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Spectral approximation of the H^1 gradient flow of a multi-well potential with bending energy*

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Abstract. We consider a fully discrete approximation of the H^1 gradient flow of an energy integral where the energy density is given by the sum of a nonnegative multi-well potential term and a bending energy term. The spatial discretization is based on a Fourier spectral method, which is combined with an implicit Euler time discretization. The numerical method is shown to be stable and to exhibit optimal orders of convergence with respect to its spatial and temporal discretization parameters in the $\ell^\infty(0,T;H^1)$ and $\ell^\infty(0,T;L^2)$ norms, without any limitations on the size of the time step in terms of the spatial discretization parameter.

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1. Introduction

This paper is concerned with the numerical approximation of the H^1 gradient flow of nonconvex energy functionals of the form

$$I[u] := \int_{\mathbb{T}^d} W(\nabla u) + \frac{\varepsilon}{2}(\Delta u)^2 \,\mathrm{d}x, \tag{1}$$

for $u : \mathbb{T}^d \to \mathbb{R}$, where $\mathbb{T}^d = (0, 2\pi)^d \subset \mathbb{R}^d$, $d \leq 3$, $W : \mathbb{R}^d \to \mathbb{R}$ is a nonnegative double- (or triple-, etc.) well potential and $\varepsilon > 0$ is a constant. A gradient flow of this type of integral is the simplest model for microstructure formation and evolution in a material where the stored energy function of the material has two low energy crystal configurations (the double-well potential) and an interfacial energy between different crystal configurations (the ε term). Functional (1) will be considered subject to periodic boundary conditions on u.

For a nonnegative real number s, by $H^s(\mathbb{T}^d) = H^s(\mathbb{T}^d;\mathbb{R})$ we denote the periodic Sobolev space of index s, consisting of all real-valued functions $v \in H^s_{\mathrm{loc}}(\mathbb{R}^d;\mathbb{R})$, which are 2π-periodic in each co-ordinate direction, i.e., $v(x + 2\pi e_i) = v(x)$ for all $x \in \mathbb{R}^d$ and all $i = 1, \ldots, d$. Further, let $\mathring{H}^s(\mathbb{T}^d) := \{v \in H^s(\mathbb{T}^d) : \fint_{\mathbb{T}^d} v(x)\,\mathrm{d}x = 0\}$.

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The H^1 gradient flow problem for the functional I defined by (1) is to find $u \in C([0,\infty); \mathring{H}^1(\mathbb{T}^d)) \cap C((0,\infty); \mathring{H}^2(\mathbb{T}^d))$ such that $u_t \in C((0,\infty); \mathring{H}^1(\mathbb{T}^d))$, $u(\cdot,0) = u_0(\cdot) \in \mathring{H}^1(\mathbb{T}^d)$ and

$$(\nabla u_t, \nabla v) = -I'[u](v) = -(\sigma(\nabla u), \nabla v) - \varepsilon(\Delta u, \Delta v), \qquad \forall\, v \in \mathring{H}^2(\mathbb{T}^d),\ t > 0, \quad (2)$$

where $(\cdot,\cdot)$ is the usual inner product in $L^2(\mathbb{T}^d) = L^2(\mathbb{T}^d;\mathbb{R})$ and $\sigma = DW$. We assume that W is such that $\sigma : \mathbb{R}^d \to \mathbb{R}^d$ is Lipschitz continuous and satisfies a coercivity condition, i.e., there exist constants $c_1 > 0$, $c_2 > 0$ and $c_3 \geq 0$ such that

$$|\sigma(p) - \sigma(q)| \leq c_1 |p - q| \quad \text{and} \quad \sigma(p) \cdot p \geq c_2 |p|^2 - c_3, \qquad \forall\, p, q \in \mathbb{R}^d. \quad (3)$$

An example of a double-well potential W that satisfies (3) for $d = 3$ is

$$W(\nabla u) := \frac{1}{2}\left[\frac{(u_x^2 - 1)^2}{u_x^2 + 1} + u_y^2 + u_z^2\right],$$

so that

$$\sigma(\nabla u) = DW(\nabla u) = \nabla u - 4\frac{u_x}{(u_x^2 + 1)^2}(1,0,0).$$

The gradient flow (2) is the weak formulation of

$$\begin{aligned} \Delta u_t - \varepsilon \Delta^2 u &= -\operatorname{div} \sigma(\nabla u) \quad \text{in } \mathbb{T}^d, \quad t > 0, \\ u &= u_0 \qquad\qquad\quad\ \ \text{in } \mathbb{T}^d, \quad t = 0, \end{aligned} \quad (4)$$

subject to 2π-periodic boundary conditions on $\partial\mathbb{T}^d$.

Another (formally) equivalent formulation of the continuous problem (2) is

$$\begin{aligned} u_t - \varepsilon \Delta u &= f(u) \quad \text{in } \mathring{H}^1(\mathbb{T}^d) \text{ for } t > 0, \\ u &= u_0 \qquad \text{when } t = 0, \end{aligned} \quad (5)$$

subject to 2π-periodic boundary conditions on $\partial\mathbb{T}^d$, where $f : \mathring{H}^1(\mathbb{T}^d) \to \mathring{H}^1(\mathbb{T}^d)$ is defined by $f(u) := (-\Delta)^{-1} \operatorname{div}(\sigma(\nabla u))$. Here,

$$(-\Delta)^{-1} : \mathring{H}^{-1}(\mathbb{T}^d) := [\mathring{H}^1(\mathbb{T}^d)]' \to \mathring{H}^1(\mathbb{T}^d)$$

is well-defined, and condition (3) implies that $f : \mathring{H}^1(\mathbb{T}^d) \to \mathring{H}^1(\mathbb{T}^d)$ is Lipschitz continuous. It is clear from the form of (5) that the H^1 gradient flow of (1) is a semilinear parabolic equation, with the particular feature that the nonlinearity f involves the nonlocal operator $(-\Delta)^{-1}$, rendering f itself nonlocal.

Thanks to standard results from semigroup theory (see e.g. [8, Corollary 3.3.5] with $X = \mathring{H}^1(\mathbb{T}^d)$, $\alpha = 0$, $A = -\varepsilon\Delta$, noting that $-\varepsilon\Delta$ is self-adjoint, densely defined and bounded below on X, so sectorial), there exists a unique solution to (5) in the sense of [8, Definition 3.3.1]; i.e., there exists a unique $u \in C([0,\infty); \mathring{H}^1(\mathbb{T}^d))$, such that $u \in C((0,\infty); \mathring{H}^2(\mathbb{T}^d))$, u_t exists and belongs to $C((0,T); \mathring{H}^1(\mathbb{T}^d))$, $t \mapsto f(u(t))$ is locally Hölder continuous in $\mathring{H}^1(\mathbb{T}^d)$, $\int_0^\rho \|f(u(t))\|_{H^1(\mathbb{T}^d)} \,\mathrm{d}t < \infty$ for some $\rho > 0$, and (5) is satisfied. By Duhamel's formula [8, Lemma 3.3.2] and [8, Theorem 3.5.2] we may express the solution $u(t)$ for all $t \geq 0$ by

$$u(t) = E(t)u_0 + \int_0^t E(t-s) f(u(s)) \,\mathrm{d}s, \quad (6)$$

where $E(t) := \exp(t\varepsilon\Delta)$, and the mapping $t \in (0,\infty) \mapsto u_t(t) \in \mathring{H}^1(\mathbb{T}^d)$ is locally Hölder continuous.

