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AN IMPLICIT MIDPOINT SPECTRAL APPROXIMATION OF NONLOCAL CAHN–HILLIARD EQUATIONS*

BARBORA BENEŠOVÁ†, CHRISTOF MELCHER†, AND ENDRE SÜLI‡

Abstract. The paper is concerned with the convergence analysis of a numerical method for nonlocal Cahn–Hilliard equations. The temporal discretization is based on the implicit midpoint rule and a Fourier spectral discretization is used with respect to the spatial variables. The sequence of numerical approximations in shown to be bounded in various norms, uniformly with respect to the discretization parameters, and optimal order bounds on the global error of the scheme are derived. The uniform bounds on the sequence of numerical solutions as well as the error bounds hold unconditionally, in the sense that no restriction on the size of the time step in terms of the spatial discretization parameter needs to be assumed.

Key words. Cahn–Hilliard equation, Ohta–Kawasaki equation, Fourier–Galerkin approximation, midpoint scheme

AMS subject classifications. 65M15, 65M70, 35Q99, 82D60

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1. Introduction.

Pattern formation processes due to phase separation of binary mixtures can conveniently be modeled by means of nonlocal Cahn–Hilliard equations. By this we mean H^{-1} gradient flows associated with functionals of Ginzburg–Landau-type, which may include a dipolar interaction term. In a spatially periodic setting, i.e., using the three-dimensional torus $\mathbb{T}^3 := 2\pi\mathbb{R}^3/\mathbb{Z}^3$ as spatial domain, such functionals typically have the form

$$E(u) = \frac{1}{2}\fint_{\mathbb{T}^3} \varepsilon^2|\nabla u|^2 + \frac{1}{2}(1-u^2)^2\,\mathrm{d}x + \frac{1}{2}\sum_{k\in\mathbb{Z}^3\setminus\{0\}} \hat{\sigma}(k)|\hat{u}(k)|^2. \tag{1.1}$$

Here, $u : \mathbb{T}^3 \to [-1,1]$ is the phase field indicator and $\hat{u}(k)$ are its Fourier coefficients (cf. section 2). In particular $u = \pm 1$ correspond to the two pure phases, respectively, while

$$m = \fint_{\mathbb{T}^3} u\,\mathrm{d}x \in (-1,1)$$

is a given relative concentration, which is preserved by the H^{-1} gradient flow. The (small) parameter $\varepsilon > 0$ reflects the width of the interface between the two pure phases, and $\hat{\sigma} : \mathbb{Z}^3 \to \mathbb{R}_{\geq 0}$ is a Fourier multiplier, which is symmetric in the sense that $\hat{\sigma}(k) = \hat{\sigma}(-k)$ for all $k \in \mathbb{Z}^3 \setminus \{0\}$ and which decays to zero as $|k| \to \infty$. In this context, a nonlocal energy term of the form

$$E_{\mathrm{dipol}}(u) = \frac{1}{2}\sum_{k\in\mathbb{Z}^3\setminus\{0\}} \hat{\sigma}(k)|\hat{u}(k)|^2$$

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†Department of Mathematics I, RWTH Aachen University, D-52056 Aachen, Germany (benesova@math1.rwth-aachen.de, melcher@math1.rwth-aachen.de).
‡Mathematical Institute, University of Oxford, Oxford OX2 6GG, UK (suli@maths.ox.ac.uk).

typically models dipolar interactions and prefers oscillations of the phase indicator, i.e., microstructure. Typical examples are multiples of negative Sobolev norms squared. The dipolar energy $E_{\text{dipol}}(u)$ represents the energy of a field, which is induced by u and depends on u in a nonlocal fashion, e.g., through a linear differential or integral equation.

Various models of energy-driven pattern formation from solid state physics and materials science fall into the framework of (1.1). For ease of presentation, we shall have two prototypical examples in mind throughout the article: first, the case when $\hat{\sigma}(k) \equiv 0$, i.e., $E(u)$ becomes the unperturbed Ginzburg–Landau energy and its H^{-1} gradient flow is then the classical Cahn–Hilliard equation derived in [2]. Second, we shall consider the case $\hat{\sigma}(k) = \frac{\sigma}{|k|^2}$ for some constant $\sigma > 0$. In this case

$$\sum_{k\in\mathbb{Z}^3\setminus\{0\}} \hat{\sigma}(k)|\hat{u}(k)|^2 = \sigma \fint_{\mathbb{T}^3} |\nabla\varphi|^2\, dx, \quad \text{where} \quad \Delta\varphi = u - m \quad \text{in } \mathbb{T}^3,$$

and $E(u)$ becomes the *Ohta–Kawasaki energy* introduced in [19] for modeling the phase separation of diblock copolymers, which are chain molecules that consist of two different and chemically incompatible segments joined together by a covalent chemical bond. Diblock copolymers find their application in diverse fields, including nanotechnology, biomedicine, and microelectronics [9]. The form corresponding to (1.1) was derived in [4, 18] and can be written as

$$E(u) = \frac{1}{2}\fint_{\mathbb{T}^3} \varepsilon^2|\nabla u|^2 + \frac{1}{2}(1-u^2)^2 + \sigma|(-\Delta)^{-\frac{1}{2}}(u-m)|^2\,\mathrm{d}x. \tag{1.2}$$

The parameter $\sigma > 0$ is inversely proportional to the lengths of the molecules involved. In this paper we shall focus on the Ohta–Kawasaki model, including the limiting case of $\sigma = 0$, which corresponds to the classical Cahn–Hilliard model. The numerical method proposed here can be adapted to more general multipliers $\hat{\sigma}$ in (1.1) with little effort, including, e.g., dipolar stray-field interaction in magnetic garnet films [14].

Let us now turn to the H^{-1} gradient flow of the Ohta–Kawasaki functional (1.2) with $\varepsilon > 0$ and $\sigma \geq 0$, including the classical Cahn–Hilliard equation when $\sigma = 0$. Since the relative concentration $m \in (-1, 1)$ is conserved along the flow, the manifold of admissible configurations is the affine space

$$M_m := \left\{ v \in H^1(\mathbb{T}^3) \ : \ \fint_{\mathbb{T}^3} v\,\mathrm{d}x = m \right\},$$

whose tangent space of admissible variations (i.e., the space of admissible test functions) is

$$\mathring{H}^1(\mathbb{T}^3) := \left\{ \phi \in H^1(\mathbb{T}^3) \ : \ \fint_{\mathbb{T}^3} \phi\,\mathrm{d}x = 0 \right\}.$$

Note that the homogeneous H^1-seminorm (cf. below) is a norm on this space.

The abstract characterization of the H^{-1} gradient flow of E over the configuration space M_n, given by

$$\langle u_t, \phi\rangle_{H^{-1}} + DE(u)\langle\phi\rangle = 0 \quad \text{for all} \quad \phi \in \mathring{H}^1(\mathbb{T}^3), \tag{1.3}$$

where $\langle\cdot,\cdot\rangle_{H^{-1}}$ denotes the homogeneous H^{-1} inner product (cf. section 2) and $\mathrm{D}E(u)\langle\phi\rangle$ is the Gâteaux derivative of E at u in the direction of ϕ, gives rise to the following fourth-order nonlinear parabolic equation, referred to as the *Ohta–Kawasaki equation*:

$$u_t + \Delta\Big(\varepsilon^2 \Delta u - (u^3 - u)\Big) + \sigma(u - m) = 0. \tag{1.4}$$

In fact, by using test functions of the form $\phi = -\Delta\varphi$, with arbitrary $\varphi \in C^\infty(\mathbb{T}^3)$, we find

$$\langle u_t, \varphi\rangle_{L^2} = \langle \mu, \Delta\varphi\rangle_{L^2},$$

where the generalized chemical potential $\mu = \varepsilon^2(-\Delta)u + (u^3 - u) + \sigma(-\Delta)^{-1}(u - m)$ is the L^2 gradient of E at u, and we recover the strong formulation $u_t = \Delta\mu$ equivalent to (1.4).

Expressed in terms of $v := u - m$, which belongs to the linear space $\mathring{H}^1(\mathbb{T}^3)$ at each time $t > 0$, (1.4) turns into

$$v_t + \Delta\Big(\varepsilon^2 \Delta v - \big((v + m)^3 - (v + m)\big)\Big) + \sigma v = 0. \tag{1.5}$$

The goal of this paper is to develop a temporally second-order, *unconditionally stable*, numerical scheme for the approximate solution of (1.4), using the implicit midpoint rule (with time step h) and a spatial discretization via the Fourier–Galerkin spectral method based on projection onto a finite-dimensional space, X_N, as defined in section 2, which exhibits spectral convergence in space. The construction of the scheme has been motivated by the work of Elliott and French [11] as well as [10], [15], and [16] where second-order schemes similar to ours were proposed. Second-order convergence was, however, only shown there under the assumption that the sequence of numerical solutions remains uniformly bounded (in L^∞) throughout temporal evolution.

In this work, we prove an a priori error bound leading to optimal-order convergence in time and space without any additional assumptions on the sequence of numerical solutions, and with no added restriction on the temporal step size h in terms of the Fourier–Galerkin spatial discretization parameter N; more precisely, we prove that the error is of order $\mathcal{O}(h^2 + N^{-s})$, where $s > 0$ is the spatial Sobolev index of the analytical solution. To this end, we exploit that the numerical scheme proposed in section 3 respects the monotonicity of the (cubic) nonlinearity. We also establish various *unconditional* uniform bounds on the sequence of approximate solutions in section 4; by this, we mean that the sequence of numerical solutions is bounded in suitable norms by data-dependent constants, which are independent of the discretization parameters h and N, and without demanding any particular relationship between h and N. Proving such uniform bounds is particularly important from the modeling point of view. Indeed, since the variable u serves as a phase indicator its values should be uniformly bounded (and ideally within the range $[-1, 1]$, which however need not be satisfied for the Cahn–Hilliard flow); this can be important, e.g., when the phase evolution is coupled to other equations. In fact, the unconditional stability of our scheme is, in a sense, a "stronger" property than its optimal convergence since the latter can be deduced from the former by invoking the results of [11], whereas optimal convergence does not necessarily imply unconditional stability. Nonetheless, we chose not to rely on [11]; instead, we present an alternative proof of optimal convergence. This is motivated by the fact that our proof of unconditional stability uses specific properties of the Fourier–Galerkin spatial approximation and generalizations to other spatial approximations seem nontrivial.

These, to the authors' knowledge, are the first results of this kind for a second-order accurate temporal discretization of Cahn–Hilliard–type flow in the spatially multivariate case. In previous works, uniform boundedness of the sequence of approximate solutions and a priori error bounds for temporally second-order discretizations of such equations were obtained for specific combinations of the spatial and temporal discretization parameters only (e.g., [8]).

For one-step schemes unconditional stability has already been established in the literature. A very convenient approach, that relates to our method of proof, is based on *convex-concave splitting*; see, e.g., [13]. Such methods amount to writing the double-well potential in the Ginzburg–Landau energy as a sum of a convex and a concave function. Then, the monotone part, which stems from a convex potential, is discretized differently from the other part of the nonlinearity that arises from the concave function (in our case this part is just linear).

Let us, at this point, briefly compare our approach to other results in the literature; alternatives to our scheme include the Crank–Nicolson scheme, which involves taking the arithmetic average of the nonlinearity at the previous and the current time level; or exploiting that the nonlinearity is actually a derivative of an underlying potential $\mathscr{W}$, which is approximated by a difference quotient (cf. [8] or [7], for example, for an adaptation of this technique to a spectral method).

Compared to these alternatives, the advantage of the implicit midpoint scheme, considered here, is that that it preserves the monotonicity of the nonlinearity under discretization (cf. section 3). On the other hand, proving conservation of energy, and thereby boundedness of the sequence of approximate solutions in the H^1 norm, is challenging, particularly when compared to the scheme from [8]. As a matter of fact, the proof of conservation of energy was not given in [11] for the fully discrete approximation, although it was shown to hold in the semidiscrete case in [12], with the temporal variable left undiscretized. Nevertheless, once H^1-boundedness of the sequence of approximate solutions has been shown for our scheme, deducing boundedness in higher-order Sobolev norms is immediate (and this is again in contrast to the scheme from [8] for which boundedness of the sequence of approximate solutions in stronger norms does not seem accessible). Thus, to show the uniform boundedness of the sequence of approximate solutions in the H^1 norm we exploit, besides the monotone growth of the nonlinear term, the fact that the L^2 orthogonal projector onto the finite-dimensional Fourier–Galerkin space X_N commutes with spatial differential operators (which then allows us to proceed with the analysis of the method as if the spatial variable were left undiscretized); cf. Theorems 4.1, 4.4, and 4.5 below.

Let us remark that the use of a Fourier–Galerkin spatial discretization seems crucial in our a priori estimates analysis. For example, in [1], in the case of a finite element spatial discretization combined with a Crank–Nicolson time stepping scheme, instability was numerically observed outside the dissipative regime. No such adverse behavior was observed for the scheme proposed herein.

The paper is structured as follows. In section 2 we review some basic results concerning Fourier–Galerkin spectral approximation in the context of the problem under consideration. In section 3 we formulate the proposed numerical method for the Ohta–Kawasaki equation and prove that the method is correctly defined, in the sense that it possesses a unique solution. Section 4 contains our proofs of the unconditional uniform a priori bounds on the sequence of numerical solutions. Section 5 is devoted to the convergence analysis of the scheme. In section 6 we discuss an iterative scheme for the solution of the system of nonlinear algebraic equations resulting at each time level. Section 7 focuses on numerical experiments, which confirm our theoretical findings.

2. Fourier–Galerkin approximation in brief. Since we aim to devise a spectral approximation (in space) of (1.4) it is natural to express the function u in terms of its Fourier series expansion

$$u(x) = \sum_{k\in\mathbb{Z}^3} \hat{u}(k)e^{ik\cdot x},$$

where $\hat{u}(k)$, $k \in \mathbb{Z}^3$, are the Fourier coefficients of u. For $N \in \mathbb{N}$ we define $\mathbb{Z}_N = \{-N,\dots,N\}$ and denote the 3-fold Cartesian product of this set by $\mathbb{Z}_N^3$. We define the following $(2N-1)^3$-dimensional subspace of $L^2(\mathbb{T}^3;\mathbb{C})$:

$$\mathrm{S}_N := \mathrm{span}_{\mathbb{C}}\{x \in \mathbb{T}^3 \mapsto \mathrm{e}^{ik\cdot x} \,:\, k \in \mathbb{Z}_N^3\},$$

and we denote by $P_N : L^2(\mathbb{T}^3;\mathbb{C}) \to \mathrm{S}_N$ the orthogonal projection operator obtained by truncating the Fourier series, i.e.,

$$P_N u(x) := \sum_{k\in\mathbb{Z}_N^3} \hat{u}(k)\,\mathrm{e}^{ik\cdot x}.$$

We further introduce the subspace of real-valued functions contained in S_N, denoted by X_N, through

$$\mathrm{X}_N := \left\{ x \in \mathbb{T}^3 \mapsto \sum_{k\in\mathbb{Z}_N^3} c(k)\,\mathrm{e}^{ik\cdot x} : c(-k) = \overline{c(k)} \right\},$$

and we consider the subspace

$$\mathring{\mathrm{X}}_N := \{\phi \in \mathrm{X}_N \,:\, \hat{\phi}(0) = 0\}, \tag{2.1}$$

consisting of all functions $\phi \in \mathrm{X}_N$ that satisfy the volume constraint

$$⨍_{\mathbb{T}^3} \phi(x)\,\mathrm{d}x = 0.$$

We refer to $P_N u$ as the *Fourier–Galerkin projection* of $u \in L^2(\mathbb{T}^3)$. We shall use the index N to emphasize, for the solution of the discretized equation, that it is an element of X_N.

