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# CONVERGENCE TO EQUILIBRIUM FOR TIME AND SPACE DISCRETIZATIONS OF THE CAHN-HILLIARD EQUATION

MATTHIEU BRACHET, PHILIPPE PARNAUDEAU, AND MORGAN PIERRE

*Dedicated to Maurizio Grasselli on the occasion of his 60th birthday*

**ABSTRACT.** We review space and time discretizations of the Cahn-Hilliard equation which are energy stable. In many cases, we prove that a solution converges to a steady state as time goes to infinity. The proof is based on Lyapunov theory and on a Łojasiewicz type inequality. In a few cases, the convergence result is only partial and this raises some interesting questions. Numerical simulations in two and three space dimensions illustrate the theoretical results. Several perspectives are discussed.

**Keywords:** Cahn-Hilliard equation, gradient flow, energy stable scheme, Lyapunov stability, Lasalle's invariance principle, Łojasiewicz-Simon inequality, Kurdyka-Łojasiewicz inequality.

## CONTENTS

1. Introduction	2
2. The time and space continuous problem	4
2.1. Functional setting and notation	4
2.2. Well-posedness and asymptotic behaviour	6
3. The space semidiscrete case	6
3.1. The convergence result	6
3.2. Examples	13
4. The time semidiscrete case	15
4.1. BDF schemes	15
4.2. Convex splitting scheme	19
4.3. Linear schemes	20
4.4. Secant scheme and related schemes	22
4.5. SAV approach	24
5. The fully discrete case	26
5.1. A general convergence result; semialgebraic functions	27
5.2. Secant scheme with Galerkin approximation	28
5.3. Linear IMEX scheme with finite difference method	30
6. Simulations	32
6.1. 2D finite element simulations	32
6.2. 3D finite difference simulations	36

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7. Conclusion and perspectives	38
7.1. Generalization to other Cahn-Hilliard equations	38
7.2. Gradient-like PDEs with inertial term	39
7.3. Conclusion	39
Acknowledgements	40
References	40

## 1. INTRODUCTION

We consider the Cahn-Hilliard system

$$\begin{cases} \partial_t u = \Delta w, \\ w = -\Delta u + \frac{1}{\varepsilon^2}(u^3 - u), \end{cases} \quad x \in \Omega, \quad t > 0, \quad (1.1)$$

where  $\Omega$  is a bounded subset of  $\mathbb{R}^d$  ( $d = 1, 2$  or  $3$ ) with Lipschitz boundary  $\partial\Omega$ . The unknowns functions are the order parameter  $u$  and the chemical potential  $w$ . The parameter  $\varepsilon > 0$  is the typical thickness of the interface between two phases. Problem (1.1) is endowed with the Neumann boundary conditions

$$\partial_n u = 0, \quad \partial_n w = 0, \quad x \in \partial\Omega, \quad t \geq 0, \quad (1.2)$$

and an initial condition

$$u|_{t=0} = u_0. \quad (1.3)$$

The Cahn-Hilliard system (1.1) can be written equivalently as

$$\partial_t u + \Delta^2 u - \frac{1}{\varepsilon^2} \Delta(u^3 - u) = 0 \quad x \in \Omega, \quad t > 0, \quad (1.4)$$

which is known as the Cahn-Hilliard equation [24]. It was originally proposed as a model of phase separation and it has been thoroughly investigated. The formulation (1.1) has been widely used for numerical purposes because it is often easier to deal with two Laplace operators rather than with one bilaplacian operator. We refer the reader to the reviews [38, 91, 92, 100] for the mathematical aspects and [14, 101, 127] for details on the model.

A solution to (1.1)-(1.2) satisfies the conservation of mass,

$$\int_{\Omega} u(x, t) dx = \int_{\Omega} u_0(x) dx, \quad t \geq 0, \quad (1.5)$$

and the energy law

$$\frac{d}{dt} \mathcal{E}(u(t)) = - \int_{\Omega} |\nabla w(x, t)|^2 dx, \quad t > 0, \quad (1.6)$$

where

$$\mathcal{E}(u(t)) = \int_{\Omega} \frac{1}{2} |\nabla u(x, t)|^2 + \frac{1}{4\varepsilon^2} (u(x, t)^2 - 1)^2 dx. \quad (1.7)$$

The relation (1.6) shows that the energy is nonincreasing. More precisely, the Cahn-Hilliard equation is a gradient flow of the energy  $\mathcal{E}$  for the  $H^{-1}$  inner product. This can be used to obtain information on the asymptotic behaviour of solutions. In particular, the  $\omega$ -limit set of a solution contains only stationary points which are

critical points of  $\mathcal{E}$  with prescribed mass. The global attractor also has a specific structure [124].

If  $\Omega$  is an interval, then the set of steady states with prescribed mass for the Cahn-Hilliard equation (1.1)-(1.2) is finite [59, 122]. As a consequence, every solution to (1.1)-(1.2) converges to a steady state as time goes to infinity; the global attractor is also well understood [59]. In two or three space dimensions, the situation regarding steady states is much more complicated and it is not yet fully understood (see, e.g. [88, 129]). In contrast with the one-dimensional case, it is possible to build a continuum of global minimizers of  $\mathcal{E}$  with prescribed mass if  $\Omega$  is a disc or a cylinder (cf. Section 6.1).

In [114], Rybka and Hoffmann proved that every classical solution to the Cahn-Hilliard equation (1.1)-(1.2) converges to a single equilibrium as time goes to infinity. Their proof, which does not require any knowledge on the set of steady states, is based on a Łojasiewicz-Simon inequality. The latter is a generalization of the celebrated Łojasiewicz inequality for analytic functions [84] introduced by Simon [121] for some nonlinear parabolic problems. We note that the approach of Simon has been extended to many PDEs with a gradient-like flow structure, thanks to the work of Jendoubi [76, 77], Haraux [66] and Chill [30] (see also [16] and the reviews [67, 73]). Without analyticity, convergence to equilibrium may fail because the  $\omega$ -limit set of a bounded solution to a gradient flow may be a cycle. We refer to [3, 103] for such examples in finite dimension and [112] for a nonconvergent bounded solution to the semilinear heat equation with a smooth nonlinearity.

Since many time and space discretizations of the Cahn-Hilliard equation are available, it is natural to ask if the discretization reproduces the longtime dynamics of the PDE. This study seems to have been initiated by Elliott [38] for the Cahn-Hilliard equation. In a seminal paper [43], Elliott and Stuart thoroughly analyzed the dynamics of several space and time discretizations of the Allen-Cahn equation. The Allen-Cahn equation is a gradient flow of  $\mathcal{E}$  for the  $L^2$  inner product and it is closely related to the Cahn-Hilliard equation.

Since the work of Elliott and Stuart, many discretizations of Cahn-Hilliard system (1.1)-(1.2) which preserve the laws (1.5) and (1.6) at the discrete level have been proposed. Following the terminology in [125], we refer to such discretizations as “energy stable”. Finite element methods [36, 46, 53], finite difference methods [20, 21, 25, 27, 48] and spectral-Galerkin approaches [119] with such properties are available. Regarding the time semidiscretization, we refer the reader to the reviews [118, 119, 125] and to the paper [18].

Our purpose in this manuscript is to review energy stable time and/or space discretizations of the Cahn-Hilliard system (1.1)-(1.2). We focus on the question of convergence of a solution to a steady state as time goes to infinity. In many situations, the answer is well-known but in some cases, some challenging questions are still open. This approach gives a new insight into energy stable schemes for Cahn-Hilliard type equations. We also want to point out some perspectives, since the Cahn-Hilliard equation is a model problem for PDEs with a gradient-like structure.

If we consider a space semidiscretization which preserves the gradient flow structure, then convergence to equilibrium is a consequence of Łojasiewicz’s convergence result for analytic functions [84, 85]. This was demonstrated for Cahn-Hilliard type equations in [29, 74]. Convergence to equilibrium for a fully discrete Cahn-Hilliard equation was first proved in [90] by means of the Łojasiewicz inequality. Several fully

discrete Allen-Cahn equations were considered in [6]. Other fully discretized PDEs with a gradient-like flow structure were analyzed in [61, 71, 75, 89, 115]. Concerning the time semidiscretization, convergence to equilibrium for the backward Euler scheme applied to the Allen-Cahn equation was considered in [90] (see also [49]). In [8], the second-order backward differentiation formula (BDF) was applied to the Cahn-Hilliard equation and in [18], BDF schemes up to order 5 were considered for the Allen-Cahn equation.

Our manuscript is organized as follows. We first recall the functional setting of the continuous problem (1.1)-(1.2). In Section 3, we consider a space semidiscretization of the Cahn-Hilliard system which includes standard finite element and finite difference approximations. We show how to use the Łojasiewicz inequality in order to prove convergence to an equilibrium. In Section 4, we consider the time semidiscrete problem. The schemes are classified according to the type of convergence result that we are able to obtain. In this regard, the BDF schemes up to order 5 and a first order convex splitting scheme turn out to be the most satisfactory. In all the other cases, the convergence result is only partial, for various reasons, and this raises some interesting questions. In Section 5, we consider the fully discrete case. Two examples illustrate that the situation in finite dimension is better understood than for the time semidiscrete problem. In particular, the Łojasiewicz inequality for semialgebraic functions proved by Kurdyka [81] is very helpful to deal with linear schemes. Numerical simulations in two and three space dimensions illustrate the theoretical results in Section 6. In the 3D case, we are able to compute the final state starting from a random initial value for a small interface thickness. This reminds the performance of Gomez, Calo, Bazilevs and Hughes in [51], but we use here a provably energy stable scheme, namely a standard finite difference linear IMEX scheme. We conclude with some perspectives in Section 7.

## 2. THE TIME AND SPACE CONTINUOUS PROBLEM

**2.1. Functional setting and notation.** Throughout the manuscript,  $\Omega$  denotes a bounded domain of  $\mathbb{R}^d$  ( $1 \leq d \leq 3$ ) which is either

- a) convex with a Lipschitz boundary (for instance, a square in  $\mathbb{R}^2$  or a cube in  $\mathbb{R}^3$ ), or
- b) of arbitrary shape with a smooth boundary (for instance, a disc or an annulus in  $\mathbb{R}^2$ ).

Additional assumptions on  $\partial\Omega$  will be specified when needed. The  $L^2(\Omega)$  inner product is denoted  $(\cdot, \cdot)$  and the associated  $L^2(\Omega)$ -norm,  $|\cdot|_0$ . The standard Sobolev space  $\mathcal{V} = H^1(\Omega)$  is equipped with the usual norm  $\|v\|_1^2 = |v|_0^2 + |\nabla v|_0^2$ , where  $|\cdot|_1 = |\nabla \cdot|_0$  is the Hilbertian seminorm in  $\mathcal{V}$ .

We denote by  $-\Delta_N : \mathcal{V} \rightarrow \mathcal{V}'$  the bounded operator associated with the inner product on  $\mathcal{V}$  through

$$\langle -\Delta_N u, v \rangle_{\mathcal{V}', \mathcal{V}} = (\nabla u, \nabla v), \quad \forall u, v \in \mathcal{V},$$

where  $\mathcal{V}'$  is the topological dual of  $\mathcal{V}$ . We will use the dense and continuous injections

$$\mathcal{V} \subset L^2(\Omega) = [L^2(\Omega)]' \subset \mathcal{V}'.$$

For a function  $u \in L^2(\Omega)$ , we denote

$$\langle u \rangle = \frac{1}{|\Omega|} \int_{\Omega} u dx \quad \text{and} \quad \dot{u} = u - \langle u \rangle,$$

where  $|\Omega| = \int_{\Omega} 1 dx$ . We also define

$$\dot{\mathcal{V}} = \left\{ u \in \mathcal{V} : \int_{\Omega} u dx = 0 \right\}.$$

By the Poincaré-Wirtinger inequality, there exists a positive constant  $C_P$  such that

$$|v - \langle v \rangle|_0 \leq C_P |v|_1, \quad \forall v \in \mathcal{V}.$$

As a consequence, the norms  $\|v\|_1$  and  $v \mapsto (|v|_1^2 + \langle v \rangle^2)^{1/2}$  are equivalent on  $\mathcal{V}$ . The operator  $-\dot{\Delta}_N : \dot{\mathcal{V}} \rightarrow \dot{\mathcal{V}}'$ , that is the restriction of  $-\Delta_N$ , is an isomorphism. The inner product in  $\dot{\mathcal{V}}'$  is given by

$$(\dot{u}, \dot{v})_{-1} = (\nabla(-\dot{\Delta}_N)^{-1}\dot{u}, \nabla(-\dot{\Delta}_N)^{-1}\dot{v}) = \langle \dot{u}, (-\dot{\Delta}_N)^{-1}\dot{v} \rangle_{\dot{\mathcal{V}}', \dot{\mathcal{V}}}$$

and the norm is given by

$$|\dot{u}|_{-1}^2 = (\dot{u}, \dot{u})_{-1} = \langle \dot{u}, (-\dot{\Delta}_N)^{-1}\dot{u} \rangle_{\dot{\mathcal{V}}', \dot{\mathcal{V}}}.$$

We recall the interpolation inequality

$$|\dot{u}|_0^2 \leq |\dot{u}|_{-1} |\dot{u}|_1, \quad \forall \dot{u} \in \dot{\mathcal{V}}. \quad (2.1)$$

We define the energy functional

$$\mathcal{E}(u) = \frac{1}{2} |u|_1^2 + \frac{1}{\varepsilon^2} (F(u), 1), \quad (2.2)$$

where  $F(s) = \frac{1}{4}(s^2 - 1)^2$ . The Sobolev injection  $\mathcal{V} \subset L^4(\Omega)$  and the polynomial growth of  $F$  ensure that  $\mathcal{E}(u) < +\infty$  for each  $u \in \mathcal{V}$ . We set

$$f(s) = F'(s) = s^3 - s \quad (s \in \mathbb{R}).$$

The corresponding map  $v \mapsto f(v)$  is Lipschitz continuous on bounded sets of  $\mathcal{V}$  with values in  $L^2(\Omega)$  and by [78, Corollaire 17.8], the functional  $\mathcal{E}$  is of class  $C^2$  on  $\mathcal{V}$ . For any  $u, v \in \mathcal{V}$ , we have

$$\langle d\mathcal{E}(u), v \rangle_{\dot{\mathcal{V}}', \dot{\mathcal{V}}} = (\nabla u, \nabla v) + \frac{1}{\varepsilon^2} (f(u), v), \quad (2.3)$$

where  $d\mathcal{E}(u) \in \dot{\mathcal{V}}'$  is the first differential of  $\mathcal{E}$  at  $u$ .

The following identity will prove useful: if  $(\cdot, \cdot)_{\mathcal{H}}$  is an inner product associated to the norm  $|\cdot|_{\mathcal{H}}$  in the space  $\mathcal{H}$ , then

$$(a, a - b)_{\mathcal{H}} = \frac{1}{2} (|a|_{\mathcal{H}}^2 - |b|_{\mathcal{H}}^2 + |a - b|_{\mathcal{H}}^2), \quad \forall a, b \in \mathcal{H}. \quad (2.4)$$

**2.2. Well-posedness and asymptotic behaviour.** The variational formulation of (1.1)-(1.2) reads: find  $(u, w) : \mathbb{R}_+ \rightarrow \mathcal{V} \times \mathcal{V}$  such that

$$\begin{cases} (\partial_t u(t), v) = -(\nabla w(t), \nabla v), & \forall v \in \mathcal{V}, \\ (w(t), z) = (\nabla u(t), \nabla z) + \frac{1}{\varepsilon^2}(f(u(t)), z), & \forall z \in \mathcal{V}, \end{cases} \quad t \geq 0, \quad (2.5)$$

where  $\mathbb{R}_+ = [0, +\infty)$ . By taking advantage of the conservation laws (1.5) and (1.6), it is straightforward to show (see, e.g., [38]) that for each  $u_0 \in \mathcal{V}$ , there exists a unique solution  $(u, w)$  of (2.5) such that

$$u \in L^\infty(\mathbb{R}_+; \mathcal{V}) \cap C^0(\mathbb{R}_+; L^2(\Omega)), \quad \partial_t u \in L^2(\mathbb{R}_+; \mathcal{V}'), \quad w \in L^2_{loc}(\mathbb{R}_+; \mathcal{V}),$$

and  $u(0) = u_0$  [38]. This can be obtained with a Galerkin approximation as in Section 3.2.2. Additional regularity can be obtained if  $u_0$  is more regular [38]. If we consider the Cahn-Hilliard equation (1.4) instead of the system (1.1), then a  $H^2$  setting is more natural [92, 124].

**Remark 2.1.** The Cahn-Hilliard equation does not satisfy the maximum principle, so that a solution starting with values in the interval  $[-1, 1]$  does not generally remain with values in  $[-1, 1]$ , as shown by the following simple counterexample, proposed in [106]. Consider the one-dimensional Cahn-Hilliard equation (1.4) in  $\Omega = (-1, 1)$ . Take  $u_0(x) = 1 - x^4$  in the neighbourhood of zero and extend this function by a smooth function with a prescribed average over  $\Omega$  and with values in  $[-1, 1]$ . We have  $u'_0(0) = u''_0(0) = 0$ , so that  $[f(u_0)]'' = 0$  at  $x = 0$ . Furthermore,  $u_0^{(4)}(0) = -24$  and so the PDE (1.4) yields  $\partial_t u(0, 0) = 24 > 0$ . Thus, by regularity of  $u$ , we have

$$u(0, t) = u(0, 0) + t\partial_t u(0, 0) + o(t) = 1 + 24t + o(t) > 1 \text{ for } t > 0 \text{ small.}$$

This counterexample can easily be extended to the 2D or 3D case. Due to curvature effects, there is also numerical evidence of solutions with initial values in  $[-1, 1]$  and which converge to a 2D or 3D steady state with values outside  $[-1, 1]$  [120, 133].

**Definition 2.2.** We say that  $(u^*, w^*) \in \mathcal{V} \times \mathcal{V}$  is a *steady state* for (2.5) if

$$(\nabla u^*, \nabla z) + \frac{1}{\varepsilon^2}(f(u^*), z) = (w^*, z), \quad \forall z \in \mathcal{V} \text{ and } w^* \text{ is constant on } \Omega. \quad (2.6)$$

Equivalently, a steady state  $u^*$  is a critical point of the energy  $\mathcal{E}$  with prescribed mass (see (2.3)).

