Big[\frac{4}{3\xi^2}\widetilde{C}_3^2 + \frac{12\gamma^2}{\xi^2}\widetilde{C}_4^2 + 64\xi^2\widehat{C}_2^2\widetilde{C}_1^2 + 9(\kappa-\xi^2)\widetilde{C}_1^2\\ &+\frac{5\xi^2}{8}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}^2 + (\kappa-\xi^2)(\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2 + \|G_h^{(0)}\Delta_{\mathcal{N}}a_h^1\|_{\mathcal{N}}^2)\Big].\end{aligned} \tag{114}$$

Based on inequality (45) in Proposition 2.1, (114) could be rewritten as

$$\begin{aligned}&\|\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}^2 - \|\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2 + \frac{\tau}{1+A\tau^3}\Big[+\frac{\xi^2}{24}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}^2\\ &+\frac{2\xi^2}{3}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2 + \frac{2\xi^2}{9}\left(\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}^2 + \|G_h^{(0)}\Delta_{\mathcal{N}}\phi_0\|_{\mathcal{N}}^2\right)\Big]\\ \le&\frac{\tau}{1+A\tau^3}\left[\frac{4}{3\xi^2}\widetilde{C}_3^2 + \frac{12\gamma^2}{\xi^2}\widetilde{C}_4^2 + 64\xi^2\widehat{C}_2^2\widetilde{C}_1^2 + 9(\kappa-\xi^2)\widetilde{C}_1^2\right].\end{aligned} \tag{115}$$

This in turn implies that

$$\|\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}^2 \le \left(\frac{4}{3}\widetilde{C}_3^2 + 12\gamma^2\widetilde{C}_4^2\right)\frac{\tau}{\xi^2} + 64\widehat{C}_2^2\widetilde{C}_1^2\xi^2\tau + 9(\kappa-\xi^2)\widetilde{C}_1^2\tau + \widetilde{C}_1^2. \tag{116}$$

Under the following $O(1)$ constraint for the time step size

$$\tau \le \left\{\frac{3}{4}\widetilde{C}_3^{-2}, \frac{1}{12\gamma^2}\widetilde{C}_4^{-2}, \frac{1}{64}\widehat{C}_2^{-2}, \frac{1}{9\kappa}\right\}, \tag{117}$$

which is a stronger requirement than (70), a rough estimate could be derived as

$$\|\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}} \le \widetilde{C}_7 := \left(2\widetilde{C}_1^2 + \frac{1}{\xi^2} + \widetilde{C}_1^2\xi^2\right)^{\frac{1}{2}}. \tag{118}$$

Notice that $\widetilde{C}_7$ is κ-independent. An application of estimate (25) in Lemma 2.5 implies that

$$\|\phi_h^1\|_\infty \le \widehat{C}_1(|\overline{a_h^1}| + \|\Delta_{\mathcal{N}}a_h^1\|_{\mathcal{N}}) \le \widehat{C}_1\widetilde{C}_7 := \widetilde{C}_8. \quad \square \tag{119}$$

A modified energy is defined at t_1 as follows:

$$\hat{E}(\phi_h^1) = E_{\mathcal{N}}(\phi_h^1) + \frac{\lambda C_L}{6}\alpha_0 \left\| \frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} \right\|_{L^2(0,t_1;\ell^2)}^2 + \frac{C_L}{12\lambda^2}\alpha_0\tau^3 \left\| \frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} \right\|_{L^2(0,t_1;\ell^2)}^2, \quad \text{with} \tag{120}$$

$$\lambda = \frac{3}{(\alpha_0+2)C_L}, \qquad \alpha_0 = \sqrt{\frac{47}{10}} + \sqrt{\frac{31}{30}}, \quad C_L = \alpha + \gamma\widetilde{C}_{10} + \frac{1}{2}\widetilde{C}_{10}^2 + \kappa, \tag{121}$$

$$\widetilde{C}_{10} = \hat{C}_1\widetilde{C}_9, \quad \widetilde{C}_9 = \left(2C_1^2 + \frac{1}{\xi^2} + C_1^2\xi^2\right)^{\frac{1}{2}}, \qquad C_1 = \frac{2}{|\xi|}\left(C_0 + \hat{C} + \left(9\gamma^4 + 3\xi^4\right)|\Omega_{\mathcal{N}}|\right)^{\frac{1}{2}}, \tag{122}$$

$$\hat{C} = \alpha_1|\Omega_{\mathcal{N}}|\widetilde{C}_L\widetilde{C}_2^2, \quad \alpha_1 = 1 + \frac{1}{\sqrt{3}}, \quad \widetilde{C}_L = \alpha + \gamma\widetilde{C}_2 + \frac{1}{2}\widetilde{C}_2^2 + \kappa. \tag{123}$$

The following theorem establishes the energy estimate at the first time step.

Theorem 3.1. *Assume that $|\alpha| \le \xi^2$, $\kappa \ge \xi^2$, and $A \ge \frac{1}{2\lambda^3}$. The time step size is taken to satisfy an $O(1)$ constraint (101). We have the following energy-stability property*

$$E_{\mathcal{N}}(\phi_h^1) \le \hat{E}(\phi_h^1) \le E_{\mathcal{N}}(\phi_0) + \hat{C} = C_0 + \hat{C}, \tag{124}$$

in which the global-in-time constants λ and $\hat{C}$ are defined in (121)–(123).

Proof. We take a discrete ℓ^2 inner product with (14) by $\frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t}$ and integrate form 0 to t_1. An application of Lemmas 2.4 and 3.4, combined with the estimates (67) and (98), reveals that

$$\begin{aligned}
&(1 + A\tau^3)\left\| \frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} \right\|_{L^2(t_1,t_2;\ell^2)}^2 + E_{\mathcal{N}}(\phi_h^1) - E_{\mathcal{N}}(\phi_h^0) \\
&\le \int_0^{t_1} \left(C_L\|\phi_h^1(t) - \phi_0\|_{\mathcal{N}} + \widetilde{C}_L\|a_h^1 - \phi_0\|_{\mathcal{N}} \right) \left\| \frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} \right\|_{\mathcal{N}} \mathrm{d}t \\
&\quad + \widetilde{C}_L \int_0^{t_1} \frac{t-\tau}{\tau}\|a_h^1 - \phi_0\|_{\mathcal{N}} \left\| \frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} \right\|_{\mathcal{N}} \mathrm{d}t \\
&\le (\frac{\alpha_1}{2} + 1)C_L\tau \left\| \frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} \right\|_{L^2(0,t_1;\ell^2)}^2 + \frac{\alpha_1}{2}\widetilde{C}_L\|a_h^1 - \phi_0\|_{\mathcal{N}}^2 \\
&\le \frac{C_L}{3}(\alpha_1 + 2)\Big(\frac{\tau^3}{2\lambda^2} + \lambda\Big) \left\| \frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} \right\|_{L^2(0,t_1;\ell^2)}^2 + \frac{\alpha_1}{2}\widetilde{C}_L\|a_h^1 - \phi_0\|_{\mathcal{N}}^2,
\end{aligned} \tag{125}$$

in which $\widetilde{C}_L \le C_L$, $\widetilde{C}_8 \le \widetilde{C}_{10}$, α_1 is defined in (123). Since $A \ge \frac{1}{2\lambda^3}$, $\lambda = \frac{3}{(\alpha_0+2)C_L}$, and $\|a_h^1\|_\infty$, $\|\phi_0\|_\infty \le \widetilde{C}_2$, we obtain

$$\begin{aligned}
&\hat{E}(\phi_h^1) + \left[1 - \frac{\lambda C_L}{6}\left(\alpha_0 + 2\alpha_1 + 4\right)\right] \left\| \frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} \right\|_{L^2(t_1,t_2;\ell^2)}^2 \\
&\quad + \left[A - \frac{C_L}{12\lambda^2}\left(\alpha_0 + 2\alpha_1 + 4\right)\right]\tau^3 \left\| \frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} \right\|_{L^2(t_1,t_2;\ell^2)}^2 \le E_{\mathcal{N}}(\phi_0) + \hat{C}. \quad \square
\end{aligned} \tag{126}$$

With the energy stability (124) theoretically justified at t_1, we are able to derive a much sharper bound for the numerical solution ϕ_h^1:

$$\|\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}} \le C_1, \tag{127}$$

$$\|\phi_h^1\|_\infty \le \|\widetilde{\phi_h^1}\|_{L^\infty} \le \hat{C}_1(|\overline{\phi_h^1}| + \|\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}}) \le \hat{C}_1C_1 := C_2, \tag{128}$$

$$\|\nabla_{\mathcal{N}}((\phi_h^1)^3)\|_{\mathcal{N}} \le 9\|\widetilde{\phi_h^1}\|_{L^\infty}^2 \cdot \hat{C}_2\|\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}} \le 9C_2^2\hat{C}_2C_1 := C_3, \tag{129}$$

$$\|\nabla_{\mathcal{N}}((\phi_h^1)^2)\|_{\mathcal{N}} \le 4\|\widetilde{\phi_h^1}\|_{L^\infty} \cdot \hat{C}_2\|\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}} \le 4C_2\hat{C}_2C_1 := C_4, \tag{130}$$

in which C_1, C_2, C_3 and C_4 are κ-independent, global-in-time constants. In fact, these constants have the following correlations:

$$\begin{aligned}
&C_0 \le \widetilde{C}_1 \le \widetilde{C}_5 \le \widetilde{C}_7 \le \widetilde{C}_9, \qquad \widetilde{C}_2 \le \widetilde{C}_6 \le \widetilde{C}_8 \le \widetilde{C}_{10}, \qquad \widetilde{C}_1 \le C_1 \le \widetilde{C}_9, \\
&\widetilde{C}_2 \le C_2 \le \widetilde{C}_{10}, \qquad \widetilde{C}_L \le C_L^{(0)} \le C_L, \qquad \widetilde{C}_3 \le C_3, \qquad \widetilde{C}_4 \le C_4, \qquad \lambda \le \lambda_1.
\end{aligned}$$

3.1.3. The estimate at the second time step

Lemma 3.5. *Under the assumption in Lemma 3.4 and the following $O(1)$ constraint for the time step size*

$$\tau \leq \left\{ \frac{3}{4} C_3^{-2}, \frac{1}{12\gamma^2} C_4^{-2}, \frac{1}{64} \hat{C}_2^{-2}, \frac{1}{9\kappa} \right\}, \tag{131}$$

the bound at time step t_2 is valid:

$$\|\Delta_{\mathcal{N}} \phi_h^2\|_{\mathcal{N}} \leq \widetilde{C}_9, \quad \|\phi_h^2\|_\infty \leq \widetilde{C}_{10}, \tag{132}$$

in which $\widetilde{C}_9$ and $\widetilde{C}_{10}$ are defined in (122), and C_i $(i = 3, 4)$ are defined in (129)–(130).

These constants are global-in-time and depend only on ξ, γ, the Sobolev inequality constants, the initial data, and the domain size.

Proof. The proof of this lemma is similar to that of Lemma 3.4 and will be skipped for the sake of brevity. □

It is obvious that the constraint (131) is stronger than (101).

We define the following modified energy functional

$$\begin{aligned}\widetilde{E}(\phi_h^{n+1}(t)) :=& E_{\mathcal{N}}(\phi_h^{n+1}(t)) + \frac{\lambda C_L}{6} \alpha_0 \left\| \frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t} \right\|^2_{L^2(t_n, t_{n+1}; \ell^2)} \\ &+ \frac{C_L}{12\lambda^2} \alpha_0 \tau^3 \left\| \frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t} \right\|^2_{L^2(t_n, t_{n+1}; \ell^2)} + \frac{\lambda C_L}{6} \sqrt{\frac{31}{30}} \left\| \frac{\mathrm{d}\phi_h^{n}(t)}{\mathrm{d}t} \right\|^2_{L^2(t_{n-1}, t_n; \ell^2)} \\ &+ \frac{C_L}{12\lambda^2} \sqrt{\frac{31}{30}} \tau^3 \left\| \frac{\mathrm{d}\phi_h^{n}(t)}{\mathrm{d}t} \right\|^2_{L^2(t_{n-1}, t_n; \ell^2)}, \qquad n \geq 1. \end{aligned} \tag{133}$$

The energy estimate at the second time step is established by the following theorem.

Theorem 3.2. *Under the assumption in Theorem 3.1. The time step size is taken to satisfy an $O(1)$ constraint (131). The following energy stability estimate is valid:*

$$E_{\mathcal{N}}(\phi_h^2) \leq \widetilde{E}(\phi_h^2) \leq \hat{E}(\phi_h^1) \leq E_{\mathcal{N}}(\phi_0) + \hat{C} = C_0 + \hat{C}, \tag{134}$$

in which the global-in-time constant $\hat{C}$ is defined in (123).