For the reader's convenience, we review some tools and notation used throughout the article. For functions u_N and v_N in X_N, i.e.,

$$u_N(x) = \sum_{k\in\mathbb{Z}_N^3} \hat{u}(k)\,\mathrm{e}^{ik\cdot x} \quad \text{and} \quad v_N(x) = \sum_{k\in\mathbb{Z}_N^3} \hat{v}(k)\,\mathrm{e}^{ik\cdot x},$$

the L^2 inner product and norm are defined by

$$\langle u_N, v_N\rangle := \sum_{k\in\mathbb{Z}_N^3} \hat{u}(k)\overline{\hat{v}(k)} \quad \text{and} \quad \|u_N\| = \sqrt{\langle u_N, u_N\rangle},$$

respectively. By virtue of Plancherel's theorem, the space $L^2(\mathbb{T}^3) = L^2(\mathbb{T}^3;\mathbb{R})$ is the closure, with respect to the L^2 norm, of the union of the spaces X_N, $N \geq 1$. In particular, for $u, v \in L^2(\mathbb{T}^3)$,

$$\begin{aligned}\langle u, v\rangle &= \sum_{k\in\mathbb{Z}^3} \hat{u}(k)\overline{\hat{v}(k)} = ⨍_{\mathbb{T}^3} u(x)\overline{v(x)}\,\mathrm{d}x \\ &= ⨍_{\mathbb{T}^3} u(x)v(x)\,\mathrm{d}x \quad \text{and hence} \quad |\langle u, v\rangle| \leq \|u\|\|v\|;\end{aligned}$$

furthermore, we set $\langle\cdot,\cdot\rangle = \langle\cdot,\cdot\rangle_{L^2}$ and $\|\cdot\| = \|\cdot\|_{L^2}$. Similarly, we define the space $\mathring{H}^{-1}(\mathbb{T}^3)$ as 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

$$\langle u, v\rangle_{H^{-1}} = \sum_{k\in\mathbb{Z}^3\setminus\{0\}} |k|^{-2}\,\hat{u}(k)\,\overline{\hat{v}(k)}.$$

Because of the volume constraint, we shall be mainly concerned with situations where test functions have zero integral. In this case the following dual estimate will be crucial: if $u_N \in \mathrm{X}_N$ and $v_N \in \mathring{\mathrm{X}}_N$, then

$$|\langle u_N, v_N\rangle| \leq \|\nabla u_N\|\|v_N\|_{H^{-1}}, \tag{2.2}$$

and hence $\langle\cdot,\cdot\rangle$ extends to a pairing between $H^1(\mathbb{T}^3) = \{u \in L^2(\mathbb{T}^3) : \nabla u \in L^2(\mathbb{T}^3)^3\}$ and $\mathring{H}^{-1}(\mathbb{T}^3)$. More generally, we may define, for $s \in \mathbb{R}$, the homogeneous H^s inner product

$$\langle u, v\rangle_{H^s} = \sum_{k\in\mathbb{Z}^3\setminus\{0\}} |k|^{2s}\,\hat{u}(k)\,\overline{\hat{v}(k)}, \tag{2.3}$$

characterizing the homogeneous Sobolev–Slobodetskiĭ space $\mathring{H}^s(\mathbb{T}^3)$ as the closure, with respect to the induced homogeneous H^s norm $[u]_{H^s} = \sqrt{\langle u, u\rangle_{H^s}}$, of the union of the spaces $\mathring{\mathrm{X}}_N$, $N \geq 1$. For $s > 0$, the norm of the Sobolev–Slobodetskiĭ space $H^s(\mathbb{T}^3)$ is obtained by adding the L^2 norm, i.e.,

$$\|u\|_{H^s} := \left(\|u\|^2 + [u]_{H^s}^2\right)^{\frac{1}{2}},$$

with the convention $H^0(\mathbb{T}^3) = L^2(\mathbb{T}^3)$. For $s \in \mathbb{N}$, this norm is equivalent to the standard Sobolev norm based on weak derivatives. Recall the following Sobolev inequality, for $u \in H^s(\mathbb{T}^3)$:

$$\|u\|_{L^\infty} \leq C(s)\|u\|_{H^s} \quad \text{for} \quad s > 3/2; \tag{2.4}$$

the inequality fails in the critical case $s = 3/2$. A critical L^∞ estimate in dimension $d = 3$ can be obtained, however, by interpolating between H^1 and H^2, which is known as Agmon's inequality: there exists a constant $C > 0$ such that

$$\|u\|_{L^\infty}^2 \leq C\|u\|_{H^1}\|u\|_{H^2} \quad \text{for all} \quad u \in H^2(\mathbb{T}^3). \tag{2.5}$$

Let us remark that the orthogonality of the Fourier system yields, for $u \in H^s(\mathbb{T}^3)$ with $s \geq 0$ and $v_N \in \mathring{\mathrm{X}}_N$, the equality

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

The following integration-by-parts formula follows easily from Fourier calculus:

$$\langle \Delta u_N, v_N\rangle = -\langle \nabla u_N, \nabla v_N\rangle \qquad \text{for all} \quad u_N, v_N \in \mathrm{X}_N. \tag{2.6}$$

We recall the following approximation property of the Fourier system (cf., e.g., [3]): assuming that $u \in H^s(\mathbb{T}^3)$, where $s > 0$, and $-\infty < r < s$, there exists a positive constant $C = C(r, s)$, independent of u, such that,

$$\|u - P_N u\|_{H^r} \leq CN^{-(s-r)}\|u\|_{H^s} \qquad \text{for all} \quad N \geq 1. \tag{2.7}$$

Remark 2.1 (Fourier collocation method). The Fourier collocation method is used for spatial discretization, in situations similar to ours (e.g., [7]), as an alternative to the Fourier–Galerkin method. Fourier collocation methods define spatial discretization by sampling the differential equation, with the analytical solution replaced by the numerical solution, at equally spaced collocation points. As has been noted in [23], for example, this is particularly useful if one needs to evaluate nonlinearities. One might be therefore tempted to use this method in our case as well. However, the projection operator P_N commutes with differential operators while the interpolation operator corresponding to the spectral collocation method does not, which, in turn, leads to significant difficulties in the analysis of the resulting collocation method, particularly in the proofs of various a priori bounds on the sequence of numerical solutions in section 4, to the extent that we were unable to show unconditional stability of such a spectral collocation version of our method.

Finite-dimensional analogues of the Lebesgue spaces L^p and Sobolev space $W^{1,\infty} = C^{0,1}$ and $W^{1,2} = H^1$ will be denoted by ℓ^p, $w^{1,\infty}$, and $\hbar^1$, respectively. We shall now formulate the proposed numerical approximation of the Ohta–Kawasaki equation, and summarize its key features.

3. The discrete scheme. The aim of this section is to formulate the proposed numerical approximation of (1.4) and to prove its well-posedness. The spatial discretization is based on a Fourier–Galerkin approximation from the finite-dimensional space X_N. The temporal discretization is performed on a uniform partition $\{0 = t^0 < t^1 < \cdots < t^M = T\}$ of the interval $[0, T]$ such that $t^{k+1} - t^k = h \equiv \Delta t := T/M$, $k = 0, 1, \ldots, M-1$, $M \geq 2$. For $k = 0, 1, \ldots, M-1$, we seek $u_N^{k+1} \in \mathrm{X}_N$ such that

$$\left\langle \frac{u_N^{k+1} - u_N^k}{h}, \phi \right\rangle_{H^{-1}} + \left\langle u_N^{k+\frac{1}{2}}, \phi \right\rangle_{\mathscr{L}} + \left\langle [u_N^{k+\frac{1}{2}}]^3, \phi \right\rangle = \left\langle u_N^{k+\frac{1}{2}}, \phi \right\rangle \quad \forall \phi \in \mathring{\mathrm{X}}_N, \tag{3.1}$$

with $u_N^0 := P_N u^0$, where u^0 is the given initial datum for the Ohta–Kawasaki equation. Here we have used the abbreviation

$$u_N^{k+\frac{1}{2}} := \frac{1}{2}\big(u_N^{k+1} + u_N^k\big),$$

$\mathscr{L}$ is the second-order elliptic operator on the configuration space M_m with range in $H^{-1}(\mathbb{T}^3)$ defined by

$$\mathscr{L}u := \varepsilon^2(-\Delta)u + \sigma(-\Delta)^{-1}(u - m)$$

and accordingly

$$\langle u, \phi \rangle_{\mathscr{L}} := \langle \mathscr{L}u, \phi \rangle \, . \tag{3.2}$$

Observe that $\mathscr{L}$ extends to $H^1(\mathbb{T}^3)$ by letting

$$\mathscr{L}u = \varepsilon^2(-\Delta)u + \sigma(-\Delta)^{-1}(\mathbf{1} - P_0)u,$$

where

$$(\mathbf{1} - P_0)u = u - m \quad \text{with} \quad m = \fint_{\mathbb{T}^3} u \, \mathrm{d}x.$$

Note that $\langle \cdot, \cdot \rangle_{\mathscr{L}}$ is an inner product, and the norm $\| \cdot \|_{\mathscr{L}}$ induced by it is equivalent to $[\cdot]_{H^1}$. Observe, however, that the norm-equivalence constants depend on ε.

Since $\phi = -\Delta\varphi \in \mathring{\mathrm{X}}_N$ for any $\varphi \in \mathrm{X}_N$, it is a valid choice of test function in (3.1). Hence, for $k = 0, 1, \ldots, M-1$, $u_N^{k+1} \in \mathrm{X}_N$ satisfies

(3.3)

$$\left\langle \frac{u_N^{k+1} - u_N^k}{h}, \varphi \right\rangle + \left\langle \nabla u_N^{k+\frac{1}{2}}, \nabla\varphi \right\rangle_{\mathscr{L}} + \left\langle \nabla [u_N^{k+\frac{1}{2}}]^3, \nabla\varphi \right\rangle = \left\langle \nabla u_N^{k+\frac{1}{2}}, \nabla\varphi \right\rangle \quad \forall \varphi \in \mathrm{X}_N.$$

Choosing in particular $\varphi \equiv 1$ in (3.3), we deduce that $P_0 u_N^{k+1} = P_0 u_N^k$ for all $k = 0, 1, \ldots, M-1$. Also, $P_0 u_N^0 = P_0(P_N u^0) = P_0 u^0 = m$. Consequently, $P_0 u_N^k = P_0 u^0 = m$, for all $k = 0, 1, \ldots, M$. In other words, necessarily,

$$\fint_{\mathbb{T}^3} u_N^k \,\mathrm{d}x = m, \quad k = 0, 1, \ldots, M,$$

and therefore $u_N^{k+\frac{1}{2}} - m \in \mathring{\mathrm{X}}_N$ for all $k = 0, 1, \ldots, M-1$; this property will play a crucial role in our analysis of the proposed numerical method. In particular, it guarantees that the sequence of numerical approximations, in analogy with the set of time slices of the analytical solution $\{u(\cdot, t) : t \in [0, T]\}$, belongs to the configuration space M_m.

Thus far we have tacitly assumed that the numerical method (3.1), with the initialization $u_N^0 := P_N u^0$, is correctly defined in the sense that it has a unique solution. Next we shall show that this is indeed the case for any $m \in (-1, 1)$ and any $\sigma \geq 0$, provided that $h < 8\varepsilon^2/(1 - 4\sigma\varepsilon^2)_+$.

Before doing so, we shall summarize for the benefit of the reader the notation for norms and inner products that we will use in the rest of the paper.

$\\|\cdot\\|_{L^p}$:	the standard norm corresponding to the Lebesgue space $L^p(\mathbb{T}^3)$;
$\langle\cdot,\cdot\rangle$, $\\|\cdot\\|$:	the inner product and the corresponding norm in the Lebesgue space $L^2(\mathbb{T}^3)$;
$\langle\cdot,\cdot\rangle_{H^s}$, $\\|\cdot\\|_{H^s}$:	the inner product in the Sobolev–Slobodetskiĭ space $H^s(\mathbb{T}^3)$ defined in (2.3) with $s \in \mathbb{R}$ and the corresponding norm;
$\langle\cdot,\cdot\rangle_{\mathscr{L}}$, $\\|\cdot\\|_{\mathscr{L}}$:	the inner product defined through (3.2) and the corresponding norm that is equivalent to $\\|\cdot\\|_{H^1}$;
$\\|\cdot\\|_*$:	$\\|\cdot\\|_* := \left(\\|\cdot\\|^2_{H^{-1}} + \\|\nabla\cdot\\|^2\right)^{1/2}$;
$\\|\cdot\\|_h^2$:	$\\|\cdot\\|_h^2 := 2\\|\cdot\\|^2_{H^{-1}} + h\\|\cdot\\|^2_{\mathscr{L}}$.

All the norms and inner products given in the above table concern the spatial variable only. To describe the temporal behavior as well, we work in standard Bochner spaces $L^p(0, T; X)$ of p-integrable functions with values in the Banach space X, and in the space $W^{k,p}(0, T; X)$ consisting of all X-valued functions that are p-integrable together with all of their derivatives of order up to k. In the time-discrete setting when, roughly speaking, integration is replaced by Riemann sums, we prefer to use the notation $\ell^p(0, T; X)$ and $w^{k,p}(0, T; X)$ instead.

THEOREM 3.1. *Suppose that $u^0 \in L^2(\mathbb{T}^3)$, with $m := P_0 u^0$, and let $h < 8\varepsilon^2/(1 - 4\sigma\varepsilon^2)_+$; then, the method (3.1), with the initialization $u_N^0 := P_N u^0$, is correctly defined in the sense that it has a unique solution $u_N^{k+1} \in \mathrm{X}_N$, with $u_N^{k+1} - m \in \mathring{\mathrm{X}}_N$, for each $k = 0, 1, \ldots, M-1$.*

Proof. That $u_N^{k+1} - m \in \mathring{\mathrm{X}}_N$ for each $k = 0, 1, \ldots, M-1$, assuming that $u_N^{k+1} \in \mathrm{X}_N$ satisfying (3.1), with the initialization $u_N^0 := P_N u^0$, exists, has already been shown above. It remains to prove the existence and uniqueness of $u_N^{k+1} \in \mathrm{X}_N$, $k = 0, 1, \ldots, M-1$.

Let $v_N^k := u_N^k - m$, $k = 0, 1, \ldots, M$, and define $v_N^{k+\frac{1}{2}} := \frac{1}{2}(v_N^{k+1} + v_N^k)$, $k = 0, 1, \ldots, M-1$. With this notation (3.1) can be rewritten as follows: Find $v_N^{k+1} \in \mathring{\mathrm{X}}_N$, such that

$$\left\langle \frac{v_N^{k+1} - v_N^k}{h}, \phi \right\rangle_{H^{-1}} + \left\langle \varepsilon^2(-\Delta) v_N^{k+\frac{1}{2}} + \sigma(-\Delta)^{-1} v_N^{k+\frac{1}{2}}, \phi \right\rangle + \left\langle [v_N^{k+\frac{1}{2}} + m]^3, \phi \right\rangle = \left\langle v_N^{k+\frac{1}{2}}, \phi \right\rangle$$

for all $\phi \in \mathring{\mathrm{X}}_N$, which can be further rewritten as

$$2\left\langle v_N^{k+\frac{1}{2}}, \phi \right\rangle_{H^{-1}} + h\left\langle \varepsilon^2(-\Delta) v_N^{k+\frac{1}{2}} + \sigma(-\Delta)^{-1} v_N^{k+\frac{1}{2}}, \phi \right\rangle + h\left\langle [v_N^{k+\frac{1}{2}} + m]^3, \phi \right\rangle - h\left\langle v_N^{k+\frac{1}{2}}, \phi \right\rangle = 2\left\langle v_N^k, \phi \right\rangle_{H^{-1}} \qquad \forall \phi \in \mathring{\mathrm{X}}_N.$$

For $v \in \mathring{\mathrm{X}}_N$ fixed, consider the linear functional $\mathscr{T}_h(v) : \mathring{\mathrm{X}}_N \to \mathbb{R}$ defined by

$$\mathscr{T}_h(v)(\phi) = 2\langle v, \phi \rangle_{H^{-1}} + h\left\langle \varepsilon^2(-\Delta) v + \sigma(-\Delta)^{-1} v, \phi \right\rangle + h\left\langle [v + m]^3, \phi \right\rangle - h\langle v, \phi \rangle \quad \forall \phi \in \mathring{\mathrm{X}}_N.$$

Therefore, the problem that is to be solved can be restated as follows:

$$\text{(3.4)} \quad \text{For a given } v_N^k \in \mathring{\mathrm{X}}_N \text{ find } v_N^{k+\frac{1}{2}} \in \mathring{\mathrm{X}}_N\text{: } \mathscr{T}_h(v_N^{k+\frac{1}{2}})(\phi) = 2\left\langle v_N^k, \phi \right\rangle_{H^{-1}} \ \ \forall \phi \in \mathring{\mathrm{X}}_N.$$

Once the existence of a unique such $v_N^{k+\frac{1}{2}}$ has been shown, the existence of a unique $v_N^{k+1} \in \mathring{\mathrm{X}}_N$ will immediately follow on noting that $v_N^{k+1} = 2v_N^{k+\frac{1}{2}} - v_N^k \in \mathring{\mathrm{X}}_N$.

