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► **To cite this version:**

Franck Davhys Reval Langa, Morgan Pierre. A DOUBLY SPLITTING SCHEME FOR THE CAGINALP SYSTEM WITH SINGULAR POTENTIALS AND DYNAMIC BOUNDARY CONDITIONS. 2019. hal-02310210

HAL Id: hal-02310210

<https://hal.science/hal-02310210>

Preprint submitted on 10 Oct 2019

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A DOUBLY SPLITTING SCHEME FOR THE CAGINALP SYSTEM WITH SINGULAR POTENTIALS AND DYNAMIC BOUNDARY CONDITIONS

FRANCK DAVHYS REVAL LANGA AND MORGAN PIERRE

Dedicated to Michel Pierre on the occasion of his 70th birthday

ABSTRACT. We propose a time semi-discrete scheme for the Caginalp phase-field system with singular potentials and dynamic boundary conditions. The scheme is based on a time splitting which decouples the equations and on a convex splitting of the energy associated to the problem. The scheme is unconditionally uniquely solvable and the energy is nonincreasing if the time step is small enough. The discrete solution is shown to converge to the energy solution of the problem as the time step tends to 0. The proof involves a multivalued operator and a monotonicity argument. This approach allows us to compute numerically singular solutions to the problem.

Keywords: Caginalp phase-field system, logarithmic potential, dynamic boundary conditions, maximal monotone operator, multivalued operator, convex splitting.

1. INTRODUCTION

The Caginalp system has been proposed in [9] to describe phase transition phenomena such as the melting-solidification in certain classes of materials. Dynamic boundary conditions have been introduced by physicists in the context of the Cahn-Hilliard equation to account for interactions of the bulk material with the walls [23, 24, 25]. In such models, the time derivative appears explicitly in the boundary conditions.

The Caginalp system with dynamic boundary conditions is the initial and boundary value problem

$$\begin{cases} \partial_t w - \Delta w = -\partial_t u, & t > 0, x \in \Omega, \\ \partial_t u - \Delta u + f(u) - \lambda u = w, & t > 0, x \in \Omega, \\ \partial_t \psi - \Delta_\Gamma \psi + g(\psi) - \alpha \psi + \partial_n u = 0, & t > 0, x \in \Gamma, \\ \partial_n w|_\Gamma = 0, \quad u|_\Gamma = \psi, \\ w|_{t=0} = w_0, \quad u|_{t=0} = u_0, \quad \psi|_{t=0} = \psi_0, \end{cases} \quad (1.1)$$

where Ω denotes a bounded domain of \mathbb{R}^2 or \mathbb{R}^3 with sufficiently smooth boundary $\partial\Omega = \Gamma$. In (1.1), λ and α are nonnegative constants, Δ_Γ is the Laplace-Beltrami operator and ∂_n is the outward normal derivative. The state variables (u, w) denote the order parameter and the temperature, respectively, and Ω is the domain which contains the material. A thermodynamically relevant choice for the nonlinearity f is the logarithmic function

$$f(s) = \ln \left(\frac{1+s}{1-s} \right), \quad s \in (-1, 1). \quad (1.2)$$

The function g is assumed to be smooth and nonincreasing. More general assumptions on f and g will be given in (2.5)-(2.6).

The well-posedness and longtime behaviour of the Caginalp system with singular potentials and dynamic boundary conditions has been thoroughly analyzed in [13, 14, 15, 17] (see also [27]). The dynamic boundary condition for the order parameter is the third equation in (1.1). For the classical Caginalp system, this equation is usually replaced by the no-flux boundary condition for u . In the latter case, if f is the logarithmic potential (1.2), a separation property holds which guarantees that u stays away from the pure phases ± 1 [16, 28]. In contrast, for problem (1.2), the solution u may take the values ± 1 on the boundary Γ , unless a sign condition holds for the nonlinearity on the boundary.

In the singular cases, solutions to (1.1) can no longer be interpreted in the usual sense. In order to remove the sign condition and to analyze the longtime behaviour of solutions, the authors used in [15] the notion of *variational solution*, by adapting to problem (1.1) the approach in [34] which was developed in the context of the Cahn-Hilliard equation. We refer the reader to the review papers [18, 33] and references therein for more information on this subject.