In [114], Rybka and Hoffmann proved that each classical solution to the Cahn-Hilliard equation (1.1)-(1.2) converges to a steady state, assuming that  $\partial\Omega$  is smooth. They also considered the case of periodic boundary conditions in  $\Omega = (0, 1)^d$ . A similar convergence result was obtained in a  $H^2$  setting for the non-autonomous Cahn-Hilliard equation by Chill and Jendoubi in [32]. In both cases, an appropriate Łojasiewicz-Simon inequality was used.

### 3. THE SPACE SEMIDISCRETE CASE

**3.1. The convergence result.** Throughout Section 3.1, we assume that the following three assumptions are satisfied:

**H1:**  $A$  is a  $M \times M$  symmetric real and positive semidefinite matrix;  $0$  is a simple eigenvalue of  $A$  associated to the eigenvector  $E_1 \in \mathbb{R}^M$ .

**H2:**  $B$  is a  $M \times M$  symmetric real and positive definite matrix;  $E_1$  is an eigenvector of  $B$ .

**H3:** The function  $G : \mathbb{R}^M \rightarrow \mathbb{R}$  is of class  $C^2$  on  $\mathbb{R}^M$  and

$$G(V) \geq 0, \quad \forall V \in \mathbb{R}^M. \quad (3.1)$$

We consider the following problem, which arises as a natural space semidiscretization of the Cahn-Hilliard equation (1.1)-(1.2): find  $(U, W) : \mathbb{R}_+ \rightarrow \mathbb{R}^M \times \mathbb{R}^M$  ( $M \geq 2$ ) such that

$$\begin{cases} BU'(t) = -AW(t) \\ BW(t) = AU(t) + \nabla G(U(t)), \end{cases} \quad t \geq 0, \quad (3.2)$$

where, for all  $V = (v_1, \dots, v_M)^T \in \mathbb{R}^M$ ,

$$\nabla G(V) = (\partial_{v_1} G(V), \dots, \partial_{v_M} G(V))^T.$$

Since  $B$  is invertible, we may eliminate  $W(t)$  from (3.2). This reads

$$U'(t) = -B^{-1}AB^{-1}(AU(t) + \nabla G(U(t))). \quad (3.3)$$

Conversely, if  $U$  satisfies (3.3), we may define  $W$  by

$$W(t) = B^{-1}(AU(t) + \nabla G(U(t))), \quad (3.4)$$

so that  $(U, W)$  solves (3.2). Thus, (3.2) and (3.3) are equivalent.

It is convenient to introduce the energy

$$E(V) = \frac{1}{2}V^T AV + G(V) \quad (V \in \mathbb{R}^M),$$

which is a Lyapunov functional for the system (3.2). We denote by  $\|\cdot\|$  the Euclidean norm in  $\mathbb{R}^M$ . We start with a useful lemma.

**Lemma 3.1.** *There exists a positive constant  $c_2$  such that for all  $V \in \mathbb{R}^M$ ,*

$$\|V\|^2 \leq c_2 \left( \frac{1}{2}V^T AV + |E_1^T V|^2 \right) \leq c_2 (E(V) + |E_1^T V|^2). \quad (3.5)$$

*Proof.* Let  $\lambda_1 = 0 < \lambda_2 \leq \dots \leq \lambda_M$  denote the eigenvalues of  $A$  associated to the eigenvectors  $(\tilde{E}_1, \tilde{E}_2, \dots, \tilde{E}_M)$  which form an orthonormal basis of  $\mathbb{R}^M$  (for the usual inner product). Let  $V \in \mathbb{R}^M$ . We have  $V = \sum_{i=1}^M v_i \tilde{E}_i$  and

$$V^T AV = \sum_{i=1}^M \lambda_i v_i^2 \geq \lambda_2 \sum_{i=2}^M v_i^2 = \lambda_2 \|V - (\tilde{E}_1^T V) \tilde{E}_1\|^2, \quad (3.6)$$

since  $\lambda_1 = 0$  and  $(\tilde{E}_1, \tilde{E}_2, \dots, \tilde{E}_M)$  is orthonormal. By the triangle inequality,

$$\|V\| \leq \|V - (\tilde{E}_1^T V) \tilde{E}_1\| + |\tilde{E}_1^T V|,$$

so we have

$$\begin{aligned} \|V\|^2 &\leq 2\|V - (\tilde{E}_1^T V) \tilde{E}_1\|^2 + 2|\tilde{E}_1^T V|^2, \\ &\leq \frac{2}{\lambda_2} V^T AV + \frac{2}{\|\tilde{E}_1\|^2} |\tilde{E}_1^T V|^2. \end{aligned}$$

In the last inequality, we have used that  $\tilde{E}_1$  is proportional to  $E_1$  (since  $\lambda_1 = 0$  is a simple eigenvalue), namely  $\tilde{E}_1 = \pm E_1 / \|E_1\|$ . This shows that first inequality in (3.5) holds. The second inequality in (3.5) follows from (3.1).  $\square$

We first prove well-posedness and a priori estimates for problem (3.2).



**Proposition 3.2.** *For every  $U_0 \in \mathbb{R}^M$ , there exists a unique*

$$(U, W) \in C^1(\mathbb{R}_+, \mathbb{R}^M \times \mathbb{R}^M)$$

*which solves (3.2) with the initial condition  $U(0) = U_0$ . Moreover,*

$$E_1^T U(t) = E_1^T U_0, \quad \forall t \geq 0, \quad (3.7)$$

$$\frac{d}{dt} \left[ \frac{1}{2} U(t)^T A U(t) + G(U(t)) \right] = -W(t)^T A W(t) \leq 0, \quad \forall t \geq 0. \quad (3.8)$$

Equation (3.7) is the discrete version of the conservation of mass (1.5) and (3.8) is the discrete version of the energy law (1.6).

*Proof.* By the Cauchy-Lipschitz theorem, equation (3.3) has a unique maximal solution  $U \in C^1([0, T^+), \mathbb{R}^M)$  such that  $U(0) = U_0$ , where  $T^+ \in (0, +\infty]$ . We define  $W \in C^1([0, T^+), \mathbb{R}^M)$  by (3.4), so that  $(U, W)$  solves (3.2), for all  $t \in [0, T^+)$ . We multiply the first line of (3.2) by  $E_1^T$  and we use assumption **H1**. This yields  $E_1^T B U'(t) = 0$ . Using assumption **H2**, we find that  $E_1^T U'(t) = 0$ , so that (3.7) holds, for all  $t \in [0, T^+)$ . Next, we multiply the second line of (3.2) by  $U'(t)^T$  and the first line by  $W(t)^T$ . We obtain (3.8), which shows that  $t \mapsto E(U(t))$  is nonincreasing, so

$$0 \leq E(U(t)) \leq E(U_0), \quad \forall t \in [0, T^+).$$

Since  $E(U(t))$  and  $E_1^T U(t)$  are bounded on  $[0, T^+)$ , the estimate (3.5) shows that  $\|U(t)\|$  is bounded as well. Thus, we have  $T^+ = +\infty$ , and the proof is complete.  $\square$

The proof above shows that every solution is bounded on  $\mathbb{R}_+$ .

We say that  $(U^*, W^*) \in \mathbb{R}^M$  is a *steady state* if

$$\begin{cases} AW^* = 0 \\ BW^* = AU^* + \nabla G(U^*). \end{cases} \quad (3.9)$$

In other words,  $(U^*, W^*)$  is a solution of (3.2) which does not depend on time.

Let  $U_0 \in \mathbb{R}^M$  and  $(U, W)$  be the solution of (3.2) such that  $U(0) = U_0$ . The  $\omega$ -limit set of  $U_0$  is the subset of  $\mathbb{R}^M$  defined by

$$\omega(U_0) = \{U^\infty \in \mathbb{R}^M : \exists t_n \rightarrow +\infty, U(t_n) \rightarrow U^\infty \text{ as } n \rightarrow +\infty\}.$$

The following result is a consequence of Lasalle's invariance principle, as pointed out in [67, Theorem 8.4.6].

**Theorem 3.3.** *Let  $U_0 \in \mathbb{R}^M$ . Then  $\omega(U_0)$  is a nonempty compact and connected subset of  $\mathbb{R}^M$  on which  $E$  is constant, and*

$$\text{dist}(U(t), \omega(U_0)) \rightarrow 0 \text{ as } t \rightarrow +\infty. \quad (3.10)$$

*Moreover, for all  $U^\infty \in \omega(U_0)$ , we have  $E_1^T U^\infty = E_1^T U_0$  and there exists  $W^\infty \in \mathbb{R}^M$  such that  $(U^\infty, W^\infty)$  is a steady state in the sense of (3.9).*

In (3.10),  $\text{dist}$  denotes the distance between a point and a set, defined by

$$\text{dist}(V, \Gamma) = \inf_{Z \in \Gamma} \|V - Z\|,$$

for  $V \in \mathbb{R}^M$  and  $\Gamma \subset \mathbb{R}^M$ .

*Proof.* It is well-known that

$$\omega(U_0) = \bigcap_{t \geq 0} \overline{U([t, +\infty))}, \quad (3.11)$$

where  $\overline{U([t, +\infty))}$  is the closure in  $\mathbb{R}^M$  of the set  $\{U(s) : s \geq t\}$ . By Proposition 3.2,  $t \mapsto \|U(t)\|$  is bounded in  $\mathbb{R}_+$ . Thus,  $\omega(U_0)$  is a nonempty compact and connected subset of  $\mathbb{R}^M$ , because it is the intersection of a decreasing family of such sets. The property (3.10) is easily proved on arguing by contradiction. By (3.8), the function  $t \mapsto E(U(t))$  is nonincreasing and since  $E$  is nonnegative (assumption **H3**), we have  $E(U(t)) \rightarrow E^\infty$  for some nonnegative real number  $E^\infty$ . As a consequence, the energy  $E$  is constant and equal to  $E_\infty$  on  $\omega(U_0)$ .

Next, we integrate (3.8) on  $[0, T]$  and we let  $T$  tend to  $+\infty$ . This yields

$$\int_0^{+\infty} W(t)^T A W(t) dt = E(U_0) - E^\infty < +\infty.$$

By arguing as in (3.6), we see that for all  $V \in \mathbb{R}^M$ ,

$$V^T A^2 V \leq \lambda_M V^T A V, \quad (3.12)$$

where  $\lambda_M > 0$  is the largest eigenvalue of  $A$ . Thus,  $\int_0^{+\infty} W(t)^T A^2 W(t) dt < +\infty$ . Using the first equation of (3.2), this yields

$$\int_0^{+\infty} \|BU'(t)\|^2 dt < +\infty. \quad (3.13)$$

Now let  $U^\infty \in \omega(U_0)$  and let  $t_n \rightarrow +\infty$  such that  $U(t_n) \rightarrow U^\infty$ . By choosing  $t = t_n$  in (3.7) and letting  $n$  tend to  $+\infty$ , we obtain that  $E_1^T U^\infty = E_1^T U_0$ . It remains to prove that  $U^\infty$  is a steady state. For every  $n$ , we denote  $U_n$  the solution of (3.3) such that  $U_n(0) = U(t_n)$ . By the Cauchy-Lipschitz theorem,  $(U_n)$  converges uniformly on  $[0, 1]$  to the solution  $\bar{U}$  of (3.3) such that  $\bar{U}(0) = U^\infty$ . By (3.13),

$$\int_0^1 \|BU'_n(t)\|^2 dt = \int_{t_n}^{t_n+1} \|BU'(t)\|^2 dt \rightarrow 0,$$

as  $n \rightarrow +\infty$ . For each  $s \in [0, 1]$ , we have

$$\begin{aligned} U(t_n + s) - U(t_n) &= \int_{t_n}^{t_n+s} U'(\sigma) d\sigma \\ &= \int_{t_n}^{t_n+s} B^{-1} B U'(\sigma) d\sigma \\ &\leq \|B^{-1}\| \left( \int_{t_n}^{t_n+1} \|B U'(\sigma)\|^2 d\sigma \right)^{1/2} \end{aligned}$$

so that  $U(t_n + s) \rightarrow U^\infty$  as  $n \rightarrow +\infty$ . In the last line above, we have used the Cauchy-Schwarz inequality. Thus, we have  $\bar{U}(t) = U^\infty$  on  $[0, 1]$ . Let

$$W^\infty = B^{-1}(A U^\infty + \nabla G(U^\infty)).$$

Since  $\bar{U} = U^\infty$  satisfies (3.3) on  $[0, 1]$ , we have  $A W^\infty = 0$ . This shows that  $(U^\infty, W^\infty)$  solves (3.9), and so  $(U^\infty, W^\infty)$  is a steady state.  $\square$

The following inequality, due to Łojasiewicz [84], is fundamental.

**Definition 3.4.** Let  $\Phi \in C^1(\mathbb{R}^M, \mathbb{R})$ . We say that  $\Phi$  satisfies the *Łojasiewicz inequality* at  $U^* \in \mathbb{R}^M$  if there exist  $\theta \in (0, 1/2)$  and  $\sigma > 0$  such that for all  $V \in \mathbb{R}^M$ ,

$$\|V - U^*\| < \sigma \Rightarrow |\Phi(V) - \Phi(U^*)|^{1-\theta} \leq \|\nabla \Phi(V)\|. \quad (3.14)$$

If  $U^*$  is not a critical point of  $\Phi$ , then (3.14) is obvious by continuity.

**Example 3.5.** For  $p \geq 2$ , the function  $\Phi(U) = \|U\|^p$  satisfies the Łojasiewicz inequality at  $U^* = 0$  with the exponent  $\theta = 1/p$ . In contrast, the function  $\Phi \in C^\infty(\mathbb{R}, \mathbb{R})$  defined by  $\Phi(x) = \exp(-1/x^2)$  if  $x \neq 0$  and  $\Phi(0) = 0$  does not satisfy the Łojasiewicz inequality at 0.

We have:

**Theorem 3.6** ([84]). *If  $\Phi : \mathbb{R}^M \rightarrow \mathbb{R}$  is real analytic, then  $\Phi$  satisfies the Łojasiewicz inequality at each point  $U^* \in \mathbb{R}^M$ .*

**Theorem 3.7.** *In addition to H1, H2 and H3, we assume that  $G$  is real analytic on  $\mathbb{R}^M$ . If  $(U, W)$  solves (3.2), there exists a steady state  $(U^*, W^*) \in \mathbb{R}^M \times \mathbb{R}^M$  such that  $(U(t), W(t)) \rightarrow (U^*, W^*)$ .*

*Proof.* Our proof is as follows: we first show that (3.2) is a gradient flow of the energy in an appropriate  $M - 1$ -dimensional subspace of  $\mathbb{R}^M$ , and then we adapt the proof of [67, Theorem 10.1.6]. Namely, we first prove that a uniform Łojasiewicz inequality holds, then we derive a convergence rate for the energy, which in turn provides a convergence rate for the solution.

**Step 1.** We may assume without loss of generality that

$$B = Id \text{ and } E_1 = (1, 0, 0, \dots, 0)^T. \quad (3.15)$$

Indeed, since  $B$  is positive definite, the bilinear form  $(V, Z) \mapsto V^T B Z$  is an inner product on  $\mathbb{R}^M$ . We choose a basis  $(F_1, \dots, F_M)$  of  $\mathbb{R}^M$  which is orthonormal for this inner product, with  $F_1$  proportional to  $E_1$ . We write  $U$  and  $W$  in this basis, namely  $U(t) = \sum_{j=1}^M v_j(t) F_j$  and  $W(t) = \sum_{j=1}^M z_j(t) F_j$ . For each  $i$ , we multiply each equation in (3.2) by the vector  $F_i^T$ . This yields

$$\begin{cases} F_i^T B U'(t) = -F_i^T A W(t), & i = 1, 2, \dots, M, \\ F_i^T B W(t) = F_i^T A U(t) + F_i^T \nabla G(U(t)), & i = 1, 2, \dots, M. \end{cases}$$

Since  $(F_1, \dots, F_M)$  is orthonormal for  $B$ , this is equivalent to

$$\begin{cases} v_i'(t) = -\sum_{j=1}^M F_i^T A F_j z_j(t), & i = 1, \dots, M, \\ z_i(t) = \sum_{j=1}^M F_i^T A v_j(t) + F_i^T \nabla G(\sum_{j=1}^M v_j(t) F_j), & i = 1, \dots, M. \end{cases} \quad (3.16)$$

The symmetric matrix  $A_B = (F_i^T A F_j)_{1 \leq i, j \leq M}$  has the same signature as  $A$  (it is positive semidefinite) and we have  $F_i^T A F_j = 0$  if  $i = 1$  or  $j = 1$  since  $F_1 = c E_1$ . By the chain rule, the function  $G_B(\varphi_1, \dots, \varphi_M) = G(\sum_{j=1}^M \varphi_j F_j)$  satisfies

$$\partial_{\varphi_i} G_B(\varphi_1, \dots, \varphi_M) = F_i^T \nabla G(\sum_{j=1}^M \varphi_j F_j).$$

Thus, the system (3.16) can be written in matrix form

$$\begin{cases} V'(t) = -A_B Z(t), \\ Z(t) = A_B V(t) + \nabla G_B(V(t)). \end{cases}$$

The matrix  $A_B$  satisfies assumption **H1** with  $E_1 = (1, 0, \dots, 0)^T$  and the function  $G_B$  is real analytic and satisfies **H3**. This is a system of the form (3.2) in which  $B = Id$  (the identity matrix) and  $E_1 = (1, 0, \dots, 0)^T$ . In the remainder of the proof, we therefore assume that (3.15) holds, so (3.2) can be written

$$\begin{cases} U'(t) = -AW(t) \\ W(t) = AU(t) + \nabla G(U(t)), \end{cases} \quad t \geq 0, \quad (3.17)$$

where

$$A = \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & \tilde{A} & \\ 0 & & \end{pmatrix} \quad (3.18)$$

and  $\tilde{A}$  is a  $(M-1) \times (M-1)$  symmetric positive definite matrix.