We shall consider to this end the finite-dimensional linear space $\mathring{\mathrm{X}}_N$, equipped with the norm $z \in \mathring{\mathrm{X}}_N \mapsto \|z\|_* := (\|z\|_{H^{-1}}^2 + \|\nabla z\|^2)^{1/2} \in \mathbb{R}_{\geq 0}$. It follows from the monotonicity of the function $x \in \mathbb{R} \mapsto (x+m)^3 \in \mathbb{R}$ and the inequality (2.2) that

$$\text{(3.5)} \quad \mathscr{T}_h(z)(z - z') - \mathscr{T}_h(z')(z - z') \geq \min\left(2 + h(\sigma - \delta), h\left(\varepsilon^2 - \frac{1}{4\delta}\right)\right) \|z - z'\|_*^2$$

for all $z, z' \in \mathring{\mathrm{X}}_N$, where δ is any positive real number, such that $1/(4\varepsilon^2) < \delta < (2/h) + \sigma$, with $\sigma \geq 0$; the existence of such a positive real number δ is the consequence of our hypothesis that

$$h < \frac{8\varepsilon^2}{(1 - 4\sigma\varepsilon^2)_+}.$$

As $\mathscr{T}_h(0)(\phi) = 0$ for all $\phi \in \mathring{\mathrm{X}}_N$, it follows from (3.5) with $z' = 0$ that

$$\text{(3.6)} \qquad \mathscr{T}_h(z)(z) \geq \min\left(2 + h(\sigma - \delta), h\left(\varepsilon^2 - \frac{1}{4\delta}\right)\right) \|z\|_*^2 \qquad \forall z \in \mathring{\mathrm{X}}_N.$$

Further, by Hölder's inequality and the Sobolev embedding theorem,

$$\text{(3.7)} \qquad |\mathscr{T}_h(z)(\phi) - \mathscr{T}_h(z')(\phi)| \leq C(\varepsilon, \sigma, h)(1 + \|z\|_{L^3}^2 + \|z'\|_{L^3}^2) \|z - z'\|_* \|\phi\|_*$$

for all $z, z' \in \mathring{X}_N$ and all $\phi \in \mathring{X}_N$. It then follows from (3.7) with $z' = 0$ that

$$|\mathcal{T}_h(z)(\phi)| \le C(\varepsilon, \sigma, h)(1 + \|z\|_{L^3}^2)\, \|z\|_*\, \|\phi\|_* \qquad \forall z, \phi \in \mathring{X}_N. \tag{3.8}$$

We deduce from (3.8) that $\mathcal{T}_h(z) \in [\mathring{X}_N]'$, where the dual space $[\mathring{X}_N]'$ of $\mathring{X}_N$ is equipped with the dual of the norm $\|\cdot\|_*$, denoted by $\|\cdot\|_{[\mathring{X}_N]'}$. It further follows from (3.8) that the operator $\mathcal{T}_h : z \in \mathring{X}_N \mapsto \mathcal{T}_h(z) \in [\mathring{X}_N]'$ is bounded. Inequality (3.5) implies that $\mathcal{T}_h$ is strongly monotone, (3.6) implies that it is coercive, and since by (3.7) we have that

$$\|\mathcal{T}_h(z) - \mathcal{T}_h(z')\|_{[\mathring{X}_N]'} \le C(\varepsilon, \sigma, h)(1 + \|z\|_{L^3}^2 + \|z'\|_{L^3}^2)\, \|z - z'\|_* \qquad \forall z, z' \in \mathring{X}_N,$$

we deduce by the Sobolev embedding of $H^1(\mathbb{T}^3)$ into $L^3(\mathbb{T}^3)$ that $\mathcal{T}_h$ is Lipschitz continuous on any bounded ball of $\mathring{X}_N$, and it is therefore continuous on $\mathring{X}_N$. It then follows by the Browder–Minty theorem (cf. Thm. 10.49 in [21]) that $\mathcal{T}_h$ is bijective as a mapping from $\mathring{X}_N$ into $[\mathring{X}_N]'$.

For $v_N^k \in \mathring{X}_N$ fixed, $\ell^k : \phi \in \mathring{X}_N \mapsto \ell^k(\phi) := 2\left\langle v_N^k, \phi \right\rangle_{H^{-1}}$ is a bounded linear functional on $\mathring{X}_N$; hence, $\ell^k \in [\mathring{X}_N]'$. For $\ell^k \in [\mathring{X}_N]'$ thus defined, we then deduce the existence of a unique $v_N^{k+1/2} \in \mathring{X}_N$ such that $\mathcal{T}_h(v_N^{k+1/2}) = \ell^k$. Thus we have shown the existence of a unique $u_N^{k+1} = v^{k+1} + m = 2v_N^{k+\frac{1}{2}} - v_N^k + m \in X_N$ that solves (3.1), for $k = 0, 1, \dots, M - 1$. ∎

4. A priori bounds on the sequence of numerical solutions.

In this section, we prove uniform bounds of the sequence of numerical solutions u_N of the scheme (3.1); recall that it reads

$$\left\langle \frac{u_N^{k+1} - u_N^k}{h}, \phi \right\rangle_{H^{-1}} + \left\langle u_N^{k+\frac{1}{2}}, \phi \right\rangle_{\mathcal{L}} + \left\langle [u_N^{k+\frac{1}{2}}]^3, \phi \right\rangle = \left\langle u_N^{k+\frac{1}{2}}, \phi \right\rangle \qquad \forall \phi \in \mathring{X}_N,$$

for $k \in \mathbb{N}_0$ and $u_N^0 = P_N u^0 \in X_N$, where $u^0 \in L^2(\mathbb{T}^3)$ with $⨍_{\mathbb{T}^3} u^0 \,\mathrm{d}x = m$. The scheme has been shown to be well-posed in X_N in the previous section, for $h < 8\varepsilon^2/(1 - 4\sigma\varepsilon^2)$. The estimates in this section rely on the uniform ellipticity of $\mathcal{L}$ for fixed $\varepsilon > 0$ and arbitrary $\sigma \ge 0$ and the monotonicity properties of the (cubic) nonlinearity.

THEOREM 4.1 (uniform boundedness in the $\ell^\infty(0,T;L^2) \cap \ell^2(0,T;H^2) \cap \ell^4(0,T;L^4)$ norm). *Let us suppose that $u^0 \in L^2(\mathbb{T}^3)$, and that $u_N^1, \dots, u_N^M$, with $h \equiv \Delta t := T/M$, $M \ge 2$, are defined by the scheme* (3.1). *Suppose further that*

$$h \le 2\varepsilon^2.$$

Then, there exists a positive constant $C = C(\varepsilon, u^0)$ such that

$$\max_{k \in \{0,\dots,M\}} \|u_N^k\|^2 \le C. \tag{4.1}$$

Proof. For the sake of clarity of the exposition we shall divide the proof into two steps.

Step 1. First, let us test (3.1) with $\phi = u_N^{k+\frac{1}{2}} - m \in \mathring{X}_N$. Then, thanks to Plancherel's theorem and a simple consequence of Young's inequality (viz. $|a|^p \le \delta a^4 + C(\delta, p)$, for any $a \in \mathbb{R}$, $\delta > 0$, and $0 < p < 4$, applied with $a = u_N^{k+\frac{1}{2}}(x)$,

$\delta = h/6$, and $p = 2, 3, 1$, in turn) we have that

$$\frac{1}{2}\left\langle u_N^{k+1} - u_N^k, u_N^{k+1} + u_N^k \right\rangle_{H^{-1}} + h\|u_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2 + h\int_{\mathbb{T}^3} [u_N^{k+\frac{1}{2}}]^4 \,\mathrm{d}x$$
$$= h\int_{\mathbb{T}^3} [u_N^{k+\frac{1}{2}}]^2 - m\left([u_N^{k+\frac{1}{2}}]^3 - u_N^{k+\frac{1}{2}}\right) \mathrm{d}x \le \frac{1}{2}h\int_{\mathbb{T}^3} [u_N^{k+\frac{1}{2}}]^4 \,\mathrm{d}x + c(m)h$$

for $k = 1, 2, \ldots, M-1$, with a positive constant $c(m)$. In other words, we have that

$$\frac{1}{2}\|u_N^{k+1}\|_{H^{-1}}^2 + h\|u_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2 + \frac{h}{2}\int_{\mathbb{T}^3} [u_N^{k+\frac{1}{2}}]^4 \,\mathrm{d}x$$
$$\le \frac{1}{2}\|u^k\|_{H^{-1}}^2 + c(m)h, \qquad k = 0, 1, \ldots, M-1.$$

Summing over $k \in \{0, 1, \ldots, M-1\}$ gives the following bounds:

$$\max_{k\in\{0,\ldots,M\}} \|u_N^k\|_{H^{-1}}^2 \le C(\varepsilon, u^0) \qquad \rightsquigarrow \ell^\infty(0, T; H^{-1}) \text{ bound,} \tag{4.2}$$

$$\sum_{k=0}^{M-1} h\|u_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2 \le C(\varepsilon, u^0) \qquad \rightsquigarrow \ell^2(0, T; H^1) \text{ bound,} \tag{4.3}$$

$$\sum_{k=0}^{M-1} h\int_{\mathbb{T}^3} [u_N^{k+\frac{1}{2}}]^4 \,\mathrm{d}x \le C(\varepsilon, u^0) \qquad \rightsquigarrow \ell^4(0, T; L^4) \text{ bound.} \tag{4.4}$$

Step 2. Next, let us test (3.1) with $\phi = -\Delta u_N^{k+\frac{1}{2}} \in \mathring{\mathrm{X}}_N$. By partial integration (cf. (2.6)) and, importantly, using in the nonlinear term that the operator P_N commutes with partial differentiation, followed by an application of Plancherel's theorem, this leads to the following equality for $k = 0, 1, \ldots, M-1$:

$$\frac{1}{2}\left\langle \nabla(u_N^{k+1} - u_N^k), \nabla(u_N^{k+1} + u_N^k) \right\rangle_{H^{-1}} + h\|\nabla u_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2$$
$$+ 3h\int_{\mathbb{T}^3} [u_N^{k+\frac{1}{2}}]^2 |\nabla u_N^{k+\frac{1}{2}}|^2 \,\mathrm{d}x = -h\left\langle u_N^{k+\frac{1}{2}}, \Delta u_N^{k+\frac{1}{2}} \right\rangle.$$

By writing $\int_{\mathbb{T}^3} [u_N^{k+\frac{1}{2}}]^2 \, |\nabla u_N^{k+\frac{1}{2}}|^2 = \|u_N^{k+\frac{1}{2}} \nabla u_N^{k+\frac{1}{2}}\|^2$ and thanks to Young's inequality (applied on the right-hand side), we obtain

$$\frac{1}{2}\left\langle \nabla(u_N^{k+1} - u_N^k), \nabla(u_N^{k+1} + u_N^k) \right\rangle_{H^{-1}} + h\|\nabla u_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2$$
$$+ 3h\|u_N^{k+\frac{1}{2}} \nabla u_N^{k+\frac{1}{2}}\|^2 \le \frac{h}{2\varepsilon^2}\|u_N^{k+\frac{1}{2}}\|^2 + \frac{h\varepsilon^2}{2}\|\Delta u_N^{k+\frac{1}{2}}\|^2.$$

As $\langle u_N^{k+\frac{1}{2}} - m, u_N^{k+\frac{1}{2}} \rangle = \langle u_N^{k+\frac{1}{2}} - m, u_N^{k+\frac{1}{2}} - m \rangle = \|u_N^{k+\frac{1}{2}} - m\|^2 \ge 0$, it follows that

$$\varepsilon^2\|\Delta u_N^{k+\frac{1}{2}}\|^2 \le \|\nabla u_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2.$$

Hence we have that

$$\frac{1}{2}\|\nabla u_N^{k+1}\|_{H^{-1}}^2 + \frac{h}{2}\|\nabla u_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2 + 3h\|u_N^{k+\frac{1}{2}} \nabla u_N^{k+\frac{1}{2}}\|^2 \le \frac{1}{2}\|\nabla u_N^k\|_{H^{-1}}^2 + \frac{h}{2\varepsilon^2}\|u_N^{k+\frac{1}{2}}\|^2.$$

Finally, summing over k and recalling (4.3) (thanks to which $\sum_{k=0}^{M-1} \frac{h}{2\varepsilon^2}\|u_N^{k+\frac{1}{2}}\|^2$ is bounded by $C = C(\varepsilon, u^0)$) we deduce the following additional a priori bounds:

$$\max_{k\in\{0,\ldots,M\}} \|\nabla u_N^k\|_{H^{-1}}^2 \le C(\varepsilon, u^0) \qquad \rightsquigarrow \ell^\infty(0,T;L^2) \text{ bound,} \tag{4.5}$$

$$\sum_{k=0}^{M-1} h\|\nabla u_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2 \le C(\varepsilon, u^0) \qquad \rightsquigarrow \ell^2(0,T;H^2) \text{ bound,} \tag{4.6}$$

$$\sum_{k=0}^{M-1} h\|u_N^{k+\frac{1}{2}}\nabla u_N^{k+\frac{1}{2}}\|^2 \le C(\varepsilon, u^0). \tag{4.7}$$

That completes the proof. □

In the rest of this section we shall derive stronger bounds under the following additional assumption: we shall fix an arbitrary constant $R > 0$ and assume that

$$u^0 \in H^3(\mathbb{T}^3) \quad \text{with} \quad \|u_N^0\|_{L^\infty} \le R. \tag{4.8}$$

Remark 4.2. The existence of such a positive constant R is easily verified: by virtue of (2.7),

$$\|u_N^0\|_{L^\infty} \le C\big(\|u_N^0 - u^0\|_{H^2} + \|u^0\|_{L^\infty}\big) \le CN^{-1}\|u^0\|_{H^3} + \|u^0\|_{L^\infty}.$$

Hence we can choose N large enough so that $\|u_N^0\|_{L^\infty} \le 2\|u^0\|_{L^\infty}$. The right-hand side of the last inequality can then be taken as R.

For convenience, we use hereafter the notation C for a generic positive constant, which may change from expression to expression, and depends only on $\varepsilon \in (0,1)$ and $u^0 \in H^3(\mathbb{T}^3)$.

LEMMA 4.3. *There exists a constant $\delta > 0$ with the following property: suppose that* (4.8) *holds and that, for $h \equiv \Delta t := T/M$, $M \ge 2$,*

$$h \le \min(2, \delta/R^4)\,\varepsilon^2;$$

then,

$$\frac{1}{h}\|u_N^1 - u_N^0\|_{H^{-1}} \le C(u^0),$$

where $C(u^0)$ depends only on $\|u^0\|_{H^3}$ but is independent of h and ε.

