Numer. Math. 63, 39–65 (1992)

Numerische Mathematik
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Numerical analysis of the Cahn-Hilliard equation with a logarithmic free energy

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Received September 21, 1991

Summary. A fully discrete finite element method for the Cahn-Hilliard equation with a logarithmic free energy based on the backward Euler method is analysed. Existence and uniqueness of the numerical solution and its convergence to the solution of the continuous problem are proved. Two iterative schemes to solve the resulting algebraic problem are proposed and some numerical results in one space dimension are presented.

Mathematics Subject Classification (1991): 65M60

1 Introduction

We shall consider the numerical approximation of the Cahn-Hilliard equation

(1.1a) $$u_t = \Delta w \quad x \in \Omega, t > 0 ,$$

(1.1b) $$w = \Psi'(u) - \gamma \Delta u \quad x \in \Omega, t > 0 ,$$

subject to the initial condition

(1.1c) $$u(x, 0) = u_0(x) \quad x \in \Omega$$

and boundary conditions

(1.1d) $$\nabla u \cdot n = \nabla w \cdot n = 0 \quad x \in \partial\Omega, t > 0$$

with $\Psi\colon [-1, 1] \to \mathbb{R}$ given by

(1.2) $$\Psi(u) = \frac{\theta}{2}[(1 + u)\ln(1 + u) + (1 - u)\ln(1 - u)] - \frac{\theta_c}{2}u^2 .$$

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Here γ, θ and θ_c are positive constants with $\theta < \theta_c$ and Ω is a bounded domain in $\mathbb{R}^d$, $d \leqq 3$, with smooth or convex Lipschitz boundary $\partial\Omega$. It follows that Ψ has a double-well form with minima at β and $-\beta$ where β is the positive root of

$$\frac{1}{\beta}\ln\left(\frac{1+\beta}{1-\beta}\right) = \frac{2\theta_c}{\theta}.$$

The points β and $-\beta$ are called binodal points and the region where $\Psi'' < 0$, $(-u_s, u_s)$, is called the spinodal interval. Since, for $|u| < 1$,

$$\Psi''(u) = \frac{\theta}{1-u^2} - \theta_c ,$$

we find that

$$u_s = \left(1 - \frac{\theta}{\theta_c}\right)^{1/2} .$$

Equation 1.1 was proposed by Cahn and Hilliard [3] to model phase separation in a binary mixture composed of species A and B which is quenched into an unstable state. Here u represents the local concentration of the species, that is, $u = X_B - X_A$, $|u| \leqq 1$, where X_A and X_B, $0 \leqq X_A, X_B \leqq 1$, $X_A + X_B = 1$, are the mass fractions of the components in the mixture, and the mean concentration u_m of the mixture is a conserved quantity.

When the quench is shallow, that is θ is close to θ_c, near $u = 0$, $\dfrac{1}{1-u^2} \approx 1 + u^2$ and this leads to the usual approximation of the free energy as a quartic polynomial in the concentration. We remark that in contrast with the quartic approximation the derivatives of the free energy defined by (1.2) become unbounded at -1 and 1.

The mathematics literature has concentrated on the quartic free energy. For a review we refer to Elliott [9] and Temam [20]. Numerical simulations are reported on in (for example) [5], [7], [10] and [19]. See also [8], [11] and [12] for the numerical analysis.

However when the quench is deep i.e. $\theta \ll \theta_c$ the form of the free energy is not at all like a polynomial. The spinodal points $\pm u_s$ are close to the singular points ± 1. Indeed Oono and Puri [17] suggested a well with infinite walls for modelling the deep quench limit. See [1, 2] for a mathematical and numerical analysis. It has been proved by Elliott and Luckhaus [13] that as $\theta/\theta_c \to 0$ the weak solution of the Cahn-Hilliard equation with the free energy given by (1.2) converges to the free boundary limit problem studied by Blowey and Elliott [1, 2]. Furthermore explicit schemes used by metallurgists can easily predict concentration values outside the interval $[-1, 1]$. This causes overflow at the next time step. Thus we are lead to study the mathematical and numerical analysis of (1.1) with the free energy (1.2). It should also be useful in the analysis of multicomponent diffusion with capillarity where models of the free energy based on formula (1.2) are used to determine the complex phase diagrams (see [16] for example).

We write

$$\Psi(u) = \psi_0(u) - \frac{\theta_c}{2}u^2 \quad |u| \leqq 1$$

and set

$$\phi(u) = \psi_0'(u) = \frac{\theta}{2}\ln\left(\frac{1+u}{1-u}\right) \quad |u| < 1 .$$

The following result concerning existence of a unique solution was proved by Elliott and Luckhaus [13].

Theorem 1.1. *Given $u_0 \in H^1(\Omega)$ and $\delta \in (0, 1)$ such that $\|u_0\|_\infty \leqq 1$ and $\frac{1}{|\Omega|}|\int_\Omega u_0| < 1-\delta$ then there exists a unique solution $\{u, w\}$ such that $u(\cdot, 0) = u_0(\cdot)$ and*

$$\begin{aligned} u &\in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H^2(\Omega)) \cap C([0, T]; L^2(\Omega)) , \\ u_t &\in L^2(0, T; H^1(\Omega))') , \\ \sqrt{t}u_t &\in L^2(0, T; H^1(\Omega)) , \\ \sqrt{t}w &\in L^\infty(0, T; H^1(\Omega)) \\ \sqrt{t}\phi(u) &\in L^\infty(0, T; L^2(\Omega)) , \end{aligned}$$

satisfying, for all $\xi \in C[0, T]$, $\eta \in H^1(\Omega)$,

$$\int_0^T \xi(t)\left(\frac{d}{dt}\langle u, \eta\rangle + (\nabla w, \nabla\eta)\right)dt = 0 , \tag{1.3a}$$

$$\int_0^T \xi(t)((w - \phi(u) + \theta_c u, \eta) - \gamma(\nabla u, \nabla\eta))\, dt = 0 \tag{1.3b}$$

with $|u| \leqq 1$ a.e..

We remark that the assumptions on u_0 allow initial data with values 1 and -1 in regions of non-zero measure and that Eqs. (1.3) make sense because $\sqrt{t}w \in L^\infty(0, T; H^1(\Omega))$ and $\sqrt{t}\phi(u) \in L^\infty(0, T; L^2(\Omega))$. This latter estimate for $\phi(u)$ means that $|u|$ cannot take the value 1 on sets of non-zero measure.

In the one dimensional case, it results from the Sobolev imbedding theorem that, for all $t > 0$, $w(\cdot, t)$ is continuous and $\|w(\cdot, t)\|_\infty \leqq C$. Letting $\tilde{x}(t)$ denote the point of maximum of u at time $t > 0$ it follows that $\gamma u''(\tilde{x}) \leqq 0$ and

$$\Psi'(u(\tilde{x})) - w(\tilde{x}) \leqq 0 .$$

Thus

$$\phi(u(\tilde{x})) \leqq C_1$$

and

$$u(\tilde{x}) < 1 .$$

A similar argument using the point of minimum of u and the fact that $-\phi(u) = \phi(-u)$ yields

$$\|u\|_\infty < 1 \quad \forall t > 0 .$$

Let Ω be a convex polygonal domain and $\mathscr{T}^h$ a quasi-uniform family of triangulations of Ω, $\Omega = \bigcup_{\tau\in\mathscr{T}^h}\tau$, with mesh size h. Let $S^h \subset H^1(\Omega)$ be the finite element space of continuous functions on $\bar{\Omega}$ which are linear on each $\tau \in \mathscr{T}^h$. Denote by $\{x_i\}_{i=1}^{N^h}$ the set of nodes of $\mathscr{T}^h$ and let $\{\chi_i\}_{i=1}^{N^h}$ be the basis for S^h defined by $\chi_i(x_j) = \delta_{ij}$.

We indicate by $(\cdot, \cdot)^h$ the discrete inner product: $\forall\chi, \eta \in C(\bar{\Omega})$

$$(\chi, \eta)^h = \int_\Omega I^h(\chi\eta)\, dx = \sum_{i=1}^{N^h} m_i\chi(x_i)\eta(x_i) ,$$

where $I^h: C(\bar{\Omega}) \to S^h$ is the interpolant defined by $I^h\chi(x_i) = \chi(x_i)$ for $i = 1, \ldots, N^h$ and $m_i = (\chi_i, \chi_i)^h \cdot |\cdot|_h = ((\cdot,\cdot)^h)^{1/2}$ is a norm on S^h which satisfies (see [6]) $\forall \chi, \eta \in S^h$

$$C_0 \|\chi\| \leqq |\chi|_h \leqq C_1 \|\chi\| , \tag{1.4}$$

$$|(\chi, \eta) - (\chi, \eta)^h| \leqq Ch^{1+r} \|\chi\|_r \|\eta\|_1 \quad r = 0, 1 , \tag{1.5}$$

where the constants are independent of h. The Poincaré inequality

$$\|\chi\| \leqq \tilde{C}_P(|\chi|_1 + |(\chi, 1)|) \quad \forall \chi \in H^1(\Omega)$$

together with (1.4) and (1.5) yields the discrete Poincaré inequality, for h sufficiently small,

$$\|\chi\|_h \leqq C_P(|\chi|_1 + |(\chi, 1)|_h) \quad \forall \chi \in S^h \tag{1.6}$$

with C_P a constant independent of h.

If we assume that $\mathcal{T}^h$ is acute, that is the angles of the triangles, in the case $d = 2$, are less than or equal to $\pi/2$ and, in the case $d = 3$, the angle made by any two faces of any tetrahedron is bounded by $\pi/2$, then, if $\alpha \in W^{1,\infty}(\mathbb{R})$ satisfies $\alpha(0) = 0$ and $0 \leqq \alpha'(s) \leqq L_\alpha < \infty$ for a.e. $s \in \mathbb{R}$, we have (see [6], [18])

$$\|\nabla I^h \alpha(\chi)\|^2 \leqq L_\alpha(\nabla \chi, \nabla I^h \alpha(\chi)) \quad \forall \chi \in S^h , \tag{1.7}$$

Let $G^h: S_0^h \to S_0^h$ be the discrete Green's operator defined by

$$(\nabla G^h v, \nabla \chi) = (v, \chi)^h \quad \forall \chi \in S^h , \tag{1.8}$$

where $S_0^h = \{\chi \in S^h: (\chi, 1)^h = 0\}$. The existence and uniqueness of $G^h v$ follows from the Lax-Milgram theorem and the Poincaré inequality (1.6).

Writing

$$|\chi|_{-h}^2 \stackrel{\text{def}}{=} |G^h \chi|_1^2$$

it follows from (1.8) that

$$|\chi|_{-h}^2 = (G^h \chi, \chi)^h = (\chi, G^h \chi)^h .$$

Finally, let us introduce the H^1-projection, $R^h: H^1(\Omega) \to S^h$, defined by

$$(\nabla R^h v, \nabla \chi) = (\nabla^v, \nabla \chi) \quad \forall \chi \in S^h ,$$

$$(R^h v, 1) = (v, 1) .$$

It holds that $R^h v \to v$ in $H^1(\Omega)$ strongly and $|R^h v|_1 \leqq |v|_1$.

An outline of the contents of this paper is as follows. In Sect. 2 we introduce the discrete finite element method for the problem and prove existence, uniqueness and stability estimates for its solution. Convergence to the solution of the continuous problem is proved in Sect. 3. In Sect. 4 we present two iterative methods that can be used to solve the algebraic problem resulting from the numerical approximation. The results of numerical experiments are presented in Sect. 5.