**Step 2.** Let  $(U, W)$  solve (3.17). From (3.18), we deduce that  $u_1'(t) = 0$ , so  $u_1(t) = u_1(0)$ , for all  $t \geq 0$ . We write

$$\tilde{U}(t) = \begin{pmatrix} u_2(t) \\ \vdots \\ u_M(t) \end{pmatrix}, \quad \tilde{W}(t) = \begin{pmatrix} w_2(t) \\ \vdots \\ w_M(t) \end{pmatrix},$$

and for  $\tilde{V} = (v_2, \dots, v_M) \in \mathbb{R}^{M-1}$ ,

$$\tilde{G}(\tilde{V}) = G(u_1(0), v_2, \dots, v_M).$$

We denote

$$\tilde{\nabla} \tilde{G}(\tilde{V}) = (\partial_{v_2} \tilde{G}(\tilde{V}), \dots, \partial_{v_M} \tilde{G}(\tilde{V}))^T.$$

Then (3.17) reads

$$\begin{cases} \tilde{U}'(t) = \tilde{A} \tilde{W}(t), \\ \tilde{W}(t) = \tilde{A} \tilde{U}(t) + \tilde{\nabla} \tilde{G}(\tilde{U}(t)), \end{cases} \quad t \geq 0. \quad (3.19)$$

The component  $w_1$  can be recovered by the formula

$$w_1(t) = \partial_{v_1} G(u_1(0), u_2(t), \dots, u_M(t)).$$

We denote the energy

$$\tilde{E}(\tilde{V}) = \frac{1}{2} \tilde{V}^T \tilde{A} \tilde{V} + \tilde{G}(\tilde{V}) = E(u_1(0), \tilde{V}) \quad (\tilde{V} \in \mathbb{R}^{M-1}).$$

We know that the map  $t \mapsto E(U(t)) = \tilde{E}(\tilde{U}(t))$  is nonincreasing and converges to  $E^\infty$  as  $t \rightarrow +\infty$ . We set  $\varphi(t) = E(U(t)) - E^\infty$ . From (3.8), we deduce that

$$\varphi'(t) = -W(t)AW(t) = -\tilde{W}(t)\tilde{A}\tilde{W}(t).$$

Thus, by (3.6) and (3.19)

$$-\varphi'(t) \geq \lambda_2 \|\tilde{W}(t)\|^2 = \lambda_2 \|\tilde{\nabla} \tilde{E}(\tilde{U}(t))\|^2. \quad (3.20)$$

On the other hand, by (3.12), we have

$$-\varphi'(t) \geq \frac{1}{\lambda_M} W(t) A^2 W(t) = \frac{1}{\lambda_M} \|\tilde{U}'(t)\|^2. \quad (3.21)$$

Let  $U_0 = U(0) = (u_1(0), \tilde{U}_0)$  and let  $\omega(\tilde{U}_0)$  denote the  $\omega$ -limit set of  $\tilde{U}_0$  in  $\mathbb{R}^{M-1}$ , i.e.

$$\omega(\tilde{U}_0) = \left\{ \tilde{U}^\infty \in \mathbb{R}^{M-1} : \exists t_n \rightarrow +\infty, \tilde{U}(t_n) \rightarrow \tilde{U}^\infty \text{ as } n \rightarrow +\infty \right\}.$$

It is clear that  $\omega(U_0) = \{u_1(0)\} \times \omega(\tilde{U}_0)$  and that  $\Gamma := \omega(\tilde{U}_0)$  inherits the properties of  $\omega(U_0)$  described in Theorem 3.3. In particular,  $\Gamma$  is compact and  $\tilde{E}$  is constant (equal to  $E^\infty$ ) on  $\Gamma$ .

Next, we show that the Łojasiewicz inequality holds uniformly on  $\Gamma$ . The function  $\tilde{E}$  is real analytic on  $\mathbb{R}^{M-1}$ , so by Theorem 3.6, for each  $\tilde{U}^\star \in \Gamma$ , there exist  $\theta_{\tilde{U}^\star} \in (0, 1/2)$  and  $\sigma_{\tilde{U}^\star} > 0$  such that

$$|\tilde{E}(\tilde{V}) - \tilde{E}(\tilde{U}^\star)|^{1-\theta_{\tilde{U}^\star}} \leq \|\tilde{\nabla} \tilde{E}(\tilde{V})\|, \quad \forall \tilde{V} \in \mathcal{B}(\tilde{U}^\star, \sigma_{\tilde{U}^\star}),$$

where  $\mathcal{B}(\tilde{Z}, \sigma)$  denotes the ball of radius  $\sigma > 0$  centered at  $\tilde{Z}$  in  $\mathbb{R}^{M-1}$ . By continuity and by choosing a smaller  $\sigma_{\tilde{U}^\star}$  if necessary, we may assume that

$$|\tilde{E}(\tilde{V}) - \tilde{E}(\tilde{U}^\star)| \leq 1, \quad \forall \tilde{V} \in \mathcal{B}(\tilde{U}^\star, \sigma_{\tilde{U}^\star}).$$

Since  $\Gamma$  is compact, there exist  $\tilde{U}_1, \dots, \tilde{U}_p$  in  $\mathbb{R}^{M-1}$  such that

$$\Gamma \subset \bigcup_{i=1}^p \mathcal{B}(\tilde{U}_i, \frac{1}{2} \sigma_{\tilde{U}_i}).$$

By choosing  $\sigma = \frac{1}{2} \min \sigma_{\tilde{U}_i}$  and  $\theta = \min \theta_i$ , we obtain that for all  $\tilde{V} \in \mathbb{R}^{M-1}$ ,

$$\text{dist}(\tilde{V}, \Gamma) < \sigma \implies |\tilde{E}(\tilde{V}) - E^\infty|^{1-\theta} \leq \|\tilde{\nabla} \tilde{E}(\tilde{V})\|.$$

By (3.10), there exists  $T > 0$  such that

$$\text{dist}(\tilde{U}(t), \Gamma) < \sigma, \quad \forall t \geq T.$$

Thus, for all  $t \geq T$ , we have

$$(\varphi(t))^{1-\theta} \leq \|\tilde{\nabla} \tilde{E}(\tilde{U}(t))\|. \quad (3.22)$$

By combining (3.22) and (3.20), we get

$$-\varphi'(t) \geq \lambda_2 (\varphi(t))^{2-2\theta}, \quad \forall t \geq T.$$

By integrating this over  $[T, t]$ , we get

$$\varphi(t) \leq C_1 t^{-\frac{1}{1-2\theta}}, \quad \forall t \geq T.$$

Now, by (3.21),

$$\int_t^{2t} \|\tilde{U}'(s)\|^2 ds \leq \lambda_M [\varphi(t) - \varphi(-2t)] \leq C_2 t^{-\frac{1}{1-2\theta}}.$$

By the Cauchy-Schwarz inequality, we have

$$\int_t^{2t} \|\tilde{U}'(s)\| ds \leq t^{1/2} \left( C_2 t^{-\frac{1}{1-2\theta}} \right)^{1/2} = \sqrt{C_2} t^{-\frac{\theta}{1-2\theta}}.$$

Thus, for all  $t \geq T$ , we have

$$\begin{aligned} \int_t^{+\infty} \|\tilde{U}'(s)\| ds &= \sum_{k=0}^{\infty} \int_{2^k t}^{2^{k+1} t} \|\tilde{U}'(s)\| ds \\ &\leq \sqrt{C_2} \sum_{k=0}^{\infty} (2^k t)^{-\frac{\theta}{1-2\theta}} \\ &= C_3 t^{-\frac{\theta}{1-2\theta}}. \end{aligned}$$

By Cauchy's criterion,  $\tilde{U}^* = \lim_{t \rightarrow +\infty} \tilde{U}(t)$  exists and

$$\|\tilde{U}(t) - \tilde{U}^*\| \leq C_3 t^{-\frac{\theta}{1-2\theta}}, \quad \forall t \geq T. \quad (3.23)$$

Thus,  $U(t) = (u_1(0), \tilde{U}(t))$  converges to  $U^* = (u_1(0), \tilde{U}^*)$  as  $t \rightarrow +\infty$ . By (3.4),  $W(t)$  converges to  $W^* = AU^* + \nabla G(U^*)$ . Theorem 3.3 shows that  $(U^*, W^*)$  is a steady state. This concludes the proof.  $\square$

**Remark 3.8.** The estimate (3.23) provides a rate of convergence to equilibrium. In case  $\theta = 1/2$ , it is possible to obtain an exponential rate [67]. However, the exponent  $\theta$  is rarely known explicitly.

### 3.2. Examples.

**3.2.1. Finite difference approximation.** Let  $\Omega = (0, 1)$ . We set  $h = 1/J$  with  $J \in \mathbb{N}^*$  and  $x_i = ih$  for  $i = 0, 1, \dots, J$ . A possible finite difference discretization of (1.1) reads (see, e.g., [120]): find  $(U, W) : \mathbb{R}_+ \rightarrow \mathbb{R}^{J+1} \times \mathbb{R}^{J+1}$  such that

$$\begin{cases} U'(t) = -A_h W(t), \\ W(t) = A_h U(t) + \frac{1}{\varepsilon^2} \nabla F_h(U), \end{cases} \quad t \geq 0, \quad (3.24)$$

where  $A_h$  is the  $(J+1) \times (J+1)$  matrix

$$A_h = \frac{1}{h^2} \begin{pmatrix} 1 & -1 & 0 & \cdots & \cdots & \cdots & 0 \\ -1 & 2 & -1 & \ddots & & & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & \cdots & \ddots & -1 & 2 & -1 \\ 0 & \cdots & \cdots & \cdots & 0 & -1 & 1 \end{pmatrix} \quad (3.25)$$

and

$$F_h(v_0, v_1, \dots, v_J) = \frac{1}{4} \sum_{i=0}^J (v_i^2 - 1)^2.$$

We have

$$\partial_{v_i} F_h(v_0, \dots, v_J) = v_i^3 - v_i \text{ for } i = 0, \dots, J.$$

The system (3.24) has the form (3.2) with  $A = A_h$ ,  $B = I_{J+1}$  (the identity matrix) and  $G(V) = \frac{1}{\varepsilon^2} F_h(V)$ . It is well-known that  $A_h$  satisfies **H1** with  $E_1 = (1, 1, \dots, 1)^T$ .

Moreover,  $B = I_{J+1}$  clearly satisfies **H2** and  $G$  is real analytic on  $\mathbb{R}^{J+1}$  (because it is a polynomial) and satisfies **H3**. Thus, we may apply Theorem 3.7.

On the square  $\Omega = (0, 1) \times (0, 1)$ , the approximation (3.24) has a natural 2D extension. Namely, we work on  $\mathbb{R}^{J+1} \otimes \mathbb{R}^{J+1}$ , which is isomorphic to  $\mathbb{R}^{(J+1)^2}$ , and with the grid

$$(x_i, y_j) = ((i-1)h, (j-1)h) \text{ for } 0 \leq i, j \leq J.$$

We set  $A = A_h \otimes I_{J+1} + I_{J+1} \otimes A_h$  and

$$F_h(v_{0,0}, \dots, v_{J,J}) = \frac{1}{4} \sum_{0 \leq i,j \leq J} (v_{i,j}^2 - 1)^2.$$

We have a system of the form (3.2) with  $B = I_{J+1} \otimes I_{J+1}$  (the identity matrix) and  $G(V) = \frac{1}{\varepsilon^2} F_h(V)$ . Again, the assumptions of Theorem 3.7 are satisfied and so the convergence result holds. The 3D case is similar, with the matrix

$$A = A_h \otimes I_{J+1} \otimes I_{J+1} + I_{J+1} \otimes A_h \otimes I_{J+1} + I_{J+1} \otimes I_{J+1} \otimes A_h. \quad (3.26)$$

**3.2.2. Galerkin method.** We assume that  $\mathcal{V}_h$  is a  $M$ -dimensional subspace of  $\mathcal{V}$  which contains the constants. The space semidiscrete scheme reads: find  $(u_h, w_h) : \mathbb{R}_+ \rightarrow \mathcal{V}_h \times \mathcal{V}_h$  such that

$$\begin{cases} (u'_h(t), v_h) = -(\nabla w_h(t), \nabla v_h), & \forall v_h \in \mathcal{V}_h, \\ (w_h(t), z_h) = (\nabla u_h(t), \nabla z_h) + \frac{1}{\varepsilon^2} (f(u_h(t)), z_h), & \forall z_h \in \mathcal{V}_h, \end{cases} \quad t \geq 0. \quad (3.27)$$

We choose a basis  $(e_1, \dots, e_M)$  of  $\mathcal{V}_h$  which is orthonormal for the  $L^2(\Omega)$  inner product and such that  $e_1$  is constant. We seek for  $u_h(t) = \sum_{i=1}^M u_i(t) e_i$  and  $w_h(t) = \sum_{i=1}^M w_i(t) e_i$ . The matrix version of (3.27) has the form (3.2) with

$$A = ((\nabla e_i, \nabla e_j))_{1 \leq i,j \leq M}, \quad B = I_M$$

and

$$G(v_1, \dots, v_M) = \frac{1}{4\varepsilon^2} \int_{\Omega} \left( \left( \sum_{i=1}^M v_i e_i(x) \right)^2 - 1 \right)^2 dx. \quad (3.28)$$

Since  $1 \leq d \leq 3$ , the Sobolev injection  $H^1(\Omega) \subset L^4(\Omega)$  holds [50]. We deduce that  $G$  is well defined and of class  $C^1$  with

$$\partial_{v_i} G(v_1, \dots, v_M) = \frac{1}{\varepsilon^2} \int_{\Omega} f \left( \sum_{i=1}^M v_i e_i(x) \right) e_i(x) dx. \quad (3.29)$$

Thus,

$$\partial_{v_i} G(u_1(t), \dots, u_M(t)) = \frac{1}{\varepsilon^2} (f(u_h(t)), e_i),$$

as claimed.

It is clear that  $A$  satisfies **H1** (since  $A$  has the form (3.18)),  $B = I_M$  satisfies **H2** and  $G$  satisfies **H3**. Moreover,  $G$  is a polynomial, so it is real analytic on  $\mathbb{R}^M$ .

Indeed, by expanding (3.28), we have

$$\begin{aligned} G(v_1, \dots, v_M) &= \frac{1}{4\varepsilon^2} \sum_{1 \leq i, j, k, l \leq M} v_i v_j v_k v_l \int_{\Omega} e_i(x) e_j(x) e_k(x) e_l(x) dx \\ &\quad - \frac{2}{4\varepsilon^2} \sum_{1 \leq i, j \leq M} v_i v_j \int_{\Omega} e_i(x) e_j(x) dx + \frac{1}{4\varepsilon^2} \int_{\Omega} dx. \end{aligned} \quad (3.30)$$

Thus, we may apply Theorem (3.7), which shows that  $(u_h(t), w_h(t))$  converges to  $(u_h^*, w_h^*)$  in  $\mathcal{V}_h \times \mathcal{V}_h$ , as  $t \rightarrow +\infty$ . Moreover,  $(u_h^*, w_h^*)$  is a steady state, which means that  $w_h^*$  is a constant function and

$$(w_h^*, z_h) = (\nabla u_h^*, \nabla z_h) + \frac{1}{\varepsilon^2} (f(u_h^*), z_h), \quad \forall z_h \in \mathcal{V}_h. \quad (3.31)$$

This asymptotic convergence result for the Galerkin method (3.27) can be applied to finite element methods such as  $P^1$  finite elements [40] or  $Q^k$  finite elements [53], but also spectral-Galerkin methods [119].

**Remark 3.9.** In (3.27), we know that  $(u_h(t), w_h(t))$  converges in  $\mathcal{V}_h \times \mathcal{V}_h$ . Thus, for any choice of a basis of  $\mathcal{V}_h$ , the coordinates of  $(u_h, w_h)$  converge in  $\mathbb{R}^M \times \mathbb{R}^M$ . For the numerical computation of  $(u_h(t), w_h(t))$ , we therefore use the most appropriate basis (for instance, a nodal basis if we have finite elements).

**Remark 3.10.** The Galerkin method (3.27) is a  $H^1$ -conforming discretization of the Cahn-Hilliard system (1.1)-(1.2). There are also several efficient space discretization of the Cahn-Hilliard equation (1.4) based on a  $H^2$  approach [7, 34, 39, 45, 51]. However, for such discretizations, it is not always clear that the energy law (1.6) is preserved. Without the energy law, the techniques used here cannot be applied and it is not known if a solution to the discretized problem converges to a steady state.

#### 4. THE TIME SEMIDISCRETE CASE

Hereafter,  $\tau > 0$  denotes the time step, which is chosen constant for sake of simplicity.

**4.1. BDF schemes.** The picture regarding convergence to a steady state is complete regarding backward differentiation formulae (BDF). The  $k$ -step BDF scheme ( $1 \leq k \leq 5$ ) applied to the Cahn-Hilliard equation (2.5) reads: let  $u^0, \dots, u^{k-1}$  in  $\mathcal{V}$  and for  $n = 0, 1, \dots$ , let  $(u^{n+k}, w^{n+k}) \in \mathcal{V} \times \mathcal{V}$  solve

$$\begin{cases} \frac{1}{\tau} (\mathcal{L}_k u^{n+k}, v) = -(\nabla w^{n+k}, \nabla v) & \forall v \in \mathcal{V}, \\ (w^{n+k}, z) = (\nabla u^{n+k}, \nabla z) + \frac{1}{\varepsilon^2} (f(u^{n+k}), z), & \forall z \in \mathcal{V}, \end{cases} \quad (4.1)$$



where the operators  $\mathcal{L}_k$  ( $1 \leq k \leq 5$ ) are given by

$$\mathcal{L}_1 u^{n+1} = u^{n+1} - u^n, \quad (4.2)$$

$$\mathcal{L}_2 u^{n+2} = \frac{3}{2}u^{n+2} - 2u^{n+1} + \frac{1}{2}u^n, \quad (4.3)$$

$$\mathcal{L}_3 u^{n+3} = \frac{11}{6}u^{n+3} - 3u^{n+2} + \frac{3}{2}u^{n+1} - \frac{1}{3}u^n, \quad (4.4)$$

$$\mathcal{L}_4 u^{n+4} = \frac{25}{12}u^{n+4} - 4u^{n+3} + 3u^{n+2} - \frac{4}{3}u^{n+1} + \frac{1}{4}u^n, \quad (4.5)$$

$$\mathcal{L}_5 u^{n+5} = \frac{137}{60}u^{n+5} - 5u^{n+4} + 5u^{n+3} - \frac{10}{3}u^{n+2} + \frac{5}{4}u^{n+1} - \frac{1}{5}u^n. \quad (4.6)$$

The  $k$ -step BDF scheme (4.1) is *nonlinear* and *uniquely solvable if the time step is small enough* (cf. Remark 4.4). Its accuracy is  $k$  if the solution is sufficiently regular (see [5] in the case of semilinear parabolic equations). For  $k = 1$ , it is the well-known *backward Euler scheme*.