From a numerical point of view, calculations for problem (1.1) with a logarithmic function were performed in [15] for regular solutions and for singular solutions, but only up to the singular time. An Allen-Cahn type problem which has some similarities with this problem (cf. Remark 4.5) was analyzed in [37], along with numerical computations of singular solutions in one space dimension. The numerical analysis and numerical computation of related problems involving dynamic boundary conditions and *regular* nonlinearities were also considered in, e.g., [1, 6, 19, 20, 26, 30, 31, 36]. Cahn-Hilliard type equations with logarithmic potential and *classical* boundary conditions have also drawn a lot of interest, cf., e.g. [4, 10, 11, 12, 21]. In these situations, one challenge is to adapt to the discretized problem the separation property which holds for the continuous time and space problem.

Up to now, the computation of singular solutions for Cahn-Hilliard type problems involving both a logarithmic potential and dynamic boundary conditions does not seem to have been addressed. Our purpose in this paper is to propose and to analyze a scheme which allows us to compute singular solutions to problem (1.1) even after the singularity occurs. A fundamental idea in our approach is to use the energy associated to the problem.

Indeed, let F and G denote an antiderivative of f and g , respectively. Then we have, assuming that (u, w) is a regular solution to (1.1),

$$\frac{d}{dt} \tilde{\mathcal{E}}(u(t), w(t)) + \int_{\Omega} |\nabla w(t)|^2 dx + \int_{\Omega} |\partial_t u(t)|^2 dx + \int_{\Gamma} |\partial_t u(t)|^2 d\sigma = 0, \quad (1.3)$$

where the energy $\tilde{\mathcal{E}}$ is defined by

$$\begin{aligned} \tilde{\mathcal{E}}(u, w) \stackrel{def}{=} & \int_{\Omega} \frac{1}{2} |\nabla u|^2 + F(u) - \frac{\lambda}{2} u^2 dx + \int_{\Omega} \frac{1}{2} |w|^2 dx \\ & + \int_{\Gamma} \frac{1}{2} |\nabla_{\Gamma} u|^2 + G(u) - \frac{\alpha}{2} u^2 d\sigma. \end{aligned}$$

Relation (1.3) shows in particular that $\tilde{\mathcal{E}}(u(t), w(t))$ is nonincreasing as t increases. It can be obtained by multiplying the first equation in (1.1) by w , the second equation

by $\partial_t u$, by summing the two resulting equations and integrating on Ω ; an integration by parts using the dynamic boundary condition yields the result.

Our time discretization is based on two ideas: a *splitting in time*, which decouples the resolution of the equations in the problem at each time step (as in, e.g. [5]), and a *convex splitting* of the energy. Thus, the scheme is unconditionally uniquely solvable (Proposition 3.1). A discrete version of (1.3) is then obtained if the time step is small enough (Lemma 3.2).

By letting the time step tend to 0 and using a monotonicity argument, we show that the time semi-discrete solution converges to an *energy solution* of problem (1.1) (Theorem 3.4, our main result). This notion of solution is adapted from [27], where a problem similar to (1.1), with dynamic boundary conditions for the temperature as well, has been considered (our “energy solutions” are called “weak solutions” in [27]; they are more regular than the variational solutions described in [15]). Singularities are taken into account thanks to duality techniques involving a multivalued operator.

For the numerical computation of solutions, we use a finite element method for the space discretization of the problem. At each time step, a constrained convex minimization problem is solved in order to compute the order parameter u , with the constraint that u has values in $[-1, 1]$. For this purpose, the logarithmic nonlinearity f (cf. (1.2)) is regularized, thus making a gradient available for the energy.

Our paper is organized as follows. In Section 2, we introduce the functional framework and the notion of energy solution to problem (1.1). We describe the time semi-discrete scheme and its behaviour in Section 3. In Section 4, we focus on the analysis and numerical computation of 1d stationary singular solutions to (1.1). This particular situation was pointed out as a counter-example in [34]. Section 5 concludes the paper with numerical computations of regular and singular solutions to the Caginalp system in two space dimension.

2. ENERGY SOLUTIONS

2.1. Main assumptions and notation. We set $H := L^2(\Omega)$ and denote by (\cdot, \cdot) the scalar product in H (and also in H^2 and H^3) and by $\|\cdot\|$ the related norm. Next, we set $V := H^1(\Omega)$ and denote by V' the (topological) dual of V . The duality between V' and V will be indicated by $\langle \cdot, \cdot \rangle$. Identifying H with H' through the scalar product of H , it is then well known that $V \subset H \subset V'$ with continuous and dense inclusions. In other words, (V, H, V') is a Hilbert triplet (see, e.g., [32]).