Proof. Taking a discrete ℓ^2 inner product of (15) with $\frac{\mathrm{d}\phi_h^2(t)}{\mathrm{d}t}$, integrating from t_1 to t_2 on both sides, and performing an analysis similar to (125), we get

$$\begin{aligned} &(1 + A\tau^3) \left\| \frac{\mathrm{d}\phi_h^2(t)}{\mathrm{d}t} \right\|^2_{L^2(t_1, t_2; \ell^2)} + E_{\mathcal{N}}(\phi_h^2) - E_{\mathcal{N}}(\phi_h^1) \\ \leq& \left(1 + \frac{1}{2\sqrt{3}}\right) C_L \tau \left\| \frac{\mathrm{d}\phi_h^2(t)}{\mathrm{d}t} \right\|^2_{L^2(t_1, t_2; \ell^2)} + \frac{C_L}{2\sqrt{3}} \tau \left\| \frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} \right\|^2_{L^2(0, t_1; \ell^2)} \\ \leq& \frac{\lambda C_L}{3} (1 + \alpha_1) \left\| \frac{\mathrm{d}\phi_h^2(t)}{\mathrm{d}t} \right\|^2_{L^2(t_1, t_2; \ell^2)} + \frac{C_L}{6\lambda^2} (1 + \alpha_1) \tau^3 \left\| \frac{\mathrm{d}\phi_h^2(t)}{\mathrm{d}t} \right\|^2_{L^2(t_1, t_2; \ell^2)} \\ &+ \frac{\lambda C_L}{3\sqrt{3}} \left\| \frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} \right\|^2_{L^2(0, t_1; \ell^2)} + \frac{C_L}{6\sqrt{3}\lambda^2} \tau^3 \left\| \frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} \right\|^2_{L^2(0, t_1; \ell^2)}. \end{aligned} \tag{135}$$

Since $A \geq \frac{1}{2\lambda^3}$, $\lambda = \frac{3}{(\alpha_0 + 2) C_L}$, we obtain

$$\begin{aligned} &\widetilde{E}(\phi_h^2) + \left[1 - \frac{\lambda C_L}{6} \alpha_2\right] \left\| \frac{\mathrm{d}\phi_h^2(t)}{\mathrm{d}t} \right\|^2_{L^2(t_1, t_2; \ell^2)} + \left[A - \frac{C_L}{12\lambda^2} \alpha_2\right] \tau^3 \left\| \frac{\mathrm{d}\phi_h^2(t)}{\mathrm{d}t} \right\|^2_{L^2(t_1, t_2; \ell^2)} \\ \leq& \hat{E}(\phi_h^1) + \frac{\lambda C_L}{6} \alpha_3 \left\| \frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} \right\|^2_{L^2(0, t_1; \ell^2)} + \frac{C_L}{12\lambda^2} \alpha_3 \tau^3 \left\| \frac{\mathrm{d}\phi_h^1(t)}{\mathrm{d}t} \right\|^2_{L^2(0, t_1; \ell^2)} \leq \hat{E}(\phi_h^1), \end{aligned} \tag{136}$$

with $\alpha_2 = \alpha_0 + 2\alpha_1 + 2$, $\alpha_3 = \frac{2}{\sqrt{3}} - \sqrt{\frac{47}{10}}$. Based on Theorem 3.1, inequality (134) is proved. □

As a consequence of Theorem 3.2, we are able to derive a much sharper bound for ϕ_h^2:

$$\|\Delta_{\mathcal{N}} \phi_h^2\|_{\mathcal{N}} \leq C_1, \tag{137}$$

$$\|\phi_h^2\|_\infty \le \|\widetilde{\phi_h^2}\|_{L^\infty} \le \widehat{C}_1(|\overline{\phi_h^2}| + \|\Delta_{\mathcal{N}}\phi_h^2\|_{\mathcal{N}}) \le \widehat{C}_1 C_1 = C_2, \tag{138}$$

$$\|\nabla_{\mathcal{N}}((\phi_h^2)^3)\|_{\mathcal{N}} \le 9\|\widetilde{\phi_h^2}\|_{L^\infty}^2 \cdot \widehat{C}_2\|\Delta_{\mathcal{N}}\phi_h^2\|_{\mathcal{N}} \le 9C_2^2\widehat{C}_2 C_1 = C_3, \tag{139}$$

$$\|\nabla_{\mathcal{N}}((\phi_h^2)^2)\|_{\mathcal{N}} \le 4\|\widetilde{\phi_h^2}\|_{L^\infty} \cdot \widehat{C}_2\|\Delta_{\mathcal{N}}\phi_h^1\|_{\mathcal{N}} \le 4C_2\widehat{C}_2 C_1 = C_4. \tag{140}$$

Remark 3.1. We notice that the H_h^2 estimate (71), (102) and (132) for a_h^1, ϕ_h^1 and ϕ_h^2, as well as the maximum norm estimate, is based on a direct analysis for the numerical scheme (13)–(15), with the help of extensive applications of discrete Sobolev embedding. However, these estimates turn out to be very rough, since the analysis does not rely on the variational energy structure. In fact, to obtain an energy dissipation at a theoretical level, an $\|\cdot\|_\infty$ bound of the numerical solution at the next time step has to be derived, due to the nonlinear term involved. Such a bound could only be possibly accomplished by a direct H^2 estimate, without using the energy structure.

3.2. Preliminary estimates of $\|\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}$ and $\|\phi_h^{n+1}\|_\infty$

In this subsection, with an a-priori assumption at the previous time steps, we perform a direct analysis for numerical scheme (16), so that the uniform-in-time $\|\cdot\|_{H_h^2}$ and $\|\cdot\|_\infty$ bound becomes available. This turn gives a global-in-time energy stability estimate for the ETD-MS scheme (19).

To proceed the global-in-time energy stability analysis, we make an a-priori assumption at the previous time steps:

$$E_{\mathcal{N}}(\phi_h^k) \le E_{\mathcal{N}}(\phi_0) \le C_0 + \widehat{C}, \qquad k = 0, 1, 2, \dots, n. \tag{141}$$

Such an a-priori assumption will be recovered at the next time step. For $k = 0, 1, 2, \dots, n$, we perform a similar analysis as in (66)–(69) and get

$$\|\Delta_{\mathcal{N}}\phi_h^k\|_\infty \le C_1, \tag{142}$$

$$\|\phi_h^k\|_\infty \le \|\widetilde{\phi_h^k}\|_{L^\infty} \le \widehat{C}_1\left(|\overline{\phi_h^k}| + \|\Delta_{\mathcal{N}}\phi_h^k\|_{\mathcal{N}}\right) \le \widehat{C}_1\widetilde{C}_1 = C_2, \tag{143}$$

$$\|\nabla_{\mathcal{N}}((\phi_h^k)^3)\|_{\mathcal{N}} \le 9\|\widetilde{\phi_h^k}\|_{L^\infty}^2 \cdot \widehat{C}_2\|\Delta_{\mathcal{N}}\phi_h^k\|_{\mathcal{N}} \le 9C_2^2\widehat{C}_2 C_1 = C_3, \tag{144}$$

$$\|\nabla_{\mathcal{N}}((\phi_h^k)^2)\|_{\mathcal{N}} \le 4\|\widetilde{\phi_h^k}\|_{L^\infty} \cdot \widehat{C}_2\|\Delta_{\mathcal{N}}\phi_h^k\|_{\mathcal{N}} \le 4C_2\widehat{C}_2 C_1 = C_4. \tag{145}$$

We aim to obtain the rough estimate for ϕ_h^{n+1}. The main theoretical result of this subsection is stated in the following theorem.

Theorem 3.3. *Assume that $|\alpha| \le \xi^2$, $\kappa \ge \xi^2$. Under the following $O(1)$ constraint for the time step size*

$$\tau \le \min\left(\frac{1}{97}\kappa^{-1}, \frac{3}{16}C_3^{-2}, \frac{1}{48\gamma^2}C_4^{-2}, \frac{1}{592}\widehat{C}_2^{-2}\right), \tag{146}$$

the bound at time step t_{n+1} is valid:

$$\|\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}} \le \widetilde{C}_9, \tag{147}$$

$$\|\phi_h^{n+1}\|_\infty \le \widetilde{C}_{10}, \tag{148}$$

in which $\widetilde{C}_9$ and $\widetilde{C}_{10}$ are defined in (122), C_i $(i = 3, 4)$ are defined in (129)–(130).

These constants are global-in-time and depend only on ξ, γ, the Sobolev inequality constants, the initial data, and the domain size.

Proof. Similarly, we denote $\phi_h^{n+1,*} = \mathrm{e}^{-K_N\tau}\phi_h^n$. The evolutionary Eq. (16) could be rewritten as the following two-substage system:

$$\frac{\phi_h^{n+1,*} - \phi_h^n}{\tau} = -K_N\mathcal{G}_0(K_N\tau)\phi_h^n, \tag{149}$$

$$\begin{aligned}\frac{\phi_h^{n+1} - \phi_h^{n+1,*}}{\tau} &= -\mathcal{G}_0(K_N\tau)F_N(\phi_h^n) - \mathcal{G}_1(K_N\tau)\left[\frac{3}{2}F_N(\phi_h^n) - 2F_N(\phi_h^{n-1}) + \frac{1}{2}F_N(\phi_h^{n-2})\right] \\ &\quad - \mathcal{G}_2(K_N\tau)\left[\frac{1}{2}F_N(\phi_h^n) - F_N(\phi_h^{n-1}) + \frac{1}{2}F_N(\phi_h^{n-2})\right].\end{aligned} \tag{150}$$

Taking a discrete ℓ^2 inner product with (149) by $\Delta_{\mathcal{N}}^2(\phi_h^{n+1,*}+\phi_h^n)$ gives the following estimate, following similar ideas as in (74)–(75):

$$\|\Delta_{\mathcal{N}}\phi_h^{n+1,*}\|_{\mathcal{N}}^2 - \|\Delta_{\mathcal{N}}\phi_h^n\|_{\mathcal{N}}^2 + \tau\left(K_N G_h\phi_h^n, \Delta_{\mathcal{N}}^2\phi_h^{n+1,*}\right)_{\mathcal{N}} + \tau\|G_h^{(5)}\phi_h^n\|_{\mathcal{N}}^2 = 0. \tag{151}$$

Meanwhile, taking a discrete ℓ^2 inner product with (150) by $2\Delta_{\mathcal{N}}^2\phi_h^{n+1}$ gives

$$\begin{aligned}(\phi_h^{n+1} - \phi_h^{n+1,*}, 2\Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}} = -2\tau\Big\{&\left(G_h F_N(\phi_h^n), \Delta_{\mathcal{N}}^2\phi_h^{n+1}\right)_{\mathcal{N}} \\ &- \left(G_h^{(1)}\left[\frac{3}{2}F_N(\phi_h^n) - 2F_N(\phi_h^{n-1}) + \frac{1}{2}F_N(\phi_h^{n-2})\right], \Delta_{\mathcal{N}}^2\phi_h^{n+1}\right)_{\mathcal{N}}\end{aligned}$$

$$- \left(G_h^{(2)} \left[\frac{1}{2} F_N(\phi_h^n) - F_N(\phi_h^{n-1}) + \frac{1}{2} F_N(\phi_h^{n-2}) \right], \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} \Big\}. \tag{152}$$

The term on the left hand side of (152) could be analyzed with the help of summation by parts:

$$(\phi_h^{n+1} - \phi_h^{n+1,*}, 2\Delta_{\mathcal{N}}^2 \phi_h^{n+1})_{\mathcal{N}} = \|\Delta_{\mathcal{N}} \phi_h^{n+1}\|_{\mathcal{N}}^2 - \|\Delta_{\mathcal{N}} \phi_h^{n+1,*}\|_{\mathcal{N}}^2 + \|\Delta_{\mathcal{N}}(\phi_h^{n+1} - \phi_h^{n+1,*})\|_{\mathcal{N}}^2. \tag{153}$$

An application of inequality (50) in Proposition 2.2 implies that

$$\tau(K_N G_h \phi_h^n, \Delta_{\mathcal{N}}^2 \phi_h^{n+1,*})_{\mathcal{N}} + \|\Delta_{\mathcal{N}}(\phi_h^{n+1} - \phi_h^{n+1,*})\|_{\mathcal{N}}^2 \geq \tau \|G_h^{(5)} \phi_h^{n+1}\|_{\mathcal{N}}^2. \tag{154}$$

Subsequently, a combination of (151)–(154) leads to

$$\begin{aligned}
&\|\Delta_{\mathcal{N}} \phi_h^{n+1}\|_{\mathcal{N}}^2 - \|\Delta_{\mathcal{N}} \phi_h^n\|_{\mathcal{N}}^2 + \tau \|G_h^{(5)} \phi_h^{n+1}\|_{\mathcal{N}}^2 + \tau \|G_h^{(5)} \phi_h^n\|_{\mathcal{N}}^2 \\
\leq & - 2\tau \left(G_h F_N(\phi_h^n), \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} \\
& - 2\tau \left(G_h^{(1)} \left[\frac{3}{2} F_N(\phi_h^n) - 2F_N(\phi_h^{n-1}) + \frac{1}{2} F_N(\phi_h^{n-2}) \right], \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} \\
& - 2\tau \left(G_h^{(2)} \left[\frac{1}{2} F_N(\phi_h^n) - F_N(\phi_h^{n-1}) + \frac{1}{2} F_N(\phi_h^{n-2}) \right], \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} \\
:= & \mathrm{I} + \mathrm{II} + \mathrm{III}.
\end{aligned} \tag{155}$$

The terms on the right hand side of the (155) will be analyzed below. Because of identity (79), the term I is divided into three parts:

$$\begin{aligned}
\mathrm{I} = \frac{\tau}{1 + A\tau^3} \Big[& -\frac{1}{3} \left(G_h (\phi_h^n)^3, \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} + \gamma \left(G_h (\phi_h^n)^2, \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} \\
& -2(\alpha - \kappa) \left(G_h \phi_h^n, \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} \Big].
\end{aligned} \tag{156}$$