Energy stability and convergence to a steady state have been proved for the two-step BDF scheme (4.1) in [8]. We also refer to [38, 90] for the BDF1 scheme and [18, 43] for the  $k$ -step BDF scheme ( $k \leq 5$ ) applied to the Allen-Cahn equation. Here, we extend the proof to the Cahn-Hilliard equation for all  $k \leq 5$ .

We denote  $\partial u^{n+1} = u^{n+1} - u^n$  and, by induction,  $\partial^j u^{n+j} = \partial(\partial^{j-1} u^{n+j})$  for  $j \geq 2$ . We readily check that  $\mathcal{L}_k = \sum_{j=1}^k \frac{1}{j} \partial^j u^{n+j}$ . As a consequence,  $\mathcal{L}_k$  is a linear combination of  $\partial u^{n+k}, \dots, \partial u^{n+1}$ . The following result was proved in [43, 123] for the BDF1, BDF2 and BDF3 schemes and [18] for the BDF4 and BDF5 schemes.

**Lemma 4.1** ([18, 43]). *Let  $(\cdot, \cdot)_{\mathcal{H}}$  be an inner product with norm  $|\cdot|_{\mathcal{H}}$  and let  $k \leq 5$ . There exist a symmetric positive definite matrix  $Q_k = (q_{ij}) \in \mathbb{R}^{(k-1) \times (k-1)}$  and a symmetric positive definite matrix  $R_k = (r_{ij}) \in \mathbb{R}^{k \times k}$  such that for all  $v^0, \dots, v^k$  in the inner space  $\mathcal{H}$ ,*

$$\begin{aligned} (\mathcal{L}_k v^k, v^k - v^{k-1})_{\mathcal{H}} &= \sum_{i,j=1}^{k-1} q_{ij} (\partial v^{i+1}, \partial v^{j+1})_{\mathcal{H}} - \sum_{i,j=1}^{k-1} q_{ij} (\partial v^i, \partial v^j)_{\mathcal{H}} \\ &\quad + \sum_{i,j=1}^k r_{ij} (\partial v^i, \partial v^j)_{\mathcal{H}} + \beta_k |\partial v^k|_{\mathcal{H}}^2, \end{aligned}$$

where the values  $\beta_k$  are given by

$$\beta_1 = \beta_2 = \frac{1}{2}, \quad \beta_3 = \frac{2}{3}, \quad \beta_4 = \frac{41}{144}, \quad \beta_5 = \frac{1}{20}. \quad (4.7)$$

The values  $\beta_k$  will appear in the restriction on the time step. It is possible to have values of  $\beta_k$  which are slightly larger than (4.7), with a different choice of the matrices  $Q_k$  and  $R_k$ . The largest possible values of  $\beta_k$  are 1 for  $k = 1, 2$  and  $95/96$  for  $k = 3$  [109]. The optimal values of  $\beta_4$  and  $\beta_5$  are given in [105]. For these optimal values, the matrix  $R_k$  is positive semi-definite instead of positive definite.

**Example 4.2.** For  $k = 1$ , the term involving  $Q_1$  is empty and  $R_1 = (1/2)$ , that is

$$(\mathcal{L}_1 u^{n+1}, \partial u^{n+1}) = \frac{1}{2} |\partial u^{n+1}|_{\mathcal{H}}^2 + \beta_1 |\partial u^{n+1}|_{\mathcal{H}}^2.$$

For  $k = 2$ , we have  $Q_2 = (1/4)$  with

$$\begin{aligned} (\mathcal{L}_2 u^{n+2}, \partial u^{n+2}) &= \frac{1}{4} |\partial u^{n+2}|_{\mathcal{H}}^2 - \frac{1}{4} |\partial u^{n+1}|_{\mathcal{H}}^2 + \frac{1}{4} |\partial u^{n+2} - \partial u^{n+1}|_{\mathcal{H}}^2 \\ &\quad + \frac{1}{2} |\partial u^{n+2}|_{\mathcal{H}}^2 + \beta_2 |\partial u^{n+2}|_{\mathcal{H}}^2. \end{aligned}$$

For  $k = 3$ , we have (for instance)

$$\begin{aligned} (\mathcal{L}_3 u^{n+3}, \partial u^{n+3}) &= \frac{5}{12} |\partial u^{n+3}|_{\mathcal{H}}^2 + \frac{1}{6} |\partial u^{n+3} - \partial u^{n+2}|_{\mathcal{H}}^2 - \frac{5}{12} |\partial u^{n+2}|_{\mathcal{H}}^2 \\ &\quad - \frac{1}{6} |\partial u^{n+2} - \partial u^{n+1}|_{\mathcal{H}}^2 + \frac{1}{6} |\partial u^{n+3} - \partial u^{n+2} + \partial u^{n+1}|_{\mathcal{H}}^2 \\ &\quad + \frac{1}{4} |\partial u^{n+3} - \partial u^{n+2}|_{\mathcal{H}}^2 + \frac{1}{6} |\partial u^{n+3}|_{\mathcal{H}}^2 + \beta_3 |\partial u^{n+3}|_{\mathcal{H}}^2. \end{aligned}$$

Using Lemma 4.1, we prove below that the  $k$ -step BDF scheme is energy stable for  $1 \leq k \leq 5$ , with a restriction on the time step. For simplicity, we assume that  $u^0, \dots, u^{k-1}$  in  $\mathcal{V}$  are such that

$$\langle u^0 \rangle = \langle u^1 \rangle = \dots = \langle u^{k-1} \rangle. \quad (4.8)$$

We obtain by induction that

$$\langle u^n \rangle = \langle u^0 \rangle, \quad \forall n \in \mathbb{N}. \quad (4.9)$$

Indeed, if we choose  $v = 1$  in (4.1), we find that  $(\mathcal{L}_k u^{n+k}, 1) = 0$ , and so

$$\mathcal{L}_k \langle u^{n+k} \rangle = 0. \quad (4.10)$$

The claim follows since  $\mathcal{L}_k$  applied to the constant sequence (1) gives 0.

We define the modified energy

$$\hat{\mathcal{E}}_k(u^{n+k}, u^{n+k-1}, \dots, u^{n+1}) = \mathcal{E}(u^{n+k}) + \frac{1}{\tau} \sum_{i,j=1}^{k-1} q_{ij} (\partial u^{n+i+1}, \partial u^{n+j+1})_{-1},$$

where  $Q_k = (q_{ij})_{1 \leq i,j \leq k-1}$  is the matrix from Lemma 4.1. Note that  $\partial u^n \in \dot{\mathcal{V}}$  for all  $n \geq 1$  by (4.9). For  $k = 1$ ,  $\hat{\mathcal{E}}_1$  is simply  $\mathcal{E}$  and (4.8) is automatically satisfied.

The stability result for the modified energy is as follows:

**Theorem 4.3.** *Let  $1 \leq k \leq 5$  and assume that  $\tau \leq 2\beta_k \varepsilon^4$ . If  $((u^n, w^n))$  is a sequence in  $\mathcal{V} \times \mathcal{V}$  which complies with (4.1) and (4.8), then we have*

$$\begin{aligned} &\hat{\mathcal{E}}_k(u^{n+k}, \dots, u^{n+1}) + \frac{1}{\tau} \sum_{i,j=1}^k r_{ij} (\partial u^{n+i}, \partial u^{n+j})_{-1} \\ &\quad + \frac{\beta_k}{2\tau} |\partial u^{n+k}|_{-1}^2 + \frac{1}{4} |\partial u^{n+k}|_1^2 \leq \hat{\mathcal{E}}_k(u^{n+k-1}, \dots, u^n), \quad \forall n \geq 0. \end{aligned} \quad (4.11)$$

**Remark 4.4.** By arguing as in [8, Proposition 2.1 and Proposition 2.2], it is easy to see that if  $\tau \leq 2\beta_k \varepsilon^4$ , there exists a unique sequence  $((u^n, w^n))$  in  $\mathcal{V} \times \mathcal{V}$  which complies with (4.1), once that  $u^0, \dots, u^{k-1}$  are given.

**Remark 4.5.** The choice of  $Q_k$  and  $R_k$  in Lemma 4.1 is not unique if  $k \geq 2$ , so that there are several choices of the modified energy for which stability holds.

*Proof.* Using (4.9), we see that the BDF scheme (4.1) is equivalent to

$$\begin{cases} \langle u^{n+k} \rangle = \langle u^0 \rangle, \\ \frac{1}{\tau}(-\dot{\Delta}_N)^{-1} \mathcal{L}_k u^{n+k} = -\dot{w}^{n+k}, \\ \dot{w}^{n+k} = -\Delta_N u^{n+k} + \frac{1}{\varepsilon^2} f(u^{n+k}) - \frac{1}{\varepsilon^2} \langle f(u^{n+k}) \rangle, \\ \langle w^{n+k} \rangle = \frac{1}{\varepsilon^2} \langle f(u^{n+k}) \rangle. \end{cases}$$

Eliminating  $w^{n+k}$  leads to

$$\frac{1}{\tau}(-\dot{\Delta}_N)^{-1} \mathcal{L}_k u^{n+k} - \Delta_N u^{n+k} + \frac{1}{\varepsilon^2} f(u^{n+k}) - \frac{1}{\varepsilon^2} \langle f(u^{n+k}) \rangle = 0, \quad (4.12)$$

for all  $n \geq 0$ . On taking the  $L^2(\Omega)$  product of (4.12) with  $\partial u^{n+k} \in \dot{\mathcal{V}}$ , we find

$$\frac{1}{\tau}(\mathcal{L}_k u^{n+k}, \partial u^{n+k})_{-1} + (\nabla u^{n+k}, \nabla \partial u^{n+k}) + \frac{1}{\varepsilon^2} (f(u^{n+k}), \partial u^{n+k}) = 0. \quad (4.13)$$

We have  $F''(s) = f'(s) = 3s^2 - 1 \geq -1$  so by the Taylor-Lagrange theorem,

$$F(r) - F(s) \geq f(s)(r - s) - \frac{1}{2}(r - s)^2, \quad \forall r, s \in \mathbb{R}.$$

Thus,

$$(f(u^{n+k}), u^{n+k-1} - u^{n+k}) \leq (F(u^{n+k-1}), 1) - (F(u^{n+k}), 1) + \frac{1}{2} |\partial u^{n+k}|_0^2. \quad (4.14)$$

Using (4.14), the well-known identity

$$(\nabla u^{n+k}, \nabla(u^{n+k} - u^{n+k-1})) = \frac{1}{2} (|u^{n+k}|_1^2 - |u^{n+k-1}|_1^2 + |u^{n+k} - u^{n+k-1}|_1^2),$$

and Lemma 4.1 with the inner product  $(\cdot, \cdot)_{-1}$ , we deduce from (4.13) that

$$\begin{aligned} & \frac{1}{\tau} \sum_{i,j=1}^{k-1} q_{ij} (\partial u^{n+i+1}, \partial u^{n+j+1})_{-1} - \frac{1}{\tau} \sum_{i,j=1}^{k-1} q_{ij} (\partial u^{n+i}, \partial u^{n+j})_{-1} \\ & + \frac{1}{\tau} \sum_{i,j=1}^k r_{ij} (\partial u^{n+i}, \partial u^{n+j})_{-1} + \frac{\beta_k}{\tau} |\partial u^{n+k}|_{-1}^2 \\ & + \frac{1}{2} (|u^{n+k}|_1^2 - |u^{n+k-1}|_1^2 + |u^{n+k} - u^{n+k-1}|_1^2) \\ & \leq \frac{1}{\varepsilon^2} \left( (F(u^{n+k-1}), 1) - (F(u^{n+k}), 1) + \frac{1}{2} |\partial u^{n+k}|_0^2 \right) \\ & \stackrel{(2.1)}{\leq} \frac{1}{\varepsilon^2} (F(u^{n+k-1}), 1) - \frac{1}{\varepsilon^2} (F(u^{n+k}), 1) + \frac{1}{2\varepsilon^2} |\partial u^{n+k}|_{-1} |\partial u^{n+k}|_1. \end{aligned} \quad (4.15)$$

By Young's inequality,

$$\begin{aligned} \frac{1}{2\varepsilon^2} |\partial u^{n+k}|_{-1} |\partial u^{n+k}|_1 & \leq \frac{1}{4} |\partial u^{n+k}|_1^2 + \frac{1}{4\varepsilon^4} |\partial u^{n+k}|_{-1}^2 \\ & \leq \frac{1}{4} |\partial u^{n+k}|_1^2 + \frac{\beta_k}{2\tau} |\partial u^{n+k}|_{-1}^2. \end{aligned} \quad (4.16)$$

The estimate (4.11) follows from (4.15) and (4.16).  $\square$

By arguing as in [8], we have:

**Corollary 4.6.** *If the assumptions of Theorem 4.3 are satisfied and if  $\Omega$  has a smooth boundary, then the whole sequence  $((u^n, w^n))$  converges to a steady state  $(u^\infty, w^\infty)$  in  $\mathcal{V} \times \mathcal{V}$ , i.e. a solution of (2.6) such that  $\langle u^\infty \rangle = \langle u^0 \rangle$ .*

This result shows that the steady states for the BDF scheme (4.1) and for the PDE (2.5) are the same. Moreover, we recover the correct energy level at infinity, since

$$\hat{\mathcal{E}}(u^{n+k}, \dots, u^{n+k-1}) \rightarrow \hat{\mathcal{E}}(u^\infty, u^\infty, \dots, u^\infty) = \mathcal{E}(u^\infty).$$

The main steps of the proof are the precompactness of trajectories, Lasalle's invariance principle and the Łojasiewicz-Simon inequality formulated in [8, Lemma 3.2]. The regularity of  $\partial\Omega$  is needed for the Łojasiewicz-Simon inequality in relation with elliptic regularity [4].

**Remark 4.7.** If assumption (4.8) is not satisfied, then the sequence  $(\langle u^n \rangle)$  satisfies the linear recurrence relation (4.10). The roots of the characteristic equation are simple roots, namely 1 and  $k-1$  complex numbers with modulus less than 1, because the  $k$ -step BDF scheme is strictly zero-stable for  $k \leq 6$  [65, 123]. Thus,  $(\langle u^n \rangle)$  converges to a constant value  $M$  with an exponential rate. By using techniques developed for asymptotically autonomous gradient systems (see, e.g., [32, 55, 56]), it is possible to prove that the whole sequence  $((u^n, w^n))$  generated by (4.1) converges to a steady state.

Lemma 4.1 cannot be extended to the 6-step BDF scheme [105], so that the order 5 seems to be a barrier. A related phenomenon occurs for the Nevanlinna-Odeh multipliers [99]. These are used to prove stability and error estimates on a finite time interval for BDF schemes applied to semilinear parabolic problems, up to order 5 [5, 87]. These considerations lead us to the following question.

**Question 1.** Is it possible to find a time semidiscretization of (2.5) which has order greater than five and which is energy stable (with a possible restriction on the time step) ? If so, does every sequence generated by the scheme converge to a steady state ?

**4.2. Convex splitting scheme.** An idea introduced in [43, Equation (5.4)] for the Allen-Cahn equation and popularized by Eyre [44] is to split the potential  $F(s)$  into the sum of a convex function and a concave function. The convex term (or contractive) is treated implicitly and the concave term (expansive) is treated explicitly. The resulting scheme is unconditionally energy stable. If we choose

$$\frac{1}{4}(s^2 - 1)^2 = \left( \frac{s^4}{4} + \frac{1}{4} \right) + \left( -\frac{s^2}{2} \right),$$

the scheme reads: let  $u^0 \in \mathcal{V}$  and for  $n = 0, 1, \dots$  let  $(u^{n+1}, w^{n+1}) \in \mathcal{V} \times \mathcal{V}$  solve

$$\begin{cases} \frac{1}{\tau}(u^{n+1} - u^n, v) = -(\nabla w^{n+1}, \nabla v), & \forall v \in \mathcal{V}, \\ (w^{n+1}, z) = (\nabla u^{n+1}, \nabla z) + \frac{1}{\varepsilon^2}((u^{n+1})^3 - u^n, z), & \forall z \in \mathcal{V}. \end{cases} \quad (4.17)$$

This is a *nonlinear* scheme with *first order accuracy* and which is *unconditionally uniquely solvable* and *energy stable* [44, 125]. The mass is conserved, as can be seen by choosing  $v = 1$  in (4.17). The stability result reads:

**Theorem 4.8** ([43, 44]). *Let  $((u^n, w^n))$  be a sequence generated by (4.17). Then*

$$\mathcal{E}(u^{n+1}) + \tau|w^{n+1}|_1^2 + \frac{1}{2}|u^{n+1} - u^n|_1^2 + \frac{1}{2\varepsilon^2}|u^{n+1} - u^n|_0^2 \leq \mathcal{E}(u^n), \quad \forall n \geq 0. \quad (4.18)$$

*Proof.* We choose  $v = \tau w^{n+1}$  and  $z = u^{n+1} - u^n$  in (4.17). We find

$$-\tau|w|_1^2 = (\nabla u^{n+1}, \nabla(u^{n+1} - u^n)) + \frac{1}{\varepsilon^2}((u^{n+1})^3, u^{n+1} - u^n) - \frac{1}{\varepsilon^2}(u^n, u^{n+1} - u^n).$$

The function  $F_+(s) = (s^4 + 1)/4$  is convex, so  $F_+''(s) \geq 0$  and by the Taylor-Lagrange theorem

$$F_+(r) - F_+(s) \geq s^3(r - s), \quad \forall r, s \in \mathbb{R}.$$

Thus,

$$(F_+(u^n), 1) - F_+(u^{n+1}), 1) \geq ((u^{n+1})^3, u^n - u^{n+1}).$$

Using (2.4), we deduce from the previous calculations that

$$\begin{aligned} & \tau|w|_1^2 + \frac{1}{2}(|u^{n+1}|_1^2 - |u^n|_1^2 + |u^{n+1} - u^n|_1^2) \\ & + \frac{1}{2\varepsilon^2}(|u^n|_0^2 - |u^{n+1}|_0^2 + |u^{n+1} - u^n|_0^2) \leq \frac{1}{\varepsilon^2}(F_+(u^n), 1) - \frac{1}{\varepsilon^2}F_+(u^{n+1}), 1). \end{aligned}$$

This is exactly (4.18), since

$$\mathcal{E}(v) = \frac{1}{2}|v|_1^2 + \frac{1}{\varepsilon^2}(F_+(v), 1) - \frac{1}{\varepsilon^2}|v|_0^2, \quad \forall v \in \mathcal{V}.$$

□

Using this stability result and arguing as in [8], we obtain convergence to equilibrium for (4.17). This means that in Corollary 4.6, we may replace the word Theorem 4.3 by the word Theorem 4.8. The convergence is valid for every choice of  $\tau$ . The proof is based on the Łojasiewicz-Simon inequality [8, Lemma 3.2] evaluated at  $u^{n+1}$ . The explicit term  $u^n$  is treated as in finite dimension [6], by writing  $u^n = u^{n+1} + (u^n - u^{n+1})$  and using the triangle inequality.