2 Numerical approximation

Let $k = T/N$ denote the time step where N is a given positive integer. The finite element approximation to (1.1) is to find U^n, $W^n \in S^h$, $n = 1, 2, \ldots, N$, such that $\forall \chi \in S^h$

$$(\partial U^n, \chi)^h + (\nabla W^n, \nabla \chi) = 0 , \tag{2.1a}$$

$$(W^n, \chi)^h = (\Psi'(U^n), \chi) + \gamma(\nabla U^n, \nabla \chi) , \tag{2.1b}$$

with $U^0 = u_0^h$, where u_0^h is some approximation of u_0 in S^h, and

$$\partial Z^n \equiv \frac{Z^n - Z^{n-1}}{k}$$

for a given sequence $\{Z^n\}_{n=0}^N$.

We observe that for $(\Psi'(U^n), \chi)^h$ to have a meaning it is necessary that $|U^n(x_i)| < 1$ for each node x_i and this is equivalent to $\| U^n \|_\infty < 1$.

Remark. Our analysis requires the condition $k < 4\gamma/\theta_c^2$. This is a consequence of the non-convexity of the free energy. Even though it is independent of the spatial mesh this condition is restrictive because $\gamma \ll 1$. One might hope to develop stable implicit schemes which allow large time steps when appropriate. However for these non-convex nonlinear partial differential equations this is as yet unrealised.

Theorem 2.1. *Suppose that* $k < \dfrac{4\gamma}{\theta_c^2}$ *and* $u_0^h \in S^h$ *satisfies* $1/|\Omega| \int_\Omega u_0^h| < 1 - \delta$, $\| u_0^h \|_\infty \leqq 1$. *Then there exists a unique solution* $\{U^n, W^n\}$ *to* (2.1) *satisfying* $\| U^n \|_\infty < 1$ *for each* $n \geqq 1$.

Proof. Uniqueness. Let $\{U_1^n, W_1^n\}$ and $\{U_2^n, W_2^n\}$ be two solutions of (2.1) and set $z^u = U_1^n - U_2^n$ and $z^w = W_1^n - W_2^n$. It follows that z^u and z^w satisfy

$$(z^u, \chi)^n + k(\nabla z^w, \nabla \chi) = 0 , \tag{2.2a}$$

$$(z^w, \chi)^h = (\Psi'(U_1^n) - \Psi'(U_2^n), \chi)^h + \gamma(\nabla z^u, \nabla \chi) . \tag{2.2b}$$

Taking $\chi = z^w$ in (2.2a) and $\chi = z^u$ in (2.2b) and subtracting the resulting equations yields

$$k|z^w|_1^2 + \gamma|z^u|_1^2 = (\Psi'(U_2^n) + \Psi'(U_1^n), z^u)^h .$$

Since

$$(\Psi'(r_2) - \Psi'(r_1))(r_1 - r_2) = -\Psi''(\xi)(r_2 - r_1)^2 \leqq \theta_c(r_2 - r_1)^2$$

it follows that

$$(\Psi'(U_2^n) - \Psi'(U_1^n), z^u)^h \leqq \theta_c |z^u|_h^2 .$$

Using equation (2.2a) with $\chi = z^u$ we obtain

$$k|z^w|_1^2 + \gamma|z^u|_1^2 \leqq \theta_c (z^u, z^u)^h \leqq k\frac{\theta_c^2}{4}|z^u|_1^2 + k|z^w|_1^2 .$$

Thus

$$\left(\gamma - k\frac{\theta_c^2}{4}\right)|z^u|_1^2 \leqq 0$$

and, since $(z^u, 1)^h = 0$, the Poincaré inequality (1.6) implies that $|z^u|_h = 0$. This concludes the proof of uniqueness.

Existence. Following the work of Elliott and Luckhaus [13] existence of a solution will be obtained by considering a regularized problem.

For $\varepsilon > 0$, ε small, we define

$$\tilde{\phi}_\varepsilon(u) = \Psi'_\varepsilon(u) + \theta_c u ,$$

$$\phi_\varepsilon(u) = \max\{-\phi(1-\varepsilon), \min\{\phi(u), \phi(1-\varepsilon)\}\} ,$$

$$\beta_\varepsilon(u) = \max\{-1+\varepsilon, \min\{u, 1-\varepsilon\}\} ,$$

where $\Psi_\varepsilon \in C^1(\mathbb{R})$,

$$\Psi_\varepsilon(u) = \begin{cases} \psi_0(1-\varepsilon) - \frac{\theta_c}{2}(1-\varepsilon)^2 + \varepsilon\tau_\varepsilon + \tau_\varepsilon(u-1) & u > 1-\varepsilon \\ \Psi(u) & |u| \leqq 1-\varepsilon \\ \psi_0(-1+\varepsilon) - \frac{\theta_c}{2}(-1+\varepsilon)^2 + \varepsilon\tau_\varepsilon - \tau_\varepsilon(u+1) & u < -1+\varepsilon , \end{cases}$$

and

$$\tau_\varepsilon = \phi(1-\varepsilon) - \theta_c(1-\varepsilon) = \frac{\theta}{2}\ln\left(\frac{2-\varepsilon}{\varepsilon}\right) - \theta_c(1-\varepsilon) .$$

We shall consider the regularized problem: find $U_\varepsilon^n, W_\varepsilon^n \in S^h$, $n = 1, 2, \ldots, N$, such that $\forall \chi \in S^h$

(2.3a) $$(\partial U_\varepsilon^n, \chi)^h + (\nabla W_\varepsilon^n, \nabla\chi) = 0 ,$$

(2.3b) $$(W_\varepsilon^n, \chi)^h = (\Psi'_\varepsilon(U_\varepsilon^n), \chi)^h + \gamma(\nabla U_\varepsilon^n, \nabla\chi) ,$$

(2.3c) $$U_\varepsilon^0 = u_0^h .$$

Note that $\tau_\varepsilon > 0$ for ε sufficiently small, ϕ is monotone increasing since $\phi' > 0$,

$$\psi_0(u) \geqq 0 \qquad |u| \leqq 1 ,$$

$$\Psi(u) \geqq -\frac{\theta_c}{2} \qquad |u| \leqq 1 ,$$

$$\Psi_\varepsilon(u) \geqq -\frac{\theta_c}{2} \qquad \forall u ,$$

$$\Psi''_\varepsilon(u) \geqq -\theta_c \qquad \forall u$$

and

$$\tilde{\phi}_\varepsilon(u) = \begin{cases} \tau_\varepsilon + \theta_c u & u > 1-\varepsilon \\ \phi(u) & |u| \leqq 1-\varepsilon \\ -\tau_\varepsilon + \theta_c u & u < -1+\varepsilon . \end{cases}$$

That $\psi_0(u) \geqq 0$ for $|u| \leqq 1$ follows from the fact that $\psi_0(0) = 0$ and the form of $\psi'_0 = \phi$. Figure 1 shows the graphs of Ψ, Ψ_ε, ϕ and $\tilde{\phi}_\varepsilon$.

Following Elliott [9] the existence of a solution to (2.3) can be shown by considering the minimization problem: find $U \in K^h$ such that

$$\mathscr{F}^h(U) = \min_{\chi \in K^h} \mathscr{F}^h(\chi) \tag{2.4}$$

where

$$\mathscr{F}^h(\chi) = (\Psi_\varepsilon(\chi), 1)^h + \frac{\gamma}{2}|\chi|_1^2 + \frac{1}{2k}|\chi - U_\varepsilon^{n-1}|_{-h}^2 ,$$

$$K^h = \{\chi \in S^h, (\chi, 1)^h = (u_0^h, 1)^h\} .$$

It follows from the definition of $\mathscr{F}^h$ that $\mathscr{F}^h$ is bounded below in K^h,

$$\mathscr{F}^h(\chi) \geqq -\frac{\theta_c}{2}|\Omega| + \frac{\gamma}{2}|\chi|_1^2 \geqq -\frac{\theta_c}{2}|\Omega| .$$

Let $d = \inf_{K^h} \mathscr{F}^h(\chi)$ and $\{\chi_n\}$ be a minimizing sequence of $\mathscr{F}^h$ in K^h, that is $\lim_{n\to\infty} \mathscr{F}^h(\chi_n) = d$. It results from the above estimate and the discrete Poincaré inequality (1.6) that $\{\chi_n\}$ is bounded in $H^1(\Omega)$. As a consequence, recalling that K^h is finite dimensional, there exists $U \in S^h$ and a subsequence $\{\chi_n\}$ such that

$$\chi_n \to U \quad \text{in } S^h .$$

Since K^h is closed, $U \in K^h$, and the continuity of $\mathscr{F}^h$ yields $\mathscr{F}^h(\chi_n) \to \mathscr{F}^h(U) = d$. Therefore, there exists a solution U to (2.4). By the calculus of variations, the minimizer U satisfies $\forall \chi \in S^h$

$$\gamma(\nabla U, \nabla \chi) + (\Psi_\varepsilon'(U), \chi)^h + \left(G^h\left(\frac{U - U_\varepsilon^{n-1}}{k}\right), \chi\right)^h - \lambda(1, \chi)^h = 0$$

where $\lambda = \dfrac{(\Psi_\varepsilon'(U), 1)^h}{|\Omega|}$ is a Lagrange multiplier. Defining

$$U_\varepsilon^n = U, \qquad W_\varepsilon^n = \lambda - G^h(\partial U_\varepsilon^n)$$

it follows that $\{U_\varepsilon^n, W_\varepsilon^n\}$ is a solution to (2.3).

We shall now proceed to obtain estimates on U_ε^n and W_ε^n, independent of ε, in order to pass to the limit.