In [14], the starting point for the construction of the numerical approximation of the problem, based on a finite element method, was (6). This was important since classical finite element spaces, such as those consisting of continuous piecewise polynomial functions, are subspaces of H^1, but not of H^2; thus, approximating (2) instead of (6) by a finite element method would have required the use of more complicated (e.g. H^2-conforming) finite element spaces, or nonconforming (or discontinuous) or indeed mixed finite element methods. Our objective in this paper is to construct and analyze a numerical method based directly on the weak formulation (2), by using a spectral spatial discretization. A second aim is to derive, in addition to an optimal order H^1 norm bound, an optimal order error bound for the method in the L^2 norm. The proof of convergence in the latter case is more complicated than in the case of the H^1 norm, as Lipschitz continuity in the L^2 norm of the nonlocal nonlinear operator $\mathcal{N} : v \in D(\mathcal{N}) := W^{2,3}(\mathbb{T}^d) \mapsto (-\Delta)^{-1}\mathrm{div}\,[\sigma(\nabla v)] \in L^2(\mathbb{T}^d)$ appearing in (5) is (unlike the case when it is considered as a mapping from H^1 into itself) *not* a straightforward consequence of the Lipschitz continuity of σ assumed in (3); this question was not considered in [14].

There is extensive literature on the finite element approximation of semilinear parabolic problems in the framework of $L^2(\Omega)$, including [13], [9], [7], [4] and [11]. A common feature of those papers is that the nonlinear term $f = f(u)$ (in [13] $f = f(t)$ and in [11] $f = f(x,u)$) is a local operator, i.e. $f : \mathbb{R} \to \mathbb{R}$, and this plays a key role in the analysis when translating assumptions on the pointwise properties of f to properties of the nonlinearity as a mapping from one function space to another. An important paper in the literature that performs error analysis for implicit Euler and semi-implicit Euler time discretization methods of semilinear parabolic problems is [3]. For the analysis of the long-time behaviour of finite element approximations of semilinear parabolic problems we refer to [10], [12] and [5]; see also [15] for a comprehensive survey. A related contribution to the spectral approximation of a different class of pattern-forming nonlinear evolution equations is [2].

The paper is structured as follows. In Section 2, we introduce relevant approximation spaces for the spectral method, which we shall define in Section 3. We also introduce periodic Sobolev spaces as well as their homogeneous counterparts and state some crucial approximation properties. In Section 3, we prove the existence of a unique solution to the numerical method. In Section 4, we study the stability of the method and in Section 5 we establish optimal bounds on the error between the analytical solution and its numerical approximation. Section 6 indicates possible extensions of the work presented herein.

2. Fourier–Galerkin approximation in Sobolev spaces

The spatial discretization of (2) is based on a spectral Galerkin method with Fourier basis functions. For a positive integer N we define

$$\mathbb{Z}_N := \{-N, \dots, N-1\},$$

and denote the d-fold Cartesian product of this set by $\mathbb{Z}_N^d$. We define the following $(2N)^d$-dimensional subspace of $L^2(\mathbb{T}^d;\mathbb{C})$:

$$\mathrm{S}_N := \mathrm{span}_{\mathbb{C}}\big\{x \in \mathbb{T}^d \mapsto \mathrm{e}^{ik\cdot x} \;:\; k \in \mathbb{Z}_N^d\big\},$$

and by $P_N : L^2(\mathbb{T}^d;\mathbb{C}) \to \mathrm{S}_N$ we denote the orthogonal projector obtained by truncating the Fourier series, i.e.,

$$P_N u(x) := \sum_{k\in\mathbb{Z}_N^d} \hat{u}(k)\,\mathrm{e}^{ik\cdot x},$$

where $\hat{u}(k)$ are the Fourier coefficients of u. Since we shall be seeking approximations to real-valued functions, we introduce the subspace of real-valued functions contained in S_N, denoted by X_N, through

$$\mathrm{X}_N := \left\{x \in \mathbb{T}^d \mapsto \sum_{k\in\mathbb{Z}_N^d} \hat{u}(k)\,\mathrm{e}^{ik\cdot x} : \hat{u}(-k) = \overline{\hat{u}(k)}\right\}.$$

With this notation, P_N maps $L^2(\mathbb{T}^d) = L^2(\mathbb{T}^d;\mathbb{R})$ onto X_N.

For functions u_N and v_N in X_N, i.e.,

$$u_N(x) = \sum_{k\in\mathbb{Z}_N^d} \hat{u}(k)\,\mathrm{e}^{ik\cdot x} \quad \text{and} \quad v_N(x) = \sum_{k\in\mathbb{Z}_N^d} \hat{v}(k)\,\mathrm{e}^{ik\cdot x},$$

consider the inner product and norm defined by

$$\langle u_N, v_N\rangle := (2\pi)^d \sum_{k\in\mathbb{Z}_N^d} \hat{u}(k)\,\overline{\hat{v}(k)} \quad \text{and} \quad \|u_N\| = \sqrt{\langle u_N, u_N\rangle}.$$

By virtue of Plancherel's theorem, the space $L^2(\mathbb{T}^d) = L^2(\mathbb{T}^d;\mathbb{R})$ is the closure, with respect to the norm $\|\cdot\|$, of the union of the spaces X_N, $N \geq 1$. In particular, for $u, v \in L^2(\mathbb{T}^d)$,

$$\langle u, v\rangle := (2\pi)^d \sum_{k\in\mathbb{Z}^d} \hat{u}(k)\,\overline{\hat{v}(k)} = \int_{\mathbb{T}^d} u\,\overline{v}\,\mathrm{d}x = \int_{\mathbb{T}^d} u\,v\,\mathrm{d}x = (u,v), \quad \text{and} \quad \|\cdot\| = \|\cdot\|_{L^2}.$$

We shall further introduce the subspace

$$\mathring{\mathrm{X}}_N := \{\phi \in \mathrm{X}_N \;:\; \hat{\phi}(0) = 0\} \tag{7}$$

consisting of all functions $\phi \in \mathrm{X}_N$ that satisfy the volume-constraint $\fint_{\mathbb{T}^d} \phi\,\mathrm{d}x = 0$.