Based on the a-priori estimate (144)–(145), the right hand side of (156) could be bounded in a similar way as in (81)–(82)

$$-\frac{1}{3} \left(G_h (\phi_h^n)^3, \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} \leq \frac{1}{3\xi^2} C_3^2 + \frac{\xi^2}{12} \|G_h^{(0)} \nabla_{\mathcal{N}} \Delta_{\mathcal{N}} \phi_h^{n+1}\|_{\mathcal{N}}^2 \tag{157}$$

$$\gamma \left(G_h (\phi_h^n)^2, \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} \leq \frac{3\gamma^2}{\xi^2} C_4^2 + \frac{\xi^2}{12} \|G_h^{(0)} \nabla_{\mathcal{N}} \Delta_{\mathcal{N}} \phi_h^{n+1}\|_{\mathcal{N}}^2. \tag{158}$$

The last term of (156), a linear inner product term, could be decomposed as two parts, and we apply a similar analysis as in (83)–(84):

$$\begin{aligned}
2(\xi^2 - \alpha) \left(G_h \phi_h^n, \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} \leq & 2(\xi^2 - \alpha) \|\nabla_{\mathcal{N}} \phi_h^n\|_{\mathcal{N}} \|G_h^{(0)} \nabla_{\mathcal{N}} \Delta_{\mathcal{N}} \phi_h^{n+1}\|_{\mathcal{N}} \\
\leq & 48\xi^2 \hat{C}_2^2 C_1^2 + \frac{\xi^2}{12} \|G_h^{(0)} \nabla_{\mathcal{N}} \Delta_{\mathcal{N}} \phi_h^{n+1}\|_{\mathcal{N}}^2,
\end{aligned} \tag{159}$$

$$\begin{aligned}
2(\kappa - \xi^2) \left(G_h \phi_h^n, \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} = & (\kappa - \xi^2) \Big(\|G_h^{(0)} \Delta_{\mathcal{N}} \phi_h^n\|_{\mathcal{N}}^2 + \|G_h^{(0)} \Delta_{\mathcal{N}} \phi_h^{n+1}\|_{\mathcal{N}}^2 \\
& - \|G_h^{(0)} \Delta_{\mathcal{N}} (\phi_h^{n+1} - \phi_h^n)\|_{\mathcal{N}}^2 \Big).
\end{aligned} \tag{160}$$

A substitution of (157)–(160) into (156) yields

$$\begin{aligned}
\mathrm{I} \leq & \frac{\tau}{1 + A\tau^3} \Big[\frac{1}{3\xi^2} C_3^2 + \frac{3\gamma^2}{\xi^2} C_4^2 + 48\xi^2 \hat{C}_2^2 C_1^2 + \frac{\xi^2}{4} \|G_h^{(0)} \nabla_{\mathcal{N}} \Delta_{\mathcal{N}} \phi_h^{n+1}\|_{\mathcal{N}}^2 \\
& + (\kappa - \xi^2) \|G_h^{(0)} \Delta_{\mathcal{N}} \phi_h^n\|_{\mathcal{N}}^2 + (\kappa - \xi^2) \|G_h^{(0)} \Delta_{\mathcal{N}} \phi_h^{n+1}\|_{\mathcal{N}}^2 - (\kappa - \xi^2) \|G_h^{(0)} \Delta_{\mathcal{N}} (\phi_h^{n+1} - \phi_h^n)\|_{\mathcal{N}}^2 \Big].
\end{aligned} \tag{161}$$

The term II is divided as follows:

$$\begin{aligned}
\mathrm{II} = \frac{\tau}{1 + A\tau^3} \Big[& -\frac{1}{2} \left(G_h^{(1)} (\phi_h^n)^3, \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} + \frac{2}{3} \left(G_h^{(1)} (\phi_h^{n-1})^3, \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} \\
& - \frac{1}{6} \left(G_h^{(1)} (\phi_h^{n-2})^3, \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} + \frac{3\gamma}{2} \left(G_h^{(1)} (\phi_h^n)^2, \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} \\
& - 2\gamma \left(G_h^{(1)} (\phi_h^{n-1})^2, \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} + \frac{\gamma}{2} \left(G_h^{(1)} (\phi_h^{n-2})^2, \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} \\
& - 3(\alpha - \kappa) \left(G_h^{(1)} (\phi_h^n - \phi_h^{n-1}), \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} + (\alpha - \kappa) \left(G_h^{(1)} (\phi_h^{n-1} - \phi_h^{n-2}), \Delta_{\mathcal{N}}^2 \phi_h^{n+1} \right)_{\mathcal{N}} \Big].
\end{aligned} \tag{162}$$

The six nonlinear inner product terms of (162) are bounded in a similar way as (107)–(110):

$$-\frac{1}{2} (G_h^{(1)} (\phi_h^n)^3, \Delta_{\mathcal{N}}^2 \phi_h^{n+1})_{\mathcal{N}} \leq \frac{3}{2\xi^2} C_3^2 + \frac{\xi^2}{48} \|G_h^{(0)} \nabla_{\mathcal{N}} \Delta_{\mathcal{N}} \phi_h^{n+1}\|_{\mathcal{N}}^2, \tag{163}$$

$$\frac{2}{3} (G_h^{(1)} (\phi_h^{n-1})^3, \Delta_{\mathcal{N}}^2 \phi_h^{n+1})_{\mathcal{N}} \leq \frac{8}{3\xi^2} C_3^2 + \frac{\xi^2}{48} \|G_h^{(0)} \nabla_{\mathcal{N}} \Delta_{\mathcal{N}} \phi_h^{n+1}\|_{\mathcal{N}}^2, \tag{164}$$

$$-\frac{1}{6} (G_h^{(1)} (\phi_h^{n-2})^3, \Delta_{\mathcal{N}}^2 \phi_h^{n+1})_{\mathcal{N}} \leq \frac{1}{6\xi^2} C_3^2 + \frac{\xi^2}{48} \|G_h^{(0)} \nabla_{\mathcal{N}} \Delta_{\mathcal{N}} \phi_h^{n+1}\|_{\mathcal{N}}^2, \tag{165}$$

$$\frac{3\gamma}{2}(G_h^{(1)}(\phi_h^n)^2, \Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}} \leq \frac{27\gamma^2}{2\xi^2}C_4^2 + \frac{\xi^2}{48}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}^2, \tag{166}$$

$$-2\gamma(G_h^{(1)}(\phi_h^{n-1})^2, \Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}} \leq \frac{24\gamma^2}{\xi^2}C_4^2 + \frac{\xi^2}{48}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}^2, \tag{167}$$

$$\frac{\gamma}{2}(G_h^{(1)}(\phi_h^{n-2})^2, \Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}} \leq \frac{3\gamma^2}{2\xi^2}C_4^2 + \frac{\xi^2}{48}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}^2. \tag{168}$$

The linear diffusion inner product on the right side of (162) is split into the following parts, and we apply a similar analysis as in (111)–(112):

$$3(\xi^2-\alpha)(G_h^{(1)}(\phi_h^n-\phi_h^{n-1}), \Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}} \leq 432\xi^2\hat{C}_2^2C_1^2 + \frac{\xi^2}{24}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}^2, \tag{169}$$

$$(\alpha-\xi^2)(G_h^{(1)}(\phi_h^{n-1}-\phi_h^{n-2}), \Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}} \leq 48\xi^2\hat{C}_2^2C_1^2 + \frac{\xi^2}{24}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}^2, \tag{170}$$

$$3(\kappa-\xi^2)(G_h^{(1)}(\phi_h^n-\phi_h^{n-1}), \Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}} \leq 72(\kappa-\xi^2)C_1^2 + \frac{\kappa-\xi^2}{8}\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}^2, \tag{171}$$

$$(\xi^2-\kappa)(G_h^{(1)}(\phi_h^{n-1}-\phi_h^{n-2}), \Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}} \leq 8(\kappa-\xi^2)C_1^2 + \frac{\kappa-\xi^2}{8}\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}^2. \tag{172}$$

The following bound is available to the second term on the right hand side of (171)–(172):

$$\begin{aligned}\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}^2 \leq& 2\|G_h^{(0)}\Delta_{\mathcal{N}}\phi_h^n\|_{\mathcal{N}}^2 + 2\|G_h^{(0)}\Delta_{\mathcal{N}}(\phi_h^{n+1}-\phi_h^n)\|_{\mathcal{N}}^2\\ \leq& 2C_1^2 + 2\|G_h^{(0)}\Delta_{\mathcal{N}}(\phi_h^{n+1}-\phi_h^n)\|_{\mathcal{N}}^2.\end{aligned} \tag{173}$$

A combination of (162)–(173) gives

$$\begin{aligned}\mathrm{II} \leq& \frac{\tau}{1+A\tau^3}\left[\frac{13}{3\xi^2}C_3^2 + \frac{39\gamma^2}{\xi^2}C_4^2 + 480\xi^2\hat{C}_2^2C_1^2 + \frac{161}{2}(\kappa-\xi^2)C_1^2\right.\\ &\left.+\frac{5\xi^2}{24}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}^2 + \frac{\kappa-\xi^2}{2}\|G_h^{(0)}\Delta_{\mathcal{N}}(\phi_h^{n+1}-\phi_h^n)\|_{\mathcal{N}}^2\right].\end{aligned} \tag{174}$$

The term III is divided into the following parts:

$$\begin{aligned}\mathrm{III} =& \frac{\tau}{1+A\tau^3}\Big[-\frac{1}{6}(G_h^{(2)}(\phi_h^n)^3, \Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}} + \frac{1}{3}(G_h^{(2)}(\phi_h^{n-1})^3, \Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}}\\ &-\frac{1}{6}(G_h^{(2)}(\phi_h^{n-2})^3, \Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}} + \frac{\gamma}{2}(G_h^{(2)}(\phi_h^n)^2, \Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}}\\ &-\gamma(G_h^{(2)}(\phi_h^{n-1})^2, \Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}} + \frac{\gamma}{2}(G_h^{(2)}(\phi_h^{n-2})^2, \Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}}\\ &-(\alpha-\kappa)(G_h^{(2)}(\phi_h^n-\phi_h^{n-1}), \Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}} + (\alpha-\kappa)(G_h^{(2)}(\phi_h^{n-1}-\phi_h^{n-2}), \Delta_{\mathcal{N}}^2\phi_h^{n+1})_{\mathcal{N}}\Big].\end{aligned} \tag{175}$$

The nonlinear inner product terms could be bounded as follows:

$$\begin{aligned}-\frac{1}{6}\left(G_h^{(2)}(\phi_h^n)^3, \Delta_{\mathcal{N}}^2\phi_h^{n+1}\right)_{\mathcal{N}} =& \frac{1}{6}\left(G_h^{(7)}G_h^{(9)}\nabla_{\mathcal{N}}((\phi_h^n)^3), G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\right)_{\mathcal{N}}\\ \leq& \frac{1}{6}\|G_h^{(7)}G_h^{(9)}\nabla_{\mathcal{N}}((\phi_h^n)^3)\|_{\mathcal{N}}\cdot\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}\\ \leq& \frac{1}{6\sqrt{3}}\|G_h^{(9)}\nabla_{\mathcal{N}}((\phi_h^n)^3)\|_{\mathcal{N}}\cdot\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}\\ \leq& \frac{1}{6\sqrt{3}}C_3\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}\\ \leq& \frac{1}{9\xi^2}C_3^2 + \frac{\xi^2}{48}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}^2,\end{aligned} \tag{176}$$

$$\frac{1}{3}\left(G_h^{(2)}(\phi_h^{n-1})^3, \Delta_{\mathcal{N}}^2\phi_h^{n+1}\right)_{\mathcal{N}} \leq \frac{4}{9\xi^2}C_3^2 + \frac{\xi^2}{48}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}^2, \tag{177}$$

$$-\frac{1}{6}\left(G_h^{(2)}(\phi_h^{n-2})^3, \Delta_{\mathcal{N}}^2\phi_h^{n+1}\right)_{\mathcal{N}} \leq \frac{1}{9\xi^2}C_3^2 + \frac{\xi^2}{48}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}^2, \tag{178}$$

$$\frac{\gamma}{2}\left(G_h^{(2)}(\phi_h^n)^2, \Delta_{\mathcal{N}}^2\phi_h^{n+1}\right)_{\mathcal{N}} \leq \frac{\gamma^2}{\xi^2}C_4^2 + \frac{\xi^2}{48}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}^2, \tag{179}$$

$$-\gamma\left(G_h^{(2)}(\phi_h^{n-1})^2, \Delta_{\mathcal{N}}^2\phi_h^{n+1}\right)_{\mathcal{N}} \leq \frac{4\gamma^2}{\xi^2}C_4^2 + \frac{\xi^2}{48}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}^2, \tag{180}$$

$$\frac{\gamma}{2}\left(G_h^{(2)}(\phi_h^{n-2})^2, \Delta_{\mathcal{N}}^2\phi_h^{n+1}\right)_{\mathcal{N}} \leq \frac{\gamma^2}{\xi^2}C_4^2 + \frac{\xi^2}{48}\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}^2, \tag{181}$$

in which Lemma 2.1, as well as the inequality (44), the first two inequalities in (48) and the estimates (144)–(145) have been applied in the analysis. The linear inner product terms of (113) is split into four parts, and we analyze them separately:

$$\begin{aligned}&(\xi^2-\alpha)(G_h^{(2)}(\phi_h^n-\phi_h^{n-1}),\Delta_{\mathcal N}^2\phi_h^{n+1})_{\mathcal N}\\ \le&(\xi^2-\alpha)\|G_h^{(7)}G_h^{(9)}\nabla_{\mathcal N}(\phi_h^n-\phi_h^{n-1})\|_{\mathcal N}\cdot\|G_h^{(0)}\nabla_{\mathcal N}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}\\ \le&\frac{\xi^2-\alpha}{\sqrt3}\|\nabla_{\mathcal N}(\phi_h^n-\phi_h^{n-1})\|_{\mathcal N}\cdot\|G_h^{(0)}\nabla_{\mathcal N}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}\\ \le&\frac{4\xi^2}{\sqrt3}\widehat C_2C_1\|G_h^{(0)}\nabla_{\mathcal N}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}\le 32\xi^2\widehat C_2^2C_1^2+\frac{\xi^2}{24}\|G_h^{(0)}\nabla_{\mathcal N}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}^2,\end{aligned}\tag{182}$$

$$(\alpha-\xi^2)(G_h^{(2)}(\phi_h^{n-1}-\phi_h^{n-2}),\Delta_{\mathcal N}^2\phi_h^{n+1})_{\mathcal N}\le 32\xi^2\widehat C_2^2C_1^2+\frac{\xi^2}{24}\|G_h^{(0)}\nabla_{\mathcal N}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}^2,\tag{183}$$

$$\begin{aligned}&(\kappa-\xi^2)(G_h^{(2)}(\phi_h^n-\phi_h^{n-1}),\Delta_{\mathcal N}^2\phi_h^{n+1})_{\mathcal N}\\ \le&(\kappa-\xi^2)\|G_h^{(7)}\Delta_{\mathcal N}(\phi_h^n-\phi_h^{n-1})\|_{\mathcal N}\cdot\|G_h^{(7)}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}\\ \le&(\kappa-\xi^2)\|G_h^{(0)}\Delta_{\mathcal N}(\phi_h^n-\phi_h^{n-1})\|_{\mathcal N}\cdot\|G_h^{(0)}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}\\ \le&2(\kappa-\xi^2)C_1\|G_h^{(0)}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}\le 8(\kappa-\xi^2)C_1^2+\frac{\kappa-\xi^2}{8}\|G_h^{(0)}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}^2,\end{aligned}\tag{184}$$

$$(\xi^2-\kappa)(G_h^{(2)}(\phi_h^{n-1}-\phi_h^{n-2}),\Delta_{\mathcal N}^2\phi_h^{n+1})_{\mathcal N}\le 8(\kappa-\xi^2)C_1^2+\frac{\kappa-\xi^2}{8}\|G_h^{(0)}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}^2,\tag{185}$$

in which the fact that $|\alpha|\le\xi^2$, and inequality (49) has been applied. A combination of (175)–(185) and the estimate (173) results in

$$\begin{aligned}\mathrm{III}\le&\frac{\tau}{1+A\tau^3}\Big[\frac{2}{3\xi^2}C_3^2+\frac{6\gamma^2}{\xi^2}C_4^2+64\xi^2\widehat C_2^2C_1^2+\frac{33}{2}(\kappa-\xi^2)C_1^2\\ &+\frac{5\xi^2}{24}\|G_h^{(0)}\nabla_{\mathcal N}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}^2+\frac{\kappa-\xi^2}{2}\|G_h^{(0)}\Delta_{\mathcal N}(\phi_h^{n+1}-\phi_h^n)\|_{\mathcal N}^2\Big].\end{aligned}\tag{186}$$

In turn, a substitution of (161), (174) and (186) into (155) yields

$$\begin{aligned}&\|\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}^2-\|\Delta_{\mathcal N}\phi_h^n\|_{\mathcal N}^2+\tau\|G_h^{(5)}\phi_h^{n+1}\|_{\mathcal N}^2+\tau\|G_h^{(5)}\phi_h^n\|_{\mathcal N}^2\\ \le&\frac{\tau}{1+A\tau^3}\Big[\frac{16}{3\xi^2}C_3^2+\frac{48\gamma^2}{\xi^2}C_4^2+592\xi^2\widehat C_2^2C_1^2+97(\kappa-\xi^2)C_1^2\\ &+\frac{2\xi^2}{3}\|G_h^{(0)}\nabla_{\mathcal N}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}^2+(\kappa-\xi^2)(\|G_h^{(0)}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}^2+\|G_h^{(0)}\Delta_{\mathcal N}\phi_h^n\|_{\mathcal N}^2)\Big].\end{aligned}\tag{187}$$

It is noticed that the term $(\kappa-\xi^2)\|G_h^{(0)}\Delta_{\mathcal N}(\phi_h^{n+1}-\phi_h^n)\|_{\mathcal N}^2$ has been balanced between (161), (174) and (186), which has played an important role in the derivation.

In addition, the two diffusion estimate terms have the following lower bounds, as given by inequality (45) in Proposition 2.1:

$$\begin{aligned}&\tau\|G_h^{(5)}\phi_h^{n+1}\|_{\mathcal N}^2+\tau\|G_h^{(5)}\phi_h^n\|_{\mathcal N}^2\\ \ge&\frac{\tau}{1+A\tau^3}\Big[\frac23\xi^2(\|G_h^{(0)}\nabla_{\mathcal N}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}^2+\|G_h^{(0)}\nabla_{\mathcal N}\Delta_{\mathcal N}\phi_h^n\|_{\mathcal N}^2)\\ &+(\kappa-\frac{7\xi^2}{9})(\|G_h^{(0)}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}^2+\|G_h^{(0)}\Delta_{\mathcal N}\phi_h^n\|_{\mathcal N}^2)\Big].\end{aligned}\tag{188}$$

Then we arrive at

$$\begin{aligned}&\|\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}^2-\|\Delta_{\mathcal N}\phi_h^n\|_{\mathcal N}^2+\frac{2}{3(1+A\tau^3)}\xi^2\tau\|G_h^{(0)}\nabla_{\mathcal N}\Delta_{\mathcal N}\phi_h^n\|_{\mathcal N}^2\\ &+\frac{2\xi^2}{9}(\|G_h^{(0)}\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}^2+\|G_h^{(0)}\Delta_{\mathcal N}\phi_h^n\|_{\mathcal N}^2)\\ \le&\tau\Big(\frac{16}{3\xi^2}C_3^2+\frac{48\gamma^2}{\xi^2}C_4^2+592\xi^2\widehat C_2^2C_1^2+97(\kappa-\xi^2)C_1^2\Big),\end{aligned}\tag{189}$$

so that the following bound becomes available:

$$\|\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}^2\le C_1^2+\Big(\frac{16}{3}C_3^2+48\gamma^2C_4^2\Big)\xi^{-2}\tau+592\xi^2\widehat C_2^2C_1^2\tau+97(\kappa-\xi^2)C_1^2\tau.\tag{190}$$

Under the following $O(1)$ constraint for the time step size

$$\tau\le\min\Big(\frac{1}{97}\kappa^{-1},\frac{3}{16}C_3^{-2},\frac{1}{48\gamma^2}C_4^{-2},\frac{1}{592}\widehat C_2^{-2}\Big),\tag{191}$$

which is a stronger requirement than (131), a rough estimate could be derived:

$$\|\Delta_{\mathcal N}\phi_h^{n+1}\|_{\mathcal N}\le\widetilde C_9=\Big(2C_1^2+\frac{1}{\xi^2}+C_1^2\xi^2\Big)^{\frac12}.\tag{192}$$

An application of estimate (25) in Lemma 2.5 implies that

$$\|\phi_h^{n+1}\|_\infty \le \widehat{C}_1(|\overline{\phi_h^{n+1}}| + \|\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}) \le \widehat{C}_1\widetilde{C}_9 = \widetilde{C}_{10}. \quad \square \tag{193}$$

3.3. Global-in-time energy stability analysis

The main result of this section is stated below.

Theorem 3.4. *Assume that $|\alpha| \le \xi^2$, $\kappa \ge \xi^2$, and*

$$A \ge \frac{1}{2\lambda^3}. \tag{194}$$

Here the global-in-time constant λ is defined in (121). If the time step size satisfies an $O(1)$ constraint (146), we have the following energy estimate:

$$\widetilde{E}(\phi_h^{n+1}) \le \widetilde{E}(\phi_h^n), \quad n \ge 2. \tag{195}$$

Proof. Taking a discrete ℓ^2 inner product with $\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}$ on both sides of (12) gives

$$\begin{aligned}
&\Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|_{\mathcal{N}}^2 + A\tau^3\Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|_{\mathcal{N}}^2 + \frac{\xi^2}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|(\Delta_{\mathcal{N}}+1)\phi_h^{n+1}(t)\|_{\mathcal{N}}^2 + \kappa\Big(\phi_h^{n+1}(t), \frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big)_{\mathcal{N}} \\
&= -\Big(f_{\mathcal{N}}(\phi_h^n), \frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big)_{\mathcal{N}} - \Big(\sum_{i=0}^{2}\ell_i(t-t_n)f_N(\phi_h^{n-i}), \frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big)_{\mathcal{N}}.
\end{aligned} \tag{196}$$

According to (59), the following identity is valid:

$$\frac{\mathrm{d}}{\mathrm{d}t}E_{\mathcal{N}}(\phi_h^{n+1}(t)) = \Big(f(\phi_h^{n+1}(t)), \frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big)_{\mathcal{N}} + \frac{\xi^2}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|(\Delta_{\mathcal{N}}+1)\phi_h^{n+1}(t)\|_{\mathcal{N}}^2. \tag{197}$$

Integrating both sides from t_n to t_{n+1}, combined with (196)–(197), we get

$$\begin{aligned}
&E_{\mathcal{N}}(\phi_h^{n+1}) - E_{\mathcal{N}}(\phi_h^n) + \Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|_{L^2(t_n,t_{n+1};\ell^2)}^2 + A\tau^3\Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|_{L^2(t_n,t_{n+1};\ell^2)}^2 \\
&\le \int_{t_n}^{t_{n+1}}\Big(g(\phi_h^{n+1}(t)) - g(\phi_h^n), \frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big)_{\mathcal{N}}\mathrm{d}t \\
&\quad - \int_{t_n}^{t_{n+1}}\Big[\frac{3(t-t_n)}{2\tau} + \frac{(t-t_n)^2}{2\tau^2}\Big]\Big(g(\phi_h^n) - g(\phi_h^{n-1}), \frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big)_{\mathcal{N}}\mathrm{d}t \\
&\quad + \int_{t_n}^{t_{n+1}}\Big[\frac{t-t_n}{2\tau} + \frac{(t-t_n)^2}{2\tau^2}\Big]\Big(g(\phi_h^{n-1}) - g(\phi_h^{n-2}), \frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big)_{\mathcal{N}}\mathrm{d}t := \mathrm{I}_1 + \mathrm{I}_2 + \mathrm{I}_3,
\end{aligned} \tag{198}$$

in which we have applied $\int_{t_n}^{t_{n+1}}\Big(1, \frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big)_{\mathcal{N}}\mathrm{d}t = (1, \phi_h^{n+1} - \phi_h^n)_{\mathcal{N}} = 0$. Regarding the I_1 term, it follows from the Hölder's inequality and (21) that

$$\begin{aligned}
\mathrm{I}_1 \le& C_L\int_{t_n}^{t_{n+1}}\|\phi_h^{n+1}(t) - \phi_h^n\| \cdot \Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|\mathrm{d}t \\
\le& C_L\tau^{\frac{1}{2}}\Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|_{L^2(t_n,t_{n+1};\ell^2)} \cdot \int_{t_n}^{t_{n+1}}\Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|\mathrm{d}t \le C_L\tau\Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|_{L^2(t_n,t_{n+1};\ell^2)}^2.
\end{aligned} \tag{199}$$

The terms I_2 and I_3 could be similarly bounded as

$$\begin{aligned}
\mathrm{I}_2 \le& C_L\int_{t_n}^{t_{n+1}}\Big[\frac{3(t-t_n)}{2\tau} + \frac{(t-t_n)^2}{2\tau^2}\Big] \cdot \|\phi_h^n - \phi_h^{n-1}\| \cdot \Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|\mathrm{d}t \\
\le& \sqrt{\frac{47}{10}}\frac{C_L\tau}{2}\Big\|\frac{\mathrm{d}\phi_h^n(t)}{\mathrm{d}t}\Big\|_{L^2(t_{n-1},t_n;\ell^2)} \cdot \Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|_{L^2(t_n,t_{n+1};\ell^2)} \\
\le& \sqrt{\frac{47}{10}}\frac{C_L\tau}{4}\Big(\Big\|\frac{\mathrm{d}\phi_h^n(t)}{\mathrm{d}t}\Big\|_{L^2(t_{n-1},t_n;\ell^2)}^2 + \Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|_{L^2(t_n,t_{n+1};\ell^2)}^2\Big),
\end{aligned} \tag{200}$$

$$\begin{aligned}
\mathrm{I}_3 \le& C_L\int_{t_n}^{t_{n+1}}\Big[\frac{t-t_n}{2\tau} + \frac{(t-t_n)^2}{2\tau^2}\Big]\|\phi_h^{n-1} - \phi_h^{n-2}\| \cdot \Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|\mathrm{d}t \\
\le& \sqrt{\frac{31}{30}}\frac{C_L\tau}{2}\Big\|\frac{\mathrm{d}\phi_h^{n-1}(t)}{\mathrm{d}t}\Big\|_{L^2(t_{n-2},t_{n-1};\ell^2)} \cdot \Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|_{L^2(t_n,t_{n+1};\ell^2)} \\
\le& \sqrt{\frac{31}{30}}\frac{C_L\tau}{4}\Big(\Big\|\frac{\mathrm{d}\phi_h^{n-1}(t)}{\mathrm{d}t}\Big\|_{L^2(t_{n-2},t_{n-1};\ell^2)}^2 + \Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|_{L^2(t_n,t_{n+1};\ell^2)}^2\Big).
\end{aligned} \tag{201}$$