**4.3. Linear schemes.** In order to have linear schemes which are energy stable, we introduce a modified potential as in [119]. Namely, we choose  $K > 1$ , we define

$$F_K(s) = \begin{cases} \frac{3K^2-1}{2}s^2 - 2K^3s + \frac{1}{4}(3K^4 + 1), & s > K, \\ \frac{1}{4}(s^2 - 1)^2, & s \in [-K, K], \\ \frac{3K^2-1}{2}s^2 + 2K^3s + \frac{1}{4}(3K^4 + 1), & s < -K, \end{cases} \quad (4.19)$$

and we replace  $f(s) = s^3 - s$  by  $F'_K(s)$  which is

$$f_K(s) = F'_K(s) = \begin{cases} (3K^2 - 1)s - 2K^3, & s > K, \\ s^3 - s, & s \in [-K, K], \\ (3K^2 - 1)s + 2K^3, & s < -K. \end{cases} \quad (4.20)$$

Thus,  $F_K \in C^2(\mathbb{R}, \mathbb{R})$  and  $f_K$  has a linear growth at  $\pm\infty$  with

$$\max_{s \in \mathbb{R}} |f'_K(s)| = 3K^2 - 1 = L. \quad (4.21)$$

The standard first-order linear implicit-explicit (IMEX) scheme reads: let  $u^0 \in \mathcal{V}$  and for  $n = 0, 1, \dots$ , let  $(u^{n+1}, w^{n+1}) \in \mathcal{V} \times \mathcal{V}$  solve

$$\begin{cases} \frac{1}{\tau}(u^{n+1} - u^n, v) = -(\nabla w^{n+1}, \nabla v), \quad \forall v \in \mathcal{V}, \\ (w^{n+1}, z) = (\nabla u^{n+1}, \nabla z) + \frac{1}{\varepsilon^2}(f_K(u^n), z), \quad \forall z \in \mathcal{V}, \end{cases} \quad \forall n \geq 0. \quad (4.22)$$

This is very efficient scheme which allows the use of FFT (Fast Fourier Transform) [25]. However, it is not clear how to choose  $K$  because the Cahn-Hilliard equation does not satisfy the maximum principle (cf. Remark 2.1 and Section 6). The modified energy is

$$\mathcal{E}_K(v) = \frac{1}{2}|v|_1^2 + (F_K(v), 1), \quad \forall v \in \mathcal{V}.$$

The dynamics of the linear IMEX scheme were first analyzed in [43] for the Allen-Cahn equation. Here, the energy stability reads:

**Proposition 4.9** ([119]). *Assume that  $\tau \leq 4\varepsilon^4/L^2$ , where  $L$  is the constant in (4.21). If  $((u^n, w^n))$  is a sequence generated by (4.22), then*

$$\mathcal{E}_K(u^{n+1}) + \frac{\tau}{2}|w^{n+1}|_1^2 \leq \mathcal{E}_K(u^n), \quad \forall n \geq 0.$$

For a sequence  $(u^n)$  in  $\mathcal{V}$ , we define the  $\omega$ -limit set

$$\omega((u^n)_{n \in \mathbb{N}}) = \{u^* \in \mathcal{V} : \exists n_k \rightarrow +\infty, u^{n_k} \rightarrow u^* \text{ strongly in } \mathcal{V}\}.$$

As a consequence, we have:

**Proposition 4.10.** *If the assumptions of Proposition 4.9 are satisfied, then the  $\omega$ -limit set  $\omega((u^n)_{n \in \mathbb{N}})$  is a nonempty compact and connected subset of  $\mathcal{V}$  on which  $\mathcal{E}_K$  is constant. Moreover, each  $u^\infty \in \omega((u^n)_{n \in \mathbb{N}})$  is a steady state for the modified potential in the sense that  $\langle u^\infty \rangle = \langle u^0 \rangle$  and*

$$(\nabla u^\infty, \nabla z) + \frac{1}{\varepsilon^2}(f_K(u^\infty), z) = (w^\infty, z), \quad \forall z \in \mathcal{V}, \quad (4.23)$$

for some constant function  $w^\infty$ .

*Proof.* On choosing  $v = 1$  in (4.22), we see that  $\langle u^{n+1} \rangle = \langle u^n \rangle$ . Thus, by induction, we have

$$\langle u^n \rangle = \langle u^0 \rangle, \quad \forall n \geq 0.$$

We deduce from (4.19) that there exist positive constants  $\kappa_1$  and  $\kappa_2$  such that

$$F_K(s) \geq \kappa_1 s^2 - \kappa_2, \quad \forall s \in \mathbb{R}.$$

We may choose for instance  $\kappa_1 = (3K^2 - 1)/4$ . Thus,  $\mathcal{E}_K$  satisfies

$$\mathcal{E}_K(v) \geq \frac{1}{2}|v|_1^2 + \kappa_1|v|_0^2 - \kappa_2|\Omega|, \quad \forall v \in \mathcal{V}.$$

On the other hand, we know by Proposition 4.9 that  $(\mathcal{E}_K(u^n))$  is nonincreasing. This shows that  $(\mathcal{E}(u^n))$  converges to a real number  $\mathcal{E}^\infty$  and that  $(u^n)$  is bounded in  $\mathcal{V}$ . Moreover,  $\mathcal{E}$  is constant and equal to  $\mathcal{E}^\infty$  on  $\omega((u^n)_{n \in \mathbb{N}})$ . Since

$$\frac{\tau}{2}|w^{n+1}|_1^2 \leq \mathcal{E}_K(u^n) - \mathcal{E}_K(u^{n+1}),$$

we also have  $\dot{w}^{n+1} \rightarrow 0$  in  $\mathcal{V}$ . The scheme (4.22) reads

$$\begin{cases} \frac{1}{\tau}(u^{n+1} - u^n) = -\Delta_N w^{n+1} \text{ in } \mathcal{V}', \\ w^{n+1} = -\Delta_N u^{n+1} + \frac{1}{\varepsilon^2} f_K(u^n) \text{ in } \mathcal{V}'. \end{cases}$$

We have

$$w^n = \dot{w}^n + \langle w^n \rangle \quad \text{with} \quad \langle w^n \rangle = \frac{1}{\varepsilon^2} \langle f_K(u^n) \rangle. \quad (4.24)$$

Since  $f_K$  has a linear growth at infinity, the sequence  $(f_K(u^n))$  is bounded in  $L^2(\Omega)$  and so  $-\Delta_N u^{n+1} = g^n$  where  $(g^n)$  is bounded in  $L^2(\Omega)$ . By elliptic regularity [60],  $(u^{n+1})$  is bounded in  $H^2(\Omega)$ . Since  $H^2(\Omega)$  is compactly embedded in  $\mathcal{V}$  [50], this shows that the set  $\{u^n : n \in \mathbb{N}\}$  is precompact in  $\mathcal{V}$ . It implies that  $\omega((u^n)_{n \in \mathbb{N}})$  is a nonempty compact subset of  $\mathcal{V}$ . Moreover,  $u^{n+1} - u^n = -\tau \Delta_N \dot{w}^{n+1}$  tends to 0 in  $\mathcal{V}'$ , and by compactness, also in  $\mathcal{V}$ . Thus,  $\omega((u^n)_{n \in \mathbb{N}})$  is also a connected subset of  $\mathcal{V}$  (see, e.g., [19, Lemma 3.1]). Now, let  $u^\infty \in \omega((u^n)_{n \in \mathbb{N}})$  and let  $(u^{n_k})$  be a subsequence such that  $u^{n_k} \rightarrow u^\infty$  in  $\mathcal{V}$  as  $k \rightarrow +\infty$ . We may let  $n = n_k$  tend to  $+\infty$  in (4.22), and we find that (4.23) holds for some constant function  $w^\infty$ . We note that  $(w^{n_k})$  converges to the constant function  $w^\infty = \langle f(u^\infty) \rangle$  in  $\mathcal{V}$  by (4.24). The proof is complete.  $\square$

Proposition 4.10 shows that, up to a subsequence,  $(u^n)$  converges to a steady state. If  $d = 1$ , by studying a phase portrait as in [122], it is possible to prove that there is a finite number of steady states with prescribed mass. Since the  $\omega$ -limit set  $\omega((u^n)_{n \in \mathbb{N}})$  is connected, it is therefore reduced to a singleton and the whole sequence  $(u^n)$  converges. However, if  $d = 2$  or  $3$ , the set of steady state is more complicated and it may even contain a continuum as in Section 6.1. In contrast with the finite dimensional case (cf. Theorem 5.9), we are not able to prove that the whole sequence converges because it is not known if a Łojasiewicz-Simon type inequality holds for  $\mathcal{E}_K$ . Indeed, the modified potential  $F_K$  is not analytic on  $\mathbb{R}$ . This raises the following question, which is related to proving a Kurdyka-Łojasiewicz-Simon inequality for  $\mathcal{E}_K$  (as defined, e.g., in [33]).

**Question 2.** If  $\tau \leq 4\varepsilon^4/L^2$ , does every sequence generated by (4.22) converge to a steady state ?

**Remark 4.11.** A similar convergence result and a similar question hold for the stabilized version of (4.22) considered in [123]. In the stabilized version, an extra dissipative term  $\frac{S}{\varepsilon^2}(u^{n+1} - u^n)$  with  $S \geq L/2$  is introduced. This makes the scheme unconditionally energy stable.

**4.4. Secant scheme and related schemes.** The secant scheme was introduced in [36] and its properties have been thoroughly investigated [38, 43, 48, 63]. It reads: let  $(u^0, w^0) \in \mathcal{V} \times \mathcal{V}$  and for  $n = 0, 1, \dots$ , let  $(u^{n+1}, w^{n+1}) \in \mathcal{V} \times \mathcal{V}$  solve

$$\begin{cases} \frac{1}{\tau}(u^{n+1} - u^n, v) = -(\nabla w^{n+1/2}, \nabla v), \quad \forall v \in \mathcal{V}, \\ (w^{n+1/2}, z) = (\nabla u^{n+1/2}, \nabla z) + \frac{1}{\varepsilon^2}(\hat{f}(u^{n+1}, u^n), z), \quad \forall z \in \mathcal{V}, \end{cases} \quad (4.25)$$

where  $w^{n+1/2} = (w^{n+1} + w^n)/2$ ,  $u^{n+1/2} = (u^{n+1} + u^n)/2$  and

$$\hat{f}(r, s) = \frac{F(r) - F(s)}{r - s}, \quad \forall r, s \in \mathbb{R}. \quad (4.26)$$

Since  $F(s) = (s^4 - 2s^2 + 1)/4$ , we can factorize and we have

$$\hat{f}(r, s) = \frac{1}{4}(r^3 + r^2s + rs^2 + s^3) - \frac{1}{2}(r + s).$$

The secant scheme is a *nonlinear* scheme with *second-order accuracy* and which is *unconditionally energy stable*. It is solvable for any  $\tau > 0$  and uniquely solvable if  $\tau < 4\varepsilon^4$  [63]. The stability property, which does not require uniqueness, reads:

**Proposition 4.12** ([36]). *Let  $\tau > 0$ . If  $((u^n, w^n))$  complies with (4.25), then*

$$\mathcal{E}(u^{n+1}) + \tau |\nabla w^{n+1/2}|_1^2 = \mathcal{E}(u^n), \quad \forall n \geq 0.$$

Remarkably, this scheme has no numerical dissipation in the sense that the energy law (1.6) holds at the discrete level. However, in contrast to the PDE (1.1), there is no regularization in finite time, since  $\Delta u^{n+1}$  has the same regularity as  $\Delta u^n$ . In particular, it is not clear that the set  $\{u^n : n \in \mathbb{N}\}$  is relatively compact in  $\mathcal{V}$ , and so we only obtain a partial convergence result.

**Proposition 4.13.** *Let  $((u^n, w^n))$  be a sequence which complies with (4.25). Then, up to a subsequence,  $((u^{n+1/2}, w^{n+1/2}))$  converges strongly in  $\mathcal{V} \times \mathcal{V}$  to a steady state  $(u^\infty, w^\infty)$ , i.e. a solution of (2.6) such that  $\langle u^\infty \rangle = \langle u^0 \rangle$ .*

*Proof.* On choosing  $v = 1$  in (4.25), we obtain by induction that

$$\langle u^n \rangle = \langle u^0 \rangle, \quad \forall n \geq 0.$$

By Proposition 4.12, the sequence  $(\mathcal{E}(u^n))$  is nonincreasing. Since

$$\mathcal{E}(v) \geq \frac{1}{2}|v|_1^2 + \kappa'_1|v|_0^2 - \kappa'_2, \quad \forall v \in \mathcal{V},$$

for some positive constants  $\kappa'_1, \kappa'_2$ , this implies that  $(u^n)$  is bounded in  $\mathcal{V}$ . Moreover,

$$\tau |w^{n+1/2}|_1^2 = \mathcal{E}(u^n) - \mathcal{E}(u^{n+1}) \rightarrow 0. \quad (4.27)$$

The first equation of (4.25) reads

$$u^{n+1} - u^n = \tau \Delta_N w^{n+1/2},$$

so that  $u^{n+1} - u^n \rightarrow 0$  in  $\mathcal{V}'$  and also weakly in  $\mathcal{V}$ , since  $u^{n+1} - u^n$  is bounded in  $\mathcal{V}$ . By the Rellich theorem,  $\mathcal{V}$  is compactly embedded in  $L^2(\Omega)$ . Thus, it is possible to find  $n_k \rightarrow +\infty$  and  $u^\infty \in \mathcal{V}$  such that

$$\begin{aligned} u^{n_k} &\rightarrow u^\infty \text{ weakly in } \mathcal{V} \text{ and a.e. in } \Omega, \\ u^{n_k+1} &\rightarrow u^\infty \text{ weakly in } \mathcal{V} \text{ and a.e. in } \Omega. \end{aligned}$$

In particular,

$$\hat{f}(u^{n_k+1}, u^{n_k}) \rightarrow \hat{f}(u^\infty, u^\infty) = f(u^\infty) \text{ a.e. in } \Omega.$$

Since the space dimension is less than or equal to 3, the space  $\mathcal{V}$  is continuously embedded in  $L^6(\Omega)$ . Thus,  $\hat{f}(u^{n_k+1}, u^{n_k})$  is bounded in  $L^2(\Omega)$ , with

$$|\hat{f}(u^{n_k+1}, u^{n_k})|_0 \leq C \left( \|u^{n_k+1}\|_{L^6(\Omega)}^3 + \|u^{n_k}\|_{L^6(\Omega)}^3 + 1 \right).$$



A classical lemma (see, e.g. [78, Lemme 4.8]) shows that  $\hat{f}(u^{n_k+1}, u^{n_k}) \rightarrow f(u^\infty)$  weakly in  $L^2(\Omega)$ . In particular, by choosing  $z = 1$  in (4.25), we have

$$(w^{n+1/2}, 1) = \frac{1}{\varepsilon^2}(\hat{f}(u^{n+1}, u^n), 1) \rightarrow \frac{1}{\varepsilon^2}(f(u^\infty), 1),$$

and so  $w^{n+1/2} = \bar{w}^{n+1/2} + \langle w^{n+1/2} \rangle$  converges strongly in  $\mathcal{V}$  to a constant function  $w^\infty$  (cf. (4.27)). We may let  $n = n_k$  tend to  $+\infty$  in (4.25), and we obtain that  $(u^\infty, w^\infty)$  is a steady state. Using the second equation in (4.25), we see that  $-\Delta_N u^{n+1/2} = g^n$  where  $(g^n)$  is bounded in  $L^2(\Omega)$ . By elliptic regularity [60],  $u^{n+1/2}$  is bounded in  $H^2(\Omega)$ . Since  $H^2(\Omega)$  is compactly embedded in  $\mathcal{V}$ , the sequence  $(u^{n_k+1/2})$  converges strongly to  $u^\infty$  in  $\mathcal{V}$ .  $\square$

In the proof above,  $(u^n)$  converges weakly in  $\mathcal{V}$  (up to a subsequence), but not necessarily strongly in  $\mathcal{V}$ . The convergence problem for the secant scheme is easier in finite dimension, as shown in Section 5.2. The lack of regularity can also be seen by examining global dynamics. In [43], it is shown that a global attractor exists for a fully discrete Allen-Cahn equation based on the secant scheme. However, the behaviour of this global attractor as the mesh step tends to 0 is not clear. A similar problem was pointed out for the Crank-Nicolson scheme applied to the 2D Navier-Stokes equation in [126]. We summarize these remarks as follows.

**Question 3.** Does every sequence  $((u^n, w^n))$  which complies with (4.25) converge strongly in  $\mathcal{V} \times \mathcal{V}$ ?

**Remark 4.14.** A similar question holds for closely related second-order one step schemes which are unconditionally energy stable, such as the Gomez-Hughes approximation [52], the Taylor expansion of the midpoint approach [79], the midpoint-BDF2 scheme [117] or the linear scheme of Wu-Van Zwieten-Van der Zee [130]. We refer the reader to the review [125] for a summary of these schemes.

**4.5. SAV approach.** Following ideas from [10], a Lagrange multiplier approach was proposed in [62, 63] to derive unconditionally energy stable linear schemes for the Cahn-Hilliard equation. The approach was generalized into the invariant energy quadratization (IEQ) method [131, 132], so as to include other situations. In [118], Shen, Xu and Yang introduced the scalar auxiliary variable (SAV) approach for gradient flows, a simplification of the IEQ method.

For the Cahn-Hilliard equation, the SAV method consists in introducing the auxiliary variable

$$r(t) = \sqrt{\int_{\Omega} \tilde{F}_{\varepsilon}(u(x, t)) dx} + C_0$$

where  $C_0 > 0$  is a fixed constant and  $\tilde{F}_{\varepsilon}(s) = \frac{1}{\varepsilon^2}F(s)$ . Then (1.1) becomes

$$\begin{cases} \partial_t u = \Delta w, \\ w = -\Delta u + \frac{r(t)}{\sqrt{(\tilde{F}_{\varepsilon}(u), 1) + C_0}} \tilde{f}_{\varepsilon}(u), \\ r'(t) = \frac{1}{2\sqrt{(\tilde{F}_{\varepsilon}(u), 1) + C_0}} (\tilde{f}_{\varepsilon}(u), \partial_t u), \end{cases} \quad (4.28)$$

with the boundary condition (1.2), where  $\tilde{f}_\varepsilon(s) = \tilde{F}'_\varepsilon(s) = \frac{1}{\varepsilon^2}f(s)$ . The system (4.28) can then be discretized by a first order or second order implicit/explicit scheme (a modified SAV method valid up to order 5 has recently been proposed in [72] for Cahn-Hilliard type equations).