Proof. We let $v_N = \frac{1}{h}(u_N^1 - u_N^0)$ and observe that $u_N^{\frac{1}{2}} = \frac{h}{2}v_N + u_N^0$. Hence, the initial step can be rewritten in terms of v_N as follows:

$$\langle v_N, \phi\rangle_{H^{-1}} + \frac{h}{2}\langle v_N, \phi\rangle_{\mathscr{L}} + \left\langle \left(\frac{h}{2}v_N + u_N^0\right)^3, \phi\right\rangle = \frac{h}{2}\langle v_N, \phi\rangle + \langle u_N^0 - \mathscr{L}u_N^0, \phi\rangle \qquad \forall \phi \in \mathring{X}_N.$$

Thus, with $\phi = v_N$, using (2.2) we have that

$$\|v_N\|_{H^{-1}}^2 + \frac{h}{2}\|v_N\|_{\mathscr{L}}^2 + \frac{h^3}{8}\|v_N\|_{L^4}^4 \le \Big(\|u_N^0\|_{H^1} + \|\mathscr{L}u_N^0\|_{H^1} + \|(u_N^0)^3\|_{H^1}\Big)\|v_N\|_{H^{-1}} + \frac{h}{2}\|v_N\|_{L^2}^2 + \frac{3h}{2}\left|\langle v_N(u_N^0)^2, v_N\rangle\right| + \frac{3h^2}{4}\left|\langle v_N^2 u_N^0, v_N\rangle\right|.$$

By virtue of Young's inequality, the fact that H^3 is an algebra and $\|u_N^0\|_{H^3} \le \|u^0\|_{H^3}$, we obtain

$$\|v_N\|_{H^{-1}}^2 + h\|v_N\|_{\mathscr{L}}^2 + \frac{h^3}{4}\|v_N\|_{L^4}^4 \le C(u^0) + h\|v_N\|_{L^2}^2 + 3h\left|\left\langle v_N(u_N^0)^2, v_N\right\rangle\right| + \frac{3h^2}{2}\left|\left\langle v_N^2 u_N^0, v_N\right\rangle\right|.$$

Moreover, using (2.2),

$$h\|v_N\|_{L^2}^2 \le h\|v_N\|_{H^{-1}}\|v_N\|_{H^1} \le \frac{h}{\varepsilon}\|v_N\|_{H^{-1}}\|v_N\|_{\mathscr{L}} \le \frac{1}{2}\sqrt{\frac{h}{\varepsilon^2}}\left(\|v_N\|_{H^{-1}}^2 + h\|v_N\|_{\mathscr{L}}^2\right),$$

which can be absorbed if $h \le 2\varepsilon^2$. Also by (2.2), (2.4), and Young's inequality we have that

$$\begin{aligned} 3h\left|\left\langle v_N(u_N^0)^2, v_N\right\rangle\right| &\le 3h\|u_N^0\|_{L^\infty}^2\|v_N\|_{L^2}^2 \le 3\frac{h}{\varepsilon}\|u_N^0\|_{L^\infty}^2\|v_N\|_{H^{-1}}\|v_N\|_{\mathscr{L}} \\ &\le CR^2\sqrt{\frac{h}{\varepsilon^2}}\left(\|v_N\|_{H^{-1}}^2 + h\|v_N\|_{\mathscr{L}}^2\right), \end{aligned}$$

which can be absorbed for $R^4h/\varepsilon^2 \le \delta$ and δ sufficiently small. Similarly, with an additional interpolation argument, we obtain

$$\begin{aligned} \left|\left\langle v_N^2 u_N^0, v_N\right\rangle\right| &\le \|u_N^0\|_{L^\infty}\|v_N\|_{L^3}^3 \le \|u_N^0\|_{L^\infty}\|v_N\|_{L^4}^2\|v_N\|_{L^2} \\ &\le \frac{CR}{\sqrt{\varepsilon}}\|v_N\|_{L^4}^2\sqrt{\|v_N\|_{H^{-1}}\|v_N\|_{\mathscr{L}}}\,. \end{aligned}$$

Hence, splitting $h^2 = h^{3/2}h^{1/2}$ and applying Young's inequality twice, we deduce that

$$\frac{3h^2}{2}\;\left|\left\langle v_N^2 u_N^0, v_N\right\rangle\right| \le \frac{h^3}{8}\|v_N\|_{L^4}^4 + CR^2\sqrt{\frac{h}{\varepsilon^2}}\left(\|v_N\|_{H^{-1}}^2 + h\|v_N\|_{\mathscr{L}}^2\right),$$

which can also be absorbed as before with an appropriate choice of δ. ∎

THEOREM 4.4. *There exist a universal constant $\delta > 0$ and a positive constant $C = C(\varepsilon, u^0)$ with the following property: suppose that* (4.8) *holds and that, for $h \equiv \Delta t := T/M$, $M \ge 2$,*

$$h \le \min(2, \delta/R^4)\,\varepsilon^2;$$

then

$$\max_{k\in\{0,\dots,M\}} \|u_N^k\|_{\mathscr{L}} \le C. \tag{4.9}$$

Proof. For the sake of clarity of the exposition we shall divide the proof into two steps.

Step 1. For $k \ge 1$, we use the test function $\phi = u_N^{k+\frac{1}{2}} - u_N^{k-\frac{1}{2}} \in \mathring{\mathrm{X}}_N$ in (3.1) leading to

$$\frac{1}{2h}\left\langle u_N^{k+1} - u_N^k, u_N^{k+1} - u_N^{k-1}\right\rangle_{H^{-1}} + \left\langle u_N^{k+\frac{1}{2}}, u_N^{k+\frac{1}{2}} - u_N^{k-\frac{1}{2}}\right\rangle_{\mathscr{L}} + \left\langle [u_N^{k+\frac{1}{2}}]^3, u_N^{k+\frac{1}{2}} - u_N^{k-\frac{1}{2}}\right\rangle = \left\langle u_N^{k+\frac{1}{2}}, u_N^{k+\frac{1}{2}} - u_N^{k-\frac{1}{2}}\right\rangle. \tag{4.10}$$

We apply the same test at the time step $k-1$, which yields

$$\text{(4.11)}\quad \frac{1}{2h}\left\langle u_N^k - u_N^{k-1}, u_N^{k+1} - u_N^{k-1}\right\rangle_{H^{-1}} + \left\langle u_N^{k-\frac12}, u_N^{k+\frac12} - u_N^{k-\frac12}\right\rangle_{\mathscr{L}} + \left\langle [u_N^{k-\frac12}]^3, u_N^{k+\frac12} - u_N^{k-\frac12}\right\rangle = \left\langle u_N^{k-\frac12}, u_N^{k+\frac12} - u_N^{k-\frac12}\right\rangle.$$

Taking the difference of (4.10) and (4.11) gives

$$\text{(4.12)}\quad \frac{1}{2h}\left\langle u_N^{k+1} - 2u_N^k + u_N^{k-1}, u_N^{k+1} - u_N^{k-1}\right\rangle_{H^{-1}} + \|u_N^{k+\frac12} - u_N^{k-\frac12}\|_{\mathscr{L}}^2 + \left\langle [u_N^{k+\frac12}]^3 - [u_N^{k-\frac12}]^3, u_N^{k+\frac12} - u_N^{k-\frac12}\right\rangle = \left\langle u_N^{k+\frac12} - u_N^{k-\frac12}, u_N^{k+\frac12} - u_N^{k-\frac12}\right\rangle.$$

The first term on the left can be written as

$$\left\langle u_N^{k+1} - 2u_N^k + u_N^{k-1}, u_N^{k+1} - u_N^{k-1}\right\rangle_{H^{-1}} = \|u_N^{k+1} - u_N^k\|_{H^{-1}}^2 - \|u_N^k - u_N^{k-1}\|_{H^{-1}}^2.$$

Moreover, we bound the right-hand side of (4.12) using (2.2) to deduce that

$$\begin{aligned}\left|\left\langle u_N^{k+\frac12} - u_N^{k-\frac12}, u_N^{k+\frac12} - u_N^{k-\frac12}\right\rangle\right| &\le \varepsilon^2\|\nabla\big(u_N^{k+\frac12} - u_N^{k-\frac12}\big)\|^2 + \frac{1}{4\varepsilon^2}\|u_N^{k+\frac12} - u_N^{k-\frac12}\|_{H^{-1}}^2 \\ &\le \|u_N^{k+\frac12} - u_N^{k-\frac12}\|_{\mathscr{L}}^2 + \frac{1}{4\varepsilon^2}\|u_N^{k+\frac12} - u_N^{k-\frac12}\|_{H^{-1}}^2.\end{aligned}$$

As, *by monotonicity*, $\langle [u_N^{k+\frac12}]^3 - [u_N^{k-\frac12}]^3, u_N^{k+\frac12} - u_N^{k-\frac12}\rangle \ge 0$, we obtain from (4.12) the following inequality:

$$\frac{1}{h}\|u_N^{k+1} - u_N^k\|_{H^{-1}}^2 \le \frac{1}{h}\|u_N^k - u_N^{k-1}\|_{H^{-1}}^2 + \frac{1}{2\varepsilon^2}\|u_N^{k+\frac12} - u_N^{k-\frac12}\|_{H^{-1}}^2.$$

Multiplying by $1/h$ and summing from $k=1$ to j, leads to

$$\text{(4.13)}\quad \frac{1}{h^2}\|u_N^{j+1} - u_N^j\|_{H^{-1}}^2 \le \frac{1}{h^2}\|u_N^1 - u_N^0\|_{H^{-1}}^2 + \frac{1}{2h\varepsilon^2}\sum_{k=1}^{j}\|u_N^{k+\frac12} - u_N^{k-\frac12}\|_{H^{-1}}^2.$$

Writing

$$u_N^{k+\frac12} - u_N^{k-\frac12} = \frac12(u_N^{k+1} - u_N^k + u_N^k - u_N^{k-1})$$

we obtain

$$\sum_{k=1}^{j}\|u_N^{k+\frac12} - u_N^{k-\frac12}\|_{H^{-1}}^2 \le \frac12\sum_{k=0}^{j-1}\|u_N^{k+1} - u_N^k\|_{H^{-1}}^2 + \frac12\|u_N^{j+1} - u_N^j\|_{H^{-1}}^2.$$

Returning to (4.13) we get

$$\text{(4.14)}\quad \frac{\|u_N^{j+1} - u_N^j\|_{H^{-1}}^2}{2h^2} \le \frac{\|u_N^1 - u_N^0\|_{H^{-1}}^2}{h^2} + \frac{1}{4\varepsilon^2}\sum_{k=0}^{j-1} h\frac{\|u_N^{k+1} - u_N^k\|_{H^{-1}}^2}{h^2}.$$

By Lemma 4.3 and the discrete Gronwall inequality, we deduce from (4.14) that

$$\text{(4.15)}\quad \max_{j\in\{0,\ldots,M-1\}} \frac{\|u_N^{j+1} - u_N^j\|_{H^{-1}}^2}{h^2} \le C \qquad \rightsquigarrow w^{1,\infty}(0,T;H^{-1}) \text{ bound.}$$

Step 2. Finally we use $\phi = u_N^{k+1} - u_N^k \in \mathring{\mathrm{X}}_N$ as a test function in (3.1) and obtain

$$\frac{2}{h}\|u_N^{k+1} - u_N^k\|_{H^{-1}}^2 + \|u_N^{k+1}\|_{\mathscr{L}}^2 - \|u_N^k\|_{\mathscr{L}}^2 + 2\left\langle [u_N^{k+\frac{1}{2}}]^3, u_N^{k+1} - u_N^k \right\rangle = 2\left\langle u_N^{k+\frac{1}{2}}, u_N^{k+1} - u_N^k \right\rangle.$$

We estimate the term on the right by

$$\left\langle u_N^{k+\frac{1}{2}}, u_N^{k+1} - u_N^k \right\rangle \leq \|\nabla u_N^{k+\frac{1}{2}}\| \, \|u_N^{k+1} - u_N^k\|_{H^{-1}} = h\, \|\nabla u_N^{k+\frac{1}{2}}\| \, \frac{\|u_N^{k+1} - u_N^k\|_{H^{-1}}}{h} \leq Ch\left(1 + \|\nabla u_N^{k+\frac{1}{2}}\|^2\right),$$

where we have used (2.2) and (4.15). Similarly,

$$\begin{aligned}
&\left\langle [u_N^{k+\frac{1}{2}}]^3, u_N^{k+1} - u_N^k \right\rangle \\
&= \left\langle P_N[u_N^{k+\frac{1}{2}}]^3, u_N^{k+1} - u_N^k \right\rangle \leq \|\nabla P_N[u_N^{k+\frac{1}{2}}]^3\| \, \|u_N^{k+1} - u_N^k\|_{H^{-1}} \\
&\leq \|\nabla [u_N^{k+\frac{1}{2}}]^3\| \, \|u_N^{k+1} - u_N^k\|_{H^{-1}} = 3h \|[u_N^{k+\frac{1}{2}}]^2 \, \nabla u_N^{k+\frac{1}{2}}\| \, \frac{\|u_N^{k+1} - u_N^k\|_{H^{-1}}}{h} \\
&\overset{(4.15)}{\leq} Ch\, \|u_N^{k+\frac{1}{2}}\|_{L^\infty} \, \|u_N^{k+\frac{1}{2}} \nabla u_N^{k+\frac{1}{2}}\| \\
&\overset{\text{Young}}{\leq} Ch\left(\|u_N^{k+\frac{1}{2}}\|_{L^\infty}^2 + \|u_N^{k+\frac{1}{2}} \nabla u_N^{k+\frac{1}{2}}\|^2\right) \\
&\overset{(2.5)}{\leq} Ch\left(\|u_N^{k+\frac{1}{2}}\|_{H^1} \, \|u_N^{k+\frac{1}{2}}\|_{H^2} + \|u_N^{k+\frac{1}{2}} \nabla u_N^{k+\frac{1}{2}}\|^2\right) \\
&\overset{\text{Young}}{\leq} Ch\left(\|u_N^{k+\frac{1}{2}}\|_{H^1}^2 + \|u_N^{k+\frac{1}{2}}\|_{H^2}^2 + \|u_N^{k+\frac{1}{2}} \nabla u_N^{k+\frac{1}{2}}\|^2\right).
\end{aligned}$$

Inserting this into the original test and summing through $k = 0, \ldots, j$, for any $j \in \{1, \ldots, M-1\}$, yields

$$\sum_{k=0}^{j} \frac{2}{h}\|u_N^{k+1} - u_N^k\|_{H^{-1}}^2 + \|u_N^{j+1}\|_{\mathscr{L}}^2 \leq \|u_N^0\|_{\mathscr{L}}^2 + C\left(1 + h\sum_{k=0}^{M-1} \|u_N^{k+\frac{1}{2}}\|_{H^1}^2 + \|u_N^{k+\frac{1}{2}}\|_{H^2}^2 + \|u_N^{k+\frac{1}{2}} \nabla u_N^{k+\frac{1}{2}}\|^2\right).$$

By combining the bounds from Steps 1 and 2 of the proof of Theorem 4.1 (in particular (4.3), (4.6), and (4.7)) and noting that $\|u_N^0\|_{\mathscr{L}}^2 \leq C(u^0, \varepsilon)$, the right-hand side is bounded by a constant, independent of the discretization parameters, which immediately yields the desired $\ell^\infty(0, T; H^1)$ bound. ∎

THEOREM 4.5. *There exist a universal constant* $\delta > 0$ *and a positive constant* $C = C(\varepsilon, u^0)$ *with the following property: suppose that* (4.8) *holds and that, for* $h \equiv \Delta t := T/M$, $M \geq 2$,

$$h \leq \min(2, \delta/R^4)\, \varepsilon^2;$$

then

$$\max_{k\in\{0,\ldots,M\}} \|\nabla u_N^k\|_{\mathscr{L}} \leq C \text{ and therefore, in particular, } \max_{k\in\{0,\ldots,M\}} \|u_N^k\|_{L^\infty} \leq C. \tag{4.16}$$

In other words, the sequence of approximate solutions is uniformly bounded in space and in time.

Proof. Again, let us divide the proof into two steps.