For $k = n-1, n, n+1$, an application of Hölder's inequality indicates that

$$\tau\Big\|\frac{\mathrm{d}\phi_h^k(t)}{\mathrm{d}t}\Big\|^2_{L^2(t_{k-1},t_k;\ell^2)} \le \frac{2\lambda}{3}\Big\|\frac{\mathrm{d}\phi_h^k(t)}{\mathrm{d}t}\Big\|^2_{L^2(t_{k-1},t_k;\ell^2)} + \frac{\tau^3}{3\lambda^2}\Big\|\frac{\mathrm{d}\phi_h^k(t)}{\mathrm{d}t}\Big\|^2_{L^2(t_{k-1},t_k;\ell^2)}. \tag{202}$$

A combination of (198)–(202) leads to

$$\begin{aligned}
&\Big[1-\alpha_4\frac{C_L\lambda}{6}\Big]\Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|^2_{L^2(t_n,t_{n+1};\ell^2)} + \Big[A-\alpha_4\frac{C_L}{12\lambda^2}\Big]\tau^3\Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|^2_{L^2(t_n,t_{n+1};\ell^2)}\\
&+E_{\mathcal{N}}(\phi_h^{n+1}) + \Big(\frac{C_L\lambda}{6}+\frac{C_L}{12\lambda^2}\Big)\sqrt{\frac{31}{30}}\Big\|\frac{\mathrm{d}\phi_h^{n}(t)}{\mathrm{d}t}\Big\|^2_{L^2(t_{n-1},t_n;\ell^2)}\\
\le&\alpha_0\Big(\frac{C_L\lambda}{6}\Big\|\frac{\mathrm{d}\phi_h^{n}(t)}{\mathrm{d}t}\Big\|^2_{L^2(t_{n-1},t_n;\ell^2)} + \frac{C_L}{12\lambda^2}\Big\|\frac{\mathrm{d}\phi_h^{n}(t)}{\mathrm{d}t}\Big\|^2_{L^2(t_{n-1},t_n;\ell^2)}\Big) + E_{\mathcal{N}}(\phi_h^n)\\
&+\Big(\frac{C_L\lambda}{6}+\frac{C_L}{12\lambda^2}\Big)\sqrt{\frac{31}{30}}\Big\|\frac{\mathrm{d}\phi_h^{n-1}(t)}{\mathrm{d}t}\Big\|^2_{L^2(t_{n-2},t_{n-1};\ell^2)},
\end{aligned} \tag{203}$$

with $\alpha_4 = 4+\sqrt{\frac{47}{10}}+\sqrt{\frac{31}{30}}$. Since $\lambda = \frac{3}{(\sqrt{\frac{31}{30}}+\sqrt{\frac{47}{10}}+2)C_L}$ and $A \ge \frac{1}{2\lambda^3}$, it is obvious that

$$1-\alpha_4\frac{C_L\lambda}{6} \ge \alpha_0\frac{C_L\lambda}{6}, \quad A-\alpha_4\frac{C_L}{12\lambda^2} \ge \alpha_0\frac{C_L}{12\lambda^2}. \tag{204}$$

By (203)–(204), we arrive at

$$\widetilde{E}(\phi_h^{n+1}) + \Big(A-\frac{1}{2\lambda^3}\Big)\tau^3\Big\|\frac{\mathrm{d}\phi_h^{n+1}(t)}{\mathrm{d}t}\Big\|^2_{L^2(t_n,t_{n+1};\ell^2)} \le \widetilde{E}(\phi_h^n). \tag{205}$$

Then we have proved the energy stability estimate (194). □

The following corollary turns out to be a direct consequence of Theorem 3.4.

Corollary 3.1. *Under the same assumption in Theorem 3.4. For any positive integer $n \ge 2$, we have the following inequality*

$$E_{\mathcal{N}}(\phi_h^{n+1}) \le \widetilde{E}(\phi_h^{n+1}) \le \widetilde{E}(\phi_h^2) \le \hat{E}(\phi_h^1) \le E_{\mathcal{N}}(\phi_0) + \hat{C} = C_0 + \hat{C}. \tag{206}$$

This corollary in turn recovers the a-priori assumption (141) at the next time step, so that an induction argument could be effectively applied.

With a theoretical justification of the energy stability estimate, we are able to obtain the much sharper $\|\cdot\|_{H_h^2}$ and $\|\cdot\|_\infty$ bound for ϕ_h^{n+1}.

Corollary 3.2. *The same assumption in Theorems 3.4 and 3.3 are made. For $n \ge 0$, we have the following bounds for the numerical solution:*

$$\|\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}} \le \frac{4}{\xi^2}\Big(C_0+\hat{C}+(9\gamma^4+3\xi^4)|\Omega_{\mathcal{N}}|\Big) = C_1, \tag{207}$$

$$\|\phi_h^{n+1}\|_\infty \le \hat{C}_1(|\overline{\phi_h^{n+1}}| + \|\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}) \le \hat{C}_1 C_1 = C_2, \tag{208}$$

in which C_1 and C_2 are κ-independent global-in-time constants.

Remark 3.2. For the time step constraint in Lemmas 3.2, 3.4 and 3.5, as well as Theorem 3.3, the overall $O(1)$ constraint for τ is (146) in Theorem 3.3, which turns out to be the strongest one. On the other hand, the rough estimate $\|\Delta_{\mathcal{N}}\phi_h^{n+1}\|_{\mathcal{N}}$ bound in (147) contains a multiple factor of the $\|\Delta_{\mathcal{N}}\phi_h^{n-k}\|_{\mathcal{N}}$ $(k=0,1,2)$ bound in (142). The reason is associated with the fact that, the value of κ has not been fixed in the rough estimate, so that we need the time step size τ to balance the quantity of κ and the rough estimate could be used in the induction.

Remark 3.3. For the gradient models without automatic Lipschitz continuity for the nonlinear part, a theoretical analysis of the maximum norm of the numerical solution is needed to establish the energy stability analysis. Thus, we have to derive a rough bound of the numerical solution. With the bound (148), we are able to choose A as in (194), so that the global-in-time energy stability becomes theoretically available. Consequently, much sharper estimates (207) and (208) become available.

Notice that the energy stability coefficient A is an $\mathcal{O}(1)$ constant. The choice of A only depends on the initial energy, the domain Ω, and constant parameters ξ^2, α and γ of the LB system (4).

4. Error estimates for the ETD-MS3 scheme

Denote $\phi_e(t)$ as the exact solution of Eq. (4). We assume that the exact solution $\phi_e(t)$ satisfies the following regularity (**A**):

$$\phi_e(t) \in H^4(0,T;C^0) \cap H^1(0,T;H^4) \cap H^3(0,T;H^{m+2}) \cap L^\infty(0,T;H^{m+6}), \quad m \ge 0. \tag{209}$$

Define Φ_N as the (spatial) Fourier projection of the exact solution into $\mathcal{B}^N$, the space of trigonometric polynomials of degree to and including N. The following projection approximation is standard:

$$\|\Phi_N - \phi_e\|_{L^\infty(0,T;H^m)} \le CN^{m-k}\|\phi_e\|_{L^\infty(0,T;H^k)}, \quad 0 \le m \le k,$$

for any $\phi_e \in L^\infty(0,T;H^k_{per})$, $k \in \mathbb{N}$. We denote $\Phi_N^n = \Phi_N(\cdot, t_n)$. Since $\Phi_N \in \mathcal{B}^N$, the mass conservation property is available at the discrete level:

$$\overline{\Phi_N^n} = \frac{1}{|\Omega|}\int_\Omega \Phi_N(\cdot, t_n)\mathrm{d}\boldsymbol{x} = \frac{1}{|\Omega|}\int_\Omega \Phi_N(\cdot, t_{n-1})\mathrm{d}\boldsymbol{x} = \overline{\Phi_N^{n-1}}, \quad \forall n \in \mathbb{N}. \tag{210}$$

Meanwhile, we denote Φ^n as the interpolation values of Φ_N at discrete grid points at time instant t_n: $\Phi^n_{i,j} := \Phi_N(x_i, y_j, t_n)$. The mass conservative projection is applied for the initial data:

$$(\phi_h^0)_{i,j} = \Phi^0_{i,j} = \Phi_N(x_i, y_j, t = 0).$$

The error grid function is defined as:

$$e^n = \Phi^n - \phi_h^n, \quad \forall n \in \{1, 2, 3, \dots\}.$$

Therefore, it follows that $\overline{e^n} = 0$, for any $n \in \{1, 2, 3, \dots\}$.

Theorem 4.1. *Given initial data Φ_N^0, Φ_N^{-1}, $\Phi_N^{-2} \in C^{m+4}_{per}(\widetilde{\Omega})$, with periodic boundary conditions, suppose the unique solution for the LB Eq. (4) is of regularity class* (**A**)*. Then, provided that $\kappa > \xi^2$, $\alpha < |\xi^2|$, and h_x, h_y and τ are sufficiently small, we have*

$$\|e(t_n)\|_{\mathcal{N}} + \Big(\xi^2\tau\sum_{i=1}^{n+1}\|\Delta_{\mathcal{N}} e^i\|^2_{\mathcal{N}}\Big)^{\frac{1}{2}} \le C(N^{-m} + \tau^3), \tag{211}$$

where $C > 0$ independent on the time step size τ and mesh size h_x and h_y.

4.1. The error evolutionary equation

For the Fourier projection solution Φ_N and its interpolation Φ, a careful consistency analysis implies that

$$\begin{aligned}\Phi^{n+1} =& \mathrm{e}^{-K_N\tau}\Phi^n - \tau\mathcal{G}_0(K_N\tau)F_N(\Phi^n)\\ &- \tau\mathcal{G}_1(K_N\tau)\Big[\frac{3}{2}F_N(\Phi^n) - 2F_N(\Phi^{n-1}) + \frac{1}{2}F_N(\Phi^{n-2})\Big]\\ &- \tau\mathcal{G}_2(K_N\tau)\Big[\frac{1}{2}F_N(\Phi^n) - F_N(\Phi^{n-1}) + \frac{1}{2}F_N(\Phi^{n-2})\Big] + \tau R^n, \ \|R^n\|_{H_h^2} \le C(h^m + \tau^3).\end{aligned} \tag{212}$$

In turn, subtracting the numerical scheme (16) from the consistency estimate (212) yields

$$\begin{aligned}e^{n+1} =& \mathrm{e}^{-K_N\tau}e^n - \tau\mathcal{G}_0(K_N\tau)\mathcal{F}(\Phi^n, \phi_h^n)\\ &- \tau\mathcal{G}_1(K_N\tau)\left[\frac{3}{2}\mathcal{F}(\Phi^n, \phi_h^n) - 2\mathcal{F}(\Phi^{n-1}, \phi_h^{n-1}) + \frac{1}{2}\mathcal{F}(\Phi^{n-2}, \phi_h^{n-2})\right]\\ &- \tau\mathcal{G}_2(K_N\tau)\left[\frac{1}{2}\mathcal{F}(\Phi^n, \phi_h^n) - \mathcal{F}(\Phi^{n-1}, \phi_h^{n-1}) + \frac{1}{2}\mathcal{F}(\Phi^{n-2}, \phi_h^{n-2})\right] + \tau R^n,\end{aligned} \tag{213}$$

with $\mathcal{F}(\Phi^k, \phi_h^k) = F_N(\Phi^k) - F_N(\phi_h^k)$, $k \ge 0$. Meanwhile, we denote $e^{n+1,*} = \mathrm{e}^{K_N\tau}e^n$, the error equation (213) could be rewritten as the following two-stage system, so that the error analysis could be carried out in a more straightforward way:

$$\frac{e^{n+1,*} - e^n}{\tau} = -K_N\mathcal{G}_0(K_N\tau)e^n, \tag{214}$$

$$\begin{aligned}\frac{e^{n+1} - e^{n+1,*}}{\tau} =& -\tau\mathcal{G}_0(K_N\tau)\mathcal{F}(\Phi^n, \phi_h^n)\\ &- \tau\mathcal{G}_1(K_N\tau)\left[\frac{3}{2}\mathcal{F}(\Phi^n, \phi_h^n) - 2\mathcal{F}(\Phi^{n-1}, \phi_h^{n-1}) + \frac{1}{2}\mathcal{F}(\Phi^{n-2}, \phi_h^{n-2})\right]\\ &- \tau\mathcal{G}_2(K_N\tau)\left[\frac{1}{2}\mathcal{F}(\Phi^n, \phi_h^n) - \mathcal{F}(\Phi^{n-1}, \phi_h^{n-1}) + \frac{1}{2}\mathcal{F}(\Phi^{n-2}, \phi_h^{n-2})\right] + \tau R^n.\end{aligned} \tag{215}$$