For instance, a first-order implicit/explicit discretization of (4.28) reads: let  $(u^0, r^0) \in \mathcal{V} \times \mathbb{R}$  and for  $n = 0, 1, \dots$ , let  $(u^{n+1}, w^{n+1}, r^{n+1}) \in \mathcal{V} \times \mathcal{V} \times \mathbb{R}$  solve

$$\begin{cases} \frac{1}{\tau}(u^{n+1} - u^n, v) = -(\nabla w^{n+1}, \nabla v), & \forall v \in \mathcal{V}, \\ (w^{n+1}, z) = (\nabla u^{n+1}, \nabla z) + \frac{r^{n+1}}{\sqrt{(\tilde{F}_\varepsilon(u^n), 1) + C_0}}(\tilde{f}_\varepsilon(u^n), z), & \forall z \in \mathcal{V}, \\ r^{n+1} - r^n = \frac{1}{2\sqrt{(\tilde{F}_\varepsilon(u^n), 1) + C_0}}(\tilde{f}_\varepsilon(u^n), u^{n+1} - u^n). \end{cases} \quad (4.29)$$

At each time step, knowing  $(u^n, r^n)$ , it is possible to compute  $(u^{n+1}, w^{n+1}, r^{n+1})$  by solving two *linear* systems involving the bilaplacian. In contrast to the linear IMEX scheme where a modified potential  $F_K$  was introduced (see (4.19)), for the SAV approach we keep the quartic potential, which is denoted  $\tilde{F}_\varepsilon$  for notational convenience. The mass is conserved and the scheme is *unconditionally energy stable* for the modified energy

$$\tilde{\mathcal{E}}(u^n, r^n) = \frac{1}{2}|u^n|_1^2 + (r^n)^2. \quad (4.30)$$

The stability result reads:

**Proposition 4.15** ([118]). *Let  $\tau > 0$  and let  $((u^n, w^n, r^n))$  be a sequence in  $\mathcal{V} \times \mathcal{V} \times \mathbb{R}$  generated by (4.29). Then for all  $n \geq 0$ , we have*

$$\tilde{\mathcal{E}}(u^{n+1}, r^{n+1}) + \tau|w^{n+1}|_1^2 + \frac{1}{2}|u^{n+1} - u^n|_1^2 + (r^{n+1} - r^n)^2 = \tilde{\mathcal{E}}(u^n, r^n) \quad (4.31)$$

*Proof.* In (4.29), we choose  $v = -\tau w^{n+1}$ ,  $z = u^{n+1} - u^n$ , we multiply the last equation by  $-2r^{n+1}$  and we add the resulting equations. We obtain

$$\tau|w^{n+1}|_1^2 + (\nabla u^{n+1}, \nabla(u^{n+1} - u^n)) + 2(r^{n+1} - r^n)r^{n+1} = 0.$$

Using twice the identity (2.4), we obtain (4.31).  $\square$

The asymptotic behaviour of sequences generated by (4.29) was studied in [19]. We say that  $(u^*, w^*, r^*) \in \mathcal{V} \times \mathcal{V} \times \mathbb{R}$  is a steady state for (4.29) if

$$(\nabla u^*, \nabla z) + \frac{r^*}{s^*}(\tilde{f}_\varepsilon(u^*), z) = (w^*, z), \quad \forall z \in \mathcal{V}, \quad (4.32)$$

where  $s^* = \sqrt{(\tilde{F}_\varepsilon(u^*), 1) + C_0}$  and  $w^*$  is a constant function on  $\Omega$ . Thus, a steady state is a solution of (4.29) which does not depend on  $n$ .

**Proposition 4.16.** *Let  $((u^n, w^n, r^n))$  be a sequence in  $\mathcal{V} \times \mathcal{V} \times \mathbb{R}$  generated by (4.29). Then, up to a subsequence,  $((u^n, w^n, r^n))$  converges in  $\mathcal{V} \times \mathcal{V} \times \mathbb{R}$  to a steady state  $(u^*, w^*, r^*)$  such that (4.32) holds with  $w^*$  constant on  $\Omega$ .*

*Proof.* By Proposition 4.15,  $(\tilde{\mathcal{E}}(u^n, r^n))$  is nonincreasing, so it converges to a non-negative real number  $\tilde{\mathcal{E}}^\infty$ . The estimate (4.31) reads

$$\tau|w^{n+1}|_1^2 + \frac{1}{2}|u^{n+1} - u^n|_1^2 + (r^{n+1} - r^n)^2 \leq \tilde{\mathcal{E}}(u^n, r^n) - \tilde{\mathcal{E}}(u^{n+1}, r^{n+1}),$$

so  $|w^{n+1}|_1 \rightarrow 0$ ,  $|u^{n+1} - u^n|_1 \rightarrow 0$  and  $r^{n+1} - r^n \rightarrow 0$  as  $n \rightarrow +\infty$ . Moreover,  $(|u^n|_1^2)$  and  $(r^n)$  are bounded, by (4.30). We also know that  $\langle u^n \rangle = \langle u^0 \rangle$  (by choosing  $v = 1$  in (4.29)). Thus, by the Poincaré-Wirtinger inequality, the sequence  $(u^n)$  is bounded in  $\mathcal{V}$ . The second equation in (4.29) reads

$$-\Delta_N u^{n+1} + \frac{r^{n+1}}{s^{n+1}} \tilde{f}_\varepsilon(u^n) = w^{n+1} \text{ in } \mathcal{V}',$$

where  $s^n = \sqrt{(\tilde{F}_\varepsilon(u^n), 1) + C_0}$ . The sequence  $(s^n)$  is bounded and satisfies  $s^n \geq \sqrt{C_0} > 0$ , for all  $n \geq 0$ , so we have  $-\Delta_N u^{n+1} = g^n$  where  $(g^n)$  is bounded in  $L^2(\Omega)$ . By elliptic regularity [60],  $(u^{n+1})$  is bounded in  $H^2(\Omega)$ . Since  $H^2(\Omega)$  is compactly embedded in  $\mathcal{V}$ , there exists a subsequence  $(u^{n_k})$  which converges strongly in  $\mathcal{V}$  to some  $u^* \in \mathcal{V}$ . We may also assume that  $(r^{n_k})$  converges to some  $r^*$  in  $\mathbb{R}$ . Concerning  $(w^n)$ , we write  $w^{n+1} = \dot{w}^{n+1} + \langle w^{n+1} \rangle$ . By choosing  $z = 1/|\Omega|$  in (4.29), we have

$$\langle w^{n_k+1} \rangle = \frac{r^{n_k+1}}{s^{n_k}} \langle \tilde{f}_\varepsilon(u^{n_k}) \rangle \rightarrow \frac{r^*}{s^*} \langle \tilde{f}_\varepsilon(u^*) \rangle,$$

where  $s^* = \sqrt{(\tilde{F}_\varepsilon(u^*), 1) + C_0}$ . Thus,  $(w^{n_k+1})$  converges to a constant function  $w^*$  in  $\mathcal{V}$ . We choose  $n = n_k$  and we let  $k$  tend to  $+\infty$  in the second equation of (4.29). This gives the steady state equation (4.32).  $\square$

It is possible to obtain information on the structure of the  $\omega$ -limit set of the sequence  $((u^n, r^n))$  [19], but we are not able to apply the techniques involving a Łojasiewicz-Simon inequality and to prove that the whole sequence converges. However, the main problem for the SAV scheme (4.29) is that the ratio  $r^*/s^*$  in (4.32) is generally not equal to 1, because the scheme is only a first-order approximation of the exact solution (see [19] for theoretical and numerical examples). Thus, the steady state equation (4.32) is only an approximation of the steady state equation (2.6) associated to the PDE.

We stress that these differences between the steady states are not limited to the first-order SAV scheme (4.29). The problem comes from the auxiliary variable. Indeed, a solution of the continuous-in-time SAV system (4.28) which does not depend on the time  $t$  also solves (4.32). It could be interesting to have a better understanding of the longtime dynamics of the SAV schemes in comparison with those of the underlying PDE. As a starter, the following question can be considered.

**Question 4.** Does every sequence  $((u^n, w^n, r^n))$  generated by (4.29) converge in  $\mathcal{V} \times \mathcal{V} \times \mathbb{R}$  ?

## 5. THE FULLY DISCRETE CASE

By combining a space discretization from Section 3 and a time discretization from Section 4, it is easy to obtain a fully discrete approximation of the Cahn-Hilliard equation which is energy stable. Sometimes, only the fully discrete scheme is

meaningful. This is the case with the forward Euler scheme [6, 25], with appropriate Runge-Kutta methods [64] or with a preconditioning as in [21, Theorem 3.3]

In this section, we focus on two examples, namely the secant scheme and the linear IMEX scheme, which show that the convergence problem in finite dimension is better understood. We start with a general convergence result and some tools related to the Łojasiewicz inequality.

**5.1. A general convergence result; semialgebraic functions.** We will use the following result, which is a direct consequence of [6, Theorem 2.4] (see also [9, Theorem 2.9] or [47, Theorem 3.1]).

**Theorem 5.1** ([6]). *Let  $\Phi \in C^1(\mathbb{R}^M, \mathbb{R})$ . Consider a bounded sequence  $(U^n)$  in  $\mathbb{R}^M$  which satisfies the following conditions:*

**H4:** *There exists a positive constant  $c_1$  such that for each  $n \in \mathbb{N}$ ,*

$$\Phi(U^n) - \Phi(U^{n+1}) \geq c_1 \|U^{n+1} - U^n\|^2;$$

**H5:** *There exists a positive constant  $c_2$  such that for each  $n \in \mathbb{N}$ ,*

$$\|\nabla \Phi(U^{n+1})\| \leq c_2 \|U^{n+1} - U^n\|.$$

*If  $\Phi$  satisfies the Łojasiewicz inequality (Definition 3.4) at an accumulation point  $U^*$  of  $(U^n)$ , then the whole sequence  $(U^n)$  converges to  $U^*$ .*

For implicit schemes, the nonlinearity is analytic and we will use Theorem 3.6. For linear IMEX schemes, the nonlinearity is no longer analytic, but it is *semialgebraic*. We recall here some definitions and properties from [9, 15, 17].

**Definition 5.2.** A subset  $S$  of  $\mathbb{R}^m$  is a *real semialgebraic set* if there exists a finite number of real polynomial functions  $P_{ij}, Q_{ij} : \mathbb{R}^m \rightarrow \mathbb{R}$  such that

$$S = \bigcup_{i=1}^p \bigcap_{j=1}^q \{x \in \mathbb{R}^m : P_{ij}(x) = 0, Q_{ij}(x) < 0\}.$$

One easily sees that the class of semialgebraic sets is stable under the operation of finite union, finite intersection, Cartesian product or complementation.

**Definition 5.3.** Let  $S_1 \subset \mathbb{R}^{m_1}$  and  $S_2 \subset \mathbb{R}^{m_2}$  be two semialgebraic sets. A mapping  $g : S_1 \rightarrow S_2$  is *semialgebraic* if its graph  $\{(x, y) \in S_1 \times S_2 : y = g(x)\}$  is a semialgebraic subset of  $\mathbb{R}^{m_1+m_2}$ .

Of course, polynomial functions are semialgebraic functions. The function  $F_K : \mathbb{R} \rightarrow \mathbb{R}$  given by (4.19) is also a semialgebraic function (see Lemma 5.8). The class of semialgebraic mappings is highly flexible thanks to the Tarski-Seidenberg principle. In particular, we have [17, Proposition 2.2.6]:

**Theorem 5.4.** *The composition  $g_2 \circ g_1$  of semialgebraic mappings  $g_1 : S_1 \rightarrow S_2$  and  $g_2 : S_2 \rightarrow S_3$  is also semialgebraic.*

As a consequence, the sum  $g_1 + g_2$  or product  $g_1 g_2$  of two semialgebraic functions on  $\mathbb{R}^m$  is also semialgebraic, by composition of  $(g_1, g_2) : \mathbb{R}^m \rightarrow \mathbb{R}^2$  with  $+: \mathbb{R}^2 \rightarrow \mathbb{R}$  or with  $\times : \mathbb{R}^2 \rightarrow \mathbb{R}$ . Kurdyka [81] generalized the Łojasiewicz inequality to *o-minimal* structures, and this includes semialgebraic functions.

**Theorem 5.5** (Theorem (LI) in [81]). *If  $\Phi : \mathbb{R}^M \rightarrow \mathbb{R}$  is of class  $C^1$  and semialgebraic, then  $\Phi$  satisfies the Łojasiewicz inequality (Definition 3.4) at each point  $U^* \in \mathbb{R}^M$ .*

**5.2. Secant scheme with Galerkin approximation.** We consider the secant scheme with variable time step, combined with a Galerkin approximation. We assume that  $\mathcal{V}_h$  is a  $(M + 1)$ -dimensional subspace of  $\mathcal{V}$  which contains the constant functions and that  $(\tau_n)$  is a bounded sequence of positive real numbers such that

$$\tau_\star \leq \tau_n \leq \tau^\star, \quad \forall n \geq 0, \quad (5.1)$$

for some positive real numbers  $\tau_\star, \tau^\star$ . If the time step is constant, then assumption (5.1) is obviously satisfied.

The scheme reads: let  $(u_h^0, w_h^0) \in \mathcal{V}_h$  and for  $n = 0, 1, \dots$ , let  $(u_h^{n+1}, w_h^{n+1}) \in \mathcal{V}_h \times \mathcal{V}_h$  solve

$$\begin{cases} \frac{1}{\tau_n}(u_h^{n+1} - u_h^n, v_h) = -(\nabla w_h^{n+1/2}, \nabla v_h), & \forall v_h \in \mathcal{V}_h, \\ (w_h^{n+1/2}, z_h) = (\nabla u_h^{n+1/2}, \nabla z_h) + \frac{1}{\varepsilon^2}(\hat{f}(u_h^{n+1}, u_h^n), z_h), & \forall z_h \in \mathcal{V}_h, \end{cases} \quad (5.2)$$

where  $u_h^{n+1/2} = (u_h^{n+1} + u_h^n)/2$ ,  $w_h^{n+1/2} = (w_h^{n+1} + w_h^n)/2$  and  $\hat{f}(r, s)$  is defined by (4.26). Convergence to equilibrium was proved in [115] for the secant scheme applied to a finite element discretization of a model of nematic liquid crystals with a Ginzburg-Landau potential. Here, we prove:

**Theorem 5.6.** *Every sequence  $((u_h^n, w_h^n))$  in  $\mathcal{V}_h \times \mathcal{V}_h$  which complies with (5.2) converges to a steady state  $(u_h^\infty, w_h^\infty)$  in  $\mathcal{V}_h \times \mathcal{V}_h$ , i.e. a solution of*

$$(\nabla u_h^\infty, \nabla z_h) + \frac{1}{\varepsilon^2}(f(u_h^\infty), z_h) = (w_h^\infty, z_h), \quad \forall z_h \in \mathcal{V}_h, \text{ with } w_h^\infty \text{ constant on } \Omega.$$

**Remark 5.7.** Uniqueness holds if  $\tau < 4\varepsilon^4$  [63]. Thus, for large  $\tau$ , there may be several sequences corresponding to a given initial value  $(u_h^0, w_h^0)$ . Each one of these sequences converges to a steady state. The scheme defines a *multivalued* dynamical system [90, 109].