Lemma 2.1. *The following stability estimates hold*

$$(\Psi_\varepsilon(U_\varepsilon^n), 1)^h + \frac{k}{2}\sum_{i=1}^{n} |W_\varepsilon^i|_1^2 + \frac{k^2}{2}\left(\gamma - \frac{k\theta_c^2}{4}\right)\sum_{i=1}^{n} |\partial U_\varepsilon^i|_1^2 + \frac{\gamma}{2}|U_\varepsilon^n|_1^2 \leqq C . \tag{2.5}$$

Proof. Choosing $\chi = W_\varepsilon^n$ in (2.3a) and $\chi = \partial U_\varepsilon^n$ in (2.3b) and subtracting the resulting equations we obtain

$$k|W_\varepsilon^n|_1^2 = -(\Psi_\varepsilon'(U_\varepsilon^n), U_\varepsilon^n - U_\varepsilon^{n-1})^h - \gamma(\nabla U_\varepsilon^n, \nabla U_\varepsilon^n - \nabla_\varepsilon^{n-1})$$

Defining $\tilde{\Psi}_\varepsilon(u) = \Psi_\varepsilon(u) + \dfrac{\theta_c}{2}u^2$ and noting that $\tilde{\Psi}_\varepsilon$ is convex we find that

$$\begin{aligned} -\Psi_\varepsilon'(r)(r-s) &= \tilde{\Psi}_\varepsilon'(r)(s-r) - \theta_c r(s-r) \\ &\leqq \tilde{\Psi}_\varepsilon(s) - \tilde{\Psi}_\varepsilon(r) - \theta_c r(s-r) \\ &\leqq \Psi_\varepsilon(s) - \Psi_\varepsilon(r) + \frac{\theta_c}{2}(r-s)^2 \end{aligned}$$

which implies

$$-(\Psi'_\varepsilon(U^n_\varepsilon), U^n_\varepsilon - U^{n-1}_\varepsilon)^h \leqq (\Psi_\varepsilon(U^{n-1}_\varepsilon) - \Psi_\varepsilon(U^n_\varepsilon), 1)^h + \frac{\theta_c}{2}|U^n_\varepsilon - U^{n-1}_\varepsilon|^2_h$$

which yields

$$k|W^n_\varepsilon|^2_1 + k^2\frac{\gamma}{2}|\partial U^n_\varepsilon|^2_1 + k\frac{\gamma}{2}\partial(|U^n_\varepsilon|^2_1 \leqq (\Psi_\varepsilon(U^{n-1}_\varepsilon) - \Psi_\varepsilon(U^n_\varepsilon), 1)^h + k^2\frac{\theta_c}{2}|\partial U^n_\varepsilon|^2_h .$$

Taking $\chi = \partial U^n_\varepsilon$ in (2.3a) gives

$$\begin{aligned} |\partial U^n_\varepsilon|^2_h &= -(\nabla W^n_\varepsilon, \nabla \partial U^n_\varepsilon) \\ &\leqq \frac{1}{k\theta_c}|W^n_\varepsilon|^2_1 + \frac{k\theta_c}{4}|\partial U^n_\varepsilon|^2_1 . \end{aligned}$$

Hence

$$(\Psi_\varepsilon(U^n_\varepsilon) - \Psi_\varepsilon(U^{n-1}_\varepsilon), 1)^h + \frac{k}{2}|W^n_\varepsilon|^2_1 + \frac{k^2}{2}\left(\gamma - \frac{k\theta_c^2}{4}\right)|\partial U^n_\varepsilon|^2_1 + k\frac{\gamma}{2}\partial(|U^n_\varepsilon|^2_1) \leqq 0 .$$

Summing over n and observing that $\|u^h_0\|_\infty \leqq 1$ it results that, for ε sufficiently small,

$$\begin{aligned} &(\Psi_\varepsilon(U^n_\varepsilon), 1)^h + \frac{k}{2}\sum_{i=1}^n |W^i_\varepsilon|^2_1 + \frac{k^2}{2}\left(\gamma - \frac{k\theta_c^2}{4}\right)\sum_{i=1}^n |\partial U^i_\varepsilon|^2_1 + \frac{\gamma}{2}|U^n_\varepsilon|^2_1 \\ &\leqq (\Psi_\varepsilon(u^h_0), 1)^h + \frac{\gamma}{2}|u^h_0|^2_1 \\ &\leqq |\Omega|(\psi_0(1-\varepsilon) + \varepsilon\tau_\varepsilon) + \frac{\gamma}{2}|u^h_0|^2_1 \\ &\leqq |\Omega|\left(\theta \ln(2) + \varepsilon\frac{\theta}{2}\ln\left(\frac{2-\varepsilon}{\varepsilon}\right)\right) + \frac{\gamma}{2}|u^h_0|^2_1 \\ &\leqq C(u^h_0) . \end{aligned}$$

which is the desired estimate. □

Remark. Recalling that $\Psi_\varepsilon(r) \geqq -\frac{\theta_c}{2}\ \forall r$ and the condition $k < \frac{4\gamma}{\theta_c^2}$ we obtain

$$k\sum_{i=1}^n |W^i_\varepsilon|^2_1 + \sum_{i=1}^n |U^i_\varepsilon - U^{i-1}_\varepsilon|^2_1 + |U^n_\varepsilon|^2_1 \leqq C . \tag{2.6}$$

From (2.5), (2.6) and the Poincaré inequality (1.6) we deduce that

$$|U^n_\varepsilon|_h \leqq C ,$$

$$(\Psi_\varepsilon(U^n_\varepsilon), 1)^h \leqq C ,$$

and the definition of Ψ_ε together with the fact that ψ_0 is positive yields, for ε sufficiently small,

$$\frac{1}{|\Omega|}([U^n_\varepsilon - 1]_+ + [-1 - U^n_\varepsilon]_+, 1)^h < \frac{C}{\tau_\varepsilon}$$

where $[v]_+ \equiv \max\{v, 0\}$. Because

$$\frac{1}{|\Omega|}\int_\Omega ([U_\varepsilon^n - 1]_+ + [-1 - U_\varepsilon^n]_+)\,dx \leqq \frac{1}{|\Omega|}\int_\Omega I^h([U_\varepsilon^n - 1]_+ + [-1 - U_\varepsilon^n]_+)\,dx$$
$$= \frac{1}{|\Omega|}([U_\varepsilon^n - 1]_+ + [-1 - U_\varepsilon^n]_+, 1)^h$$

it follows that

$$\frac{1}{|\Omega|}\int_\Omega ([U_\varepsilon^n - 1]_+ + [-1 - U_\varepsilon^n]_+)\,dx < \frac{C}{\tau_\varepsilon}\,. \tag{2.7}$$

Lemma 2.2. *For $t_n > 0$, where $t_n \equiv nk$, we have*

$$t_n |W_\varepsilon^n|_1^2 + k\sum_{i=1}^n t_i |\partial U_\varepsilon^i|_1^2 \leqq C\,. \tag{2.8}$$

Proof. From Eq. (2.3b) we have

$$(\partial W_\varepsilon^n, \chi)^h = (\partial \Psi_\varepsilon'(U_\varepsilon^n), \chi)^h + \gamma(\nabla \partial U_\varepsilon^n, \nabla \chi)$$
$$= (\partial \tilde{\phi}_\varepsilon(U_\varepsilon^n), \chi)^h - \theta_c(\partial U_\varepsilon^n, \chi)^h + \gamma(\nabla \partial U_\varepsilon^n, \nabla \chi)\,.$$

Taking $\chi = \partial U_\varepsilon^n$ in the above equation and $\chi = \partial W_\varepsilon^n$ in (2.3a) it results

$$(\nabla W_\varepsilon^n, \nabla \partial W_\varepsilon^n) + (\partial \tilde{\phi}_\varepsilon(U_\varepsilon^n), \partial U_\varepsilon^n)^h + \gamma|\partial U_\varepsilon^n|_1^2 = \theta_c |\partial U_\varepsilon^n|_h^2.$$

Using the fact that $\tilde{\phi}_\varepsilon$ is monotone and Eqn. (2.3a) we obtain

$$\frac{1}{2k}|W_\varepsilon^n|_1^2 - \frac{1}{2k}|W_\varepsilon^{n-1}|_1^2 + \frac{1}{2k}|W_\varepsilon^n - W_\varepsilon^{n-1}|_1^2 + \gamma|\partial U_\varepsilon^n|_1^2 \leqq -\theta_c(\nabla W_\varepsilon^n, \nabla \partial U_\varepsilon^n)$$
$$\leqq \frac{\theta_c^2}{2\gamma}|W_\varepsilon^n|_1^2 + \frac{\gamma}{2}|\partial U_\varepsilon^n|_1^2\,.$$

Therefore

$$|W_\varepsilon^n|_1^2 - |W_\varepsilon^{n-1}|_1^2 + k\gamma|\partial U_\varepsilon^n|_1^2 \leqq \frac{k\theta_c^2}{\gamma}|W_\varepsilon^n|_1^2.$$

Multiplying by t_n yields

$$t_n|W_\varepsilon^n|_1^2 - t_{n-1}|W_\varepsilon^{n-1}|_1^2 + kt_n\gamma|\partial U_\varepsilon^n|_1^2 \leqq kT\frac{\theta_c^2}{2\gamma}|W_\varepsilon^n|_1^2 + k|W_\varepsilon^{n-1}|_1^2\,.$$

Summing over n we obtain from (2.6)

$$t_n|W_\varepsilon^n|_1^2 + k\gamma\sum_{i=2}^n t_i|\partial U_\varepsilon^i|_1^2 \leqq C + t_1|W_\varepsilon^1|_1^2\,.$$

Inequality (2.6) with $n = 1$ yields the result. □

Lemma 2.3. *For $t_n > 0$*

$$t_n\left|I^h\phi_\varepsilon(U_\varepsilon^n) - \frac{1}{|\Omega|}\int_\Omega I^h\phi_\varepsilon(U_\varepsilon^n)\,dx\right|_h^2 \leqq C\,. \tag{2.9}$$

Proof. Observing that

$$(\Psi'_\varepsilon(U^n_\varepsilon), \chi)^h = (I^h\phi_\varepsilon(U^n_\varepsilon) - \theta_c I^h\beta_\varepsilon(U^n_\varepsilon), \chi)^h$$

and taking $\chi = I^h\phi_\varepsilon(U^n_\varepsilon) - \frac{1}{|\Omega|}\int_\Omega I^h\phi_\varepsilon(U^n_\varepsilon)\,dx$ in (2.3b) gives

$$\begin{aligned}
&\left(W^n_\varepsilon, I^h\phi_\varepsilon(U^n_\varepsilon) - \frac{1}{|\Omega|}\int_\Omega I^h\phi_\varepsilon(U^n_\varepsilon)\,dx\right)^h \\
&= \left(I^h\phi_\varepsilon(U^n_\varepsilon), I^h\phi_\varepsilon(U^n_\varepsilon) - \frac{1}{|\Omega|}\int_\Omega I^h\phi_\varepsilon(U^n_\varepsilon)\,dx\right)^h \\
&\quad - \theta_c\left(I^h\beta_\varepsilon(U^n_\varepsilon), I^h\phi_\varepsilon(U^n_\varepsilon) - \frac{1}{|\Omega|}\int_\Omega I^h\phi_\varepsilon(U^n_\varepsilon)\,dx\right)^h + \gamma(\nabla U^n_\varepsilon, \nabla I^h\phi_\varepsilon(U^n_\varepsilon))\,.
\end{aligned}$$

The inequality (1.7) implies that $\gamma(\nabla U^n_\varepsilon, \nabla I^h\phi_\varepsilon(U^n_\varepsilon)) \geqq 0$ and the fact that $(\chi, 1)^h = (\chi, 1)\forall\chi\in S^h$ yields

$$\begin{aligned}
\left|I^h\phi_\varepsilon(U^n_\varepsilon) - \frac{1}{|\Omega|}\int_\Omega I^h\phi_\varepsilon(U^n_\varepsilon)\,dx\right|^2_h &\leqq \theta_c\left(I^h\beta_\varepsilon(U^n_\varepsilon), I^h\phi_\varepsilon(U^n_\varepsilon) - \frac{1}{|\Omega|}\int_\Omega I^h\phi_\varepsilon(U^n_\varepsilon)\,dx\right)^h \\
&\quad + \left(W^n_\varepsilon - \frac{1}{|\Omega|}\int_\Omega W^n_\varepsilon\,dx, I^h\phi_\varepsilon(U^n_\varepsilon)\,dx - \frac{1}{|\Omega|}\int_\Omega I^h\phi_\varepsilon(U^n_\varepsilon)\,dx\,dx\right)^h \\
&\leqq C\left(\left|W^n_\varepsilon - \frac{1}{|\Omega|}\int_\Omega W^n_\varepsilon\,dx\right|^2_h + |I^h\beta_\varepsilon(U^n_\varepsilon)|^2_h\right).
\end{aligned}$$

Using the Poincaré inequality (1.6) and recalling the definition of β_ε and the boundedness of $|U^n_\varepsilon|_h$ we deduce that

$$\left|I^h\phi_\varepsilon(U^n_\varepsilon) - \frac{1}{|\Omega|}\int_\Omega I^h\phi_\varepsilon(U^n_\varepsilon)\,dx\right|^2_h \leqq C|W^n_\varepsilon|^2_1 + C$$

and the result follows from (2.8). □

In order to prove the theorem we will need the following lemma which has been proved by Elliott and Luckhaus [13].