4.2. The $\ell^\infty(0,T;\ell^2) \cap \ell^2(0,T;H_h^2)$ error estimate

Now we proceed into the convergence estimate. An application of the linear operator $G_0 = (\mathcal{G}_0(K_N\tau))^{-1}$ to (214)–(215) gives

$$\frac{G_0(e^{n+1,*} - e^n)}{\tau} = -K_N e^n, \tag{216}$$

$$\begin{aligned}\frac{G_0(e^{n+1} - e^{n+1,*})}{\tau} =& -\tau\mathcal{F}(\Phi^n, \phi_h^n) + \tau G_0 R^n\\ &- \tau G_h^{(3)}\Big[\frac{3}{2}\mathcal{F}(\Phi^n, \phi_h^n) - 2\mathcal{F}(\Phi^{n-1}, \phi_h^{n-1}) + \frac{1}{2}\mathcal{F}(\Phi^{n-2}, \phi_h^{n-2})\Big]\end{aligned}$$

$$- \tau G_h^{(4)} \Big[\frac{1}{2} \mathcal{F}(\Phi^n, \phi_h^n) - \mathcal{F}(\Phi^{n-1}, \phi_h^{n-1}) + \frac{1}{2} \mathcal{F}(\Phi^{n-2}, \phi_h^{n-2}) \Big]. \tag{217}$$

Taking a discrete ℓ^2 inner product with (216) by $e^{n+1,*} + e^n$ results in

$$\|G_0^{(0)} e^{n+1,*}\|_{\mathcal{N}}^2 - \|G_0^{(0)} e^n\|_{\mathcal{N}}^2 + \tau(K_N e^n, \mathrm{e}^{-K_N \tau} e^n)_{\mathcal{N}} + \tau(K_N e^n, e^n)_{\mathcal{N}} = 0, \tag{218}$$

in which the summation by parts identity (40) has been applied. Similarly, taking a discrete ℓ^2 inner product with (217) by $2e^{n+1}$ yields

$$\begin{aligned}
&\|G_0^{(0)} e^{n+1}\|_{\mathcal{N}}^2 - \|G_0^{(0)} e^{n+1,*}\|_{\mathcal{N}}^2 + \|G_0^{(0)} (e^{n+1} - e^{n+1,*})\|_{\mathcal{N}}^2 \\
=& 2\tau(G_0 R^n, e^{n+1})_{\mathcal{N}} - 2\tau(\mathcal{F}(\Phi^n, \phi_h^n), e^{n+1})_{\mathcal{N}} \\
&- \tau(G_h^{(3)}(3\mathcal{F}(\Phi^n, \phi_h^n) - 4\mathcal{F}(\Phi^{n-1}, \phi_h^{n-1}) + \mathcal{F}(\Phi^{n-2}, \phi_h^{n-2})), e^{n+1})_{\mathcal{N}} \\
&- \tau(G_h^{(4)}(\mathcal{F}(\Phi^n, \phi_h^n) - 2\mathcal{F}(\Phi^{n-1}, \phi_h^{n-1}) + \mathcal{F}(\Phi^{n-2}, \phi_h^{n-2})), e^{n+1})_{\mathcal{N}}.
\end{aligned} \tag{219}$$

Meanwhile, an application of inequality (51) in Proposition 2.2 reveals that

$$\tau(K_N e^n, e^{n+1,*})_{\mathcal{N}} + \|G_0^{(0)} (\phi_h^{n+1} - e^{n+1,*})\|_{\mathcal{N}}^2 \geq \tau(K_N e^{n+1}, e^{n+1})_{\mathcal{N}}. \tag{220}$$

Subsequently, a combination of (218)–(220) leads to

$$\begin{aligned}
&\|G_0^{(0)} e^{n+1}\|_{\mathcal{N}}^2 - \|G_0^{(0)} e^n\|_{\mathcal{N}}^2 + \tau(K_N e^{n+1}, e^{n+1})_{\mathcal{N}} + \tau(K_N e^n, e^n)_{\mathcal{N}} \\
\leq& 2\tau(G_0 R^n, e^{n+1})_{\mathcal{N}} - 2\tau(\mathcal{F}(\Phi^n, \phi_h^n), e^{n+1})_{\mathcal{N}} \\
&- \tau(G_h^{(3)}(3\mathcal{F}(\Phi^n, \phi_h^n) - 4\mathcal{F}(\Phi^{n-1}, \phi_h^{n-1}) + \mathcal{F}(\Phi^{n-2}, \phi_h^{n-2})), e^{n+1})_{\mathcal{N}} \\
&- \tau(G_h^{(4)}(\mathcal{F}(\Phi^n, \phi_h^n) - 2\mathcal{F}(\Phi^{n-1}, \phi_h^{n-1}) + \mathcal{F}(\Phi^{n-2}, \phi_h^{n-2})), e^{n+1})_{\mathcal{N}}.
\end{aligned} \tag{221}$$

A bound for the truncation error term is straightforward:

$$2\tau(G_0 R^n, e^{n+1})_{\mathcal{N}} \leq \tau\|G_0^{(0)} R^n\|_{\mathcal{N}}^2 + \tau\|G_0^{(0)} e^{n+1}\|_{\mathcal{N}}^2. \tag{222}$$

In terms of the first nonlinear inner product, an application Lemma 2.5 and the first inequality in (46) indicates that

$$\begin{aligned}
- 2\tau(\mathcal{F}(\Phi^n, \phi_h^n), e^{n+1})_{\mathcal{N}} \leq& \frac{2\hat{C}_5 \tau}{1 + A\tau^3} \|e^n\|_{\mathcal{N}} \|e^{n+1}\|_{\mathcal{N}} \leq \frac{2\hat{C}_5 \tau}{1 + A\tau^3} \|e^n\|_{\mathcal{N}} \|G_0^{(0)} e^{n+1}\|_{\mathcal{N}} \\
\leq& \frac{\tau}{1 + A\tau^3} \Big(\frac{2\xi^2}{9} \|e^n\|_{\mathcal{N}}^2 + \frac{9\hat{C}_5^2}{2\xi^2} \|G_0^{(0)} e^{n+1}\|_{\mathcal{N}}^2 \Big),
\end{aligned} \tag{223}$$

with $\hat{C}_5 = 2\alpha + \kappa + \xi^2 + 2\gamma\hat{C}_6 + \hat{C}_6^2$ and $\hat{C}_6 = \max\{\|\phi_e\|_{L^\infty((0,T)\times\Omega)}, C_2\}$. The nonlinear inner product involving $G_h^{(3)}$ could be bounded as follows:

$$\begin{aligned}
- 3\tau G_h^{(3)}(\mathcal{F}(\Phi^n, \phi_h^n), e^{n+1})_{\mathcal{N}} \leq& 3\hat{C}_3 \tau\|\mathcal{F}(\Phi^n, \phi_h^n)\|_{\mathcal{N}}^2 \|e^{n+1}\|_{\mathcal{N}}^2 \leq \frac{3\hat{C}_3 \hat{C}_5}{1 + A\tau^3} \tau\|e^n\|_{\mathcal{N}} \|G_0^{(0)} e^{n+1}\|_{\mathcal{N}} \\
\leq& \frac{\tau}{1 + A\tau^3} \Big(\frac{2\xi^2}{9} \|e^n\|_{\mathcal{N}}^2 + \frac{81}{8\xi^2} \hat{C}_3^2 \hat{C}_5^2 \|G_0^{(0)} e^{n+1}\|_{\mathcal{N}}^2 \Big),
\end{aligned} \tag{224}$$

with the inequality (49) applied in the first step. The other nonlinear inner product terms could be analyzed in a similar way, and the following results are available:

$$4\tau G_h^{(3)}(\mathcal{F}(\Phi^{n-1}, \phi_h^{n-1}), e^{n+1})_{\mathcal{N}} \leq \frac{\tau}{1 + A\tau^3} \Big(\frac{\xi^2}{8} \|e^{n-1}\|_{\mathcal{N}}^2 + \frac{32}{\xi^2} \hat{C}_3^2 \hat{C}_5^2 \|G_0^{(0)} e^{n+1}\|_{\mathcal{N}}^2 \Big), \tag{225}$$

$$- \tau G_h^{(3)}(\mathcal{F}(\Phi^{n-2}, \phi_h^{n-2}), e^{n+1})_{\mathcal{N}} \leq \frac{\tau}{1 + A\tau^3} \Big(\frac{\xi^2}{8} \|e^{n-2}\|_{\mathcal{N}}^2 + \frac{2}{\xi^2} \hat{C}_3^2 \hat{C}_5^2 \|G_0^{(0)} e^{n+1}\|_{\mathcal{N}}^2 \Big), \tag{226}$$

$$- \tau G_h^{(4)}(\mathcal{F}(\Phi^n, \phi_h^n), e^{n+1})_{\mathcal{N}} \leq \frac{\tau}{1 + A\tau^3} \Big(\frac{2\xi^2}{9} \|e^n\|_{\mathcal{N}}^2 + \frac{9}{8\xi^2} \hat{C}_3^2 \hat{C}_5^2 \|G_0^{(0)} e^{n+1}\|_{\mathcal{N}}^2 \Big), \tag{227}$$

$$2\tau G_h^{(4)}(\mathcal{F}(\Phi^{n-1}, \phi_h^{n-1}), e^{n+1})_{\mathcal{N}} \leq \frac{\tau}{1 + A\tau^3} \Big(\frac{\xi^2}{8} \|e^{n-1}\|_{\mathcal{N}}^2 + \frac{8}{\xi^2} \hat{C}_3^2 \hat{C}_5^2 \|G_0^{(0)} e^{n+1}\|_{\mathcal{N}}^2 \Big), \tag{228}$$

$$- \tau G_h^{(4)}(\mathcal{F}(\Phi^{n-2}, \phi_h^{n-2}), e^{n+1})_{\mathcal{N}} \leq \frac{\tau}{1 + A\tau^3} \Big(\frac{\xi^2}{8} \|e^{n-2}\|_{\mathcal{N}}^2 + \frac{2}{\xi^2} \hat{C}_3^2 \hat{C}_5^2 \|G_0^{(0)} e^{n+1}\|_{\mathcal{N}}^2 \Big). \tag{229}$$

A substitution of (222)–(229) into (221) results in

$$\begin{aligned}
&\|G_0^{(0)} e^{n+1}\|_{\mathcal{N}}^2 - \|G_0^{(0)} e^n\|_{\mathcal{N}}^2 + \tau(K_N e^{n+1}, e^{n+1})_{\mathcal{N}} + \tau(K_N e^n, e^n)_{\mathcal{N}} \\
\leq& \tau\|G_0^{(0)} R^n\|_{\mathcal{N}}^2 + \Big(\frac{\hat{C}_5^2 (5 + 56\hat{C}_3^2)}{(1 + A\tau^3)\xi^2} + 1 \Big) \tau\|G_0^{(0)} e^{n+1}\|_{\mathcal{N}}^2 \\
&+ \frac{2\xi^2 \tau}{3(1 + A\tau^3)} \|e^n\|_{\mathcal{N}}^2 + \frac{\xi^2 \tau}{4(1 + A\tau^3)} \Big(\|e^{n-1}\|_{\mathcal{N}}^2 + \|e^{n-2}\|_{\mathcal{N}}^2 \Big).
\end{aligned} \tag{230}$$

Table 1
Temporal convergence.

τ	$A = 0.1$	
	Error	Order
r/2	1.0060×10^{-6}	
r/4	1.0670×10^{-7}	3.2371
r/8	1.2227×10^{-8}	3.1253
r/16	1.4605×10^{-9}	3.0655
r/32	1.7828×10^{-10}	3.0343
r/64	2.1982×10^{-11}	3.0198

Since $\kappa > \xi^2$ and $K_N = (1 + A\tau^3)^{-1}(\Delta_{\mathcal{N}} + I)^2 + \kappa I$, we have

$$\begin{aligned}\tau(K_N v, v)_{\mathcal{N}} =& \frac{\tau}{1 + A\tau^3}\left(\xi^2\|(\Delta_{\mathcal{N}} + I)v\|_{\mathcal{N}}^2 + \kappa\|v\|_{\mathcal{N}}^2\right)\\ \geq& \frac{\tau}{1 + A\tau^3}\left(\frac{\xi^2}{4}\|\Delta_{\mathcal{N}} v\|_{\mathcal{N}}^2 + \frac{2\xi^2}{3}\|v\|_{\mathcal{N}}^2\right), \qquad \forall v \in \mathcal{M}_0^{\mathcal{N}}.\end{aligned} \tag{231}$$

A combination of (230) and (231) gives

$$\begin{aligned}&\|G_0^{(0)} e^{n+1}\|_{\mathcal{N}}^2 - \|G_0^{(0)} e^n\|_{\mathcal{N}}^2 + \frac{\tau}{1 + A\tau^3}\left(\frac{\xi^2}{4}\|\Delta_{\mathcal{N}} e^{n+1}\|_{\mathcal{N}}^2 + \frac{2\xi^2}{3}\|e^{n+1}\|_{\mathcal{N}}^2\right)\\ \leq& \tau\|G_0^{(0)} R^n\|_{\mathcal{N}}^2 + \left(\frac{\widehat{C}_5^2(5 + 56\widehat{C}_3^2)}{(1 + A\tau^3)\xi^2} + 1\right)\tau\|G_0^{(0)} e^{n+1}\|_{\mathcal{N}}^2 + \frac{\xi^2\tau}{2(1 + A\tau^3)}(\|e^{n-1}\|_{\mathcal{N}}^2 + \|e^{n-2}\|_{\mathcal{N}}^2).\end{aligned} \tag{232}$$

In turn, an application of discrete Gronwall inequality leads to the desired convergence estimate:

$$\|G_0^{(0)} e^{n+1}\|_{\mathcal{N}}^2 + \frac{\tau}{1 + A\tau^3}\left(\frac{\xi^2}{4}\sum_{i=1}^{n+1}\|\Delta_{\mathcal{N}} e^i\|_{\mathcal{N}}^2 + \frac{\xi^2}{6}\sum_{i=1}^{n+1}\|e^i\|_{\mathcal{N}}^2\right) \leq C^*(N^{-2m} + \tau^6), \tag{233}$$

in which C^* is independent of τ, h_x and h_y. In addition, by the preliminary estimate (46), we obtain an $\ell^\infty(0, T; \ell^2) \cap \ell^2(0, T; H_h^2)$ error estimate:

$$\|e^{n+1}\|_{\mathcal{N}}^2 + \tau\left(\xi^2\sum_{i=1}^{n+1}\|\Delta_{\mathcal{N}} e^i\|_{\mathcal{N}}^2 + \frac{2\xi^2}{3}\sum_{i=1}^{n+1}\|e^i\|_{\mathcal{N}}^2\right) \leq C^{**}(N^{-2m} + \tau^6), \tag{234}$$

with C^{**} independent on τ, h_x and h_y. This finishes the proof of Theorem 4.1.