*Proof.* We first choose  $v_h = 1$  in (5.2) and we obtain by induction that

$$\langle u_h^n \rangle = \langle u_h^0 \rangle, \quad \forall n \geq 0.$$

We choose  $v_h = -\tau_n w_h^{n+1/2}$  and  $z_h = u_h^{n+1} - u_h^n$  in (5.2) and we add the resulting equations. This yields

$$\mathcal{E}(u_h^{n+1}) - \mathcal{E}(u_h^n) + \tau_n |w_h^{n+1/2}|_1^2 = 0, \quad \forall n \geq 0. \quad (5.3)$$

Thus,  $(\mathcal{E}(u_h^n))$  is bounded and so the sequence  $(u_h^n)$  is bounded in  $\mathcal{V}_h$ , by the Poincaré-Wirtinger inequality. Next, we apply Theorem 5.1. We choose a basis  $(e_0, e_1, \dots, e_M)$  of  $\mathcal{V}_h$  which is orthonormal for the inner product in  $L^2(\Omega)$  and such that  $e_0$  is constant. We write  $u_h^n = \sum_{i=0}^M u_i^n e_i$  and  $w_h^n = \sum_{i=0}^M w_i^n e_i$ . The scheme (5.2) implies that  $(u_0^n)$  is constant and that

$$\begin{cases} \frac{1}{\tau_n}(U^{n+1} - U^n) = -A_h W^{n+1/2}, \\ W^{n+1/2} = A_h U^{n+1/2} + \frac{1}{\varepsilon^2} \hat{F}_h(U^{n+1}, U^n), \end{cases}, \quad \forall n \geq 0, \quad (5.4)$$

where  $U^n = (u_i^n)_{1 \leq i \leq M}$ ,  $W^n = (w_i^n)_{1 \leq i \leq M}$ ,  $A_h = (\nabla e_i, \nabla e_j)_{1 \leq i, j \leq M}$  and

$$\hat{F}_h(U^{n+1}, U^n) = (\hat{f}(u_h^{n+1}, u_h^n), e_i)_{1 \leq i \leq M}.$$

The  $M \times M$  matrix  $A_h$  is symmetric positive definite since  $(\nabla \cdot, \nabla \cdot)$  is an inner product on  $\dot{\mathcal{V}}_h = \mathcal{V}_h \cap \dot{\mathcal{V}}$ . We define

$$\Phi(V) = \Phi(v_1, \dots, v_M) = \mathcal{E}(u_0 e_0 + \sum_{i=1}^M v_i e_i).$$

Then (5.3) shows that for all  $n \geq 0$ , we have

$$\begin{aligned} \Phi(U^n) - \Phi(U^{n+1}) &= \tau_n (W^{n+1/2})^T A_h W^{n+1/2} \\ &= \frac{1}{\tau_n} (U^{n+1} - U^n)^T A_h^{-1} (U^{n+1} - U^n), \\ &\geq \frac{1}{\tau^* \lambda_M} \|U^{n+1} - U^n\|^2, \end{aligned}$$

where  $\lambda_M > 0$  is the largest eigenvalue of  $A_h$ . Thus, assumption **H4** is satisfied. Now, we turn to **H5**. We note that (5.4) is equivalent to

$$-\frac{1}{\tau_n} A_h^{-1} (U^{n+1} - U^n) = A_h U^{n+1/2} + \frac{1}{\varepsilon^2} \hat{F}_h(U^{n+1}, U^n). \quad (5.5)$$

Since all norms are equivalent in  $\mathcal{V}_h$ , there is a constant  $C$  such that

$$\|u_h^n\|_{L^\infty(\Omega)} \leq C, \quad \forall n \geq 0.$$

By Taylor's formula, for all  $r, s \in \mathbb{R}$ , there exists  $\xi \in [r, s]$  such that

$$F(s) = F(r) + (s - r)f(r) + \frac{(s - r)^2}{2} f'(\xi).$$

Thus, for all  $r, s \in [-C, C]$ , we have

$$\left| \hat{f}(r, s) - f(r) \right| \leq \frac{|s - r|}{2} L_C,$$

where  $L_C = \sup_{\xi \in [-C, C]} |f'(\xi)|$ . It is clear that (cf. (3.29))

$$\nabla \Phi(U^{n+1}) = A_h U^{n+1} + \frac{1}{\varepsilon^2} ((f(u_h^{n+1}), e_i))_{1 \leq i \leq M},$$

so we have

$$\begin{aligned} &\left\| A_h U^{n+1/2} + \frac{1}{\varepsilon^2} \hat{F}_h(U^{n+1}, U^n) - \nabla \Phi(U^{n+1}) \right\| \\ &\leq \frac{1}{2} \|A_h(U^{n+1} - U^n)\| + \frac{L_C}{2\varepsilon^2} \|U^{n+1} - U^n\|. \end{aligned} \quad (5.6)$$

Using the triangle inequality, we deduce from (5.5) and (5.6) that

$$\|\nabla \Phi(U^{n+1})\| \leq C' \|U^n - U^{n+1}\|, \quad \forall n \geq 0,$$

for some constant  $C' = C'(\tau_*, \varepsilon, \|A_h\|, \|A_h^{-1}\|, L_C)$  independent of  $n$ . This shows that assumption **H5** is satisfied. Moreover, the function  $\Phi$  is a polynomial (see (3.30)). Thus, by Theorem 3.6,  $\Phi$  satisfies the Łojasiewicz inequality at each point in  $\mathbb{R}^M$ . We are in position to apply Theorem 5.1 and we obtain that  $(U^n)$  converges. Finally, we may pass to the limit in (5.2) and the proof is complete.  $\square$

**5.3. Linear IMEX scheme with finite difference method.** We consider the linear IMEX scheme (4.22) combine with the finite difference space discretization from Section 3.2.1. It reads: let  $U^0 \in \mathbb{R}^M$  and for  $n = 0, 1, \dots$ , let  $(U^{n+1}, W^{n+1}) \in \mathbb{R}^M \times \mathbb{R}^M$  solve

$$\begin{cases} \frac{1}{\tau}(U^{n+1} - U^n) = -AW^{n+1}, \\ W^{n+1} = AU^{n+1} + \frac{1}{\varepsilon^2} \nabla F_{K,M}(U^n), \end{cases} \quad (5.7)$$

where  $A$  satisfies assumption **H1** from Section 3.1 and  $F_{K,M} : \mathbb{R}^M \rightarrow \mathbb{R}$  is defined by

$$F_{K,M}(v_1, \dots, v_M) = \sum_{i=1}^M F_K(v_i)$$

with  $F_K$  given by (4.19). For the standard difference scheme, 0 is a simple eigenvalue of  $A$  associated to the eigenvector  $E_1 = (1, 1, \dots, 1)^T$  and  $M = J + 1$  if  $\Omega = (0, 1)$  (see (3.25)),  $M = (J + 1)^2$  if  $\Omega = (0, 1)^2$  and  $M = (J + 1)^3$  if  $\Omega = (0, 1)^3$  (see (3.26)), where  $h = 1/J$  is the step size.

We first point out:

**Lemma 5.8.** *The function  $F_{K,M} \in C^2(\mathbb{R}^M, \mathbb{R})$  is semialgebraic.*

*Proof.* We have  $F_{K,M} = l \circ g$  where  $g : \mathbb{R}^M \rightarrow \mathbb{R}^M$  is defined by

$$g(v_1, \dots, v_M) = (F_K(v_1), \dots, F_K(v_M)),$$

and  $l : \mathbb{R}^M \rightarrow \mathbb{R}$  is given by  $l(z_1, \dots, z_M) = z_1 + \dots + z_M$ . Since  $l$  is a polynomial function, it is semialgebraic. We claim that  $g$  is semialgebraic and so, by Theorem 5.4,  $l \circ g$  is semialgebraic. In order to prove the claim, we write the graph of  $g$  as the finite intersection of the sets  $S_i$  ( $i = 1, \dots, M$ ) defined by

$$S_i = \{(v_1, \dots, v_M, z_1, \dots, z_M) \in \mathbb{R}^M \times \mathbb{R}^M : z_i = F_K(v_i)\}.$$

Using (4.19), we see that  $S_i \subset \mathbb{R}^{2M}$  can be written as

$$\begin{aligned} S_i = & \left\{ \frac{1}{4}(v_i^2 - 1)^2 - z_i = 0, v_i^2 - K^2 < 0 \right\} \\ & \cup \left\{ \frac{3K^2 - 1}{2}v_i^2 - 2K^3v_i + \frac{1}{4}(3K^4 + 1) - z_i = 0, K - v_i < 0 \right\} \\ & \cup \left\{ \frac{3K^2 - 1}{2}v_i^2 + 2K^3v_i + \frac{1}{4}(3K^4 + 1) - z_i = 0, v_i + K < 0 \right\} \\ & \cup \left( \{v_i^2 - K^2 = 0, -1 < 0\} \cap \left\{ \frac{1}{4}(v_i^2 - 1)^2 - z_i = 0, -1 < 0 \right\} \right). \end{aligned}$$

This shows that each  $S_i$  is a semialgebraic subset of  $\mathbb{R}^{2M}$  (Definition 5.2), and the proof is complete.  $\square$

**Theorem 5.9.** *Assume that  $\tau \leq 4\varepsilon^4/L^2$  where  $L$  is given by (4.21). Then every sequence  $((U^n, W^n))$  generated by (5.7) converges to a steady state  $(U^\infty, W^\infty)$  in  $\mathbb{R}^M \times \mathbb{R}^M$ , i.e. a solution of*

$$AW^\infty = 0, \quad AU^\infty + \frac{1}{\varepsilon^2} \nabla F_{K,M}(U^\infty) = W^\infty. \quad (5.8)$$

*Proof.* We multiply the first equation in (5.7) by  $E_1^T$  and we obtain by induction that  $E_1^T U^n = E_1^T U^0$ , for all  $n \geq 0$ . Thus, we only have to deal with the remaining  $M - 1$  degrees of freedom. By using an orthonormal basis of  $\mathbb{R}^M$  starting with  $E_1/\|E_1\|$  as in the Proof of Theorem 3.7 (Step 1), we may assume that  $A$  has the form (3.18) and that  $E_1 = (1, 0, \dots, 0)^T$ . The system (5.7) becomes

$$\begin{cases} \frac{1}{\tau}(\tilde{U}^{n+1} - \tilde{U}^n) = -\tilde{A}\tilde{W}^{n+1}, \\ \tilde{W}^{n+1} = \tilde{A}\tilde{U}^{n+1} + \frac{1}{\varepsilon^2}\nabla\tilde{F}_{K,M}(\tilde{U}^n), \end{cases}$$

where  $\tilde{A}$  is a  $(M - 1) \times (M - 1)$  symmetric positive definite matrix,

$$\tilde{U} = (U_2, \dots, U_M)^T, \quad \tilde{W} = (w_2, \dots, w_M)^T$$

and  $\tilde{F}_{K,M} : \mathbb{R}^{M-1} \rightarrow \mathbb{R}$  is a nonnegative semialgebraic function of class  $C^2$ , obtained by composition of  $F_{K,M}$  and of a linear mapping. In the remainder of the proof, we omit the tilde symbol and we change  $M - 1$  into  $M$ . That is, we deal with the system (5.7) but we assume this time that  $A$  is a  $M \times M$  symmetric positive definite matrix.

The energy stability of the scheme reads (cf. Proposition 4.9)

$$\frac{\tau}{2}(W^{n+1})^T A W^{n+1} + \Phi(U^{n+1}) \leq \Phi(U^n), \quad \forall n \geq 0, \quad (5.9)$$

where the energy  $\Phi : \mathbb{R}^M \rightarrow \mathbb{R}$  is defined by

$$\Phi(V) = \frac{1}{2}V^T A V + \frac{1}{\varepsilon^2}F_{K,M}(V) \quad (V \in \mathbb{R}^M).$$

By Lemma 3.1, the sequence  $(U^n)$  is bounded. We note that the function  $\Phi$  is semialgebraic by composition of the semialgebraic maps

$$\mathbb{R}^M \ni V \mapsto \left(\frac{1}{2}V^T A V, \frac{1}{\varepsilon^2}F_{K,M}(V)\right) \in \mathbb{R}^2$$

and  $+$  :  $\mathbb{R}^2 \rightarrow \mathbb{R}$ . Thus, by Theorem 5.5,  $\Phi$  satisfies the Łojasiewicz inequality at every point in  $\mathbb{R}^M$ . Using the first equation in (5.7), we deduce from (5.9) that

$$\begin{aligned} \Phi(U^n) - \Phi(U^{n+1}) &\geq \frac{1}{2\tau}(U^{n+1} - U^n)^T A^{-1}(U^{n+1} - U^n) \\ &\geq \frac{1}{2\tau\lambda_M}\|U^{n+1} - U^n\|^2, \end{aligned}$$

for all  $n \geq 0$ , where  $\lambda_M > 0$  is the largest eigenvalue of  $A$ . Thus, assumption **H4** holds. On the other hand, by applying to  $F_K$  the Taylor inequality, we deduce that

$$\left\| \nabla\Phi(U^{n+1}) - \left( A U^{n+1} + \frac{1}{\varepsilon^2}\nabla F_{K,M}(U^n) \right) \right\| \leq \frac{L}{\varepsilon^2}\|U^{n+1} - U^n\|, \quad (5.10)$$

for all  $n \geq 0$ . By eliminating  $W^{n+1}$  from (5.7), we have

$$A U^{n+1} + \frac{1}{\varepsilon^2}\nabla F_{K,M}(U^n) = -\frac{1}{\tau}A^{-1}(U^{n+1} - U^n). \quad (5.11)$$

Using the triangle inequality, we deduce from (5.10) and (5.11) that **H5** also holds. Thus, we may apply Theorem 5.1, and we obtain that  $(U^n)$  converges. By continuity, the limit is necessarily a steady state, and the proof is complete.  $\square$



**Remark 5.10.** If we replace the finite difference by a finite element discretization with numerical integration, a similar proof shows that the whole sequence generated by the linear IMEX scheme converges to a steady state (see, e.g. [6]).

## 6. SIMULATIONS

We show 2D and 3D examples which illustrate our convergence results. For the 2D finite element computation, we used the **FreeFem++** software [69]. The 3D finite difference computation was performed with a **Python**<sup>1</sup> code. Concerning the visualization, we used **Visit**<sup>2</sup> for the 3D figures and **MATLAB**<sup>®</sup> for the other figures.

**6.1. 2D finite element simulations.** We have performed numerical simulations for the Cahn-Hilliard equation (2.5) on the disc  $\Omega$  of radius  $1/2$  centered at  $(0, 0)$ . This situation is interesting because there is a continuum of global minimizers by rotational invariance of the steady state equation. We first point out a symmetry breaking due to the space discretization. Then, we discuss a numerical solution to the secant scheme with adaptive time step.

**6.1.1. Symmetry breaking.** For the space discretization, we use the Galerkin approximation (3.27) with a  $P^1$  finite element approximation. We note that the space discretization induces a symmetry breaking. Indeed, the disc  $\Omega$  is approximated by a convex polygonal  $\Omega_h$  whose vertices lie on  $\partial\Omega$ . The conformal triangulation  $\mathcal{T}_h$  of  $\Omega_h$  into triangles has no rotational invariance (see Figure 1). The finite element space  $\mathcal{V}_h$  is a subspace of  $H^1(\Omega_h)$ , namely

$$\mathcal{V}_h = \{v_h \in C^0(\overline{\Omega}_h) : \forall K \in \mathcal{T}_h, (v_h)|_K \in P^1\}.$$

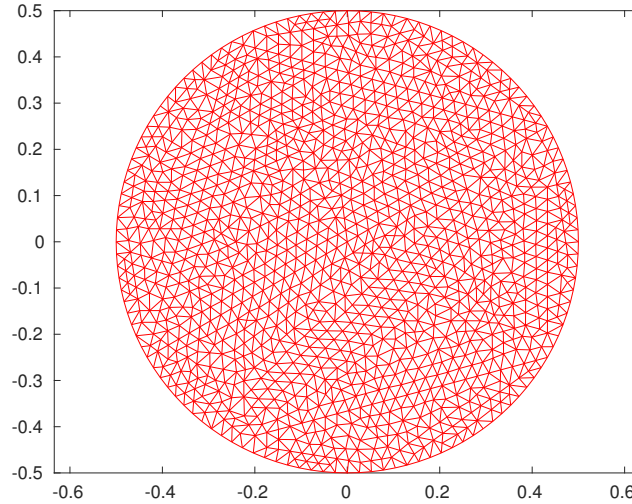


FIGURE 1. Mesh used for (6.1)

<sup>1</sup>Python is freely available at <https://www.python.org/>

<sup>2</sup>Visit is freely available at <https://wci.llnl.gov/simulation/computer-codes/visit>

We expect that the symmetry breaking results in many local minimizers with the same prescribed mean value, which are steady states in the sense of (3.31). In order to support this affirmation, we have computed the asymptotic state  $u_h^\infty$  and the energy level  $\mathcal{E}(u_h^\infty)$  for different initial values. The initial value is a rotation of the  $\tanh(x)$  profile, namely

$$u_0(x, y) = 0.9 \tanh((\cos(\theta)x + \sin(\theta)y)/0.01) \quad (6.1)$$

with  $\theta \in [0, \pi]$ . For each  $\theta$ , we use the  $P^1$  interpolate of  $u_0$  and we subtract its mean value so that the mean value of the discrete approximate is zero.

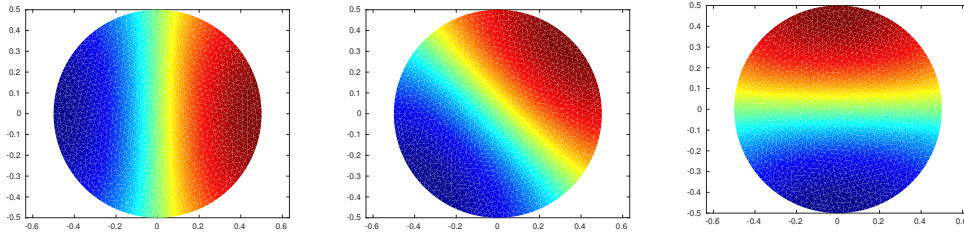


FIGURE 2. Final value for (6.1) with  $\theta = 0$  (left),  $\theta = \pi/4$  (middle) and  $\theta = \pi/2$  (right). The thickness parameter  $\varepsilon$  is equal to 0.2.

The thickness parameter  $\varepsilon$  in (3.27) is equal to 0.2. The mesh  $\mathcal{T}_h$ , shown in Figure 1, is a conforming triangulation of a regular polygon with 120 sides. It has 1333 vertices and 2544 triangles with  $h_{min} = 0.021$  and  $h_{max} = 0.043$ , where  $h_{min}$  and  $h_{max}$  are respectively the minimum and maximum diameter of all the triangles in  $\mathcal{T}_h$ . Thus, the typical interface thickness  $\varepsilon = 0.2$  is computed with a sufficient resolution (5-10 triangles per  $\varepsilon$ ).

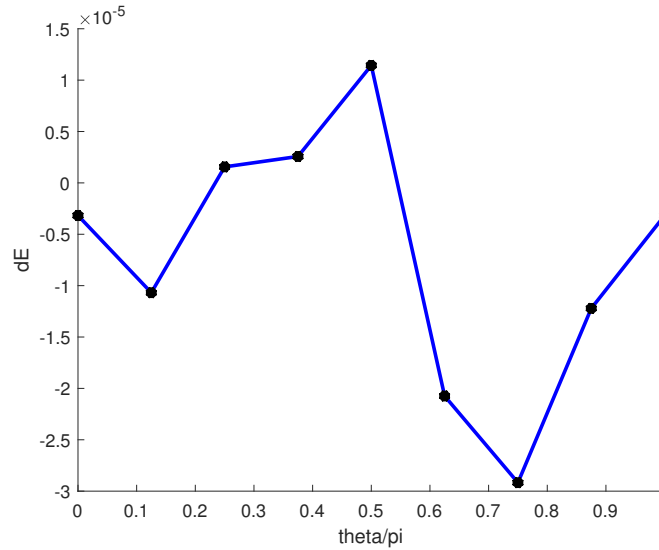


FIGURE 3. Final energy level vs. angle  $\theta$  for (6.1)

In Figure 3, we have represented the final state corresponding to the initial value (6.1) for the parameters  $\theta = 0, \pi/4$  and  $\pi/2$ . For the time resolution, we used the unconditionally stable convex splitting scheme (4.17) with time step  $\tau = 0.04$ . By arguing as in Theorem 5.6, it is easy to prove that for every initial value, the sequence uniquely generated by the scheme converges to a steady state. This asymptotic convergence result does not say *which* steady state will be reached. Remarkably, the final state has the same orientation as the initial state. This is rather expected but it is difficult to prove. As a consequence of the Łojasiewicz inequality, it is known that a local minimizer is stable with respect to the time discretization (see [90, Proposition 2.6] and [6, Theorem 2.12]).