The space $\mathring{H}^{-1}(\mathbb{T}^d) := [\mathring{H}^1(\mathbb{T}^d)]'$ can be identified with the closure of the union of $\mathring{\mathrm{X}}_N$, $N \geq 1$, with respect to the homogeneous H^{-1} norm induced by the inner product

$$\langle u, v\rangle_{\mathring{H}^{-1}} = (2\pi)^d \sum_{k\in\mathbb{Z}^d\setminus\{0\}} |k|^{-2}\,\hat{u}(k)\,\overline{\hat{v}(k)}.$$

More generally, for $s \in \mathbb{R}$ we consider the homogeneous H^s inner products

$$\langle u, v\rangle_{\mathring{H}^s} := (2\pi)^d \sum_{k\in\mathbb{Z}^d\setminus\{0\}} |k|^{2s}\, \hat{u}(k)\, \overline{\hat{v}(k)},$$

associated with the homogeneous Sobolev spaces $\mathring{H}^s(\mathbb{T}^d)$ as the closures, with respect to the induced homogeneous H^s norms $[u]_{H^s} = \sqrt{\langle u, u\rangle_{\mathring{H}^s}}$, of the union of the spaces $\mathring{\mathrm{X}}_N$, $N \geq 1$. For any $s \in \mathbb{R}$, the "full" Sobolev space $H^s(\mathbb{T}^d)$ consists of all periodic tempered distributions u such that

$$\|u\|_{H^s} := \left((2\pi)^d \sum_{k\in\mathbb{Z}^d} (1+|k|^2)^s |\hat{u}(k)|^2\right)^{\frac{1}{2}} < \infty.$$

For $s > 0$, the norm $\|\cdot\|_{H^s}$ thus defined is equivalent to the norm $\left(\|\cdot\|^2 + [\,\cdot\,]^2_{H^s}\right)^{\frac{1}{2}}$; we shall therefore not distinguish between them and we shall use the same notation for both. For $s = 0$, we adopt the convention that $H^0(\mathbb{T}^d) = L^2(\mathbb{T}^d)$. For $s \in \mathbb{N}$, the two H^s norms defined above are equivalent to the standard Sobolev norm based on weak derivatives.

The following Poincaré inequalities will be helpful:

$$\|v\|^2 \leq \|\nabla v\|^2, \qquad \forall\, v \in \mathring{H}^1,$$
$$\|\nabla v\|^2 = (v, -\Delta v) \leq \|v\|\|\Delta v\| \leq \|\nabla v\|\|\Delta v\| \leq \|\Delta v\|^2, \qquad \forall\, v \in \mathring{H}^2.$$

The orthogonality of the Fourier system yields, for $u \in H^s(\mathbb{T}^d)$ with $s \geq 0$ and $v_N \in \mathring{\mathrm{X}}_N$, the equality

$$\langle u, v_N\rangle_{H^s} = \langle P_N u, v_N\rangle_{H^s}.$$

We recall from [1] the following crucial approximation property of the projector P_N: assuming that $u \in \mathring{H}^s(\mathbb{T}^d)$, where $s > 0$ and $-\infty < r < s$, there exists a positive constant $C = C(r, s)$, independent of u, such that,

$$\|u - P_N u\|_{H^r} \leq C N^{-(s-r)} \|u\|_{H^s}, \qquad \forall\, N \geq 1. \tag{8}$$

For $p \in [1, \infty)$ and a Banach space $\mathfrak{X}$, consider the set $\ell^p(0, T; \mathfrak{X})$ of all $\mathfrak{X}$-valued functions v defined on the set $\{0 = t^0, t^1, \ldots, t^M = T\}$, where $t^{k+1} - t^k = h \equiv \Delta t := T/M$, $k = 0, 1, \ldots, M-1$, $M \geq 2$, such that

$$\|v\|_{\ell^p(0,T;\mathfrak{X})} := \left(h \sum_{k=0}^{M} \|v(t^k)\|^p_{\mathfrak{X}}\right)^{\frac{1}{p}} \leq Const. < \infty,$$

uniformly in h, with the usual modification for $p = \infty$.

For a real number x, we shall write $(x)_+$ for the nonnegative part of x, i.e., we define $(x)_+ := \max(x, 0)$.

After these preparatory considerations we are now ready to formulate our numerical approximation of the gradient flow problem (2).

3. Definition of the numerical method

The aim of this section is to define the proposed discretization of (2). The spatial discretization is based on a Fourier–Galerkin approximation from the finite-dimensional space $\mathring{\mathrm{X}}_N$, while the temporal discretization of the equation is performed on a uniform partition $\{0 = t^0, t^1, \ldots, t^M = T\}$ of the interval $[0, T]$ such that $t^{k+1} - t^k = h \equiv \Delta t := T/M$, $k = 0, 1, \ldots, M-1$, $M \geq 2$, using the implicit Euler scheme. For $k = 0, 1, \ldots, M-1$, we seek $u_N^{k+1} \in \mathring{\mathrm{X}}_N$ such that

$$\left(\nabla\left(\frac{u_N^{k+1} - u_N^k}{h}\right), \nabla\phi\right) + (\sigma(\nabla u_N^{k+1}), \nabla\phi) + \varepsilon(\Delta u_N^{k+1}, \Delta\phi) = 0, \qquad \forall\, \phi \in \mathring{\mathrm{X}}_N, \quad (9)$$

where $u_N^0 := P_N u_0$, with $u_0 \in \mathring{H}^1(\mathbb{T}^d)$.

We begin with the analysis of the numerical method by showing the existence and uniqueness of the numerical solution. To this end, we rewrite (9) as follows:

$$\frac{1}{h}(-\Delta)u_N^{k+1} - P_N\left[\operatorname{div}\sigma(\nabla u_N^{k+1})\right] + \varepsilon\Delta^2 u_N^{k+1} - \frac{1}{h}(-\Delta)u_N^k = 0.$$

We shall invoke the following corollary of Brouwer's fixed point theorem (cf. Girault & Raviart [6, Corollary 1.1, p.279]).

Lemma 1. *Let $\mathscr{H}$ be a finite-dimensional Hilbert space whose inner product is denoted by $(\cdot,\cdot)_{\mathscr{H}}$ and the corresponding norm by $\|\cdot\|_{\mathscr{H}}$. Let $\mathscr{F}$ be a continuous mapping from $\mathscr{H}$ into $\mathscr{H}$ with the following property: there exists a $\mu > 0$ such that $(\mathscr{F}(v), v)_{\mathscr{H}} > 0$ for all $v \in \mathscr{H}$ with $\|v\|_{\mathscr{H}} = \mu$. Then, there exists an element $u \in \mathscr{H}$ such that $\|u\|_{\mathscr{H}} \leq \mu$ and $\mathscr{F}(u) = 0$.*

Theorem 1 (Existence and uniqueness)**.** *For all $h > 0$ and $N \geq 1$, the solution to (9) exists. If, in addition, $h < h_0 := 1/(c_1 - \varepsilon)_+$, then the solution is unique.*

Proof. We apply Lemma 1 with $\mathscr{H} = \mathring{\mathrm{X}}_N$, equipped with the inner product $(\cdot,\cdot)_{\mathscr{H}} = (\cdot,\cdot)$ and norm $\|\cdot\|_{\mathscr{H}} = \|\cdot\|$, and with the operator $\mathscr{F} : \mathring{\mathrm{X}}_N \to \mathring{\mathrm{X}}_N$ defined by

$$\mathscr{F}(v) := \frac{1}{h}(-\Delta)v - P_N\left[\operatorname{div}\sigma(\nabla v)\right] + \varepsilon\Delta^2 v - \frac{1}{h}(-\Delta)u_N^k, \qquad v \in \mathring{\mathrm{X}}_N.$$