Lemma 2.4. *Let $v\in L^1(\Omega)$ such that there exist positive constants δ and δ' satisfying*

$$\left|\frac{1}{|\Omega|}\int_\Omega v\,dx\right| < 1 - \delta\,,$$

$$\frac{1}{|\Omega|}\int_\Omega([v-1]_+ + [-1-v]_+)\,dx < \delta'\,.$$

If $\delta' < \frac{\delta^2}{16}$ then

$$|\Omega^+_\delta| = \left|\left\{x: v(x) > 1 - \frac{\delta}{4}\right\}\right| < \left(1 - \frac{\delta}{4}\right)|\Omega|$$

and

$$|\Omega_\delta^-| = \left|\left\{x\colon v(x) < -1 + \frac{\delta}{4}\right\}\right| < \left(1 - \frac{\delta}{4}\right)|\Omega|\,.$$

Letting $\chi = 1$ in (2.3a) it results that

$$(U_\varepsilon^n, 1)^h = (u_0^h, 1)^h$$

and noting that $(\chi, 1)^h = (\chi, 1)\,\forall\chi\in S^h$ we obtain

$$\left.\frac{1}{|\Omega|}\int_\Omega U_\varepsilon^n\,dx\right| = \frac{1}{|\Omega|}\left|\int_\Omega u_0^h\,dx\right| < 1 - \delta\,.$$

Thus, recalling (2.7), for ε sufficiently small, Lemma 2.4 can be applied for U_ε^n in order to obtain a measure for the sets

$$\left\{x\colon U_\varepsilon^n(x) > 1 - \frac{\delta}{4}\right\},$$

$$\left\{x\colon U_\varepsilon^n(x) < -1 + \frac{\delta}{4}\right\}.$$

Lemma 2.5. *For $t_n > 0$ the a priori estimate is satisfied*

$$t_n\|I^h\phi_\varepsilon(U_\varepsilon^n)\|^2 \leqq C\,.$$

Proof. Using that $I^h\phi_\varepsilon(U_\varepsilon^n) \leqq \max\phi_\varepsilon(U_\varepsilon^n)$ and the monotonicity of ϕ_ε we obtain from Lemma 2.4

$$\frac{1}{|\Omega|}(1, I^h\phi_\varepsilon(U_\varepsilon^n))^h = \frac{1}{|\Omega|}\int_{U_\varepsilon^n \leqq 1-\frac{\delta}{4}} I^h\phi_\varepsilon(U_\varepsilon^n)\,dx + \frac{1}{|\Omega|}\int_{U_\varepsilon^n > 1-\frac{\delta}{4}} I^h\phi_\varepsilon(U_\varepsilon^n)\,dx$$

$$\leqq \phi_\varepsilon\left(1 - \frac{\delta}{4}\right) + \frac{\left(1 - \frac{\delta}{4}\right)^{1/2}}{|\Omega|^{1/2}}\|I^h\phi_\varepsilon(U_\varepsilon^n)\|\,.$$

In the same way we have

$$\frac{1}{|\Omega|}(1, I^h\phi_\varepsilon(U_\varepsilon^n))^h \geqq -\phi_\varepsilon\left(1 - \frac{\delta}{4}\right) - \frac{\left(1 - \frac{\delta}{4}\right)^{1/2}}{|\Omega|^{1/2}}\|I^h\phi_\varepsilon(U_\varepsilon^n)\|\,.$$

Therefore, using that $(a + b)^2 \leqq a^2\left(1 + \frac{8}{\delta}\right) + b^2\left(1 + \frac{\delta}{8}\right)$,

$$\left(\frac{1}{|\Omega|}\int_\Omega I^h\phi_\varepsilon(U_\varepsilon^n)\,dx\right)^2 \leqq \left(1 + \frac{8}{\delta}\right)\left(\phi_\varepsilon\left(1 - \frac{\delta}{4}\right)\right)^2 + \left(1 - \frac{\delta}{8} - \frac{\delta^2}{32}\right)\frac{1}{|\Omega|}\|I^h\phi_\varepsilon(U_\varepsilon^n)\|^2\,. \tag{2.10}$$

Observing that

$$\frac{1}{|\Omega|}\left\| I^h\phi_\varepsilon(U_\varepsilon^n) - \frac{1}{|\Omega|}\int_\Omega I^h\phi_\varepsilon(U_\varepsilon^n)\,dx \right\|^2 = \frac{1}{|\Omega|}\,\|I^h\phi_\varepsilon(U_\varepsilon^n)\|^2 - \left(\frac{1}{|\Omega|}\int_\Omega I^h\phi_\varepsilon(U_\varepsilon^n)\,dx\right)^2$$

it results, from (2.10), that

$$\left(\frac{\delta}{8}+\frac{\delta^2}{32}\right)\frac{1}{|\Omega|}\,\|I^h\phi_\varepsilon(U_\varepsilon^n)\|^2 \leqq \frac{1}{|\Omega|}\left\| I^h\phi_\varepsilon(U_\varepsilon^n) - \frac{1}{|\Omega|}\int_\Omega I^h\phi_\varepsilon(U_\varepsilon^n)\,dx \right\|^2 + \left(1+\frac{8}{\delta}\right)\left(\phi_\varepsilon\left(1-\frac{\delta}{4}\right)\right)^2 .$$

For ε sufficiently small $\phi_\varepsilon\left(1-\frac{\delta}{4}\right) = \phi\left(1-\frac{\delta}{4}\right)$ and (2.9) gives

$$t_n\,\|I^h\phi_\varepsilon(U_\varepsilon^n)\|^2 \leqq C . \quad \Box$$

Lemma 2.5 yields, for h fixed,

$$\|I^h\phi_\varepsilon(U_\varepsilon^n)\|_\infty \leqq C(h, t_n) \quad \text{independently of } \varepsilon$$

and

$$|\phi_\varepsilon(U_\varepsilon^n(x_i))| \leqq C(h, t_n) \quad \text{independently of } \varepsilon .$$

Furthermore, from (2.8) and the discrete Poincaré inequality, we find that $|W_\varepsilon^n|_h$ is bounded independently of ε. The uniform bounds on U_ε^n and W_ε^n imply the existence of subsequences $\{U_\varepsilon^n\}$, $\{W_\varepsilon^n\}$ such that

$$U_\varepsilon^n(x_i) \to U^n(x_i) ,$$

$$W_\varepsilon^n(x_i) \to W^n(x_i) ,$$

for U^n, $W^n \in S^h$.

Let us fix β so that $\phi(1-\beta) > C(h, t_n)$. Since

$$\phi_\varepsilon(r) = \phi(r) \quad \text{for } |r| \leqq 1-\varepsilon ,$$

it follows that for $\varepsilon < \beta$

$$|\phi_\varepsilon(U_\varepsilon^n(x_i))| \leqq C(h, t_n) < \phi(1-\beta) = \phi_\varepsilon(1-\beta) .$$

The monotonicity of $\phi_\varepsilon(\cdot)$ implies that

$$|U_\varepsilon^n(x_i)| \leqq 1-\beta \quad \text{for all } \varepsilon < \beta .$$

Thus $|U^n(x_i)| \leqq 1-\beta$ and $\phi_\varepsilon(U_\varepsilon^n(x_i)) \to \phi(U^n(x_i))$ as $\varepsilon \to 0$.

The existence of a solution to (2.1) is established by passing to the limit as ε goes to zero in (2.3). $\Box$

Theorem 2.2. *The sequences $\{U^n, W^n\}$ generated by (2.1) satisfy the stability estimates*

$$k\sum_{i=1}^{n} |W^i|_1^2 + \sum_{i=1}^{n} |U^i - U^{i-1}|_1^2 + |U^n|_1^2 \leqq C ,$$

$$t_n\,\|I^h\phi(U^n)\|^2 + t_n\,|W^n|_1^2 + k\sum_{i=1}^{n} t_i\,|\partial U^i|_1^2 \leqq C .$$

Proof. This result is a consequence of the stability estimates for $\{U_\varepsilon^n, W_\varepsilon^n\}$. $\Box$

3 Convergence

Given $u_0 \in H^1(\Omega)$, $\|u_0\|_\infty \leqq 1$, $\frac{1}{|\Omega|}\left|\int_\Omega u_0\right| < 1-\delta$, let us take $u_0^h = P^h u_0$ where $P^h u_0$ is the unique solution of

$$(P^h u_0, \chi)^h = (u_0, \chi) \quad \forall \chi \in S^h . \tag{3.1}$$

Since $(u_0^h, 1)^h = (u_0, 1)$ it follows that

$$\frac{1}{|\Omega|}\left|\int_\Omega u_0^h\right| < 1-\delta .$$

Also, because

$$u_0^h(x_i) = \frac{(u_0, \chi_i)}{(1, \chi_i)^h}$$

and $\|u_0\|_\infty \leqq 1$ it results that $\|u_0^h\|_\infty \leqq 1$. Therefore u_0^h satisfies the assumptions of Theorem 2.1.

For $t \in (t_{n-1}, t_n)$, $1 \leqq n \leqq N$, we define

$$u_k^h(t) = U^n ,$$

$$w_k^h(t) = W^n ,$$

$$\phi_k^h(t) = I^h \phi_\varepsilon(U^n) ,$$

$$\xi_k(t) = \xi(t_{n-1}) \equiv \xi^{n-1}, \quad \xi \in C^\infty(0, T) ,$$

and denote by $\hat{u}_k^h$, $\hat{\xi}_k$ the piecewise linear continuous functions on $[0, T]$ defined by

$$\hat{u}_k^h(t_n) = U^n \quad n = 0, \dots, N ,$$

$$\hat{\xi}_k(t_n) = \xi^n \quad n = 0, \dots, N-1 ,$$

$$\hat{\xi}_k(T) = \xi^{N-1} .$$

The stability estimates given by Theorem 2.2 imply that

$$u_k^h \text{ is bounded in } L^\infty(0, T; H^1(\Omega)) ,$$

$$\hat{u}_k^h \text{ is bounded in } L^\infty(0, T; H^1(\Omega)) ,$$

$$\sqrt{t}\frac{d}{dt}\hat{u}_k^h \text{ is bounded in } L^2(0, T; H^1(\Omega)) ,$$

$$\sqrt{t}\, w_k^h \text{ is bounded in } L^\infty(0, T; H^1(\Omega)) ,$$

$$\sqrt{t}\, \phi_k^h \text{ is bounded in } L^\infty(0, T; L^2(\Omega)) .$$

Thus there exists $\{u, \hat{u}, w, \zeta\}$ such that, for $\tau > 0$,

$$u \in L^\infty(0, T; H^1(\Omega)) ,$$

$$\hat{u} \in L^\infty(0, T; H^1(\Omega)) ,$$

$$\sqrt{t}\frac{d}{dt}\hat{u} \in L^2(0, T; H^1(\Omega)) ,$$

$$\sqrt{t} w \in L^\infty(0, T; H^1(\Omega)) ,$$

$$\zeta \in L^\infty(\tau, T; L^2(\Omega)) ,$$

$$\sqrt{t}\zeta \in L^\infty(0, T; L^2(\Omega)) ,$$

and for subsequences $\{u_k^h, \hat{u}_k^h, w_k^h, \phi_k^h\}$

$$u_k^h \to u \quad \text{in } L^\infty(0, T; H^1(\Omega)) \text{ weak–star} ,$$

$$\hat{u}_k^h \to \hat{u} \quad \text{in } L^\infty(0, T; H^1(\Omega)) \text{ weak–star} ,$$

$$\sqrt{t}\frac{d}{dt}\hat{u}_k^h \to \sqrt{t}\frac{d}{dt}\hat{u} \quad \text{in } L^2(0, T; H^1(\Omega)) \text{ weakly} ,$$

$$\sqrt{t} w_k^h \to \sqrt{t} w \quad \text{in } L^\infty(0, T; H^1(\Omega)) \text{ weak–star} ,$$

$$\sqrt{t}\phi_k^h \to \sqrt{t}\zeta \quad \text{in } L^\infty(0, T; L^2(\Omega)) \text{ weak–star} .$$