Step 1. In this first step we shall derive a uniform bound in the $\ell^2(0,T;H^3)$ norm. To this end we use the test function $\phi = \Delta^2 u_N^{k+\frac{1}{2}} \in \mathring{\mathrm{X}}_N$ in (3.1). Integrating by parts twice leads to

$$\frac{1}{2}\left\langle \nabla^2(u_N^{k+1}-u_N^k), \nabla^2(u_N^{k+1}+u_N^k)\right\rangle_{H^{-1}} + h\|\nabla^2 u_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2 + h\left\langle \nabla^2[u_N^{k+\frac{1}{2}}]^3, \nabla^2 u_N^{k+\frac{1}{2}}\right\rangle = h\|\nabla^2 u_N^{k+\frac{1}{2}}\|^2.$$

We now expand the term $\langle \nabla^2[u_N^{k+\frac{1}{2}}]^3, \nabla^2 u_N^{k+\frac{1}{2}}\rangle$. Since

$$\nabla^2[u_N^{k+\frac{1}{2}}]^3 = 3\nabla\left([u_N^{k+\frac{1}{2}}]^2\nabla u_N^{k+\frac{1}{2}}\right) = 6u_N^{k+\frac{1}{2}}\,\nabla u_N^{k+\frac{1}{2}}\otimes\nabla u_N^{k+\frac{1}{2}} + 3[u_N^{k+\frac{1}{2}}]^2\,\nabla^2 u_N^{k+\frac{1}{2}},$$

we deduce from Plancherel's theorem (note that we exploit the commutativity of the Fourier–Galerkin projectors with differential operators here)

$$\left\langle \nabla^2[u_N^{k+\frac{1}{2}}]^3, \nabla^2 u_N^{k+\frac{1}{2}}\right\rangle = 3\int_{\mathbb{T}^3}[u_N^{k+\frac{1}{2}}]^2|\nabla^2 u_N^{k+\frac{1}{2}}|^2\,\mathrm{d}x + 6\int_{\mathbb{T}^3} u_N^{k+\frac{1}{2}}(\nabla u_N^{k+\frac{1}{2}}\otimes\nabla u_N^{k+\frac{1}{2}}) : \nabla^2 u_N^{k+\frac{1}{2}}\,\mathrm{d}x.$$

Hence,

$$\begin{aligned}\frac{1}{2}\|\nabla^2 u_N^{k+1}\|_{H^{-1}}^2 &+ h\|\nabla^2 u_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2 + 3h\|u_N^{k+\frac{1}{2}}\nabla^2 u_N^{k+\frac{1}{2}}\|^2 \\ &\le \frac{1}{2}\|\nabla^2 u_N^k\|_{H^{-1}}^2 + h\|\nabla^2 u_N^{k+\frac{1}{2}}\|^2 \\ &\quad + 6h\underbrace{\left|\int_{\mathbb{T}^3} u_N^{k+\frac{1}{2}}(\nabla u_N^{k+\frac{1}{2}}\otimes\nabla u_N^{k+\frac{1}{2}}) : \nabla^2 u_N^{k+\frac{1}{2}}\,\mathrm{d}x\right|}_{(+)}.\end{aligned} \tag{4.17}$$

It remains to bound the term (+); to this end, we proceed as follows:

$$\begin{aligned}(+) &\overset{\text{Hölder}}{\le} \||\nabla u_N^{k+\frac{1}{2}}|^2\|\,\|u_N^{k+\frac{1}{2}}\nabla^2 u_N^{k+\frac{1}{2}}\| \\ &\overset{\text{Young}}{\le} \frac{1}{4}\|u_N^{k+\frac{1}{2}}\nabla^2 u_N^{k+\frac{1}{2}}\|^2 + \||\nabla u_N^{k+\frac{1}{2}}|^2\|^2 \\ &\le \frac{1}{4}\|u_N^{k+\frac{1}{2}}\nabla^2 u_N^{k+\frac{1}{2}}\|^2 + \|\nabla u_N^{k+\frac{1}{2}}\|_{L^\infty}^2\|\nabla u_N^{k+\frac{1}{2}}\|^2 \\ &\overset{(2.5)}{\le} \frac{1}{4}\|u_N^{k+\frac{1}{2}}\nabla^2 u_N^{k+\frac{1}{2}}\|^2 + C\|\nabla u_N^{k+\frac{1}{2}}\|_{H^1}\|\nabla u_N^{k+\frac{1}{2}}\|_{H^2} \\ &\overset{\text{Young}}{\le} \frac{1}{4}\|u_N^{k+\frac{1}{2}}\nabla^2 u_N^{k+\frac{1}{2}}\|^2 + \frac{1}{12}\|\nabla^2 u_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2 + C\|u_N^{k+\frac{1}{2}}\|_{H^2}^2,\end{aligned}$$

where in the transition from the third line to the fourth line we have used that $\|\nabla u_N^{k+\frac{1}{2}}\|^2$ is uniformly bounded thanks to Theorem 4.4. Inserting this into (4.17) yields

$$\frac{1}{2}\|\nabla^2 u_N^{k+1}\|_{H^{-1}}^2 + \frac{h}{2}\|\nabla^2 u_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2 + \frac{3h}{2}\|u_N^{k+\frac{1}{2}}\nabla^2 u_N^{k+\frac{1}{2}}\|^2 \le \frac{1}{2}\|\nabla^2 u_N^k\|_{H^{-1}}^2 + Ch\|\nabla^2 u_N^{k+\frac{1}{2}}\|^2.$$

Summing over $k = 0, \dots, j$ for some $j \in \{1, \dots, M-1\}$ yields

$$\frac{1}{2}\|\nabla^2 u_N^{j+1}\|_{H^{-1}}^2 + \sum_{k=0}^{j} \frac{h}{2}\|\nabla^2 u_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2 + \sum_{k=0}^{j} \frac{3h}{2}\|u_N^{k+\frac{1}{2}}\nabla^2 u_N^{k+\frac{1}{2}}\|^2 \\ \leq \frac{1}{2}\|\nabla^2 u_N^0\|_{H^{-1}}^2 + C\sum_{k=0}^{M-1} h\|\nabla^2 u_N^{k+\frac{1}{2}}\|^2 \leq C,$$

where the last inequality follows from (4.6). We thus deduce that

$$\sum_{k=0}^{M-1} h\|\nabla^2 u_N^{k+\frac{1}{2}}\|_{\mathscr{L}} \leq C \qquad \rightsquigarrow \ell^2(0,T;H^3) \text{ bound,} \tag{4.18}$$

$$\sum_{k=0}^{M-1} h\|u_N^{k+\frac{1}{2}}\nabla^2 u_N^{k+\frac{1}{2}}\|_{L^2}^2 \leq C. \tag{4.19}$$

Step 2. Using $\phi = -\Delta(u_N^{k+1} - u_N^k) \in \mathring{\mathrm{X}}_N$ in (3.1) we obtain

$$\frac{\|u_N^{k+1} - u_N^k\|^2}{h} + \frac{1}{2}\Big(\|\nabla u_N^{k+1}\|_{\mathscr{L}}^2 - \|\nabla u_N^k\|_{\mathscr{L}}^2\Big) = \Big\langle \Delta\big([u_N^{k+\frac{1}{2}}]^3 - u_N^{k+\frac{1}{2}}\big), u_N^{k+1} - u_N^k \Big\rangle.$$

Using (2.2)

$$\Big|\Big\langle \Delta\big([u_N^{k+\frac{1}{2}}]^3 - u_N^{k+\frac{1}{2}}\big), u_N^{k+1} - u_N^k)\Big\rangle\Big| \leq h\|\nabla^3\big([u_N^{k+\frac{1}{2}}]^3 - u_N^{k+\frac{1}{2}}\big)\|\frac{\|u_N^{k+1} - u_N^k\|_{H^{-1}}}{h} \\ \leq Ch\|\nabla^3\big([u_N^{k+\frac{1}{2}}]^3 - u_N^{k+\frac{1}{2}}\big)\|,$$

where the last inequality follows from (4.15). Let us now evaluate the third-order tensor $\nabla^3[u_N^{k+\frac{1}{2}}]^3$; we obtain componentwise, relying on Step 1,

$$\begin{aligned}\big[\nabla^3[u_N^{k+\frac{1}{2}}]^3\big]_{ijk} &= \frac{\partial}{\partial x_i}\left(6u_N^{k+\frac{1}{2}}\frac{\partial u_N^{k+\frac{1}{2}}}{\partial x_j}\frac{\partial u_N^{k+\frac{1}{2}}}{\partial x_k} + 3[u_N^{k+\frac{1}{2}}]^2\frac{\partial^2 u_N^{k+\frac{1}{2}}}{\partial x_j \partial x_k}\right) \\ &= 6u_N^{k+\frac{1}{2}}\left(\frac{\partial u_N^{k+\frac{1}{2}}}{\partial x_i}\frac{\partial^2 u_N^{k+\frac{1}{2}}}{\partial x_j \partial x_k} + \frac{\partial u_N^{k+\frac{1}{2}}}{\partial x_j}\frac{\partial^2 u_N^{k+\frac{1}{2}}}{\partial x_i \partial x_k} + \frac{\partial u_N^{k+\frac{1}{2}}}{\partial x_k}\frac{\partial^2 u_N^{k+\frac{1}{2}}}{\partial x_i \partial x_j}\right) \\ &\quad + 6\frac{\partial u_N^{k+\frac{1}{2}}}{\partial x_i}\frac{\partial u_N^{k+\frac{1}{2}}}{\partial x_j}\frac{\partial u_N^{k+\frac{1}{2}}}{\partial x_k} + 3[u_N^{k+\frac{1}{2}}]^2\frac{\partial^3 u_N^{k+\frac{1}{2}}}{\partial x_i \partial x_j \partial x_k}.\end{aligned}$$

We shall bound the individual terms in this expression as follows:

$$\begin{aligned}\||\nabla u_N^{k+\frac{1}{2}}|^3\| &\leq \|\nabla u_N^{k+\frac{1}{2}}\|_{L^\infty}^2\|\nabla u_N^{k+\frac{1}{2}}\| \\ &\overset{\text{Thm. 4.4}}{\leq} C\|\nabla u_N^{k+\frac{1}{2}}\|_{L^\infty}^2 \\ &\overset{(2.5)}{\leq} C\|\nabla^2 u_N^{k+\frac{1}{2}}\|\|\nabla^3 u_N^{k+\frac{1}{2}}\| \\ &\overset{\text{Young}}{\leq} C\big(\|\nabla^2 u_N^{k+\frac{1}{2}}\|^2 + \|\nabla^3 u_N^{k+\frac{1}{2}}\|^2\big);\end{aligned}$$

similarly,

$$\begin{aligned}\| \, |u_N^{k+\frac{1}{2}} \nabla^2 u_N^{k+\frac{1}{2}}| \, |\nabla u_N^{k+\frac{1}{2}}| \, \| &\leq \|\nabla u_N^{k+\frac{1}{2}}\|_{L^\infty} \|u_N^{k+\frac{1}{2}} \nabla^2 u_N^{k+\frac{1}{2}}\| \\ &\overset{\text{Young}}{\leq} C\big(\|\nabla u_N^{k+\frac{1}{2}}\|_{L^\infty}^2 + \|u_N^{k+\frac{1}{2}} \nabla^2 u_N^{k+\frac{1}{2}}\|^2\big) \\ &\overset{(2.5)}{\leq} C\big(\|\nabla^2 u_N^{k+\frac{1}{2}}\| \|\nabla^3 u_N^{k+\frac{1}{2}}\| + \|u_N^{k+\frac{1}{2}} \nabla^2 u_N^{k+\frac{1}{2}}\|^2\big), \\ &\overset{\text{Young}}{\leq} C\big(\|\nabla^2 u_N^{k+\frac{1}{2}}\|^2 + \|\nabla^3 u_N^{k+\frac{1}{2}}\|^2 + \|u_N^{k+\frac{1}{2}} \nabla^2 u_N^{k+\frac{1}{2}}\|^2\big);\end{aligned}$$

and, finally,

$$\begin{aligned}\|[u_N^{k+\frac{1}{2}}]^2 \, \nabla^3 u_N^{k+\frac{1}{2}}\| &\leq \|u_N^{k+\frac{1}{2}}\|_{L^\infty}^2 \|\nabla^3 u_N^{k+\frac{1}{2}}\| \\ &\overset{\text{Young}}{\leq} C\big(\|u_N^{k+\frac{1}{2}}\|_{L^\infty}^4 + \|\nabla^3 u_N^{k+\frac{1}{2}}\|^2\big) \\ &\overset{(2.5)}{\leq} C\big(\|\nabla u_N^{k+\frac{1}{2}}\|^2 \, \|\nabla^2 u_N^{k+\frac{1}{2}}\|_{L^2}^2 + \|\nabla^3 u_N^{k+\frac{1}{2}}\|^2 + 1\big) \\ &\overset{\text{Thm. 4.4}}{\leq} C\big(\|\nabla^2 u_N^{k+\frac{1}{2}}\|^2 + \|\nabla^3 u_N^{k+\frac{1}{2}}\|^2\big).\end{aligned}$$

Thus, we have that

$$\begin{aligned}&\sum_{k=0}^{M-1} \left| \left\langle \Delta\big([u_N^{k+\frac{1}{2}}]^3 - u_N^{k+\frac{1}{2}}\big), u_N^{k+1} - u_N^k)\right\rangle \right| \\ &\qquad \leq C \sum_{k=0}^{M-1} h\Big(\|\nabla^2 u_N^{k+\frac{1}{2}}\|^2 + \|\nabla^3 u_N^{k+\frac{1}{2}}\|^2 + \|u_N^{k+\frac{1}{2}} \nabla^2 u_N^{k+\frac{1}{2}}\|^2 + 1\Big);\end{aligned}$$

the right-hand side is bounded thanks to (4.6), (4.18), and (4.19).

All in all, by summing from 0 to some arbitrary $j \in \{1, \dots, M-1\}$, we obtain

$$\begin{aligned}\sum_{k=0}^{j} h \frac{\|u_N^{k+1} - u_N^k\|^2}{2h^2} + \|\nabla u_N^{j+1}\|_{\mathscr{L}}^2 &\leq \|\nabla u_N^0\|_{\mathscr{L}}^2 \\ &\quad + \sum_{k=0}^{M-1} \left| \left\langle \Delta\big([u_N^{k+\frac{1}{2}}]^3 - u_N^{k+\frac{1}{2}}\big), u_N^{k+1} - u_N^k)\right\rangle \right|,\end{aligned}$$

which yields the desired uniform $\ell^\infty(0, T; H^2)$ bound. ∎

Remark 4.6. The a priori bounds imply uniform bounds on sequences of interpolants

$$\left(u_N^{(h)}\right) \subset H^1(0, T; L^2(\mathbb{T}^3)) \cap L^\infty(0, T; H^2(\mathbb{T}^3))$$

as $N \to \infty$ and $h \searrow 0$. It is routine now to obtain, for $u^0 \in H^3(\mathbb{T}^3)$ with $⨍_{\mathbb{T}^3} u \, \mathrm{d}x = m$ and by virtue of suitable compactness arguments, a weak limit function u in the above function space satisfying

$$u_t + \Delta\Big(\varepsilon^2 \Delta u - (u^3 - u)\Big) + \sigma(u - m) = 0 \quad \text{and} \quad u(0) = u^0$$

in the weak sense. The weak solution u is unique in the class in which it exists. Indeed, one easily obtains from Sobolev embeddings the following stability result:

$$\|(u - v)(t)\|_{H^{-1}}^2 + \frac{1}{2} \int_0^t \|u - v\|_{\mathscr{L}}^2 \, \mathrm{d}s \leq \|u^0 - v^0\|_{H^{-1}}^2 + C(R) \int_0^t \|(u - v)(t)\|_{H^{-1}}^2 \mathrm{d}s,$$

valid for all $t \in (0,T]$ and all such solutions u and v with $L^\infty(0,T;H^2)$ norms smaller than $R > 0$. Observe that by a standard approximation procedure, we obtain such solutions for $u^0 \in H^2(\mathbb{T}^3)$ only. Moreover, for solutions in this class we have $u_t + \varepsilon^2\Delta^2 u \in L^\infty(0,T;L^2) \cap H^1(0,T;H^{-2})$. Hence, for $u^0 \in H^3(\mathbb{T}^3)$, $D_x^3 u \in L^\infty(0,T;L^2)$ and $u_{tt} \in L^2(0,T;L^2)$ (for finite T), which can be deduced, e.g., from Duhamel's formula and the mapping properties of $\mathrm{e}^{-\varepsilon^2\Delta^2 t}$. This enables a bootstrapping argument, and we obtain, for smooth initial data u^0, a smooth solution $u : \mathbb{T}^3 \times [0,T] \to \mathbb{R}$, which may be extended to all $T < \infty$.