By noting (3) and the chain of inequalities

$$\begin{aligned}\|P_N\left[\operatorname{div}\sigma(\nabla v_1)\right] - P_N\left[\operatorname{div}\sigma(\nabla v_2)\right]\| &\leq d^{\frac{1}{2}} N \|\sigma(\nabla v_1) - \sigma(\nabla v_2)\| \\ &\leq c_1 d^{\frac{1}{2}} N \|\nabla v_1 - \nabla v_2\| \\ &\leq c_1 d N^2 \|v_1 - v_2\|,\end{aligned}$$

for all $v_1, v_2 \in \mathring{\mathrm{X}}_N$, we obtain that

$$\|\mathscr{F}(v_1) - \mathscr{F}(v_2)\| \leq \left(\frac{dN^2}{h} + c_1 dN^2 + \varepsilon d^2 N^4\right)\|v_1 - v_2\| \qquad \forall\, v_1, v_2 \in \mathring{\mathrm{X}}_N;$$

therefore $\mathscr{F}$ is (Lipschitz) continuous. Further, by (3) and Poincaré's inequality,

$$\begin{aligned}(\mathscr{F}(v), v) &= \frac{1}{h}\|\nabla v\|^2 + (\sigma(\nabla v), \nabla v) + \varepsilon\|\Delta v\|^2 - \frac{1}{h}(\nabla u_N^k, \nabla v)\\ &\geq \left(\frac{1}{2h} + c_2 + \varepsilon\right)\|\nabla v\|^2 - \frac{1}{2h}\|\nabla u_N^k\|^2 - (2\pi)^d c_3\\ &\geq \left(\frac{1}{2h} + c_2 + \varepsilon\right)\|v\|^2 - \left(\frac{1}{2h}\|\nabla u_N^k\|^2 + (2\pi)^d c_3\right).\end{aligned}$$

By taking any $\mu > 0$ such that $\left(\frac{1}{2h} + c_2 + \varepsilon\right)\mu^2 > \left(\frac{1}{2h}\|\nabla u_N^k\|^2 + (2\pi)^d c_3\right)$ the existence of a solution to (9) follows from Lemma 1.

Further, we note that for $h < h_0 := 1/(c_1 - \varepsilon)_+$ we have

$$(\mathscr{F}(v_1) - \mathscr{F}(v_2), v_1 - v_2) \geq \left(\frac{1}{h} - c_1 + \varepsilon\right)\|\nabla(v_1 - v_2)\|^2, \qquad \forall\, v_1, v_2 \in \mathring{\mathrm{X}}_N.$$

The uniqueness of the solution to (9) thus follows for all $h \in (0, h_0)$. □

4. Stability analysis of the numerical method

The purpose of this section is to show that method (9) is nonlinearly stable, uniformly in the discretization parameters, in a sense that will be made precise below. To this end, we consider, in conjunction with (9), the following discrete problem. For $k = 0, 1, \ldots, M-1$, we seek $v_N^{k+1} \in \mathring{\mathrm{X}}_N$ such that

$$\left(\nabla\left(\frac{v_N^{k+1} - v_N^k}{h}\right), \nabla\phi\right) + (\sigma(\nabla v_N^{k+1}), \nabla\phi) + \varepsilon(\Delta v_N^{k+1}, \Delta\phi) = 0, \qquad \forall\, \phi \in \mathring{\mathrm{X}}_N. \quad (10)$$

We define $v_N^0 := P_N v_0$, with $v_0 \in \mathring{H}^1(\mathbb{T}^d)$.

Theorem 2 (Stability). *Suppose that $h \leq \frac{1}{4}h_0$, where $h_0 := 1/(c_1 - \varepsilon)_+$. Then, the following inequality holds, with $c_0 := 2(c_1 - \varepsilon)_+ = 2/h_0$:*

$$\max_{1\leq k\leq M}\|\nabla(u_N^k - v_N^k)\| \leq \mathrm{e}^{c_0 T}\|\nabla(u_0 - v_0)\|, \qquad \forall\, u_0, v_0 \in \mathring{H}^1(\mathbb{T}^d).$$

This theorem expresses the stability of the numerical method (9) in the norm appearing on the left-hand side of the last inequality, without any condition constraining the time step h in terms of the spatial discretization parameter N, the only restriction being that $h \leq \frac{1}{4}h_0$. Stability is to be understood in the usual sense of continuous dependence of the solution on the (initial) data.

Proof. We introduce $w_0 := u_0 - v_0$ and $w_N^k := u_N^k - v_N^k$ for $k = 0, 1, \ldots, M$. Hence, after subtracting (10) from (9) and taking $\phi = w_N^{k+1}$, we have

$$\left(\nabla\left(\frac{w_N^{k+1} - w_N^k}{h}\right), \nabla w_N^{k+1}\right) + (\sigma(\nabla u_N^{k+1}) - \sigma(\nabla v_N^{k+1}), \nabla w_N^{k+1}) + \varepsilon\|\Delta w_N^{k+1}\|^2 = 0.$$

Thus, by (3) and Poincaré's inequality, we deduce that

$$\frac{1}{2h}\left(\|\nabla w_N^{k+1}\|^2 - \|\nabla w_N^k\|^2\right) + \varepsilon\|\nabla w_N^{k+1}\|^2 \leq c_1\|\nabla w_N^{k+1}\|^2, \qquad k = 0, 1, \ldots, M-1.$$

Suppose that $h \leq \frac{1}{4}h_0$, where $h_0 := 1/(c_1 - \varepsilon)_+$. Then,

$$\|\nabla w_N^{k+1}\|^2 \leq (1 + 2c_0 h)\|\nabla w_N^k\|^2, \qquad k = 0, 1, \ldots, M-1,$$

where $c_0 := 2(c_1 - \varepsilon)_+ = 2/h_0$. Consequently, by noting that

$$\|\nabla w_N^0\| = \|\nabla(P_N w_0)\| = \|P_N(\nabla w_0)\| \leq \|\nabla w_0\|,$$

we have that

$$\max_{1\leq k\leq M} \|\nabla w_N^k\|^2 \leq (1 + 2c_0 h)^{T/h}\|\nabla w_N^0\|^2 \leq \mathrm{e}^{2c_0 T}\|\nabla w_0\|^2.$$

We have thus shown that, if $h \leq \frac{1}{4}h_0$, where $h_0 := 1/(c_1 - \varepsilon)_+$, then the following inequality holds, with $c_0 := 2(c_1 - \varepsilon)_+ = 2/h_0$:

$$\max_{1\leq k\leq M} \|\nabla(u_N^k - v_N^k)\| \leq \mathrm{e}^{c_0 T}\|\nabla(u_0 - v_0)\|, \qquad \forall\, u_0, v_0 \in \mathring{H}^1(\mathbb{T}^d).$$

That completes the proof. □

5. Convergence analysis of the numerical method

We shall now embark on the convergence analysis of the proposed method.