Also, as $k \to 0$,

$$\xi_k \to \xi \quad \text{in } L^2(0, T) \text{ strongly} ,$$

$$\frac{d}{dt}\hat{\xi}_k \to \frac{d}{dt}\xi \quad \text{in } L^2(0, T) \text{ strongly} .$$

Defining $\Omega_T = \Omega \times (0, T)$ and observing that

$$\|\hat{u}_k^h - u_k^h\|_{L^2(\Omega_T)}^2 = \sum_{i=1}^{N} \int_{(i-1)k}^{ik} \|\hat{u}_k^h - u_k^h\|^2 \, dt$$

$$\leqq k \sum_{i=1}^{N} \|U^i - U^{i-1}\|^2$$

it results from Theorem 2.2 that $\hat{u} = u$.

Given $\eta \in H^1(\Omega)$ we set $\chi = R^h\eta$ and multiply equations (2.1a) and (2.1b) by $k\xi^{n-1}$. Summing over n the resulting equations it results

$$-k\sum_{i=1}^{N-1} \partial\xi^i (U^i, \chi)^h + (U^N, \chi)^h \xi^{N-1} - (U^0, \chi)^h \xi^0 + k\sum_{i=1}^{N} \xi^{i-1}(\nabla W^i, \nabla\chi) = 0 ,$$

$$k\sum_{i=1}^{N} \xi^{i-1}\big((W^i - \phi(U^i) + \theta_c U^i, \chi)^h - \gamma(\nabla U^i, \nabla\chi)\big) = 0 ,$$

or, equivalently,

(3.2a) $$-\int_0^T \hat{\xi}_k'(t)(u_k^h, \chi)^h \, dt + (U^N, \chi)^h \xi^{N-1} - (u_0, \chi)\xi^0 + \int_0^T \xi_k(t)(\nabla w_k^h, \nabla\chi) \, dt = 0 ,$$

(3.2b) $$\int_0^T \xi_k(t)\big((w_k^h - \phi_k^h + \theta_c u_k^h, \chi)^h - \gamma(\nabla u_k^h, \nabla\chi)\big) \, dt = 0 .$$

Rewriting these equations as

$$-\int_0^T \hat{\xi}_k'(t)(u_k^h,\chi)\,dt + (U^N,\chi)^h\xi^{N-1} - (u_0,\chi)\xi^0 + \int_0^T \xi_k(t)(\nabla w_k^h,\nabla\chi)\,dt$$
$$+\int_0^T \hat{\xi}_k'(t)\big((u_k^h,\chi)-(u_k^h,\chi)^h\big)\,dt = 0\,,$$

$$\int_0^T \xi_k(t)\big((w_k^h-\phi_k^h+\theta_c u_k^h,\chi)-\gamma(\nabla u_k^h,\nabla\chi)\big)\,dt$$
$$+\int_0^T \xi_k(t)\big((w_k^h-\phi_k^h+\theta_c u_k^h,\chi)^h-(w_k^h-\phi_k^h+\theta_c u_k^h,\chi)\big)\,dt = 0\,,$$

are recalling the error (1.5) due to numerical integration we have that

$$\left|\int_0^T \hat{\xi}_k'(t)\big((u_k^h,\chi)^h-(u_k^h,\chi)\big)\,dt\right| \leqq Ch^2\int_0^T \|\chi\|_1\,\|u_k^h\|_1\,dt$$

and

$$\left|\int_0^T \xi_k(t)\big((w_k^h-\phi_k^h+\theta_c u_k^h,\chi)^h-(w_k^h-\phi_k^h+\theta_c u_k^h,\chi)\big)\,dt\right|$$
$$\leqq Ch\int_0^T \|\chi\|_1\,\|\phi_k^h\|\,dt + Ch^2\int_0^T \|\chi\|_1(\|w_k^h\|_1+\theta_c\|u_k^h\|_1)\,dt\,.$$

Choosing ξ such that $\xi(T)=0$, $\xi(0)\neq 0$, using the bounds on u_k^h, $\sqrt{t}w_k^h$ and $\sqrt{t}\phi_k^h$ and observing that $\|\chi\|_1$ remains bounded as $k,h\to 0$ and $\xi^{N-1}\to\xi(T)$ we can pass to the limit as $k,h\to 0$ to obtain

(3.3a) $$-\int_0^T \xi'(t)(u,\eta)\,dt + \int_0^T \xi(t)(\nabla w,\nabla\eta)\,dt - (u_0,\eta)\xi(0) = 0\,,$$

(3.3b) $$\int_0^T \xi(t)\big((w-\zeta+\theta_c u,\eta)-\gamma(\nabla u,\nabla\eta)\big)\,dt = 0$$

which implies

$$\langle u_t,\eta\rangle + (\nabla w,\nabla\eta) = 0 \quad \text{a.e. in } (0,T)\,,$$
$$(w-\zeta+\theta_c u,\eta)(-\gamma(\nabla u,\nabla\eta) = 0 \quad \text{a.e. in } (0,T)\,.$$

An integration by parts of (3.3a) gives

$$(u(0)-u_0,\eta)=0 \quad \forall\eta\in H^1(\Omega)$$

and therefore $u(0)=u_0$.

It remains to show that

(3.4) $$\zeta=\phi(u)\,.$$

Given $M>0$, let us define

$$F_M(v)=\max\{-M,\min\{M,v\}\}\,,$$
$$\phi_M(v)=F_M(\phi(v))$$

and

$$\Omega_M^{h,k}=\{x:|\phi_k^h(x,t)|>M\}\,.$$

It follows from Theorem 2.2 that for each t

$$t \int_{\Omega_M^{h,k}} |\phi_k^h(x,t)|^2\,dx \leqq t\,\|\phi_k^h(x,t)\|^2 \leqq C$$

which yields

$$|\Omega_M^{h,k}| < \frac{C}{M^2}\,.$$

Thus, $\forall \eta \in L^\infty(\Omega) \cap H^1(\Omega)$, $\tau > 0$,

$$\left|\int_\tau^T \xi(t)(\phi_k^h - F_M(\phi_k^h), \eta)\,dt\right| = \left|\int_\tau^T \xi(t) \int_{\Omega_M^{h,k}} (\phi_k^h - F_M(\phi_k^h))\eta\,dx\,dt\right|$$

$$\leqq \|\xi\|_\infty \|\eta\|_\infty \int_\tau^T \int_{\Omega_M^{h,k}} (|\phi_k^h| + M)\,dx\,dt$$

$$\leqq \|\xi\|_\infty \|\eta\|_\infty \left(\int_\tau^T |\Omega_M^{h,k}|^{1/2} \|\phi_k^h\|\,dt + \frac{C(\tau)}{M}\right)$$

and the boundedness of ϕ_k^h in $L^\infty(\tau, T; L^2(\Omega))$ yields

$$\left|\int_\tau^T \xi(t)(\phi_k^h - F_M(\phi_k^h), \eta)\,dt\right| \leqq \frac{C(\tau)}{M} \|\xi\|_\infty \|\eta\|_\infty\,.$$

For $\tau > 0$ $\hat{u}_k^h$ is bounded in $H^1((\tau, T)\times\Omega)$ and the fact that the injection of $H^1((\tau, T)\times\Omega)$ into $L^2((\tau, T)\times\Omega)$ is compact guarantees the existence of some subsequence u_k^h such that

$$u_k^h \to u \quad \text{in } L^2(\tau, T; L^2(\Omega)) \text{ strongly}\,. \tag{3.5}$$

Observing that

$$\left|\int_\tau^T \xi(t)\big(F_M(\phi_k^h) - \phi_M(u), \eta\big)\,dt\right| = \left|\int_\tau^T \xi(t)\big(\phi_M(u_k^h) - \phi_M(u), \eta\big)\,dt\right.$$

$$\left. + \int_\tau^T \xi(t)\Big(\big(F_M(\phi_k^h) - \phi_M(u_k^h), \eta\big) - \big(F_M(\phi_k^h) - \phi_M(u_k^h), \eta\big)^h\Big)\,dt\right|$$

$$\leqq Ch\,\|F_M(\phi_k^h) - \phi_M(u_k^h)\|\;\|\eta\|_1 + \left|\int_\tau^T \xi(t)\big(\phi_M(u_k^h) - \phi_M(u), \eta\big)\,dt\right|$$

it results that, since ϕ_M is Lipschitz continuous and (3.5) holds true,

$$\int_\tau^T \xi(t)\big(F_M(\phi_k^h) - \phi_M(u), \eta\big)\,dt \to 0 \quad \text{as } k, h \to 0\,.$$

Therefore

$$\left|\int_\tau^T \xi(t)\big(\phi_k^h - F_M(\phi_k^h), \eta\big)\,dt\right| \to \left|\int_\tau^T \xi(t)(\zeta - \phi_M(u), \eta)\,dt\right| \quad \text{as } k, h \to 0$$

and

$$\left|\int_\tau^T \xi(t)(\zeta - \phi_M(u), \eta)\,dt\right| \leqq \frac{C(\tau)}{M} \|\xi\|_\infty \|\eta\|_\infty\,. \tag{3.6}$$

Taking $\eta = \phi_M(u)$ we obtain

$$\left| \int_\tau^T \xi(t) \| \phi_M(u) \|^2 \, dt \right| \leqq C(\tau) \| \xi \|_\infty + \left| \int_\tau^T \xi(t)(\zeta, \phi_M(u)) \, dt \right| .$$

Choosing $\xi(t) = 1$ and recalling that $\zeta \in L^\infty(\tau, T; L^2(\Omega))$ it results that $\forall M > 0$

$$\int_\tau^T \| \phi_M(u) \|^2 \, dt \leqq C(\tau)$$

which implies

$$\int_\tau^T \| \phi(u) \|^2 \, dt \leqq C(\tau) .$$

As $M \to \infty$,

$$\phi_M(u) \to \phi(u) \quad \text{in } L^2(\tau, T; L^2(\Omega)) \text{ strongly}$$

and (3.6) gives

$$\zeta = \phi(u) \quad \text{on } (\tau, T) .$$

Since τ is arbitrary (3.4) follows.

Because the limit is independent of the subsequence and Eq. (1.3) has a unique solution we conclude that the whole sequence converges.