The regularity obtained in the above remark is independent of the nonlocal term and the parameter σ. This is so, because we rely on the regularizing properties of $\varepsilon^2\Delta^2 u$ with $\varepsilon > 0$ fixed. Therefore, assuming sufficiently regular initial data, we obtain smoothness of the analytical solution of the Cahn–Hilliard/Ohta–Kawasaki equation; this will be essential in Theorem 5.1.

5. Convergence analysis. In the two previous sections we established the existence of a unique solution to the proposed numerical method (cf. Theorem 3.1) and derived various bounds on norms of the sequence of approximate solutions. We shall now derive an a priori bound on the error between the analytical solution and its numerical approximation, assuming sufficient smoothness of the analytical solution (cf. Remark 4.6). Our main result is stated in the following theorem.

THEOREM 5.1. *Suppose that $u^0 \in H^2(\mathbb{T}^3)$ with $⨍_{\mathbb{T}^3} u^0 \,\mathrm{d}x = m$, and that, for $T > 0$, the corresponding unique solution $u \in H^1(0,T;L^2(\mathbb{T}^3)) \cap L^\infty(0,T;H^2(\mathbb{T}^3))$ to* (1.4)*, satisfying $u(0) = u^0$, has the following additional regularity:*

$$u \in H^3(0,T;H^{-1}(\mathbb{T}^3)) \cap L^\infty(0,T;H^s(\mathbb{T}^3))$$

with some $s \geq 2$. Suppose, in addition, that for a fixed $\alpha \in (0,2)$ and $h = T/M$,

$$h \leq \alpha\varepsilon^2.$$

Then, there exists a constant $C = C(\varepsilon, u^0)$ such that

$$\max_{k\in\{0,1,\dots,M\}} \|u_N^k - u(t^k)\|_{H^{-1}} + \left(h\sum_{k=0}^{M-1} \|u_N^{k+\frac{1}{2}} - u(t^{k+\frac{1}{2}})\|^4\right)^{\frac{1}{4}} \leq C\big(h^2 + N^{-s}\big)$$

and

$$\left(h\sum_{k=0}^{M-1} \|\nabla u_N^{k+\frac{1}{2}} - \nabla u(t^{k+\frac{1}{2}})\|^2\right)^{\frac{1}{2}} \leq C\big(h^2 + N^{1-s}\big).$$

Remark 5.2. The bound on the second term in the first displayed error bound is optimal in terms of our assumption on the spatial regularity of the analytical solution $u \in L^\infty(0,T;H^s(\mathbb{T}^3))$.

Proof. The proof proceeds as in [11, 7]; i.e., we compare the discrete solution $u_N^{k+\frac{1}{2}}$ with the analytical solution $u(t^{k+\frac{1}{2}})$ evaluated at $t^{k+\frac{1}{2}} = \frac{1}{2}(t^k + t^{k+1})$. In addition to the bounds outlined in [11, 7], we exploit the monotonicity of the nonlinearity. This, combined with the fact that we are using a spatial discretization based on a Fourier spectral method, allows us to *avoid assuming* uniform bounds on the sequence of approximate solutions, which were essential, for example, in [11].

First, let us consider the partial differential equation (1.4) at time $t^{k+\frac{1}{2}}$ tested with some $\varphi = (-\Delta)^{-1}\phi$, where $\phi \in \mathring{\mathrm{X}}_N$; thus,

$$\left\langle u_t(t^{k+\frac{1}{2}}), \phi \right\rangle_{H^{-1}} + \left\langle u(t^{k+\frac{1}{2}}), \phi \right\rangle_{\mathscr{L}} + \left\langle [u(t^{k+\frac{1}{2}})]^3, \phi \right\rangle = \left\langle u(t^{k+\frac{1}{2}}), \phi \right\rangle.$$

Reordering and, by orthogonality, truncating the Fourier series of the analytical solution leads to

$$\begin{aligned}
&\frac{1}{h}\left\langle P_N u(t^{k+1}) - P_N u(t^k), \phi \right\rangle_{H^{-1}} + \left\langle \frac{P_N u(t^k) + P_N u(t^{k+1})}{2}, \phi \right\rangle_{\mathscr{L}} \\
&\quad + \left\langle P_N \Big[\frac{P_N u(t^k) + P_N u(t^{k+1})}{2} \Big]^3, \phi \right\rangle \\
&\quad = \left\langle \frac{P_N u(t^k) + P_N u(t^{k+1})}{2}, \phi \right\rangle \\
&\quad - \left\langle P_N u_t(t^{k+\frac{1}{2}}) - \frac{P_N u(t^{k+1}) - P_N u(t^k)}{h}, \phi \right\rangle_{H^{-1}} \\
&\quad + \frac{1}{2}\left\langle P_N u(t^k) - 2P_N u(t^{k+\frac{1}{2}}) + P_N u(t^{k+1}), \phi \right\rangle_{\mathscr{L}} \\
&\quad - \frac{1}{2}\left\langle P_N u(t^k) - 2P_N u(t^{k+\frac{1}{2}}) + P_N u(t^{k+1}), \phi \right\rangle \\
&\quad + \left\langle P_N [P_N u(t^{k+\frac{1}{2}})]^3, \phi - P_N [u(t^{k+\frac{1}{2}})]^3 \right\rangle \\
&\quad + \left\langle P_N \Big[\frac{P_N u(t^k) + P_N u(t^{k+1})}{2} \Big]^3 - P_N [P_N u(t^{k+\frac{1}{2}})]^3, \phi \right\rangle.
\end{aligned} \tag{5.1}$$

In order to abbreviate various long expressions, we define, with $\phi \in \mathring{\mathrm{X}}_N$,

$$\begin{aligned}
\langle \mathrm{Err}_0(u), \phi \rangle &:= -\left\langle P_N u_t(t^{k+\frac{1}{2}}) - \frac{P_N u(t^{k+1}) - P_N u(t^k)}{h}, \phi \right\rangle_{H^{-1}}, \\
\langle \mathrm{Err}_1(u), \phi \rangle &:= -\frac{1}{2}\left\langle P_N u(t^k) - 2P_N u(t^{k+\frac{1}{2}}) + P_N u(t^{k+1}), \phi \right\rangle \\
&\qquad + \left\langle P_N \Big[\frac{P_N u(t^k) + P_N u(t^{k+1})}{2} \Big]^3 - P_N [P_N u(t^{k+\frac{1}{2}})]^3, \phi \right\rangle \\
&\qquad + \left\langle P_N [P_N u(t^{k+\frac{1}{2}})]^3 - P_N [u(t^{k+\frac{1}{2}})]^3, \phi \right\rangle, \\
\langle \mathrm{Err}_2(u), \phi \rangle &:= \frac{1}{2}\left\langle P_N u(t^k) - 2P_N u(t^{k+\frac{1}{2}}) + P_N u(t^{k+1}), \phi \right\rangle_{\mathscr{L}}.
\end{aligned}$$

To bound the error due to time discretization, we introduce the difference e_N^k between the numerical solution and the projection of the analytical solution evaluated at t^k onto $\mathring{\mathrm{X}}_N$, i.e.,

$$e_N^k := u_N^k - P_N u(t^k) \in \mathring{\mathrm{X}}_N.$$

Consistently with our earlier notational conventions, we define $e_N^{k+\frac{1}{2}} := \frac{1}{2}(e_N^k + e_N^{k+1})$. Subtracting (5.1) from the discrete equation (3.1) and testing the result with $\phi = e_N^{k+\frac{1}{2}}$

leads to

(5.2)

$$\frac{1}{2}\Big(\|e_N^{k+1}\|_{H^{-1}}^2 - \|e_N^k\|_{H^{-1}}^2\Big) + h\|e_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2$$
$$\le \frac{1}{2}\Big(\|e_N^{k+1}\|_{H^{-1}}^2 - \|e_N^k\|_{H^{-1}}^2\Big) + h\|e_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2$$
$$+ h\underbrace{\left\langle P_N[u_N^{k+\frac{1}{2}}]^3 - P_N\left[\frac{P_N u(t^k) + P_N u(t^{k+1})}{2}\right]^3, \overbrace{u_N^{k+\frac{1}{2}} - \frac{P_N u(t^k) + P_N u(t^{k+1})}{2}}^{e_N^{k+\frac{1}{2}}}\right\rangle}_{\ge 0}$$
$$= h\left\langle e_N^{k+\frac{1}{2}}, e_N^{k+\frac{1}{2}}\right\rangle + h\left\langle \mathrm{Err}_0(u), e_N^{k+\frac{1}{2}}\right\rangle_{H^{-1}}$$
$$+ h\left\langle \mathrm{Err}_1(u), e_N^{k+\frac{1}{2}}\right\rangle + h\left\langle \mathrm{Err}_2(u), e_N^{k+\frac{1}{2}}\right\rangle_{\mathscr{L}}$$
$$\le \frac{h}{2\varepsilon^2}\|e_N^{k+\frac{1}{2}}\|_{H^{-1}}^2 + \frac{3h}{4}\|e_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2 + C\Big(\|\mathrm{Err}_0(u)\|_{H^{-1}}^2 + \|\mathrm{Err}_1(u)\|^2 + \|\mathrm{Err}_2(u)\|_{\mathscr{L}}^2\Big),$$

where, in the last line, we exploited (2.2). Insofar as the error terms are concerned, the following bounds can be deduced from Taylor expansion, as in [11, 7]:

$$\|\mathrm{Err}_0(u)\|_{H^{-1}}^2 = \left\|P_N\Big(u_t(t^{k+\frac{1}{2}}) - \frac{u(t^{k+1}) - u(t^k)}{h}\Big)\right\|_{H^{-1}}^2 \le Ch^3 \int_{t^k}^{t^{k+1}} \|u_{ttt}(t)\|_{H^{-1}}^2 \,\mathrm{d}t,$$
$$\|\mathrm{Err}_2(u)\|_{\mathscr{L}}^2 = \left\|P_N\big(u(t^k) - 2u(t^{k+\frac{1}{2}}) + u(t^{k+1})\big)\right\|_{\mathscr{L}}^2 \le Ch^3 \int_{t^k}^{t^{k+1}} \|u_{tt}(t)\|_{\mathscr{L}}^2 \,\mathrm{d}t.$$

Let us now consider $\|\mathrm{Err}_1(u)\|$; for its first term we have that

$$\|P_N u(t^k) - 2P_N u(t^{k+\frac{1}{2}}) + P_N u(t^{k+1})\|^2 \le Ch^3 \int_{t^k}^{t^{k+1}} \|u_{tt}(t)\|^2 \,\mathrm{d}t,$$

similarly as in the bound on $\mathrm{Err}_2(u)$. For the second term of $\|\mathrm{Err}_1(u)\|$ we proceed similarly (cf. also [11]):

$$\left\|P_N\left[\frac{P_N u(t^k) + P_N u(t^{k+1})}{2}\right]^3 - P_N[P_N u(t^{k+\frac{1}{2}})]^3\right\|^2$$
$$\le C(1 + \|P_N u\|_{L^\infty(0,T;H^s(\mathbb{T}^3))}^4)\|P_N u(t^k) - 2P_N u(t^{k+\frac{1}{2}}) + P_N u(t^{k+1})\|^2$$
$$\le Ch^3(1 + \|u\|_{L^\infty(0,T;H^s(\mathbb{T}^3))}^4)\int_{t^k}^{t^{k+1}} \|u_{tt}(t)\|^2 \,\mathrm{d}t,$$

where, again, the last inequality follows by Taylor expansion. Finally, for the last term of $\|\mathrm{Err}_1(u)\|$ we have that

$$\|P_N[P_N u(t^{k+\frac{1}{2}})]^3 - P_N[u(t^{k+\frac{1}{2}})]^3\|^2$$
$$\le C\big(1 + \|P_N u\|_{L^\infty(0,T;H^s(\mathbb{T}^3))}^4\big)\|u(t^{k+\frac{1}{2}}) - P_N u(t^{k+\frac{1}{2}})\|^2$$
$$\le C\big(1 + \|u\|_{L^\infty(0,T;H^s(\mathbb{T}^3))}^4\big)\|u - P_N u\|_{L^\infty(0,T;L^2(\mathbb{T}^3))}^2$$
$$\le C\big(1 + \|u\|_{L^\infty(0,T;H^s(\mathbb{T}^3))}^6\big)N^{-2s},$$

where we used (2.4) and (2.7). Taking all of the above into account and summing (5.2) from 0 to some arbitrary $j \in \{0, 1, \dots, M-1\}$, with $h \equiv \Delta t := T/M$, $M \geq 2$, we get that

$$\begin{aligned}
&\|e_N^{j+1}\|_{H^{-1}}^2 + \frac{h}{2}\sum_{k=0}^{j} \|e_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2 \\
&\quad \leq \|e_N^0\|_{H^{-1}}^2 + \frac{h}{2\varepsilon^2}\sum_{k=0}^{j+1} \|e_N^k\|_{H^{-1}}^2 + C\big(h^4 + N^{-2s}\big) \\
&\quad \leq \|e_N^0\|_{H^{-1}}^2 + \frac{h}{2\varepsilon^2}\sum_{k=0}^{j} \|e_N^k\|_{H^{-1}}^2 + \frac{h}{2\varepsilon^2}\|e_N^{j+1}\|_{H^{-1}}^2 + C\big(h^4 + N^{-2s}\big),
\end{aligned}$$

where $C = C(\varepsilon, u^0)$. Thanks to the hypothesis $h \leq \alpha\varepsilon^2$, with $\alpha \in (0, 2)$ fixed, we get that

(5.3)
$$\Big(1 - \frac{\alpha}{2}\Big)\|e_N^{j+1}\|_{H^{-1}}^2 + \frac{h}{2}\sum_{k=0}^{j} \|e_N^{k+\frac{1}{2}}\|_{\mathscr{L}}^2 \leq \|e_N^0\|_{H^{-1}}^2 + \frac{h}{2\varepsilon^2}\sum_{k=0}^{j} \|e_N^k\|_{H^{-1}}^2 + C\big(h^4 + N^{-2s}\big).$$

As $e_N^0 = 0$, the discrete Gronwall inequality then implies that

$$\max_{j \in \{1,2,\dots,M\}} \|e_N^j\|_{H^{-1}} + \left(h\sum_{k=0}^{M-1} \|e^{k+\frac{1}{2}}\|_{\mathscr{L}}^2\right)^{\frac{1}{2}} \leq C\big(h^2 + N^{-s}\big). \tag{5.4}$$

The bound on the first term on the left-hand side implies that

$$\max_{k \in \{0,1,\dots,M-1\}} \|e_N^{k+\frac{1}{2}}\|_{H^{-1}} \leq C\big(h^2 + N^{-s}\big).$$

Thus, by function space interpolation between this last bound and the bound on the second term on the left-hand side of (5.4), noting that $e_N^0 = 0$ and therefore $e_N^{\frac{1}{2}} = \frac{1}{2}e_N^1$, we have that

$$\max_{j \in \{0,1,\dots,M\}} \|e_N^j\|_{H^{-1}} + \left(h\sum_{k=0}^{M-1} \|e^{k+\frac{1}{2}}\|^4\right)^{\frac{1}{4}} \leq C\big(h^2 + N^{-s}\big).$$

Finally, by the triangle inequality,

$$\begin{aligned}
\|u_N^k - u(t^k)\|_{H^{-1}} &\leq \|e_N^k\|_{H^{-1}} + \|P_N u(t^k) - u(t^k)\|_{H^{-1}}, \qquad k = 0, 1, \dots, M, \quad \text{and} \\
\|u_N^{k+\frac{1}{2}} - u(t^{k+\frac{1}{2}})\| &\leq \|e_N^{k+\frac{1}{2}}\| + \|P_N u(t^{k+\frac{1}{2}}) - u(t^{k+\frac{1}{2}})\|, \qquad k = 0, 1, \dots, M-1.
\end{aligned}$$

By combining the last three displayed inequalities and noting the approximation result (2.7), we deduce the desired error bound, with $C = C(\varepsilon, u^0)$:

$$\max_{k \in \{0,1,\dots,M\}} \|u_N^k - u(t^k)\|_{H^{-1}} + \left(h\sum_{k=0}^{M-1} \|u_N^{k+\frac{1}{2}} - u(t^{k+\frac{1}{2}})\|^4\right)^{\frac{1}{4}} \leq C\big(h^2 + N^{-s}\big).$$

This proves the first displayed error bound in the statement of the theorem.