Theorem 3 (Convergence in the $\ell^\infty(0,T;H^1(\mathbb{T}^d))$ norm)**.** *Suppose that $h \leq \frac{1}{4}h_1$, where $h_1 := 1/(2c_1 - \varepsilon)_+$. Suppose, further, that $u \in L^\infty(0,T;H^s(\mathbb{T}^d))$ for some $s > 1$ and $\nabla u_{tt} \in L^2(0,T;L^2(\mathbb{T}^d))$. Then,*

$$\max_{1\leq m\leq M} \|\nabla(u(\cdot,t^m) - u_N^m)\| \leq C_1 N^{1-s}\|u\|_{L^\infty(0,T;H^s(\mathbb{T}^d))} + C_2 h\,\|\nabla u_{tt}\|_{L^2(0,T;L^2(\mathbb{T}^d))}\,,$$

where C_1 and C_2 are positive constants, which are independent of the discretization parameters h and N.

Proof. We begin by decomposing the discretization error

$$u(\cdot,t^k) - u_N^k = (u(\cdot,t^k) - P_N u(\cdot,t^k)) - (u_N^k - P_N u(\cdot,t^k)) =: \eta_N^k - \xi_N^k.$$

Note that

$$\begin{aligned}(u(\cdot,t^k) - P_N u(\cdot,t^k), \phi) &= 0, &&\forall\, \phi \in \mathring{\mathrm{X}}_N,\\ (\nabla(u(\cdot,t^k) - P_N u(\cdot,t^k)), \nabla\phi) = -(\Delta u(\cdot,t^k) - P_N(\Delta u(\cdot,t^k)), \phi) &= 0, &&\forall\, \phi \in \mathring{\mathrm{X}}_N,\\ (\Delta(u(\cdot,t^k) - P_N u(\cdot,t^k)), \Delta\phi) = (\Delta^2 u(\cdot,t^k) - P_N(\Delta^2 u(\cdot,t^k)), \phi) &= 0, &&\forall\, \phi \in \mathring{\mathrm{X}}_N.\end{aligned}$$

Hence,

$$(\eta_N^k, \phi) = (\nabla\eta_N^k, \nabla\phi) = (\Delta\eta_N^k, \Delta\phi) = 0, \qquad \forall\, \phi \in \mathring{\mathrm{X}}_N.$$

Next, we observe that

$$\begin{aligned}
&\left(\nabla\left(\frac{\xi_N^{k+1}-\xi_N^k}{h}\right),\nabla\phi\right)+\varepsilon(\Delta\xi_N^{k+1},\Delta\phi)\\
&\quad=\left(\nabla\left(\frac{u_N^{k+1}-u_N^k}{h}\right),\nabla\phi\right)+\varepsilon(\Delta u_N^{k+1},\Delta\phi)\\
&\qquad-\left(\nabla P_N\left(\frac{u(\cdot,t^{k+1})-u(\cdot,t^k)}{h}\right),\nabla\phi\right)-\varepsilon(\Delta P_N u(\cdot,t^{k+1}),\Delta\phi)\\
&\quad=-(\sigma(\nabla u_N^{k+1}),\nabla\phi)\\
&\qquad-\left(\nabla\left(\frac{u(\cdot,t^{k+1})-u(\cdot,t^k)}{h}\right),\nabla\phi\right)-\varepsilon(\Delta u(\cdot,t^{k+1}),\Delta\phi)\\
&\quad=\Big[(\sigma(\nabla u(\cdot,t^{k+1})),\nabla\phi)-(\sigma(\nabla u_N^{k+1}),\nabla\phi)\Big]\\
&\qquad+\left(\nabla\left[u_t(\cdot,t^{k+1})-\left(\frac{u(\cdot,t^{k+1})-u(\cdot,t^k)}{h}\right)\right],\nabla\phi\right)\\
&\quad=:\mathcal{T}_1(\phi)+\mathcal{T}_2(\phi),\qquad\forall\,\phi\in\mathring{\mathrm{X}}_N.
\end{aligned}\tag{11}$$

Now,

$$\begin{aligned}
|\mathcal{T}_1(\phi)|&=|(\sigma(\nabla u(\cdot,t^{k+1}))-\sigma(\nabla P_N u(\cdot,t^{k+1})),\nabla\phi)\\
&\qquad+(\sigma(\nabla P_N u(\cdot,t^{k+1}))-\sigma(\nabla u_N^{k+1}),\nabla\phi)|\\
&\le c_1\big(\|\nabla\eta_N^{k+1}\|+\|\nabla\xi_N^{k+1}\|\big)\|\nabla\phi\|,\qquad\forall\,\phi\in\mathring{\mathrm{X}}_N,
\end{aligned}\tag{12}$$

and

$$\begin{aligned}
|\mathcal{T}_2(\phi)|&=\left|\left(\frac{1}{h}\int_{t^k}^{t^{k+1}}\left[\int_s^{t^{k+1}}\nabla u_{tt}(\cdot,t)\,\mathrm{d}t\right]\mathrm{d}s,\nabla\phi\right)\right|\\
&\le h^{\frac12}\left(\int_{t^k}^{t^{k+1}}\|\nabla u_{tt}(\cdot,t)\|^2\,\mathrm{d}t\right)^{\frac12}\|\nabla\phi\|,\qquad\forall\,\phi\in\mathring{\mathrm{X}}_N.
\end{aligned}\tag{13}$$

We take $\phi=\xi_N^{k+1}$ in (11), (12) and (13), and substitute the resulting inequalities (12) and (13) into (11) to deduce that

$$\begin{aligned}
&\left(\nabla\left(\frac{\xi_N^{k+1}-\xi_N^k}{h}\right),\nabla\xi_N^{k+1}\right)+\varepsilon(\Delta\xi_N^{k+1},\Delta\xi_N^{k+1})\\
&\quad\le c_1\big(\|\nabla\eta_N^{k+1}\|+\|\nabla\xi_N^{k+1}\|\big)\|\nabla\xi_N^{k+1}\|+h^{\frac12}\left(\int_{t^k}^{t^{k+1}}\|\nabla u_{tt}(\cdot,t)\|^2\,\mathrm{d}t\right)^{\frac12}\|\nabla\xi_N^{k+1}\|.
\end{aligned}$$

Thanks to Poincaré's inequality, we then have that

$$\begin{aligned}\left(\frac{1}{2h}+\varepsilon-c_1\right)\|\nabla\xi_N^{k+1}\|^2 \\ &\le \frac{1}{2h}\|\nabla\xi_N^k\|^2 + c_1\|\nabla\eta_N^{k+1}\|\,\|\nabla\xi_N^{k+1}\| + h^{\frac12}\left(\int_{t^k}^{t^{k+1}}\|\nabla u_{tt}(\cdot,t)\|^2\,\mathrm{d}t\right)^{\frac12}\|\nabla\xi_N^{k+1}\| \\ &\le \frac{1}{2h}\|\nabla\xi_N^k\|^2 + c_1\|\nabla\xi_N^{k+1}\|^2 + \frac12 c_1\|\nabla\eta_N^{k+1}\|^2 + \frac{h}{2c_1}\int_{t^k}^{t^{k+1}}\|\nabla u_{tt}(\cdot,t)\|^2\,\mathrm{d}t,\end{aligned}$$

which implies that

$$\begin{aligned}&(1-2h(2c_1-\varepsilon))\,\|\nabla\xi_N^{k+1}\|^2 \\ &\qquad\le \|\nabla\xi_N^k\|^2 + c_1h\|\nabla\eta_N^{k+1}\|^2 + \frac{h^2}{c_1}\int_{t^k}^{t^{k+1}}\|\nabla u_{tt}(\cdot,t)\|^2\,\mathrm{d}t.\end{aligned}$$