4 Iterative method

We shall now discuss two iterative procedures used to solve (2.1) in the one dimensional case.

Method I. Representing the solution in terms of the basis functions as

$$U^n = \sum_{i=1}^{N^h} c_i^n \chi_i, \qquad W^n = \sum_{i=1}^{N^h} d_i^n \chi_i ,$$

Eqs. (2.1) lead to the following system,

$$M(\boldsymbol{c}^n - \boldsymbol{c}^{n-1}) + kK\boldsymbol{d}^n = \boldsymbol{0} ,$$

$$M\boldsymbol{d}^n = \boldsymbol{f}(\boldsymbol{c}^n) + \gamma K \boldsymbol{c}^n ,$$

where

$$\boldsymbol{c}^n = \{c_i^n\}, \qquad \boldsymbol{d}^n = \{d_i^n\} ,$$

$$K_{ij} = (\nabla \chi_i, \nabla \chi_j) ,$$

$$\{\boldsymbol{f}(\boldsymbol{c}^n)\}_i = (\Psi'(U^n), \chi_i)^h ,$$

with $M_{ii} = m_i$, $M_{ij} = 0$ $i \neq j$, and the resulting algebraic problem to be solved is

$$M(\boldsymbol{c}^n - \boldsymbol{c}^{n-1}) + k\gamma K M^{-1} M \boldsymbol{c}^n + kKM^{-1}\boldsymbol{f}(\boldsymbol{c}^n) = \boldsymbol{0} . \tag{4.1}$$

Given $\boldsymbol{c}_0^n$, an initial guess to $\boldsymbol{c}^n$, we solved the linear problem for $j \geqq 1$

$$M(\boldsymbol{c}_j^n - \boldsymbol{c}^{n-1}) + k\gamma K M^{-1} K \boldsymbol{c}_j^n + kKM^{-1}\boldsymbol{f}(\boldsymbol{c}_{j-1}^n) = \boldsymbol{0} . \tag{4.2}$$

Provided that k is sufficiently small it is possible to show that the mapping associated with this iterative scheme is a contraction with respect to $|\cdot|_h$. If

$\|c_j^n\|_\infty < 1 \, \forall j$ then the sequence $\{c_j^n\}_{j=0}^\infty$ obtained from (4.2) converges to the unique solution of (4.1). Unfortunately, we have no guarantee that $\|c_{j-1}^n\|_\infty < 1$ implies $\|c_j^n\|_\infty < 1$. However, by decreasing the time step if $\|c_j^n\|_\infty \geqq 1$ and computing a new c_j^n until $\|c_j^n\|_\infty < 1$, a sequence $\{c_j^n\}$ that satisfies $\|c_j^n\|_\infty < 1$ was always generated when $\|U^0\|_\infty < 1$. Alternatively, if $\|c_j^n\|_\infty \geqq 1$ we can truncate c_j^n to the binodal values and continue the iteration. The problem here is that we may not have convergence.

Method II. Let us denote by q the number of nodes of $\mathscr{T}^h$, that is $q = N^h$, and rewrite (2.1) as

$$(G^h(\partial U^h), \chi)^h + \gamma(\nabla U^n), \nabla\chi) + (\phi(U^n), \chi)^h - \theta_c(U^n, \chi)^h - \lambda^n(1, \chi)^h = 0$$

where $\lambda^n = \dfrac{(\Psi'(U^n), 1)^h}{|\Omega|}$.

Given $y \in S = \{y \in \mathbb{R}^q \colon \mathbf{1}^T M y = 0\}$, the existence of G^h defines, implicitly, the invertible linear transformation $T\colon S \to S$ by

$$T(y) = \tilde{y} \tag{4.3}$$

where $\tilde{y}$ is the solution of

$$K\tilde{y} = My\,, \qquad \mathbf{1}^T M\tilde{y} = 0 \tag{4.4}$$

and $\mathbf{1}$ is the vector with components 1.

As a consequence, given U^{n-1}, the algebraic problem to be solved is

$$T\left(\frac{c^n - c^{n-1}}{k}\right) + \gamma M^{-1}Kc^n + \boldsymbol{\phi}(c^n) - \theta_c c^n - \lambda^n \mathbf{1} = \mathbf{0}\,,$$

which can be written as

$$T\left(\frac{c^n - c^{n-1}}{k}\right) + T(\gamma M^{-1}KM^{-1}Kc^n - \theta_c M^{-1}Kc^n) + \boldsymbol{\phi}(c^n) - \tilde{\lambda}^n \mathbf{1} = \mathbf{0}\,, \tag{4.5}$$

where

$$\{\boldsymbol{\phi}(c^n)\}_i = \frac{\theta}{2}\ln\left(\frac{1 + c_i^n}{1 - c_i^n}\right)$$

and $\tilde{\lambda}^n = \dfrac{1}{|\Omega|}\,\mathbf{1}^T M\boldsymbol{\phi}(c^n)$.

Letting $v = \sum_{i=1}^q y_i\chi_i$ we observe that for $\varepsilon > 0$

$$\begin{aligned} (v, v)^h &= (\nabla G^h, \nabla v)^h \\ &\leqq |G^h v|_1 |v|_1 \\ &\leqq \frac{1}{2\varepsilon}|G^h v|_1^2 + \frac{\varepsilon}{2}|v|_1^2\,. \end{aligned} \tag{4.6}$$

Let us define the operators A and B,

$$A: (-1, 1)^q \to \mathbb{R}^q$$

$$A(y) = \phi(y) ,$$

$$B: D(B) \to S$$

$$B(y) = T\left(\frac{y - c^{n-1}}{k}\right) + T(\gamma M^{-1}KM^{-1}Ky - \theta_c M^{-1}Ky) ,$$

where $D(B) = \{y \in \mathbb{R}^q : \mathbf{1}^T My = (u_0^h, 1)^h\}$, so that c^n satisfies

$$B(c^n) + A(c^n) - \tilde{\lambda}^n \mathbf{1} = \mathbf{0} .$$

It follows from the monotonicity of ϕ that A is monotone and, since range$(I + \mu A) = \mathbb{R}^q$ $\forall \mu > 0$, A is maximal. If $k < \frac{4\gamma}{\theta_c^2}$ then B is coercive: given $z, y \in D(B)$ and denoting by $(\cdot, \cdot)$ the inner product of $\mathbb{R}^q$ defined by $(z, y) = y^T Mz$ it results that

$$(B(z) - B(y), z - y) = \frac{1}{k}(z - y)^T MT(z - y) - \theta_c(z - y)^T M(z - y)$$

$$+ \gamma(z - y)^T K(z - y) .$$

Defining $\chi = \sum_{i=1}^q z_i \chi_i$, $\eta = \sum_{i=1}^q y_i \chi_i$, it follows that

$$(B(z) - B(y), z - y) = \frac{1}{k}|G^h(\chi - \eta)|_1^2 - \theta_c|\chi - \eta|_h^2 + \gamma|\chi - \eta|_1^2$$

and the inequality (4.6) yields

$$(B(z) - B(y), z - y) = \frac{1}{k}|G^h(\chi - \eta)|_1^2 - \frac{\theta_c}{2\varepsilon}|G^h(\chi - \eta)|_1^2 + \left(\gamma - \frac{\theta_c \varepsilon}{2}\right)|\chi - \eta|_1^2 .$$

Taking $\varepsilon = \frac{\theta_c k}{2}$, the Poincaré inequality yields

$$(B(z) - B(y), z - y) \geqq C|\chi - \eta|_h^2 \geqq C(z - y)^T M(z - y))$$

and therefore B is coercive.

A natural iteration to find c^n and $\tilde{\lambda}^n$ is

(4.7a) $$c_{j+\frac{1}{2}}^n + \mu A(c_{j+\frac{1}{2}}^n) = c_j^n - \mu B(c_j^n) + \mu \tilde{\lambda}_j^n \mathbf{1} ,$$

(4.7b) $$c_{j+1}^n + \mu B(c_{j+1}^n) - \mu \tilde{\lambda}_{j+1}^n \mathbf{1} = c_{j+\frac{1}{2}}^n - \mu A(c_{j+\frac{1}{2}}^n) ,$$

with $\mu > 0$ and $\{\tilde{\lambda}_j^n\}_{j=1}^\infty$ a sequence of Lagrange multipliers. Recalling that $\mathbf{1}^T MB(c_{j+1}^n) = \mathbf{0}$ we find that

$$\tilde{\lambda}_{j+1}^n = \frac{1}{\mu|\Omega|}(\mathbf{1}^T Mc_{j+1}^n - \mathbf{1}^T Mc_{j+\frac{1}{2}}^n + \mu \mathbf{1}^T MA(c_{j+\frac{1}{2}}^n)) .$$

We remark that solving (4.7b) is equivalent to solving

$$K(c^n_{j+1} + \mu B(c^n_{j+1})) = K(c^n_{j+\frac{1}{2}} - \mu A(c^n_{j+\frac{1}{2}}))$$

because 0 is a simple eigenvalue of K with eigenvector $\mathbf{1}$. Equation (4.4) yields

$$\text{(4.8)}\quad kKc^n_{j+1} + \mu(M - k\theta_c K + k\gamma KM^{-1}K)c^n_{j+1} = \mu Mc^{n-1} + kK(c^n_{j+\frac{1}{2}} - \mu A(c^n_{j+\frac{1}{2}}))\,.$$

For $k < \dfrac{4\gamma}{\theta_c^2}$ the matrix $M - \theta_c kK + k\gamma KM^{-1}K$ is symmetric positive definite, since in this case the eigenvalues of $I - \theta_c kM^{-1}K + k\gamma M^{-1}KM^{-1}K$ are positive. It follows that (4.8) has a unique solution.

Proposition 4.1. *Let* $k < \dfrac{4\gamma}{\theta_c^2}$. *Given* $\{\tilde{\lambda}^n_1, c^n_1\}$ *the sequence* $\{c^n_1\}_{j=1}^{\infty}$ *generated by the algorithm* (4.7) *converges to the unique solution of* (4.5).

Proof. We have adapted the proof given by Lions and Mercier [15] where the algorithm, without Lagrange multipliers, is analysed for more general operators A and B (see also [14]).