Remark 4.1. The $\mathcal{O}(\tau^3)$ convergence is unconditional in the following sense: there is no restriction for τ in terms of N to guarantee the convergence estimate.

On the other hand, the first two steps of numerical scheme (17)–(19) will not lead to a loss of accuracy [32]. Instead, some alternate explicit high-order numerical algorithms could be used, such as RK2 and RK3, to update the numerical solutions at t_1 and t_2, so that the third order numerical accuracy is preserved in the first few time steps. This approach enables one to derive the full third order temporal convergence estimate in the above theorem. In particular, we notice that the first two time steps in the initial approximation will not cause any stability concern, since they are treated as the initial values in the numerical scheme.

5. Numerical results

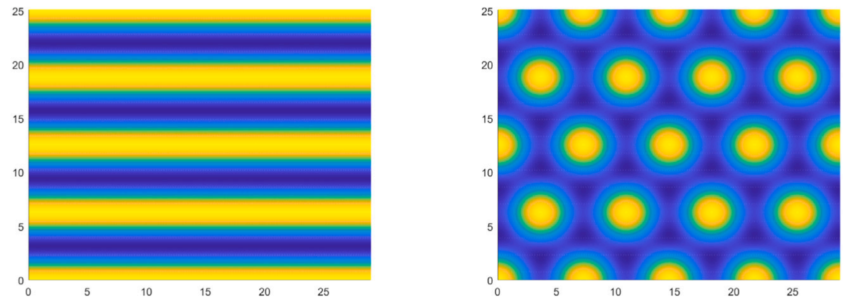
This section is devoted to some numerical experiments conducted by the developed scheme. The convergence rate, the energy stability and mass conservation property of the ETD-MS3 scheme (16)–(19) are verified. A few different equilibrium stable phases and structures are simulated in the 3D space.

5.1. Temporal accuracy

The temporal accuracy of the ETD-MS3 scheme (16)–(19) is verified. The computational domain is $\Omega = [0, 16\pi/\sqrt{3}] \times [0, 8\pi]$, and the parameters of LB model (1) are set as $\xi^2 = 1$, $\alpha = -0.15$, $\gamma = 0.25$. The initial condition is given by

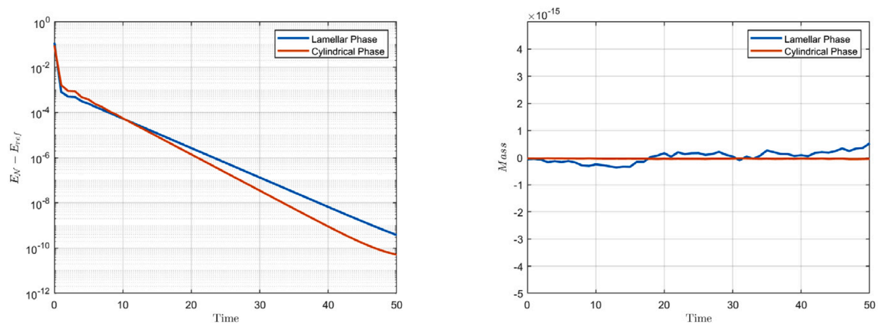
$$\phi_0(x, y) = \sin\sqrt{3}x \sin y. \tag{235}$$

Let $A = 0.1$, $\kappa = 0.01$ and a uniform $N \times N$ spatial mesh is taken. To test the temporal convergence rate, we fix $N = 256$ and choose $\tau = r/[2, 4, 8, 16, 32, 64]$, with $r = 0.05$. The temporal accuracy order is displayed in Table 1. The ℓ^2-errors $\|\phi^{N_t} - \phi_\tau^{N_t}\|_{\mathcal{N}}$ at $t = 1$ are calculated between the numerical solution and benchmark solution, which is obtained by the proposed numerical scheme (16)–(19) with $N = 256$ and $\tau = \frac{r}{512}$. By Table 1, the third-order temporal accuracy is clearly observed for the ETD-MS3 scheme.



(a) Lamellar phase (b) Cylindrical phase

Fig. 1. The 2D periodic crystals in LB model with $\alpha = -0.15$, $\gamma = 0.25$.



(a) Energy (b) Mass

Fig. 2. Numerical behavior for Lamellar (Fig. 1(a)) and cylindrical (Fig. 1(b)) phases of ETD-MS3 method with $\tau = 1$.

5.2. Energy stability and mass conservation property

This example is to verify the energy stability and mass conservation property of the ETD-MS3 method. The computational domain is $\Omega = [0, 16\pi/\sqrt{3}] \times [0, 8\pi]$, and the parameters are set as $\xi^2 = 1$, $\alpha = -0.15$ and $\gamma = 0.25$. The initial condition to the lamellar and cylindrical phases are chosen as [53]

$$\phi_0(\boldsymbol{x}) = 2a_1 \cos(\mathbf{G}_1 \cdot \boldsymbol{x}) + 2a_2 \left(\cos(\mathbf{G}_2 \cdot \boldsymbol{x}) + \cos(\mathbf{G}_3 \cdot \boldsymbol{x})\right), \tag{236}$$

$$\text{with} \quad \mathbf{G}_1 = (0, 1), \quad \mathbf{G}_2 = (-\sqrt{3}/2, 1/2), \quad \mathbf{G}_3 = (-\sqrt{3}/2, -1/2), \quad \boldsymbol{x} = (x, y)^T. \tag{237}$$

The lamellar phase is described by $a_1 = \sqrt{-2\alpha}$, $a_2 = 0$, and the cylindrical phase is described by $a_1 = a_2 = (\gamma + \sqrt{\gamma^2 - 10\alpha})/5$. Notice that $\overline{\phi_0} = 0$.

Let $A = 1$, $\kappa = 0.01$, $\tau = 1$ and a uniform 512×512 spatial mesh is taken. We calculate 2D periodic crystals of lamellar phase and cylindrical phase, as shown in Fig. 1, to demonstrate the performance of ETD-MS3 method.

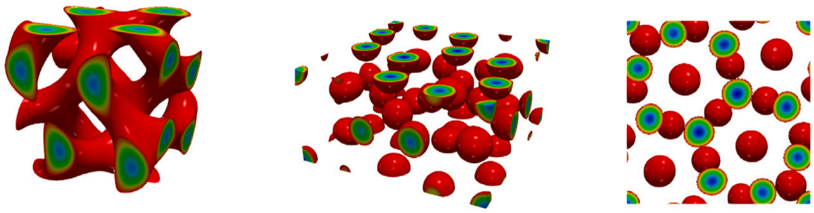
Figs. 1(a) and 1(b) display the stationary solutions of the lamellar and cylindrical phases, respectively. Corresponding evolution of the energy and the average mass of two phases are plotted in Figs. 2(a) and 2(b). In this numerical test, the reference energy values (12 significant decimal digits) of lamellar and cylindrical phases are given by $E_{ref} = -16.5320740920$ and $E_{ref} = -17.3241033761$, respectively, which are the finally convergent values. The reference energies are obtained at time $t = 50$ under the same parameters and numerical scheme. It is clear that the ETD-MS3 method is energy stable and mass conservative. Specifically, we notice that when A and κ are lower than the restriction in Theorem 3.4, the energy also gradually decreases and is dissipative over time.

5.3. Periodic crystals

In this example, we simulate some 3D periodic crystals to demonstrate the numerical performance of the proposed method and the richness of the model structure.

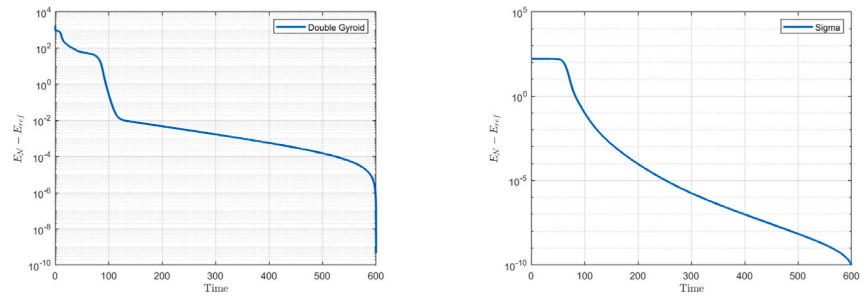
5.3.1. Double gyroid (GYR) phase

The double gyroid structure belongs to the cubic crystal system. Therefore, the 3-order invertible matrix can be chosen as $\mathbf{B} = (1/\sqrt{6})\mathbf{I}_3$. Accordingly, the computational domain in physical space becomes $\Omega = [0, 2\sqrt{6}\pi)^3$, and the initial data can be



(a) (b) (c)

Fig. 3. The stationary periodic crystals in the LB model. 3D perspective view of the (a) GYR, (b) sigma phases. (c) 2D top view of the sigma phase.



(a) GYR phase (b) Sigma phase

Fig. 4. The relative energy $E_{\mathcal{N}} - E_{ref}$ evolution of GYR (Fig. 3(a)) and sigma (Figs. 3(b) and 3(c)) phases.

chosen as

$$\phi_0(x, y, z) = \sum_{\boldsymbol{k}\in\Lambda^0} \hat{\phi}_{\boldsymbol{k}} e^{i\left[(\mathbf{B}\boldsymbol{k})^T (x,y,z)^T\right]},$$

where initial lattice points set $\Lambda^0 \subset \mathbb{Z}^3$ contains only the ones on which the located Fourier coefficients are nonzero. The corresponding Λ^0 of the double gyroid phase can be found in Table 1 in [54]. The parameters of LB model (4) are set as $\xi^2 = 1$, $\alpha = -0.47$, $\gamma = 0.46$.

Let $A = 1$, $\kappa = 0.01$, $\tau = 0.1$ and a uniform $256 \times 256 \times 256$ spatial mesh is taken. Fig. 3(a) displays the final composition profiles of the double gyroid phase in a diblock copolymer melt. The double gyroid phase is a continuous network periodic phase [6]. Fig. 4(a) plots the evolution of the relative energy difference. The reference energy value is given by $E_{ref} = -894.816819028$, which is obtained at time $t = 600$ under the same set of parameters and numerical scheme.

5.3.2. Sigma phase

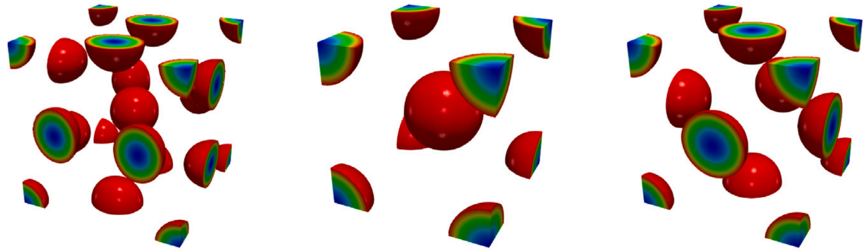
The second periodic structure considered here is the sigma phase, which is a spherical packed phase recently discovered in a block copolymer experiment [55], and in the self-consistent mean-field simulation [56]. For such a pattern, we implement the proposed algorithm on $\Omega = [0, 27.7884) \times [0, 27.7884) \times [0, 14.1514)$. In fact, the initial values could be found in [56–58], and the parameters are set as $\xi^2 = 0.65$, $\alpha = -0.025$, $\gamma = 0.7$.

Let $A = 1$, $\kappa = 0.01$, $\tau = 0.1$, and a uniform $256 \times 256 \times 128$ spatial mesh is taken. Figs. 3(b) and 3(c) display the 3D and 2D view of the volume fraction profile of the sigma phase within a unit cell. As expected, all the particles are spheres of equal size. The sigma phase has a larger, much more complicated tetragonal unit cell with 30 atoms [59]. In this unit cell, there are five non-equivalent types of lattice sites [60]. The relative energy evolution is plotted in Fig. 4(b). The reference energy value of $E_{ref} = -168.393863312$ is obtained at time $t = 600$ under the same set of parameters and numerical scheme.