Now, suppose that $h \le \frac14 h_1$, where $h_1 := 1/(2c_1-\varepsilon)_+$. Then, letting $c_* := 2/h_1$, we have that

$$[1-2h(2c_1-\varepsilon)]^{-1} \le 1+2c_*h \le 2,$$

and therefore

$$\|\nabla\xi_N^{k+1}\|^2 \le (1+2c_*h)\|\nabla\xi_N^k\|^2 + 2c_1h\|\nabla\eta_N^{k+1}\|^2 + \frac{2h^2}{c_1}\int_{t^k}^{t^{k+1}}\|\nabla u_{tt}(\cdot,t)\|^2\,\mathrm{d}t.$$

Summing the last inequality through $k = 0,\dots,m-1$, where $m \in \{1,\dots,M\}$, on noting that $\xi_N^0 = 0$ we have the following inequality:

$$\|\nabla\xi_N^m\|^2 \le 2c_*h\sum_{k=0}^{m-1}\|\nabla\xi_N^k\|^2 + 2c_1h\sum_{k=1}^{M}\|\nabla\eta_N^k\|^2 + \frac{2h^2}{c_1}\int_0^T\|\nabla u_{tt}(\cdot,t)\|^2\,\mathrm{d}t.$$

Hence, by a discrete Gronwall inequality,

$$\max_{1\le m\le M}\|\nabla\xi_N^m\|^2 \le \left(2c_1h\sum_{k=1}^{M}\|\nabla\eta_N^k\|^2 + \frac{2h^2}{c_1}\int_0^T\|\nabla u_{tt}(\cdot,t)\|^2\,\mathrm{d}t\right)\mathrm{e}^{2c_*T},$$

and therefore, by (8),

$$\max_{1\le m\le M}\|\nabla\xi_N^m\| \le C_1N^{1-s}\|u\|_{L^\infty(0,T;H^s(\mathbb{T}^d))} + C_2h\,\|\nabla u_{tt}\|_{L^2(0,T;L^2(\mathbb{T}^d))},$$

where C_1 and C_2 are positive constants, independent of h and N. Hence, by the triangle inequality $\|\nabla(u(\cdot,t^m)-u_N^m)\| \le \|\nabla\xi_N^m\| + \|\nabla\eta_N^m\|$, we have that

$$\max_{1\le m\le M}\|\nabla(u(\cdot,t^m)-u_N^m)\| \le C_1N^{1-s}\|u\|_{L^\infty(0,T;H^s(\mathbb{T}^d))} + C_2h\,\|\nabla u_{tt}\|_{L^2(0,T;L^2(\mathbb{T}^d))}$$

with possibly different positive constants C_1 and C_2, which are independent of the discretization parameters h and N. □

Next, we shall prove a second convergence theorem in another norm. To this end, we require three preparatory lemmas.

Lemma 2. *Suppose that* $u_0 \in \mathring{H}^3(\mathbb{T}^d)$*,* $d \in \{1,2,3\}$*. Then* $\|u\|_{L^\infty(0,T;W^{2,3}(\mathbb{T}^d))} \le C(T, \|u_0\|_{H^3})$*, and* $\|P_N u\|_{L^\infty(0,T;W^{2,3}(\mathbb{T}^d))} \le C(T, \|u_0\|_{H^3})$*.*

Proof. We shall prove that $\|u\|_{L^\infty(0,T;H^\ell(\mathbb{T}^d))} \le C(T, \|u_0\|_{H^\ell})$, for $\ell = 1,2,3$. The first assertion will then follow from the continuous embedding of the Sobolev space $H^3(\mathbb{T}^d) = W^{3,2}(\mathbb{T}^d)$ into $W^{2,3}(\mathbb{T}^d)$ (i.e., $\|w\|_{W^{2,3}} \le C\|w\|_{H^3}$, $d = 1,2,3$, applied with $w = u(\cdot,t)$, $t \in [0,T]$), and the second assertion will follow with $w = P_N u(\cdot,t)$, $t \in [0,T]$, from the same Sobolev embedding by noting that

$$\|P_N u(\cdot,t)\|_{H^3} \le \|u(\cdot,t)\|_{H^3} \le C(T, \|u_0\|_{H^3}), \quad t \in [0,T].$$

(a) Let us first show that $\|u\|_{L^\infty(0,T;H^1(\mathbb{T}^d))} \le C(T, \|u_0\|_{H^1})$. We do so by taking $v = u$ in (2), to deduce, using (4), that

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\nabla u(t)\|^2 \le c_3(2\pi)^d,$$

and therefore $\|\nabla u(t)\|^2 \le \|\nabla u_0\|^2 + 2c_3(2\pi)^d T$. By Poincaré's inequality,

$$\|u(t)\|_{H^1}^2 \le 2\left(\|\nabla u_0\|^2 + 2c_3(2\pi)^d T\right) \text{ for all } t \in [0,T],$$

which implies the desired bound.

(b) Next, we prove that $\|u\|_{L^\infty(0,T;H^2(\mathbb{T}^d))} \le C(T, \|u_0\|_{H^2})$. We do so by taking $v = u_t$ in (2), to deduce, using (4), that

$$\begin{aligned}
\|\nabla u_t(t)\|^2 + \frac{\varepsilon}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\Delta u(t)\|^2 &= -(\sigma(\nabla u(t)), \nabla u_t(t)) \\
&= (\sigma(0) - \sigma(\nabla u(t)), \nabla u_t(t)) \le c_1\|\nabla u(t)\|\,\|\nabla u_t(t)\| \\
&\le \frac{1}{2}c_1^2\|\nabla u(t)\|^2 + \frac{1}{2}\|\nabla u_t(t)\|^2,
\end{aligned}$$

and therefore $\|\Delta u(t)\|^2 \le \|\Delta u_0\|^2 + (c_1^2/\varepsilon)\int_0^T \|\nabla u(s)\|^2\,\mathrm{d}s$ for all $t \in [0,T]$. By part (a) above, $\|\Delta u(t)\|^2 \le C(T, \|u_0\|_{H^2})$ for all $t \in [0,T]$, and finally, by Poincaré's inequality, we have the desired bound.