Let us drop the dependence on n and set $c \equiv c^n$, $c_j \equiv c^n_j$, $\tilde{\lambda} \equiv \tilde{\lambda}^n$, $\tilde{\lambda}_j \equiv \tilde{\lambda}^n_j$. We define

$$\begin{aligned} v &= c + \mu B(c) - \mu\tilde{\lambda}\mathbf{1}\,, \\ z &= c + \mu A(c)\,, \\ a &= A(c)\,, \\ v_j &= c_j + \mu B(c_j) - \mu\tilde{\lambda}_j\mathbf{1}\,, \\ z_j &= 2c_j - v_j\,, \\ a_j &= \frac{z_j - v_{j+1}}{2\mu}\,. \end{aligned}$$

It results that

$$v + z = 2c\,,$$

$$a = \frac{z - v}{2\mu}\,,$$

and the iteration (4.7) can be written as

$$\begin{aligned} v_{j+1} &= (I - \mu A)(I + \mu A)^{-1} z_j \\ &= (2J^\mu_A - I)z_j \end{aligned}$$

where $J^\mu_A = (I + \mu A)^{-1}$. As a consequence we have

$$\frac{v_{j+1} + z_j}{2} = J^\mu_A(z_j)$$

and therefore

$$a_j = A\left(\frac{v_{j+1} + z_j}{2}\right).$$

The monotonicity of A yields

$$0 \leqq \left(\boldsymbol{a}_j - \boldsymbol{a}, \frac{\boldsymbol{v}_{j+1} + \boldsymbol{z}_j}{2} - c \right) = \frac{1}{4\mu}(\boldsymbol{z}_j - \boldsymbol{z} - \boldsymbol{v}_{j+1} + \boldsymbol{v}, \boldsymbol{v}_{j+1} - \boldsymbol{v} + \boldsymbol{z}_j - \boldsymbol{z}) \tag{4.9}$$

$$= \frac{1}{4\mu}(|\boldsymbol{z}_j - \boldsymbol{z}|^2 - |\boldsymbol{v}_{j+1} - \boldsymbol{v}|^2) .$$

Also, the monotonicity of B together with the fact that $(\boldsymbol{c}_j - \boldsymbol{c}, \mathbf{1}) = 0$ gives

$$0 \leqq (B(\boldsymbol{c}_j) - B(\boldsymbol{c}), \boldsymbol{c}_j - \boldsymbol{c}) \tag{4.10}$$

$$= \left(\frac{\boldsymbol{v}_j - \boldsymbol{c}_j}{\mu} + \tilde{\lambda}_j \mathbf{1} - \frac{\boldsymbol{v} - \boldsymbol{c}}{\mu} - \tilde{\lambda}\mathbf{1}, \boldsymbol{c}_j - \boldsymbol{c} \right)$$

$$= \frac{1}{4\mu}(\boldsymbol{v}_j - \boldsymbol{v} - \boldsymbol{z}_j + \boldsymbol{z}, \boldsymbol{z}_j - \boldsymbol{z} + \boldsymbol{v}_j - \boldsymbol{v})$$

$$= \frac{1}{4\mu}(|\boldsymbol{v}_j - \boldsymbol{v}|^2 - |\boldsymbol{z}_j - \boldsymbol{z}|^2)$$

Equations (4.9) and (4.10) imply

$$|\boldsymbol{v}_{j+1} - \boldsymbol{v}|^2 \leqq |\boldsymbol{v}_j - \boldsymbol{v}|^2$$

which shows that $\{|\boldsymbol{v}_j - \boldsymbol{v}|\}$ is a decreasing sequence bounded below. Adding (4.9) and (4.10) we obtain

$$0 \leqq (B(\boldsymbol{c}_j) - B(\boldsymbol{c}), \boldsymbol{c}_j - \boldsymbol{c}) + \left(\boldsymbol{a}_j - \boldsymbol{a}, \frac{\boldsymbol{v}_{j+1} + \boldsymbol{z}_j}{2} - c \right)$$

$$\leqq \frac{1}{4\mu}(|\boldsymbol{v}_j - \boldsymbol{v}|^2 - |\boldsymbol{v}_{j+1} - \boldsymbol{v}|^2) \to 0 \quad \text{as } j \to \infty .$$

This yields

$$(B(\boldsymbol{c}_j) - B(\boldsymbol{c}), \boldsymbol{c}_j - \boldsymbol{c}) \to 0 \quad \text{as } j \to \infty$$

and, since B is coercive, we conclude that

$$\boldsymbol{c}_j \to \boldsymbol{c} \quad \text{as } j \to \infty . \quad \square$$

To compare the two iterative procedures the simulations described below were performed using the two methods. When u_b was not close to 1 the iterative method I was faster than method II. However, for u_b close to 1 method I required a very small time step and, in this case, the superiority of method II was evident. Also, when the initial data took values 1 or -1, method II always gave a solution while this was not true for method I since sometimes convergence was not obtained due to the fact that the iterative process returned a solution which satisfied $\| \boldsymbol{c}_j^n \|_\infty \geqq 1$.

5 Numerical simulations

A one-phase homogeneous binary mixture with average composition u_m inside the spinodal interval is unstable with respect to infinitesimally small fluctuations in composition and separates into regions of higher and lower concentrations of A and B. Such a system evolves towards an equilibrium state with phases having concentrations β or $-\beta$ where β is defined in Sect. 1.

Numerical simulations in one space dimension were performed with $\Omega = (0, 1)$. Note that (4.7a) may be rewritten as

$$c^n_{j+\frac{1}{2}} + \mu A(c^n_{j+\frac{1}{2}}) = 2c^n_j - (c^n_j + \mu B(c^n_j) - \mu\tilde{\lambda}^n_j \mathbf{1})$$

and, due to (4.7b), an explicit expression for T is not needed. To start the computations, as an initial guess to c^1 we took c^0 if $\| U^0 \|_\infty < 1$. When $\| U^0 \|_\infty = 1$ the initial guess to U^1 was U^1_0 defined by

$$U^1_0(x_i) = U^0(x_i) \qquad \text{if } -1 < U(x_i) < 1\ ,$$

$$U^1_0(x_i) = 0.99 \qquad \text{if } U(x_i) = 1\ ,$$

$$U^1_0(x_i) = -0.99 \qquad \text{if } U(x_i) = -1\ .$$

Then $\{\tilde{\lambda}^1_1, c^1_1\}$ was the solution of $c^1_1 + \mu B(c^1_1) - \mu\tilde{\lambda}^1_1 \mathbf{1} = c^0 - \mu A(c^0)$. For $n \geqq 2$, $\{\tilde{\lambda}^n_1, c^n_1\}$ was $\{\tilde{\lambda}^{n-1}, c^{n-1}\}$.

To solve (4.7a), for each node, the bisection method was used. The Cholesky decomposition can be employed to find the unique solution of (4.8). If we multiply Eq. (4.7b) by $kM^{-1}K$ then, as explained by Blowey and Elliott [2], it is possible to use a discrete cosine transform to solve the resulting system. On the square $\Omega = (0, L) \times (0, L)$ with a uniform triangulation it requires I^h to be the piecewise bilinear interpolant.

In order to decide which μ to take we run one experiment with different values of μ: $\mu = 0.01$, $\mu = 0.1$, $\mu = 1$, $\mu = 2$. The value that required, on average, fewer iterations was $\mu = 1$. However we cannot be conclusive about this value since, probably, the best choice would depend on the problem.

In all simulations we let $\mu = 1$ and the maximum number of iterations, for most of the experiments, was smaller than 50. The exceptions were the cases with $\theta = 0.2$ and $\theta = 0.15$ when, for some times, about 250 iterations were needed. However, the number of iterations required to obtain convergence of the algorithm, in all experiments, was usually small.

Finally, the simulations were stopped when a solution that did not change for a long time and whose associated discrete chemical potential was constant up to 4 decimals was obtained.

5.1 Comparison with quartic free energy

As explained in the introduction, if $\theta_c \approx \theta$ and u is small, the logarithmic free energy can be approximated by a quartic polynomial. In this experiment we choose $\theta_c = 2.2$ and $\theta = 2.17$ so that $\theta_c \approx \theta$, and compared the evolution of the system from an initial condition which was a random perturbation of the uniform state $u = 0$ with the evolution when $\Psi'(u) = \frac{\theta}{3}u^3 - (\theta_c - \theta)u$. No significant difference was observed and the error in the maximum norm was smaller than 5.7×10^{-3} for the times computed. We let $\gamma = 2 \times 10^{-4}$, $k = 1 \times 10^{-4}$, $h = \frac{1}{100}$ and judged that

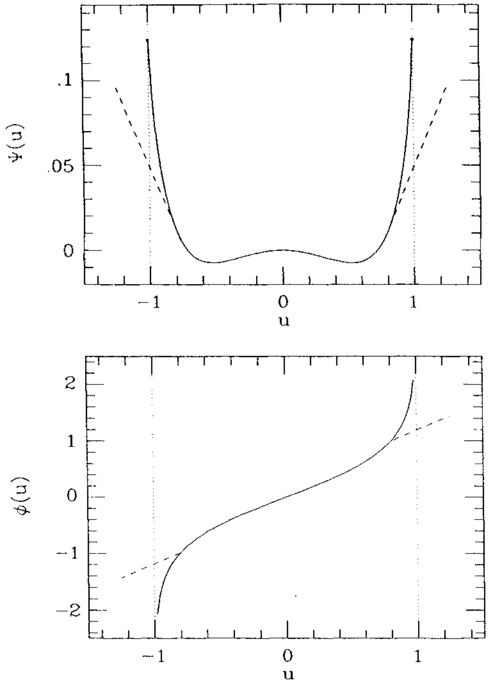

Fig. 1. The solid lines represent Ψ and ϕ and the broken lines represent Ψ_ε and $\tilde{\phi}_\varepsilon$

the iterative process converged when $\|c_j^n - c_{j-1}^n\|_\infty < \mathrm{TOL}$ with $\mathrm{TOL} = 1\times 10^{-7}$. The results were virtually the same when the initial data was interpolated up to 201 nodes.

5.2 Initial data satisfying $\| U^0 \|_\infty = 1$

We have shown in Sect. 2 that the numerical approximation has a solution even when $\| U^0 \|_\infty = 1$. We run two simulations with initial data satisfying $\| U^0 \|_\infty = 1$. In the first experiment the initial condition is a piecewise linear continuous function which is equal to 1 over an interval I, equal to -1 over an interval J and a random perturbation of zero on $(0, 1)\backslash(I \bigcup J)$. In the second experiment, the initial condition does not assume the value -1. The parameters were $\theta_c = 1$, $\theta = 0.5$, $\gamma = 5 \times 10^{-3}$, $k = \gamma$ and $\mathrm{TOL} = 1 \times 10^{-7}$ with $0.957 < \beta < 0.96$.

To compute U^1, 19 iterations were required to obtain convergence in the first case and 23 in the second one. The subsequent number of iterations was much smaller in both experiments.

The results are shown in Fig. 2 and the final state is a single-interface solution.

5.3 The limit $\dfrac{\theta}{\theta_c} \to 0$

We shall now describe some simulations to investigate the limit $\dfrac{\theta}{\theta_c} \to 0$. It was remarked in the introduction that Elliott and Luckhaus [13] have shown that the

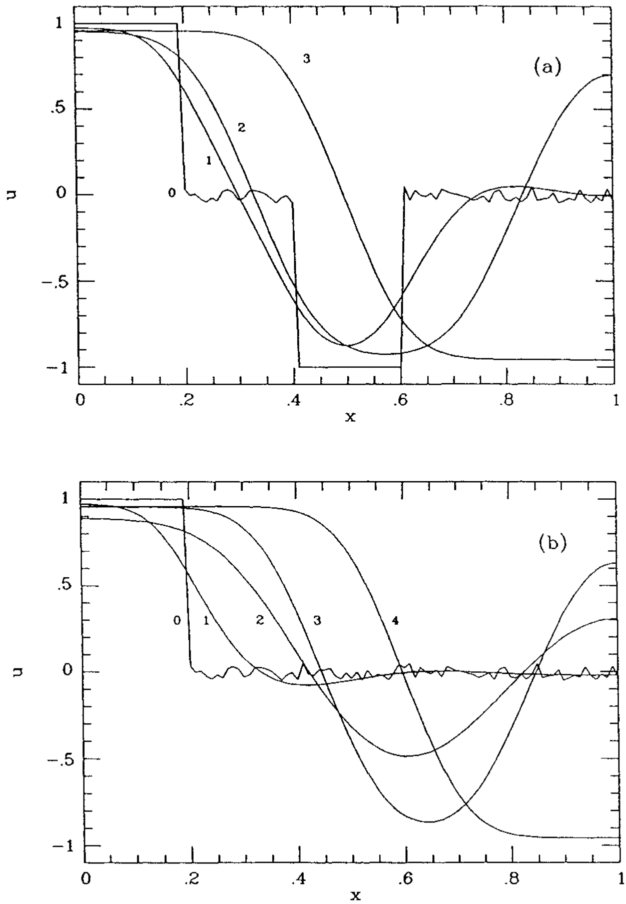

Fig. 2a, b. The evolution from initial condition that takes values 1 and −1 in regions of non-zero measure. The numbers indicate the direction of increasing time; this applies throughout. **a** $t = 0$, 0.005, 0.1, 3; **b** $t = 0$, 0.005, 0.1, 0.5, 3

weak solution of the Cahn-Hilliard equation with the logarithmic free energy converges to the weak solution of the free-boundary problem studied by Blowey and Elliott [1]. It is our aim to compare the results of our simulations for $\frac{\theta}{\theta_c} \to 0$ with the numerical results obtained by Blowey and Elliott [2]. To this end, we fixed $\gamma = 5 \times 10^{-3}$ and $\theta_c = 1$ which correspond to the parameters used by Blowey and Elliott [2] and performed two experiments with the same initial data they have taken. In both experiments, we obtained, for the smallest θ considered, a solution similar to the stationary solution of Blowey and Elliott [2]. We remark that (see Introduction), for γ, θ_c and u_m fixed, β increases when θ decreases.