For the second bound, we return to (5.4) and note that the bound on the second term on the left-hand side implies that

$$\left(h\sum_{k=0}^{M-1}\|\nabla e_N^{k+\frac{1}{2}}\|^2\right)^{\frac{1}{2}} \le C\big(h^2+N^{-s}\big).$$

Also,

$$\|\nabla(u_N^{k+\frac{1}{2}}-u(t^{k+\frac{1}{2}}))\| \le \|\nabla e_N^{k+\frac{1}{2}}\|+\|\nabla(P_N u(t^{k+\frac{1}{2}})-u(t^{k+\frac{1}{2}}))\|, \qquad k=0,1,\dots,M-1.$$

By noting the approximation result (2.7) to bound the second term on the right-hand side of the last inequality, the desired error bound then follows by the triangle inequality. ∎

6. Iteration scheme for the discrete problem. Theorem 3.1 guarantees the existence of a unique solution defined by the scheme (3.1), with $u_N^0 := P_N u^0$, provided that $h < 8\varepsilon^2/(1-4\sigma\varepsilon^2)_+$. Theorems 4.4 and 4.5 imply that the sequence of numerical solutions defined by the scheme (3.1) is bounded in various norms, uniformly with respect to the discretization parameters $h \equiv \Delta t := T/M$, $M \ge 2$, and $N \ge 1$, provided that $h \le 2\varepsilon^2$ (cf. Theorem 4.1) and $h \le \min(2,\delta/R^4)\varepsilon^2$ (cf. Theorems 4.4 and 4.5), respectively. We have also shown in Theorem 5.1 that the sequence of numerical approximations converges to the analytical solution in various norms, under the assumption that $h \le \alpha\varepsilon^2$, where $\alpha \in (0,2)$ is a fixed positive constant.

Before embarking on our numerical experiments, we shall develop an iterative method for the numerical solution of the system of nonlinear equations arising at a given time level of the scheme (3.1). It is based on splitting the nonlinear operator into a monotone nonlinear part and a (noncoercive) linear part. The monotone part of the operator will then be dealt with using ideas from the theory of monotone operators, similarly as in section 3, while the (noncoercive) linear part is handled via fixed point theory. The practical relevance of this "convex splitting" is that one can rely in the implementation of the method on well-developed techniques from convex optimization and fixed point methods (cf. Remark 6.3). For ease of exposition, we shall concentrate here on the case when

$$m = \fint_{\mathbb{T}^3} u \,\mathrm{d}x = 0; \tag{6.1}$$

the case of $m \neq 0$ can be dealt with by shifting u by its integral mean over $\mathbb{T}^3$, as in section 3. This shift only has a consequence on the cubic nonlinearity but does not affect its monotonicity properties and the argument for $m = 0$ can be therefore easily adapted to the case of $m \neq 0$.

Recall that the equation (3.1) under consideration reads as follows:

$$\left\langle \frac{u_N^{k+1}-u_N^k}{h},\phi\right\rangle_{H^{-1}} + \left\langle u_N^{k+\frac{1}{2}},\phi\right\rangle_{\mathscr{L}} + \left\langle [u_N^{k+\frac{1}{2}}]^3,\phi\right\rangle = \left\langle u_N^{k+\frac{1}{2}},\phi\right\rangle \qquad \forall \phi \in \mathring{\mathrm{X}}_N,$$

and can be rewritten as

$$2\left\langle u_N^{k+\frac{1}{2}},\phi\right\rangle_{H^{-1}} + h\left\langle u_N^{k+\frac{1}{2}},\phi\right\rangle_{\mathscr{L}} + h\left\langle [u_N^{k+\frac{1}{2}}]^3,\phi\right\rangle = h\left\langle u_N^{k+\frac{1}{2}},\phi\right\rangle + 2\left\langle u_N^k,\phi\right\rangle_{H^{-1}} \qquad \forall \phi \in \mathring{\mathrm{X}}_N.$$

It will be convenient for computational purposes to reformulate the problem by means of the operator $\mathscr{A}_h : \mathring{\mathrm{X}}_N \to \mathring{\mathrm{X}}_N$ defined by

$$\langle \mathscr{A}_h(u), \phi \rangle = 2 \langle u, \phi \rangle_{H^{-1}} + h \langle u, \phi \rangle_{\mathscr{L}} + h \langle u^3, \phi \rangle \qquad \forall \phi \in \mathring{\mathrm{X}}_N; \tag{6.2}$$

therefore we are to solve

$$\text{for } u_N^k \in \mathring{\mathrm{X}}_N \text{ find } u_N^{k+\frac{1}{2}} \in \mathring{\mathrm{X}}_N \quad \text{s.t.} \left\langle \mathscr{A}_h(u_N^{k+\frac{1}{2}}), \phi \right\rangle = h \left\langle u_N^{k+\frac{1}{2}}, \phi \right\rangle + 2 \left\langle u_N^k, \phi \right\rangle_{H^{-1}} \quad \forall \phi \in \mathring{\mathrm{X}}_N. \tag{6.3}$$

Let us note that in (6.3) we are not solving for u_N^{k+1}, but seek $u_N^{k+\frac{1}{2}} := \frac{1}{2}(u_N^{k+1} + u_N^k)$ instead. Clearly, this is not a drawback because, given u_N^k, once $u_N^{k+\frac{1}{2}}$ has been found, u_N^{k+1} is also determined uniquely.

Remark 6.1 (properties of $\mathscr{A}_h$). The operator $\mathscr{A}_h$ is strongly monotone on $\mathring{\mathrm{X}}_N$ in the sense that

$$\begin{aligned} \langle \mathscr{A}_h(z) - \mathscr{A}_h(z'), z - z' \rangle &\geq 2\|z - z'\|_{H^{-1}}^2 + h\|z - z'\|_{\mathscr{L}}^2 \\ &=: \|z - z'\|_h^2 \qquad \forall z, z' \in \mathring{\mathrm{X}}_N. \end{aligned} \tag{6.4}$$

As $\mathscr{A}_h(0) = 0$, it follows from (6.4) with $z' = 0$ that $\langle \mathscr{A}_h(z), z \rangle \geq \|z\|_h^2$ for all $z \in \mathring{\mathrm{X}}_N$, and therefore $\mathscr{A}_h$ is coercive on $\mathring{\mathrm{X}}_N$. Further, by Hölder's inequality and Sobolev's embedding theorem,

$$| \langle \mathscr{A}_h(z) - \mathscr{A}_h(z'), \phi \rangle | \leq C(\varepsilon, u^0)(1 + \|z\|_{L^3}^2 + \|z'\|_{L^3}^2) \|z - z'\|_h \|\phi\|_h \qquad \forall z, z' \in \mathring{\mathrm{X}}_N,$$

and therefore

$$\|\mathscr{A}_h(z) - \mathscr{A}_h(z')\|_{[\mathring{\mathrm{X}}_N]'} \leq C(\varepsilon, u^0)(1 + \|z\|_{L^3}^2 + \|z'\|_{L^3}^2) \|z - z'\|_h \qquad \forall z, z' \in \mathring{\mathrm{X}}_N, \tag{6.5}$$

where the dual space $[\mathring{\mathrm{X}}_N]'$ is equipped with the dual of the norm $\| \cdot \|_h$. Thus, in particular, viewed as a mapping from $\mathring{\mathrm{X}}_N$ into $[\mathring{\mathrm{X}}_N]'$, $\mathscr{A}_h$ is continuous and (again, since $\mathscr{A}_h(0) = 0$) bounded. Thanks to the Browder–Minty theorem (cf. Thm. 10.49 in [21]), $\mathscr{A}_h$ is therefore bijective as a mapping from $\mathring{\mathrm{X}}_N$ into $[\mathring{\mathrm{X}}_N]'$. By identifying, via the Riesz representation theorem, $[\mathring{\mathrm{X}}_N]'$ with $\mathring{\mathrm{X}}_N$, we deduce that $\mathscr{A}_h$ is bijective as a mapping on $\mathring{\mathrm{X}}_N$; i.e., for any $f \in \mathring{\mathrm{X}}_N$ there exists a unique $z \in \mathring{\mathrm{X}}_N$ such that

$$\mathscr{A}_h(z) = f. \tag{6.6}$$

In fact, (6.6) can be equivalently understood as a minimization problem corresponding to a strictly convex objective function $\mathscr{I}_h : \mathring{\mathrm{X}}_N \to \mathbb{R}$, whose Gâteaux derivative is $\mathscr{A}_h(z) - f$. It is important to note that $\mathscr{A}_h$ is bijective for all $h > 0$, regardless of ε; in particular, in contrast with the proof of Theorem 3.1 where the nonlinear operator under consideration only satisfied the hypotheses of the Browder–Minty theorem for $h < 8\varepsilon^2/(1 - 4\sigma\varepsilon^2)_+$, here no such condition on h is needed.

By virtue of (6.6), for a given $u_N^k \in \mathring{\mathrm{X}}_N$ and any $z \in \mathring{\mathrm{X}}_N$ we may find a unique $T_h(z) \in \mathring{\mathrm{X}}_N$ such that

$$\langle \mathscr{A}_h(T_h(z)), \phi \rangle = h \langle z, \phi \rangle + 2 \left\langle u_N^k, \phi \right\rangle_{H^{-1}} \qquad \forall \phi \in \mathring{\mathrm{X}}_N. \tag{6.7}$$

This then defines a (nonlinear) operator $T_h : \mathring{\mathrm{X}}_N \to \mathring{\mathrm{X}}_N$, and solving (6.3) is equivalent to finding the unique fixed point $z = u_N^{k+\frac{1}{2}}$ of T_h.

THEOREM 6.2. *Suppose that $\alpha \in (0,2)$ is a fixed real number such that*

$$h \le \alpha\varepsilon^2$$

and that the assumptions of Theorem 4.4 hold. Then, the sequence $\{z^l\}_{l\in\mathbb{N}} \subset \mathring{\mathrm{X}}_N$ generated by the iteration

$$z^{l+1} = T_h(z^l) \quad \forall l \in \mathbb{N}_0 \quad \textit{with} \quad z^0 := u_N^k,$$

converges in $\mathring{\mathrm{X}}_N$ to the unique fixed point $z = u_N^{k+\frac{1}{2}}$ of T_h, and there exists a positive constant $q = q(\alpha) \in (0,1)$, independent of h and N, such that

$$\|z - z^l\|_h \le \frac{q^l}{1-q}\, C(\varepsilon, u^0)\, h^{\frac{1}{2}}, \qquad l = 1, 2, \dots. \tag{6.8}$$

Proof. The proof will be accomplished in two steps.

Step 1. First we prove that $T_h : \mathring{\mathrm{X}}_N \to \mathring{\mathrm{X}}_N$ is a contraction. To this end take any z, z' in $\mathring{\mathrm{X}}_N$, define $Z := T_h(z)$, $Z' := T_H(z')$ and, relying on the strong monotonicity of $\mathscr{A}_h$, we note that, for any $\beta > 0$,

$$\begin{aligned}\|Z - Z'\|_h^2 &\le \langle \mathscr{A}_h(Z) - \mathscr{A}_h(Z'), Z - Z'\rangle = h\,\langle z - z', Z - Z'\rangle \\ &\le \beta\|z - z'\|_{H^{-1}}^2 + \frac{h^2}{4\beta}\|\nabla(Z - Z')\|^2 \le \frac{\beta}{2}\|z - z'\|_h^2 + h\frac{h}{4\varepsilon^2\beta}\|Z - Z'\|_{\mathscr{L}}^2.\end{aligned}$$

As $\frac{h}{4\varepsilon^2} \le \frac{\alpha}{4}$, it follows that

$$\left(1 - \frac{\alpha}{4\beta}\right)\|Z - Z'\|_h^2 \le \frac{\beta}{2}\|z - z'\|_h^2.$$

Suppose that β is a positive real number, independent of h and N, such that $\beta > \alpha/4$ and $|1 - \beta| < \sqrt{1 - (\alpha/2)}$. Clearly, the set of such δ is nonempty; for example, $\beta = 1$ satisfies these conditions for any $\alpha \in (0,2)$. Let $q := [2\beta^2/(4\beta - \alpha)]^{\frac{1}{2}}$. Then, $0 < q < 1$, and we have the contraction property

$$\|Z - Z'\|_h \le q\|z - z'\|_h.$$

Step 2. It follows from Step 1 that

$$\|z - z^l\|_h \le \frac{q^l}{1-q}\|z^1 - z^0\|_h, \qquad l = 1, 2, \dots.$$

In order to complete the proof it remains to bound $\|z^1 - z^0\|_h = \|z^1 - u_N^k\|_h$, where $z_1 = T_h(u_N^k)$. To this end, we rewrite

$$\begin{aligned}\|z^1 - u_N^k\|_h^2 &\le \left\langle \mathscr{A}_h(z^1) - \mathscr{A}_h(u_N^k), z^1 - u_N^k\right\rangle \\ &= h\left\langle u_N^k - [u_N^k]^3, z^1 - u_N^k\right\rangle - h\left\langle u_N^k, z^1 - u_N^k\right\rangle_{\mathscr{L}} \\ &\le Ch\Big\{\|[u_N^k]^3\|^2 + \|u_N^k\|^2 + \|u_N^k\|_{\mathscr{L}}^2\Big\} + \frac{1}{2}\|z^1 - u_N^k\|_h^2 \\ &\le Ch + \frac{1}{2}\|z^1 - u_N^k\|_h^2,\end{aligned}$$

where in the last inequality we used that the expression in the curly brackets in the penultimate line is uniformly bounded thanks to Theorem 4.4. We thus deduce, by absorbing a factor 2 into $C = C(\varepsilon, u^0)$, that $\|z^1 - z^0\|_h \le C(\varepsilon, u^0)\, h^{\frac{1}{2}}$, and thereby

$$\|z - z^l\|_h \le \frac{q^l}{1-q}\, C(\varepsilon, u^0)\, h^{\frac{1}{2}}.$$

That completes the proof. ∎

Remark 6.3.

- On bounding $h^{\frac{1}{2}}$ by $T^{\frac{1}{2}}$, it follows from (6.8) that the convergence of the fixed point iteration $z^{l+1} := T_h(z_l)$, $l = 0, 1, \ldots$, $z^0 := u_N^k$, is uniform in h and N.
- We only needed the results of Theorem 4.4 in the proof of Theorem 6.2; the uniform bound obtained in Theorem 4.5 was not required. This is because of the monotonicity argument used.
- According to (6.7) and our definition of the sequence $\{z^l\}_{l\in\mathbb{N}} \subset \mathring{\mathrm{X}}_N$,

$$\left\langle \mathscr{A}_h(z^{l+1}), \phi \right\rangle = h \left\langle z^l, \phi \right\rangle + 2 \left\langle u_N^k, \phi \right\rangle_{H^{-1}} \qquad \forall \phi \in \mathring{\mathrm{X}}_N.$$

  Thanks to the strong monotonicity and continuous differentiability of the nonlinear operator $\mathscr{A}_h$ on $\mathring{\mathrm{X}}_N$, the unique solution $z^{l+1} \in \mathring{\mathrm{X}}_N$ can be computed, for a given $u_N^k \in \mathring{\mathrm{X}}_N$, from $z^l \in \mathring{\mathrm{X}}_N$, to within a given tolerance, by Newton's method, which in this case exhibits global quadratic convergence on the finite-dimensional vector space $\mathring{\mathrm{X}}_N$; see, [22], for example, and references therein.