(c) To prove that $\|u\|_{L^\infty(0,T;H^3(\mathbb{T}^d))} \le C(T, \|u_0\|_{H^3})$, we take $v = -\Delta u_t$ in (2), to deduce, using (4), that

$$\begin{aligned}
\|\Delta u_t(t)\|^2 + \frac{\varepsilon}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\nabla\Delta u(t)\|^2 &= -(\operatorname{div}\sigma(\nabla u(t)), \Delta u_t(t)) \\
&\le |\sigma|_{W^{1,\infty}}|u(t)|_{H^2}\|\Delta u_t(t)\| \\
&\le \frac{1}{2}c_1^2|u(t)|_{H^2}^2 + \frac{1}{2}\|\Delta u_t(t)\|^2,
\end{aligned}$$

and therefore $\|\nabla\Delta u(t)\|^2 \le \|\nabla\Delta u_0\|^2 + (c_1^2/\varepsilon)\int_0^T |u(s)|_{H^2}^2\,\mathrm{d}s$ for all $t \in [0,T]$. By part (b) above, $\|\nabla\Delta u(t)\|^2 \le C(T, \|u_0\|_{H^3})$ for all $t \in [0,T]$, and finally, by Poincaré's inequality, we have the desired bound. $\square$

Lemma 3. *Suppose that* $u_0 \in \mathring{H}^3(\mathbb{T}^d)$. *Then*

$$\max_{1\le k\le M} \|u_N^k\|_{W^{2,3}} \le C(T, \|u_0\|_{H^3}).$$

Proof. The proof is analogous to that of Lemma 2, the only difference being that in the argument that yields the analogues of (a), (b), (c) in the proof of Lemma 2 above instead of the identity $(w_t(t), w(t)) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|w(t)\|^2$, we use that

$$(w(t) - w(s), w(t)) \ge \frac{1}{2}(\|w(t)\|^2 - \|w(s)\|^2), \quad t, s \in [0, T],$$

for any sufficiently smooth function, and in particular for any element of the linear space $\mathring{\mathrm{X}}_N$. □

Lemma 4. *Let* $v, w \in \mathring{W}^{2,3}(\mathbb{T}^d) = \{\phi \in W^{2,3}(\mathbb{T}^d) : \fint_{\mathbb{T}^d} \phi \,\mathrm{d}x = 0\}$. *Suppose also, in addition to* (3), *that* $\sigma \in W^{2,\infty}(\mathbb{R}^d)$. *Then, there exists a positive constant* $C \ge 1$, *independent of* v *and* w, *such that*

$$\|(-\Delta)^{-1}\mathrm{div}[\sigma(\nabla v) - \sigma(\nabla w)]\| \le c_4\|v - w\|,$$

where

$$c_4 = c_4(v, w) := C\Big(|\sigma|_{W^{1,\infty}} + |\sigma|_{W^{2,\infty}}\big(|v|_{W^{2,3}} + |w|_{W^{2,3}}\big)\Big).$$

Proof. We begin by noting that

$$\begin{aligned}
\|(-\Delta)^{-1}\mathrm{div}[\sigma(\nabla v) - \sigma(\nabla w)]\| &= \|\mathrm{div}[\sigma(\nabla v) - \sigma(\nabla w)]\|_{\mathring{H}^{-2}} \\
&\le C\|\sigma(\nabla v) - \sigma(\nabla w)\|_{\mathring{H}^{-1}} \\
&\le C\|\sigma(\nabla v) - \sigma(\nabla w)\|_{H^{-1}},
\end{aligned}$$

where $C \ge 1$ is a constant, independent of v and w. Now, for each $i = 1, \dots, d$,

$$\begin{aligned}
\|\sigma_i(\nabla v) - \sigma_i(\nabla w)\|_{H^{-1}} &= \sup_{\phi\in\mathring{H}^1(\mathbb{T}^d)} \frac{(\sigma_i(\nabla v) - \sigma_i(\nabla w), \phi)}{\|\nabla\phi\|} \\
&= \sup_{\phi\in\mathring{H}^1(\mathbb{T}^d)} \frac{\left(\int_0^1 \nabla\sigma_i(\theta\nabla v + (1-\theta)\nabla w)\,\mathrm{d}\theta \cdot \nabla(v - w), \phi\right)}{\|\nabla\phi\|} \\
&= \sup_{\phi\in\mathring{H}^1(\mathbb{T}^d)} \frac{\left(v - w, \mathrm{div}\left[\phi\left(\int_0^1 \nabla\sigma_i(\theta\nabla v + (1-\theta)\nabla w)\,\mathrm{d}\theta\right)\right]\right)}{\|\nabla\phi\|} \\
&\le \|v - w\| \sup_{\phi\in\mathring{H}^1(\mathbb{T}^d)} \frac{\left\|\mathrm{div}\left[\phi\left(\int_0^1 \nabla\sigma_i(\theta\nabla v + (1-\theta)\nabla w)\,\mathrm{d}\theta\right)\right]\right\|}{\|\nabla\phi\|}.
\end{aligned}$$

Let us consider the numerator in the fraction in the last line:

$$\begin{aligned}
&\left\|\operatorname{div}\left[\phi\left(\int_0^1 \nabla\sigma_i(\theta\nabla v+(1-\theta)\nabla w)\,\mathrm{d}\theta\right)\right]\right\| \\
&\quad\le \left\|\nabla\phi\cdot\int_0^1 \nabla\sigma_i(\theta\nabla v+(1-\theta)\nabla w)\,\mathrm{d}\theta\right\| \\
&\qquad + \left\|\phi\int_0^1 \operatorname{div}\left[\nabla\sigma_i(\theta\nabla v+(1-\theta)\nabla w)\right]\,\mathrm{d}\theta\right\| \\
&\quad\le \|\nabla\phi\|\left\|\int_0^1 \nabla\sigma_i(\theta\nabla v+(1-\theta)\nabla w)\,\mathrm{d}\theta\right\|_{L^\infty} \\
&\qquad + \|\phi\|_{L^6}\left\|\int_0^1 \operatorname{div}\left[\nabla\sigma_i(\theta\nabla v+(1-\theta)\nabla w)\right]\,\mathrm{d}\theta\right\|_{L^3} \\
&\quad\le C\|\nabla\phi\|\left[\left\|\int_0^1 \nabla\sigma_i(\theta\nabla v+(1-\theta)\nabla w)\,\mathrm{d}\theta\right\|_{L^\infty}\right. \\
&\qquad \left. + \left\|\int_0^1 \operatorname{div}\left[\nabla\sigma_i(\theta\nabla v+(1-\theta)\nabla w)\right]\,\mathrm{d}\theta\right\|_{L^3}\right] \\
&\quad\le C\|\nabla\phi\|\Big[|\sigma_i|_{W^{1,\infty}}+|\sigma_i|_{W^{2,\infty}}\big(|v|_{W^{2,3}}+|w|_{W^{2,3}}\big)\Big].
\end{aligned}$$

We thus deduce that

$$\|\sigma(\nabla v)-\sigma(\nabla w)\|_{H^{-1}}\le C\Big[|\sigma|_{W^{1,\infty}}+|\sigma|_{W^{2,\infty}}\big(|v|_{W^{2,3}}+|w|_{W^{2,3}}\big)\Big]\,\|v-w\|.$$

That completes the proof. □

In the proof of Theorem 4 below Lemma 4 will be applied first with $v=u(\cdot,t^{k+1})$ and $w=P_N u(\cdot,t^{k+1})$, and then with $v=P_N u(\cdot,t^{k+1})$ and $w=u_N^{k+1}$. Since c_4, as defined in the statement of Lemma 4, is required to be a constant in the context of the proof of Theorem 4, we need bounds on the $W^{2,3}$ seminorms of $u(\cdot,t^{k+1})$, $P_N u(\cdot,t^{k+1})$ and u_N^{k+1}, independent of the discretization parameters; those bounds are, in turn, furnished by Lemmas 2 and 3. Thus, hereafter, c_4 will signify a positive constant, independent of the discretization parameters, which can be computed by tracking the constants in Lemmas 2, 3 and 4, and such that $c_4\ge c_1$.