In the first simulation, the initial condition was a random perturbation of the uniform state $u = 0$ and the values of θ were 0.8, 0.5, 0.35, 0.2. The other parameters

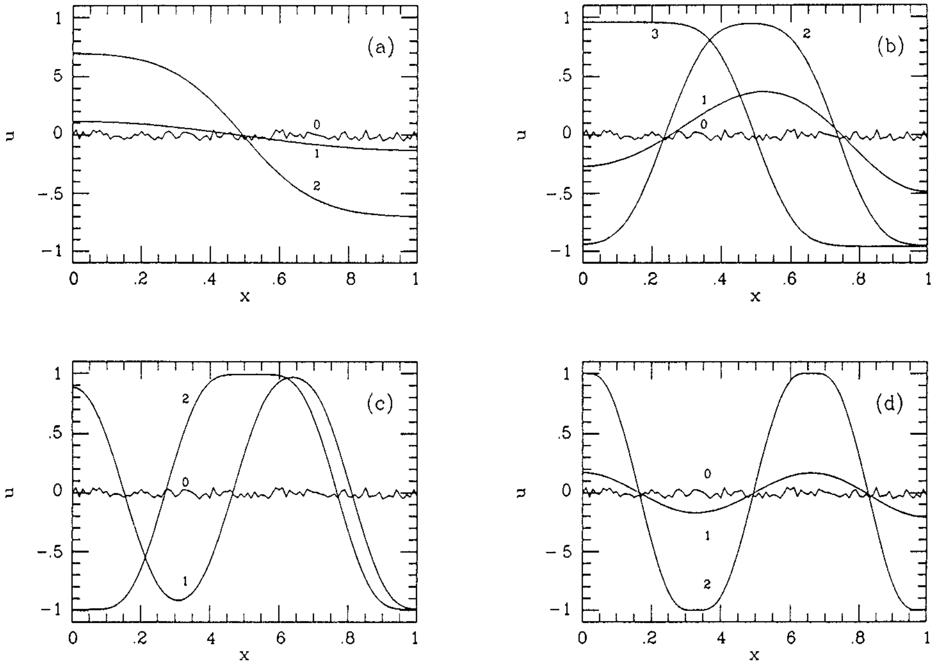

Fig. 3a–d. The evolution from initial condition which is a random perturbation of the uniform state $u = 0$ for different values of θ. **a** $\theta = 0.8$, $t = 0, 2, 6$; **b** $\theta = 0.5$, $t = 0, 0.5, 1, 40$; **c** $\theta = 0.35$, $t = 0, 0.5, 2$; **d** $\theta = 0.2$, $t = 0, 0.1, 2$

were $k = \gamma$, $h = \dfrac{1}{100}$ and $\mathrm{TOL} = 1 \times 10^{-7}$. In the case of $\theta = 0.35$ the initial condition was interpolated up to 201 nodes and the results were virtually the same.

In the second simulation we took $\theta = 0.5$, $\theta = 0.3$, $\theta = 0.2$, $\theta = 0.15$ and the initial condition was a random perturbation of $u = -0.6$. We let $k = \gamma$, $h = \dfrac{1}{100}$ and $\mathrm{TOL} = 1 \times 10^{-7}$ for the first three values of θ. When $\theta = 0.15$, we have $0.999995 < \beta < 0.999999$ and for this reason TOL was decreased to $\mathrm{TOL} = 1 \times 10^{-8}$.

Figures 3 and 4 show the results. In Fig. 3 the "stable" patterns shown in (c) and (d) could be approximations of steady-state solutions. We run these two simulations for long time and a slightly movement along the interfaces was observed in case (d) indicating that the pattern will eventually change under longer time scales. The "stable" pattern shown in Fig. 4c should not remain because it is not an approximation of a solution of the steady-state equation as described by Carr et al. [4].

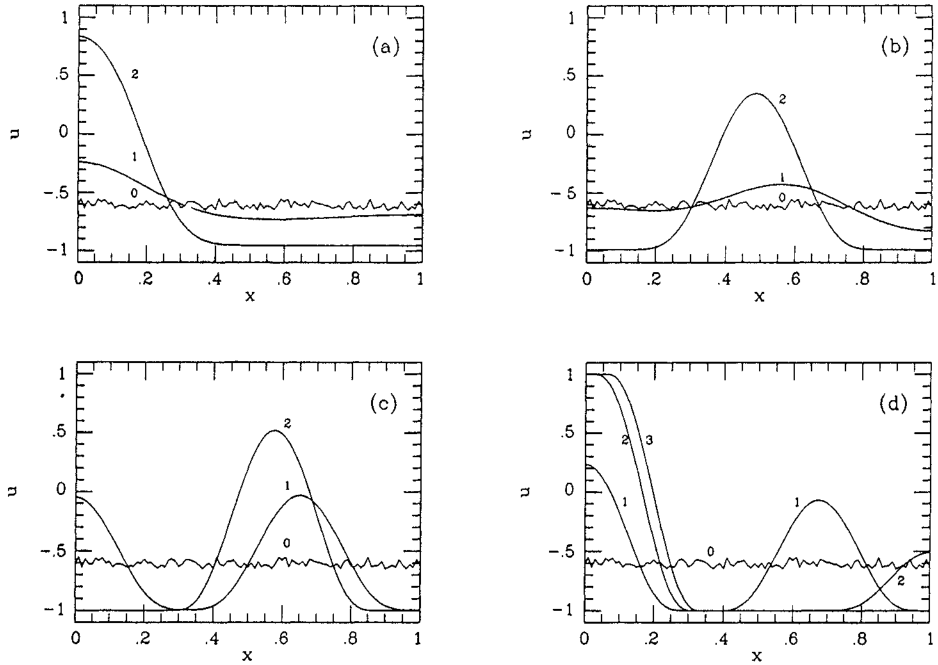

Fig. 4a–d. The evolution from initial condition which is a random perturbation of the uniform state $u = -0.6$ for different values of θ. **a** $\theta = 0.5$, $t = 0, 2, 4$; **b** $\theta = 0.3$, $t = 0, 0.4, 1$; **c** $\theta = 0.2$, $t = 0, 0.4, 1$; **d** $\theta = 0.15$, $t = 0, 0.4, 0.6, 2$

Acknowledgement. This work was partially supported by the Brazilian institution CAPES.

References

1. Blowey, J.F., Elliott, C.M. (1991): The Cahn-Hilliard gradient theory for phase separation with non-smooth free energy. Part I: Mathematical analysis. Eur. J. Appl. Math. **2**, 233–280
2. Blowey, J.F., Elliott, C.M. (1992): The Cahn-Hilliard gradient theory for phase separation with non-smooth free energy. Part II: Numerical analysis. Eur. J. Appl. Math. **3**, 147–179
3. Cahn, J.W., Hilliard, J.E. (1958): Free energy of a non-uniform system. I. Interfacial free energy. J. Chem. Phys. **28**, 258–267
4. Carr, J., Gurtin, M.E., Slemrod, M. (1984): Structured phase transitions on a finite interval. Arch. Rat. Mech. Anal. **86**, 317–351
5. Chakrabarti, A., Toral, R. (1989): Late stages of spinodal decomposition in a three dimensional model system. Phys. Rev. B **39**, 4386–4394
6. Ciavaldini, J.F. (1975): Analyse numérique d'un problème de Stefan à deux phases par une méthode d'elements finis. SIAM J. Numer. Anal. **12**, 464–487
7. Copetti, M.I.M., Elliott, C.M. (1990): Kinetics of phase decomposition processes: numerical solutions to Cahn-Hilliard equation. Materials Sci. Technol. **6**, 273–283
8. Qiang Du, Nicolaides, R.A. (1991): Numerical analysis of a continuum model of phase transition. SIAM J. Numer. Anal. **28**, 1310–1322
9. Elliott, C.M. (1989): The Cahn-Hilliard model for the kinetics of phase separation. In: Mathematical models for phase change problems, In: J. Rodrigues (ed.), International Series of Numerical Mathematics, Vol. 88. Birkhäuser, Basel, pp. 35–74

10. Elliott, C.M., French, D.A. (1987): Numerical studies of the Cahn-Hilliard equation for phase separation. I.M.A. J. Appl. Math. **38**, 97–128
11. Elliott, C.M., French, D.A., Milner, F.A. (1989): A second order splitting method for the Cahn-Hilliard equation. Numer. Math. **54**, 575–590
12. Elliott, C.M., Larsson, S. (1992): Error estimates with smooth and nonsmooth data for a finite element method for the Cahn-Hilliard equation. Math. Comput. **58**, 603–630
13. Elliott, C.M., Luckhaus, S. (1991): A generalised diffusion equation for phase separation of a multi-component mixture with interfacial free energy. I.M.A. (Minnesota) Preprint Series **887**
14. Glowinski, R., Lions, J.L., Trémolières, R. (1981): Numerical analysis of variational inequalities. North-Holland, Amsterdam
15. Lions, P.L., Mercier, B. (1979): Splitting algorithms for the sum of two nonlinear operators. SIAM J. Numer. Anal. **16**, 964–979
16. Meijer, P., Napiorkowski, M. (1987): The three-state lattice gas, a model for binary gas-liquid systems. J. Chem. Phys. **86**, 5771–5777
17. Oono, Y., Puri, S. (1988): Study of phase separation by use of cell dynamical systems. I. Modelling. Phys. Rev. A **38**, 434–453
18. Nochetto, R. (1991): Finite elements for free and moving boundary problems. In: W. Light, ed., Proceedings of the SERC summer school on numerical analysis. Advances in Numerical Analysis, Vol. 1. Clarendon Press, Oxford
19. Rogers, T.G., Elder, K.R., Desai, R.C. (1988): Numerical study of the late stages of spinodal decomposition. Phys. Rev. B **37**, 9638–9649
20. Temam, R. (1988): Infinite dimensional dynamical systems in mechanics and physics. Applied Mathematical Sciences Series 68. Springer, Berlin Heidelberg New York