The energy level  $\mathcal{E}(u_h^\infty)$  of the asymptotic state is computed for  $\theta = k\pi/8$  ( $k = 0, 1, \dots, 8$ ) in Figure 3. The graphic represents the difference  $\mathcal{E}(u_h^\infty) - 4.28992$  with respect to  $\theta$ , where 4.28992 is chosen as a reference energy level. We see that the energy levels are all different even if the relative difference is very small (less than  $10^{-5}$ ). Thus, the asymptotic states are most likely *local minimizers* of the energy  $\mathcal{E}$  in  $\mathcal{V}_h$  with prescribed zero mean value.

**6.1.2. Secant scheme with adaptive time stepping.** We have computed a numerical solution to the secant scheme with variable time step and finite element discretization (5.2). The thickness parameter is smaller than previously, namely  $\varepsilon = 0.04$ . Accordingly, the mesh  $\mathcal{T}_h$  is much finer than in Figure 1. It is a conforming triangulation of a regular polygon with 500 sides;  $\mathcal{T}_h$  has 43256 triangles and 21879 vertices, with  $h_{\min} = 0.0047$  and  $h_{\max} = 0.011$  (4-10 triangles per  $\varepsilon$ ).

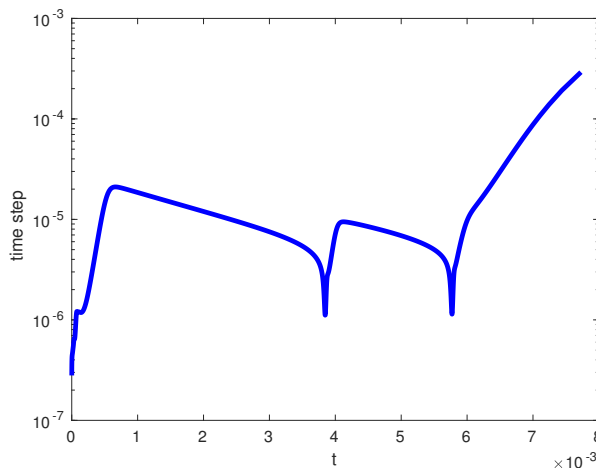


FIGURE 4. Time step vs. time for the 2D secant scheme

In order to reduce the number of iterations, we have used the time step adaptive strategy described in [51, Algorithm 1]. The idea is to combine the second-order secant scheme with a first order scheme in order to estimate the error due to the time discretization. The first-order scheme here is Eyre's convex splitting (4.17), which is unconditionally energy stable. The values for the safety coefficient  $\rho$  and the tolerance  $tol$  are the same as in [51, Equation (29)], that is  $\rho = 0.9$  and  $tol = 10^{-3}$ . The maximum value of the time step is 0.1. At every iteration, the two nonlinear

systems associated to the secant scheme and to Eyre's scheme are solved by a Newton algorithm.

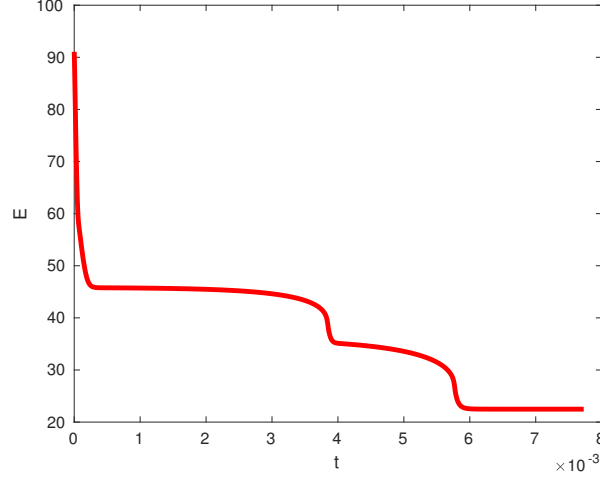


FIGURE 5. Energy vs. time for the 2D secant scheme

We start with a uniformly distributed random initial value with mean value close to 0.3 and amplitude 1, which is regularized by a few steps of Eyre's algorithm, so that the initial state takes values in the interval  $[-0.82, 0.65]$ . As shown in Figure 4, the time step  $\tau_n$  varies between  $10^{-7}$  and  $10^{-3}$  for  $t < 8 \times 10^{-3}$ . Once the steady state is reached numerically (around time  $t = 0.01$ ), the time step rapidly reaches its maximum value 0.1 and remains equal to 0.1 thereafter. The time step adaptive strategy results in a huge gain in the computational time. The energy ( $\mathcal{E}(u_h^n)$ ) is nonincreasing with respect to time (Figure 5), as predicted. The mean value  $\langle u_h^n \rangle$  remains constant and equal to 0.300197.

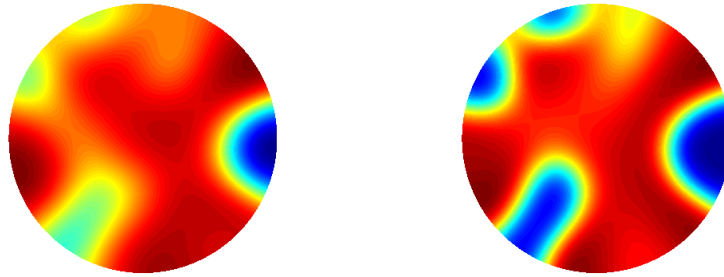
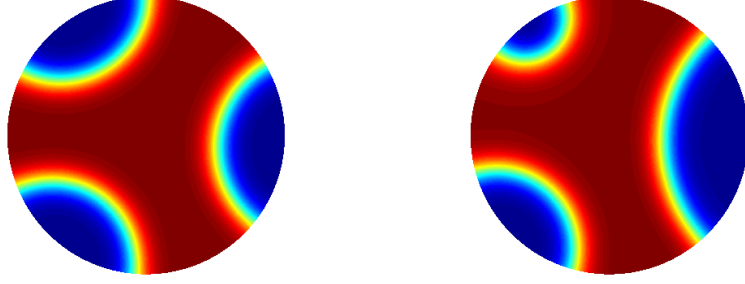
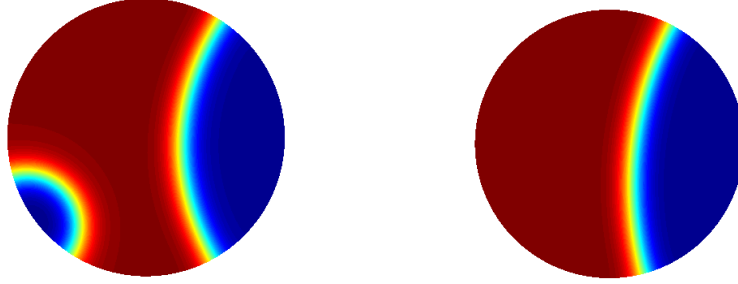


FIGURE 6. Time  $t = 0.03 \cdot 10^{-5}$  (left) and  $t = 2.3 \cdot 10^{-5}$  (right)

The iterates of the solution  $u_h^n$  are presented in Figures 6-8. The solution converges to a steady state, as proved in Theorem 5.6. By the Modica-Mortola theorem [95, 96], the interface of the steady state is an approximation of an arc. The minimum value of the final state is equal to  $-1.007$  and its maximum value is  $0.993$  (see Remark 2.1).

FIGURE 7. Time  $t = 40 \cdot 10^{-5}$  (left) and  $t = 357 \cdot 10^{-5}$  (right)FIGURE 8. Time  $t = 532 \cdot 10^{-5}$  (left) and steady state (right). The thickness parameter  $\varepsilon$  is equal to 0.04.

**6.2. 3D finite difference simulations.** We show numerical simulations for the finite difference linear IMEX scheme (5.7) on the unit cube  $\Omega = (0, 1)^3$ . At each iteration, the linear system is solved by a Fourier-spectral space discretization of the differential operators (Discrete Cosine Transform) and the parallelization strategy is based on a slab decomposition which is the same as in [104]. The thickness parameter is set to  $\varepsilon = 0.04$  and the fixed time step is  $\tau = 10^{-7}$ . The mesh step is  $h = 1/256$  with  $257^3 \approx 17 \times 10^6$  degrees of freedom (see (3.25)-(3.26)), allowing typically 10 points per  $\varepsilon$ . The initial value is a uniformly distributed random variable in the interval  $[-0.06, 0.06]$ .

The mass of the iterates remains equal to 0 up to  $\pm 10^{-16}$ , that is up to double precision accuracy. The minimum and maximum value of the iterates ( $U^n$ ) of the discrete solution over all iterations  $n$  are equal to  $-1.052$  and  $+1.042$  respectively. In particular, they are outside the interval  $[-1, 1]$ , in agreement with Remark 2.1. Moreover, since the values of ( $U^n$ ) remain in the interval  $[-1.06, 1.06]$ , we may choose  $K = 1.06$  in the definition (4.19) of the modified potential  $F_K$ . For this particular solution,  $F_K$  coincides with  $F$  and the stability restriction on the time step reads

$$\tau \leq 4\varepsilon^4/L^2 = 1.8 \cdot 10^{-6}.$$

It is satisfied for our choice  $\tau = 10^{-7}$ . Thus, we have performed the numerical simulation with  $F$  instead of  $F_K$ , because it is much faster. In fact, for the choice  $\tau = 10^{-7}$  and  $\varepsilon = 0.04$  and for other trials of the initial condition with values in

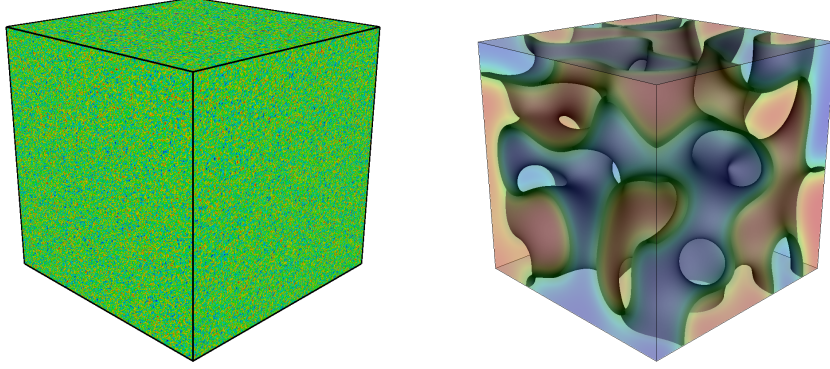


FIGURE 9. Time  $t = 0$  (left) and  $t = 2 \cdot 10^{-5}$  (right)

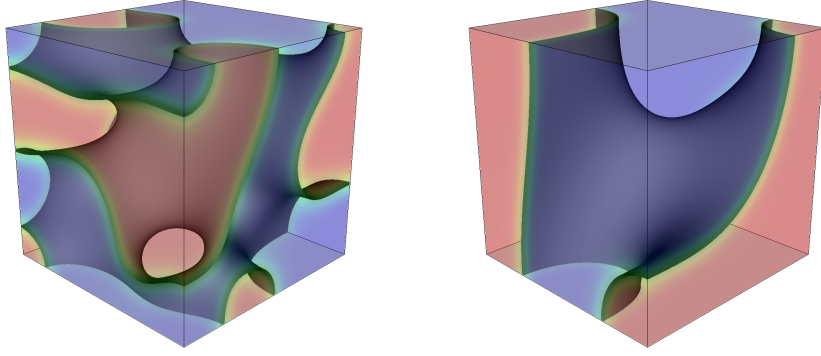


FIGURE 10. Time  $8 \cdot 10^{-5}$  (left) and  $t = 36 \cdot 10^{-5}$  (right)

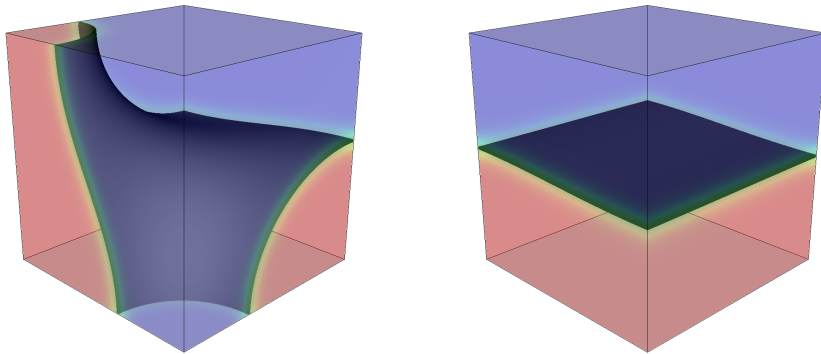


FIGURE 11. Time  $875 \cdot 10^{-5}$  (left) and steady state (right). The thickness parameter  $\varepsilon$  is equal to 0.04.

$[-1, 1]$ , we never observed any blow-up with the quartic potential  $F$  instead of  $F_K$ . A strategy to deal with the cubic nonlinearity has recently been proposed in [83].

Several iterates are represented in Figures 9-11. In the final state (which is chosen as the solution at time  $t = 1875 \times 10^{-5}$ ), the two phases are completely separated by a horizontal plane which has a thickness close to  $\varepsilon = 0.04$ . The minimum and maximum value of the numerical final state are equal to  $-1.001$  and  $+1.001$  respectively.

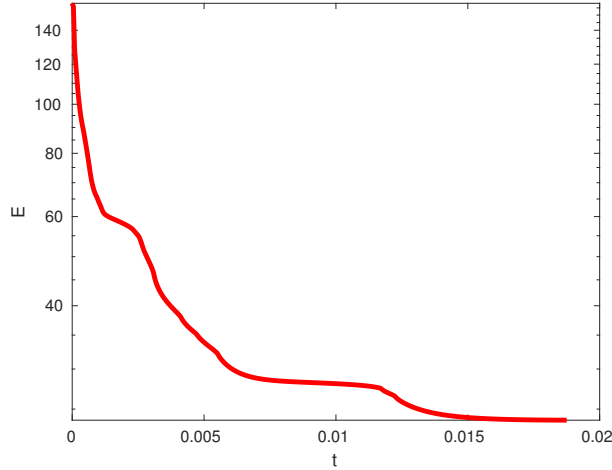


FIGURE 12. Energy vs. time for 3D linear IMEX scheme

In Figure 12, the energy decreases with respect to time, as predicted by the stability analysis.

## 7. CONCLUSION AND PERSPECTIVES

**7.1. Generalization to other Cahn-Hilliard equations.** Most of the convergence results proved above also hold if we replace the double-well polynomial potential  $F(s)$  by a suitable analytic potential with  $H^1$  subcritical growth, as in [8]. The potential may also depend on the variable  $x$  [114]. We can also replace the Neumann boundary conditions (1.2) by periodic boundary conditions or Dirichlet boundary conditions. For Dirichlet boundary conditions, the mass is no longer preserved, but the analysis is generally easier because the Laplace operator is invertible from  $H_0^1(\Omega)$  into its dual. Some types of dynamic boundary conditions which preserve a gradient-like flow structure at the continuous and discrete level are also possible [29, 31, 68, 97, 98, 102].

If we consider the Cahn-Hilliard equation with a logarithmic potential, the situation is more complex. In [1], Abels and Wilke proved that a solution converges to a steady state. In particular, they proved a separation property: a solution remains bounded away from the pure states  $\pm 1$ . The Cahn-Hilliard equation with logarithmic potential and a degenerate mobility is even more difficult (see [41] and [92, Section 4.5]). To the best of our knowledge, there is no proof that solutions converge to an equilibrium in this case.

The numerical analysis and simulations of the Cahn-Hilliard equation with logarithmic nonlinearity can be found, e.g., in [12, 13, 26, 35, 51]. It could be interesting to address the question of convergence to equilibrium in these situations. The Cahn-Hilliard equation with logarithmic potential and dynamic boundary conditions could

also be investigated. In this case, the separation property does not hold any more [94] (see also [28, 82] for a Caginalp system and [110] for an Allen-Cahn-Gurtin equation).

**7.2. Gradient-like PDEs with inertial term.** The convergence result of Simon [121] has been adapted to a huge number of PDEs with a gradient-like structure. We focus here on the damped wave equation, pointed out in the review [67]. It reads

$$\partial_{tt}u + \alpha \partial_t u - \Delta u + \frac{1}{\varepsilon^2}(u^3 - u) = 0, \quad x \in \Omega, \quad t > 0, \quad (7.1)$$

where  $\alpha > 0$ , with Dirichlet or Neumann boundary conditions. If  $d = 1$  or  $2$ , then convergence to equilibrium holds [67, 76]. If  $d = 3$ , this case is critical, but it is possible to have an analytic nonlinearity with subcritical growth. The PDE (7.1) can be seen as an Allen-Cahn equation with inertial term. Convergence to a steady state for space and/or time discretizations of (7.1) has been studied in [6, 55, 66, 111] by means of a Łojasiewicz inequality (see also [70] for a nonlocal damping). Related PDEs have also been considered, such as the Cahn-Hilliard equation with inertial term [54, 57] or the modified phase-field crystal equation [56, 58].

If we consider the time semidiscretization of (7.1), a first-order approximation has been considered in [111]. However, we have the following

**Question 5.** Is it possible to find a second-order time semidiscretization of (7.1) which is energy stable and such that every sequence generated by the scheme converges to a steady state ?

In contrast to what happens for gradient flows,  $k$ -step BDF schemes with  $k \geq 2$  do not seem to preserve the gradient-like flow structure for (7.1). A second-order energy stable SAV scheme was considered in [19], but the steady state equation is modified by the auxiliary variable, as in Section 4.5.

**7.3. Conclusion.** We have reviewed energy stable methods for time and space discretizations of the Cahn-Hilliard equation, with a focus on the asymptotic behaviour of solutions. In many cases, it is possible to prove that every solution converges to a steady state. Some questions are still challenging, in particular for the time semidiscrete problem (cf. Questions 1-5).

As pointed out in [2, 93], the Łojasiewicz-Simon inequality can be used to prove the stability of local minimizers. This was shown for perturbations with respect to the time discretization in [90, Proposition 2.6] and [6, Theorem 2.12], but it seems out of reach for perturbations with respect to the space discretization. In fact, single trajectories are generally not very robust objects with respect to perturbations, and in this regard, it is generally best to consider global dynamics and attractors (see, e.g., [123, 124, 128]). The stability of the global attractor as the time step or the mesh step tends to 0 has been considered, e.g., in [11, 42, 43, 116], for discretized Allen-Cahn or Cahn-Hilliard equations. Exponential attractors have also been explored in [37, 86, 107, 108]. These aspects could be further investigated. In particular, it is not clear how Crank-Nicolson type schemes or SAV schemes behave in this matter. Other fascinating aspects of the dynamics such as the coarsening process [22, 23, 80, 113] could also be analyzed for discretized Cahn-Hilliard type equations.



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