We are now ready to state and prove our second convergence result.

Theorem 4 (Convergence in the $\ell^\infty(0,T;L^2(\mathbb{T}^d))$ norm)**.** *Suppose that $h\le\frac{1}{4}h_2$, where $h_2:=1/(2c_4-\varepsilon)_+$. Suppose, further, that*

$$\sigma\in W^{2,\infty}(\mathbb{R}^d),\ u_0\in \mathring{H}^3(\mathbb{T}^d),\ u\in L^\infty(0,T;H^s(\mathbb{T}^d)),$$

for some $s\ge 3$ and $u_{tt}\in L^2(0,T;L^2(\mathbb{T}^d))$. Then,

$$\max_{1\le m\le M}\|u(\cdot,t^m)-u_N^m\|\le C_1N^{-s}\|u\|_{L^\infty(0,T;H^s(\mathbb{T}^d))}+C_2h\,\|u_{tt}\|_{L^2(0,T;L^2(\mathbb{T}^d))},$$

where C_1 and C_2 are positive constants, which are independent of h and N.

Proof. We proceed identically as in the proof of Theorem 3, except that we now take $\phi = (-\Delta)^{-1}\xi_N^{k+1}$ in (11), and note that

$$\left(\left(\frac{\xi_N^{k+1} - \xi_N^k}{h}\right), \xi_N^{k+1}\right) + \varepsilon(\nabla\xi_N^{k+1}, \nabla\phi)$$
$$= \mathcal{T}_1((-\Delta)^{-1}\xi_N^{k+1}) + \mathcal{T}_2((-\Delta)^{-1}\xi_N^{k+1}), \qquad \forall\,\phi \in \mathring{\mathrm{X}}_N, \tag{14}$$

with $\mathcal{T}_1$ and $\mathcal{T}_2$ as defined in (11); further,

$$\begin{aligned}|\mathcal{T}_1((-\Delta)^{-1}\xi_N^{k+1})| &= |((-\Delta)^{-1}\mathrm{div}[\sigma(\nabla u(\cdot,t^{k+1})) - \sigma(\nabla P_N u(\cdot,t^{k+1}))], \xi_N^{k+1}) \\ &\quad +((-\Delta)^{-1}\mathrm{div}[\sigma(\nabla P_N u(\cdot,t^{k+1})) - \sigma(\nabla u_N^{k+1})], \xi_N^{k+1})| \\ &\le c_4\big(\|\eta_N^{k+1}\| + \|\xi_N^{k+1}\|\big)\|\xi_N^{k+1}\|, \end{aligned} \tag{15}$$

where, in the transition to the last line, Lemma 4 was used (c_4 being a positive constant here, independent of the discretization parameters, thanks to Lemmas 2 and 3, $c_4 \ge c_1$), and

$$\begin{aligned}|\mathcal{T}_2((-\Delta)^{-1}\xi_N^{k+1})| &= \left|\left(\frac{1}{h}\int_{t^k}^{t^{k+1}}\left[\int_s^{t^{k+1}} u_{tt}(\cdot,t)\,\mathrm{d}t\right]\mathrm{d}s, \xi_N^{k+1}\right)\right| \\ &\le h^{\frac{1}{2}}\left(\int_{t^k}^{t^{k+1}} \|u_{tt}(\cdot,t)\|^2\,\mathrm{d}t\right)^{\frac{1}{2}}\|\xi_N^{k+1}\|. \end{aligned} \tag{16}$$

We substitute (15) and (16) into (14), and then proceed in the same way as in the proof of Theorem 3, *mutatis mutandis.* □

The error bounds stated in Theorems 3 and 4 are of optimal order with respect to both the spatial and the temporal discretization parameter.

6. Conclusions and outlook

We have constructed a numerical method for the approximate solution of the H^1 gradient flow of the nonconvex functional $I[u]$ defined by (2), involving a nonnegative multi-well potential term and a bending energy term, based on a spatial Fourier–Galerkin spectral discretization and implicit Euler time discretization. The numerical method was shown to have a solution for any choice of the spatial and temporal discretization parameters, N and h, respectively, and it was also shown that for h sufficiently small the solution is unique (cf. Theorem 1). For h sufficiently small, the method was shown to be stable in the norm $\ell^\infty(0,T;H^1(\mathbb{T}^d))$, uniformly with respect to N (cf. Theorem 2). Granted sufficient smoothness, the sequence of numerical solutions was further shown to converge, with optimal orders of convergence, to the analytical solution in both the $\ell^\infty(0,T;H^1(\mathbb{T}^d))$ norm (cf. Theorem 3) and the $\ell^\infty(0,T;L^2(\mathbb{T}^d))$ norm (cf. Theorem 4). A notable feature of Theorem 4 is that its proof requires the Lipschitz continuity of the zeroth order nonlocal nonlinear operator $v \mapsto (-\Delta)^{-1}\mathrm{div}\,[\sigma(\nabla v)]$; this was shown in Lemma 4 to hold, in the L^2 norm, on bounded balls of the Sobolev space $\mathring{W}^{2,3}(\mathbb{T}^d)$ for $d = 1, 2, 3$.

All of our results, with the exception of Lemma 4 and our second convergence result stated in Theorem 4, which requires Lemma 4, hold in any number of space dimensions. The proof of Lemma 4 relies on various Sobolev inequalities, some of which hold in the (physically relevant) space dimensions, $d = 1, 2, 3$, only. For this reason, the number of space dimensions was limited to three or less from the outset. The precise form of the second term in the functional $I[u]$ defined by (2) is of no particular significance (except for its physical interpretation as a simple model of bending energy) up to and including Theorem 3; similar results could have been shown to hold had $(\Delta u)^2$ been replaced, for example, by $[(-\Delta)^\alpha u]^2$, with $\alpha \in (0, 1]$. The results presented herein also hold for the vectorial version of the functional

$$u \mapsto I[u] := \int_{\mathbb{T}^d} W(\nabla u) + \frac{\varepsilon}{2}|\Delta u|^2 \,\mathrm{d}x,$$

where

$$u : \mathbb{T}^d \to \mathbb{R}^d,\ \nabla u : \mathbb{T}^d \to \mathbb{R}^{d\times d},\ \Delta u : \mathbb{T}^d \to \mathbb{R}^d,$$

$|\cdot|$ denotes the 2-norm on $\mathbb{R}^d$, and W is a nonnegative potential satisfying (3) (with $p, q \in \mathbb{R}^{d\times d}$, $|\cdot|$ on the left-hand side of the first inequality in (3) denoting the 2-norm on $\mathbb{R}^{d\times d\times d}$ and on its right-hand side the 2-norm on $\mathbb{R}^{d\times d}$).

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