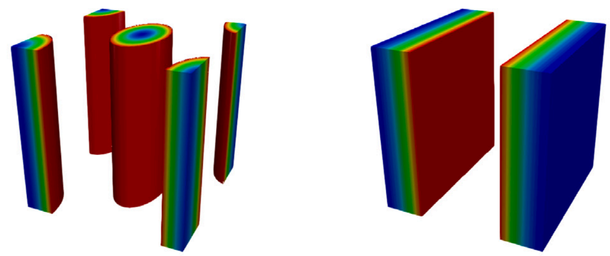
5.3.3. Other phase structures

Other 3D periodic crystal structures are also simulated, such as the A15 phase, the body-centered cubic (BCC) phase and the face-centered-cubic (FCC) phase, the Hexagonal (HEX) phase and the Lamellar (LAM) phase. These structures have been discovered in a wide range of soft matter systems; the associated initial values can be found in [54].

The A15 phase is a cubic phase with two nonequivalent types of lattice sites: atoms sit at the edges and center of the conventional unit cell in the first type lattice site, and atoms are placed along lines subdividing the cubic faces into two congruent parts in the other type lattice site [60]. This phase is shown in Fig. 5(a), and the corresponding relative energy evolution is plotted in Fig. 6(a). The reference energy value of $E_{ref} = -321.103297630$ is obtained at $t = 1000$.

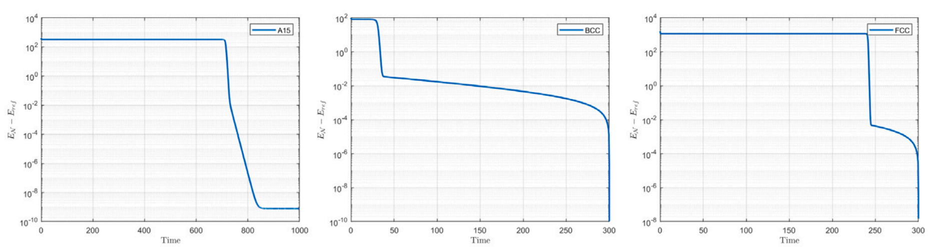


(a) A15 (b) BCC (c) FCC

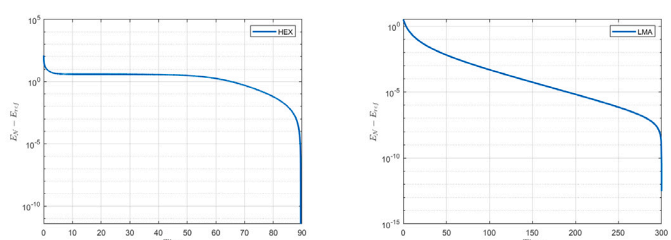


(d) HEX (e) LAM

Fig. 5. Most frequently observed macrolattices. (a) A15, (b) BCC, (c) FCC, (d) HEX, and (e) LAM.



(a) A15 (b) BCC (c) FCC



(d) HEX (e) LAM

Fig. 6. The relative energy $E_{\mathcal{N}} - E_{ref}$ evolution. (a) A15, (b) BCC, (c) FCC, (d) HEX, and (e) LAM.

The BCC phase has one lattice point in the center of the unit cell in addition to the eight corner points [61]. This phase is displayed in Fig. 5(b), and the corresponding relative energy evolution is shown in Fig. 6(b). The reference energy value of $E_{ref} = -80.9718979044$ is obtained at $t = 300$.

The FCC phase has lattice points on the faces of the cube, each giving exactly one-half contribution, in addition to the corner lattice points, giving a total of 4 lattice points per unit cell [61]. The phase structure and energy evolution are shown in Figs. 5(c) and 6(c), respectively. The reference energy value of $E_{ref} = -1174.38427666$ is obtained at $t = 300$.

The HEX and LAM phase consists of periodic sheets and cylinders packed on a hexagonal lattice, respectively [6]. The HEX structure is shown in Fig. 5(d), with energy evolution in Fig. 6(d). The reference energy value of $E_{ref} = -5.03108865057$ is obtained at $t = 90$. The LAM structure is displayed in Fig. 5(e), with the corresponding energy evolution in Fig. 6(e). the reference energy value of $E_{ref} = -0.02486398137$ is obtained at $t = 300$.

Specifically, the final simulation times for A15, BCC, FCC, HEX, and LAM phases are $t = 1000$, 300, 300, 90, and 300, respectively. These are the physical times at which the structures in Fig. 5 are obtained.

Based on these results, it is evident that the ETD-MS3 method is an efficient approach to simulate the GYR and sigma phases while ensuring energy dissipation. In particular, the ETD-MS3 approach has been shown to be highly effective in computing various phases.

6. Conclusions

In this article, a third-order accurate in time, stabilized ETD scheme for the LB equation is presented. The numerical scheme is proposed by combining the ETD method with second-order Lagrange interpolation. Moreover, a continuous version of Dupont-Douglas type stabilization term $A\tau^3 \frac{\partial \phi}{\partial t}$ is added to ensure the energy stability. The Fourier collocation spectral spatial approximation is adopted. Various global operators involved in the third-order ETD-based numerical scheme, as well as their inverse operators, have been preliminarily estimated with the help Fourier eigenvalue analysis. The mass conservation property becomes a direct consequence. In addition, we have established a global-in-time energy stability analysis for the ETD-MS3 scheme by directly estimating the uniform-in-time $\|\cdot\|_{H_h^2}$ bound for the numerical solution. In particular, a uniform-in-time $\|\cdot\|_\infty$ bound for the numerical solution and A are recovered using the Sobolev embedding from H^2 to L^∞. The $\mathcal{O}(\tau^3)$ convergence analysis, in the $\ell^\infty(0,T;\ell^2)\cap\ell^\infty(0,T;H_h^2)$ norm, is also provided. Extensive computational results for 2D and 3D periodic crystals have demonstrated the advantages. Furthermore, this global-in-time energy estimate is the first such result of a third-order accurate, stabilized numerical scheme for this physical model. This result will inspire us to explore the method for the Lifshitz–Petrich model, which is widely applied to compute quasiperiodic structures, such as the bi-frequency excited Faraday wave [62], and explain the stability of soft-matter quasicrystals [63]. We also believe that this approach will be of benefit to the studies of other polymeric systems.

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Appendix A. Proof of Proposition 2.1

An application of Parseval equality to the discrete Fourier expansions for f, $G_h^{(0)} f$ and $G_h^{(5)} f$ given by (33), (38) and (41), respectively, leads to

$$\|f\|_{\mathcal{N}}^2 = L_x L_y \sum_{k\in\mathcal{K}} |\hat{f}_k|^2, \qquad \|G_h^{(0)} f\|_{\mathcal{N}}^2 = L_x L_y \sum_{k\in\mathcal{K}} \frac{1-e^{-\tau\Lambda_k}}{\tau\Lambda_k} |\hat{f}_k|^2, \tag{A.1}$$

$$\|G_h^{(5)} f\|_{\mathcal{N}}^2 = L_x L_y \sum_{k\in\mathcal{K}} \frac{1-e^{-\tau\Lambda_k}}{\tau\Lambda_k} \Lambda_k \lambda_k^2 |\hat{f}_k|^2. \tag{A.2}$$

To prove the inequality (45), we begin with the following observation:

$$\begin{aligned}(1+A\tau^3)\Lambda_k &= \xi^2(-1+\lambda_k)^2 + \kappa \\ &= \xi^2(\lambda_k - \frac{4}{3})^2 + \frac{2}{3}\xi^2\lambda_k + (\kappa - \frac{7\xi^2}{9}) \geq \frac{2}{3}\xi^2\lambda_k + (\kappa - \frac{7\xi^2}{9}),\end{aligned} \tag{A.3}$$

$$\text{so that} \quad \Lambda_k\lambda_k^2 \geq \frac{2\xi^2}{3(1+A\tau^3)}\lambda_k^3 + \frac{\kappa - \frac{7\xi^2}{9}}{1+A\tau^3}\lambda_k^2. \tag{A.4}$$

This in turn gives the following inequality

$$\|G_h^{(5)} f\|_{\mathcal{N}}^2 \geq L_x L_y \sum_{k\in\mathcal{K}} \frac{1-e^{-\tau\Lambda_k}}{\tau\Lambda_k} \Big(\frac{2\xi^2}{3(1+A\tau^3)}\lambda_k^3 + \frac{\kappa - \frac{7\xi^2}{9}}{1+A\tau^3}\lambda_k^2 \Big) |\hat{f}_k|^2. \tag{A.5}$$

Meanwhile, an application of Parseval equality to the discrete Fourier expansion of $G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} f$ and $G_h^{(0)}\Delta_{\mathcal{N}} f$ indicates that

$$\|G_h^{(0)}\nabla_{\mathcal{N}}\Delta_{\mathcal{N}} f\|_{\mathcal{N}} f^2 = L_x L_y \sum_{k\in\mathcal{K}} \frac{1-e^{-\tau\Lambda_k}}{\tau\Lambda_k} \lambda_k^3 |\hat{f}_k|^2, \tag{A.6}$$

$$\|G_h^{(0)}\Delta_{\mathcal{N}} f\|_{\mathcal{N}} f^2 = L_x L_y \sum_{k\in\mathcal{K}} \frac{1-e^{-\tau\Lambda_k}}{\tau\Lambda_k} \lambda_k^2 |\hat{f}_k|^2. \tag{A.7}$$

A comparison of (A.5)–(A.7) leads to the inequality of (45). The inequalities in (46) could be analyzed in a similar way as (45).

Inequalities in (47)–(49) can be directly obtained from the estimates in Lemma 2.6, and the last two inequalities in (49) comes from Proposition 2.5 in [31]; the details are left to interested readers.

Appendix B. Proof of Proposition 2.2

The inequality (50) comes from the article [35]; the details are skipped for the sake of brevity.

Next, the inequality (51) is proved. The corresponding expansion of the grid function g takes a standard form as

$$g_{i,j} = \sum_{\boldsymbol{k}\in\mathcal{K}} \widehat{g}_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}\left[(\mathbf{B}\boldsymbol{k})^T (x_i,y_j)^T\right]}, \tag{B.1}$$

which in turn gives the discrete inner product as

$$\tau(K_N f, \mathrm{e}^{-K_N\tau} f)_{\mathcal{N}} = L_x L_y \sum_{\boldsymbol{k}\in\mathcal{K}} (\tau\Lambda_{\boldsymbol{k}}) \mathrm{e}^{-\tau\Lambda_{\boldsymbol{k}}} |\widehat{f}_{\boldsymbol{k}}|^2. \tag{B.2}$$

Meanwhile, an application of Parseval equality to the discrete Fourier expansion of $G_0^{(0)}(g - \mathrm{e}^{-K_N\tau})$ implies that

$$\|G_0^{(0)}(g - \mathrm{e}^{-K_N\tau})\|_{\mathcal{N}}^2 = L_x L_y \sum_{\boldsymbol{k}\in\mathcal{K}} \frac{\tau\Lambda_{\boldsymbol{k}}}{1 - \mathrm{e}^{-\tau\Lambda_{\boldsymbol{k}}}} |\widehat{g}_{\boldsymbol{k}} - \mathrm{e}^{-\tau\Lambda_{\boldsymbol{k}}} \widehat{f}_{\boldsymbol{k}}|^2. \tag{B.3}$$

On the other hand, for each fixed mode frequency $\boldsymbol{k}$, the following lower bound is valid:

$$\begin{aligned} \mathrm{e}^{\tau\Lambda_{\boldsymbol{k}}} a^2 + \frac{1}{1 - e^{-\tau\Lambda_{\boldsymbol{k}}}} b^2 &= a^2 + b^2 + (\mathrm{e}^{-\tau\Lambda_{\boldsymbol{k}}} - 1)a^2 + (\frac{1}{1 - \mathrm{e}^{-\tau\Lambda_{\boldsymbol{k}}}} - 1)b^2 \\ &\geq a^2 + b^2 + 2ab \geq (a+b)^2, \quad \text{for any } a, b \geq 0, \end{aligned} \tag{B.4}$$

in which the Cauchy inequality has been applied. Then we arrive at

$$\mathrm{e}^{\tau\Lambda_{\boldsymbol{k}}} |\mathrm{e}^{-\tau\Lambda_{\boldsymbol{k}}} \widehat{f}_{\boldsymbol{k}}|^2 + \frac{1}{1 - \mathrm{e}^{-\tau\Lambda_{\boldsymbol{k}}}} |\widehat{g}_{\boldsymbol{k}} - \mathrm{e}^{-\tau\Lambda_{\boldsymbol{k}}} \widehat{f}_{\boldsymbol{k}}|^2 \geq |\widehat{g}_{\boldsymbol{k}}|^2, \tag{B.5}$$

so that

$$\tau(K_N f, \mathrm{e}^{-K_N\tau} f)_{\mathcal{N}} + \|G_0^{(0)}(g - \mathrm{e}^{-K_N\tau})\|_{\mathcal{N}}^2 \geq L_x L_y \sum_{\boldsymbol{k}\in\mathcal{K}} (\tau\Lambda_{\boldsymbol{k}}) |\widehat{g}_{\boldsymbol{k}}|^2 = \tau(K_N g, g)_{\mathcal{N}}. \tag{B.6}$$

The proof of Proposition 2.2 is complete.

Data availability

No data was used for the research described in the article.

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