7. Numerical experiments. In order to assess the performance of the numerical method formulated in section 3, we implemented it in MATLAB. For the sake of computational efficiency, in our numerical experiments the computational domain was taken to be the d-dimensional torus $\mathbb{T}^d$, with $d = 1, 2$, rather than $\mathbb{T}^3$. We have assumed in the numerical experiments that the initial datum has zero integral mean, whereby (6.1) holds.

Even though the flow to the optimum of the Ohta–Kawasaki energy is a motivation for designing unconditionally stable schemes, within this numerical section (and, in fact, in the whole contribution) we concentrate *only* on solving the Ohta–Kawasaki equation itself. Therefore, it may well happen that the stationary states computed here are metastable (cf., for example, the wiggly lamellar states in [20]). Nevertheless, because of our focus on the flow equation, we do not implement any advanced techniques such as those from [5] to escape from these, possibly metastable, states.

We need to solve (3.1) for $k = 1, \ldots, M-1$. As has been explained in section 6, to this end we have to solve (6.3), which we do by expressing the problem in Fourier transform space. Thus, given any function $w \in \mathring{\mathrm{X}}_N$, we denote by $\hat{w}(l)$ its Fourier coefficients, with $l \in \mathbb{Z}_N^d$. The constraint (1.4) then corresponds to requiring that $\hat{w}_N^k(0) = 0$ for all $k = 0, 1, \ldots, M$. We further have that

$$\begin{aligned}(7.1)\quad \langle \mathscr{A}_h(w), \mathrm{e}^{il\cdot x}\rangle &= [\widehat{\mathscr{A}_h(w)}](l) \\ &= \frac{2}{|l|^2}\hat{w}(l) + \varepsilon^2 |l|^2 \hat{w}(l) + \frac{\sigma}{|l|^2}\hat{w}(l) + [\hat{w} \star \hat{w} \star \hat{w}](l), \quad l \in \mathbb{Z}_N^d \setminus \{0\},\end{aligned}$$

and for $l = 0$ we set $[\widehat{\mathscr{A}_h(w)}](l) = 0$ so that $\mathscr{A}_h : \mathring{\mathrm{X}}_N \to \mathring{\mathrm{X}}_N$. In (7.1) we denoted by $\hat{f} \star \hat{g}$ the discrete convolution defined by

$$[\hat{f} \star \hat{g}](l) = \sum_{n\in\mathbb{Z}^d} \hat{f}(l-n)\hat{g}(n), \qquad l \in \mathbb{Z}_N^d,$$

with the convention of *zero padding*; i.e., for any $\hat{w} \in \mathring{\mathrm{X}}_N$, whose Fourier coefficients are $\hat{w}(l)$ for $l \in \mathbb{Z}_N^d$, we set $\hat{w}(l) = 0$ for all $l \in \mathbb{Z}^d \setminus \mathbb{Z}_N^d$.

As was noted in the discussion preceding (6.6), the operator $\mathscr{A}_h$ is invertible and thus for any $f \in \mathring{\mathrm{X}}_N$ there exists a unique $u \in \mathring{\mathrm{X}}_N$ such that

$$[\widehat{\mathscr{A}_h(u)}](l) - \hat{f}(l) = 0, \qquad l \in \mathbb{Z}^d_N. \tag{7.2}$$

As $\mathscr{A}_h$ is strongly monotone, solving (7.2) is equivalent to solving the following (unconstrained) minimization problem

$$\sum_{l \in \mathbb{Z}^d_N} \Big([\widehat{\mathscr{A}_h(u)}](l) - 2\hat{f}(l) \Big) \overline{\hat{u}(l)} \to \min.$$

We exploit this fact in the one-dimensional case ($d = 1$) by employing the MATLAB built-in function `fsolve`, with a trust-region option in the algorithm, to solve the system of nonlinear equations (7.2). In the two-dimensional case, because of the squared number of degrees of freedom, we have used instead the MATLAB optimization software TOMLAB/CONOPT to solve the convex optimization problem resulting from the proposed discretization, and to calculate $\mathscr{A}_h^{-1}$.

Remark 7.1 (convolution). The most costly part of evaluating $\mathscr{A}_h$ for the iterations leading to the solution of (7.1) is the computation of the convolutions involved in the Fourier transform of the cubic nonlinearity. To reduce the associated computational cost, we have used a fast convolution based on FFT of longer vectors than those that enter into the convolution in order to avoid aliasing errors; cf. [17].

After calculating $\mathscr{A}_h^{-1}$, (6.3) was solved by the fixed point iteration

$$\begin{aligned} \Big[u^{k+\frac{1}{2}}_{N,[0]}\Big]^{\wedge}(l) &= \Big[u^k_N\Big]^{\wedge}(l), && l \in \mathbb{Z}^d_N \setminus \{0\}, \\ \big[\mathscr{A}_h(u^{k+\frac{1}{2}}_{N,[\ell+1]})\big]^{\wedge}(l) &= \Big[u^{k+\frac{1}{2}}_{N,[\ell]}\Big]^{\wedge}(l) + \frac{2}{|l|^2}\Big[u^{k+\frac{1}{2}}_{N,[\ell]}\Big]^{\wedge}(l), && l \in \mathbb{Z}^d_N \setminus \{0\}, \quad \ell = 0, 1, \dots, \end{aligned}$$

where the last equation was solved as was indicated in connection with (7.2) above. The stopping criterion for the fixed point iteration was

$$\max_{l \in \mathbb{Z}^d_N} \left| \Big[u^{k+\frac{1}{2}}_{N,[\ell+1]}\Big]^{\wedge}(l) - \Big[u^{k+\frac{1}{2}}_{N,[\ell]}\Big]^{\wedge}(l) \right| < \mathtt{TOL},$$

where the termination tolerance `TOL` was taken to be 10^{-7} in our numerical experiments.

7.1. Accuracy and stability analysis in 1D. To assess the accuracy and stability of the proposed method, we have conducted a series of numerical experiments; they were performed in one space dimension ($d = 1$) because of shorter run times.

To test the temporal accuracy of the method (as the accuracy of a Fourier spectral method in the case of a smooth solution is well known to be "exponential" (cf. [17], for example)) we used a smooth initial datum, $u^0(x) = \cos(x)/2$, and took $\varepsilon = 0.5$ and $N = 211$; the time steps of the time interval $[0, 10]$ were chosen as $h = 2^{-j}$ with $j = 0 \to 7$. Note that N was intentionally taken to be relatively large, so that the inaccuracy of the method really stems from the temporal discretization. Let us denote by u^j_{Acc} the numerical solutions corresponding to the parameter values above. We then compared u^j_{Acc} to u_{Acc}, the latter being a highly accurate reference numerical solution (corresponding to $h = 2^{-10}$) playing the role of the exact solution of the Ohta–Kawasaki equation for the parameter values above.

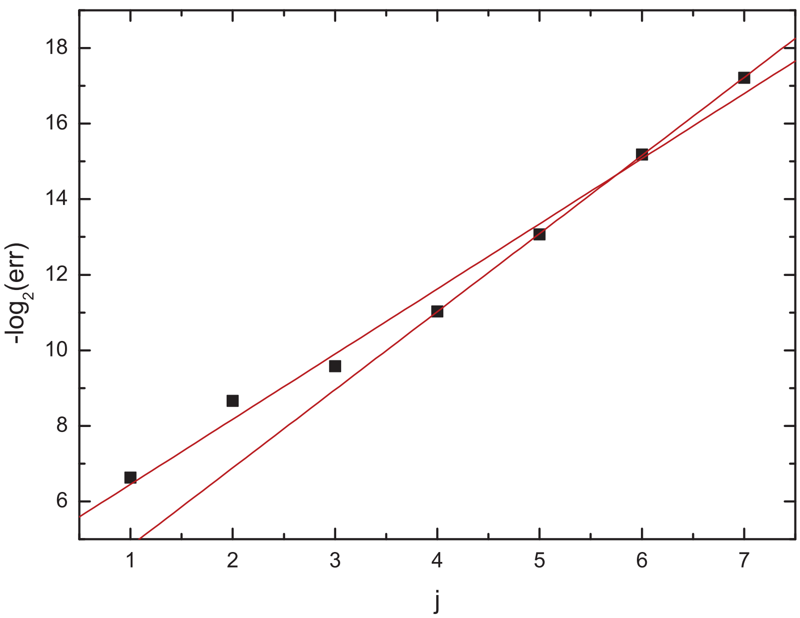

FIG. 1. *Plot of* $-\log_2(\mathtt{err}_j)$ *(black squares) with an affine fit through all points, and an affine fit only through the last four points (higher slope).*

Let us define

$$\mathtt{err}_j := \|u^j_{\mathrm{Acc}} - u_{\mathrm{Acc}}\|_{\ell^\infty([0,10];H^{-1}(\mathbb{T}^3))}, \tag{7.3}$$

and plot $-\log_2(\mathtt{err}_j)$ versus j to verify the second-order convergence of the proposed method; we expect a linear growth of $-\log_2(\mathtt{err}_j)$ as a function of j, with slope 2.

The results of this test can be read from Figure 1 where the black squares are the values of $-\log_2(\mathtt{err}_j)$. Using ORIGINLab we fitted two affine functions to the data; the first fit includes all data points and has slope 1.7, which is lower than what would correspond to second-order convergence. We believe that this is due to the fact that choices of h with $h > 2\varepsilon^2$, i.e., those that do not fulfill the assumptions of Theorem 5.1, are outside the asymptotic range for second-order convergence. This is confirmed by the second fit for which only the points corresponding to $h < \varepsilon^2$ were considered—the slope of the fitted curve is 2.07, which is very close to the theoretically predicted value of 2. We note that no numerical instabilities were observed for any of the values of h considered; in particular, we did not observe any numerical instabilities for $h > 2\varepsilon^2$.

Remark 7.2 (adaptive time stepping). In view of the computational results presented in the numerical experiment we have just described, we also implemented an adaptive time-stepping method. Whenever the iterative scheme from section 6 failed to converge in a given number of iterations (we chose 40, but in our experiments we did not even encounter such a situation), we halved the time step while if the ℓ^∞ norm of the difference of two consecutive solutions was smaller than a chosen tolerance value then we doubled the time step.

7.2. Morphological evolution in two dimensions. We shall now present the results of two-dimensional ($d = 2$) simulations of pattern evolution for the Ohta–Kawasaki equation ($\sigma > 0$) using the proposed algorithm. When starting from a

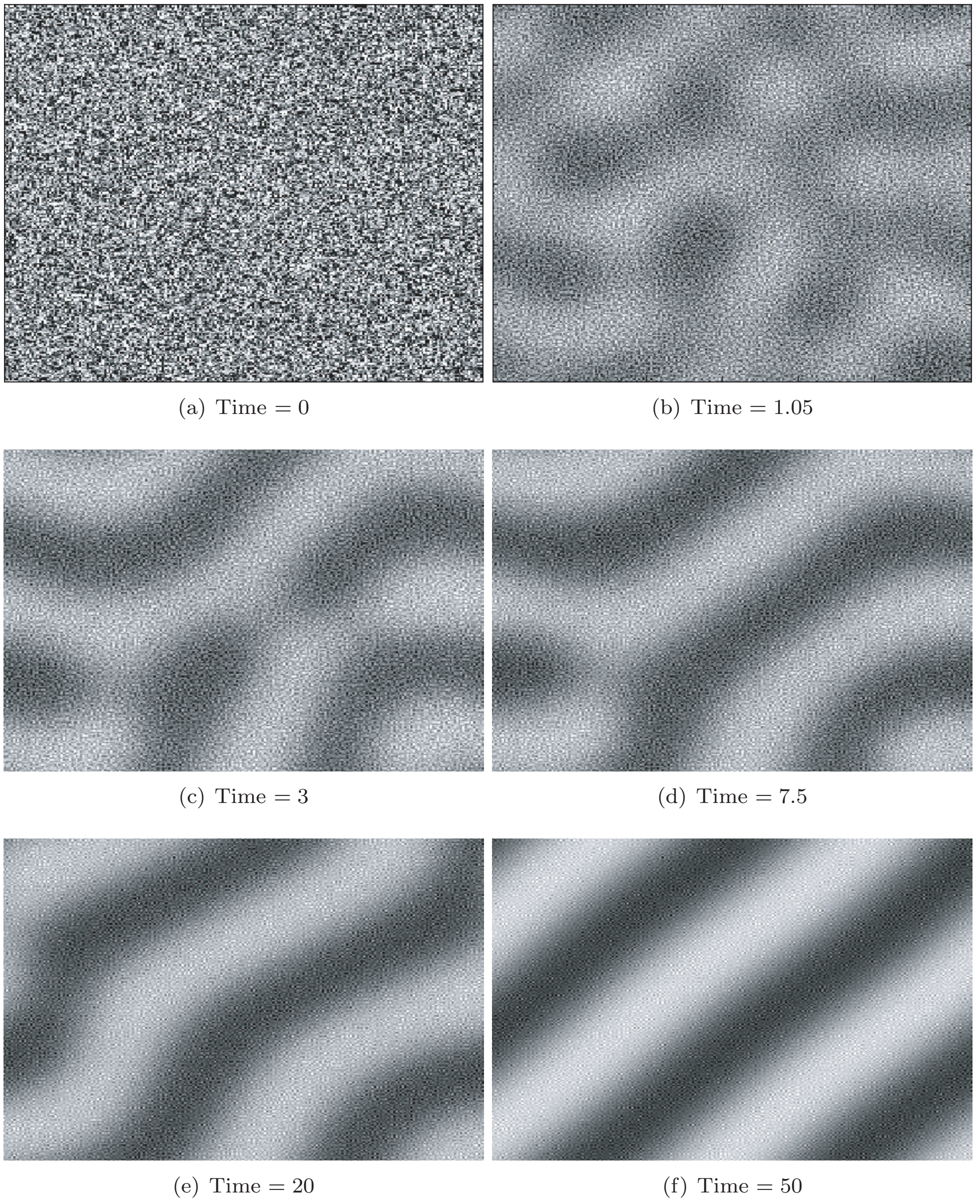

Fig. 2. *Pattern evolution in the Ohta–Kawasaki model starting from a uniformly distributed random initial datum.*

uniformly distributed random initial datum, morphological evolution is expected to exhibit several time scales (cf. [6]): first, on a rather fast scale, phase separation should be observed, i.e., regions where either of the two phases is favored are formed. Then, on a slow scale, the morphology of this pattern changes until a stable state is reached. In our case, since we work with the constraint (6.1), the only stable state is a lamellar like pattern, so we can expect evolution towards such a state.

This is indeed confirmed by the computations presented in Figure 2, where black represents the positive values (which, at later times, take a value near +1) while white corresponds to negative values around -1. It can be observed that after a very short time (which, in our computations, was 3 units of time) phase separation becomes noticeable while it takes another 50 time units for the solution to reach the unique stable state, exhibiting a pattern with lamellae.

For completeness, we specify the exact parameter values that were used in the computations whose results are depicted in Figure 2. The calculation was performed with $N = 243$. We used $\varepsilon = 0.2$ and $\sigma = 3$ so as to exclude the case when the unique minimizer of the Ohta–Kawasaki functional to which the gradient flow of the functional, described by the Ohta–Kawasaki equation, evolves is identically zero (cf. [6, Thm. 3.1]). The time step was fixed at $h = 1/200$ throughout the computation so that $h < 2\varepsilon^2$, as is required in Theorem 6.2. Notice, however, that h is several orders larger than $1/N^2$ which shows that our method performs well also in this case while usually $h \sim 1/N^2$ is required for stability elsewhere in the literature; see, e.g., [24].

For an animated evolution corresponding to this calculation and for the original source files, the reader is referred to http://www.math1.rwth-aachen.de/files/benesova-webFiles/OhtaKaw.php

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