Since the system (1.1) also includes equations defined on Γ , we introduce some further spaces. Thus, we set $H_\Gamma := L^2(\Gamma)$ and $V_\Gamma := H^1(\Gamma)$ and denote by $(\cdot, \cdot)_\Gamma$ the scalar product in H_Γ , by $\|\cdot\|_\Gamma$ the corresponding norm, and by $\langle \cdot, \cdot \rangle_\Gamma$ the duality between V'_Γ and V_Γ . In general, the symbol $\|\cdot\|_X$ indicates the norm in the generic (real) Banach space X and $\langle \cdot, \cdot \rangle_X$ stands for the duality between X and X' . We also denote by ∇_Γ the tangential gradient on Γ . We can thus define the spaces

$$\mathcal{H} := H \times H_\Gamma \quad \text{and} \quad \mathcal{V} := \{z \in V : z|_\Gamma \in V_\Gamma\}.$$

We introduce the \mathcal{H} -scalar product in the following natural way,

$$((u, \psi), (v, \varphi))_{\mathcal{H}} := (u, v) + (\psi, \varphi)_\Gamma,$$

and the associated norm is denoted $\|\cdot\|_{\mathcal{H}}$. Next, we set, on \mathcal{V} ,

$$((u, v))_{\mathcal{V}} := \int_{\Omega} (\nabla u \cdot \nabla v) dx + \int_{\Gamma} u|_\Gamma v|_\Gamma + \nabla_\Gamma u|_\Gamma \cdot \nabla_\Gamma v|_\Gamma d\sigma$$

and, analogously, we set, on V ,

$$((u, v))_V := \int_{\Omega} (\nabla u \cdot \nabla v) dx + \int_{\Gamma} u|_{\Gamma} v|_{\Gamma} d\sigma.$$

Here and below, the restriction $|_{\Gamma}$ is understood in the sense of traces. We note that the norm $\|\cdot\|_V$ related to the scalar product $((\cdot, \cdot))_V$ is equivalent to the usual one. It is not difficult to prove (see, e.g. [35, Lemma 2.1]) that the space \mathcal{V} is dense in \mathcal{H} . A characterization of the spaces V' and \mathcal{V}' has been given in [27, Proposition 2.1].

We also define the continuous elliptic operators

$$\begin{aligned} A : V &\rightarrow V', & \langle Av_1, v_2 \rangle &:= \int_{\Omega} \nabla v_1 \cdot \nabla v_2 dx, \\ A_{\Gamma} : V_{\Gamma} &\rightarrow V'_{\Gamma}, & \langle A_{\Gamma} \xi_1, \xi_2 \rangle_{\Gamma} &:= \int_{\Gamma} \nabla \xi_1 \cdot \nabla \xi_2 d\sigma, \\ \mathcal{A} : \mathcal{V} &\rightarrow \mathcal{V}', & \langle \mathcal{A} v_1, v_2 \rangle_{\mathcal{V}} &:= \langle Av_1, v_2 \rangle + \langle A_{\Gamma} \xi_1, \xi_2 \rangle_{\Gamma}, \end{aligned}$$

where $\xi_i = v_i|_{\Gamma}$ for $i = 1, 2$. In particular, for $v \in V$, we have,

$$\|Av\|_{V'} \stackrel{\text{def}}{=} \sup_{\|\varphi\|_V \leq 1} \langle Av, \varphi \rangle_V = \sup_{\|\varphi\|_V \leq 1} (\nabla v, \nabla \varphi) \leq \|\nabla v\|, \quad (2.1)$$

where we used the Cauchy-Schwarz inequality.

For $v \in V'$, we denote

$$\langle v \rangle := \frac{1}{|\Omega|} \langle v, 1 \rangle,$$

where $|\Omega|$ is the measure of Ω . We notice that there exists a positive constant c_{Ω} such that

$$|\langle v \rangle| \leq c_{\Omega} \|v\|_{V'}, \quad \forall v \in V', \quad (2.2)$$

$$\|v - \langle v \rangle\|_{V'} \leq c_{\Omega} \|v\|_{V'}, \quad \forall v \in V', \quad (2.3)$$

$$\|v - \langle v \rangle\|_V \leq c_{\Omega} \|\nabla v\|, \quad \forall v \in V. \quad (2.4)$$

Next, we state our hypotheses on the nonlinearities (cf. [15]). We assume that

$$\begin{cases} 1. f \in C^2(-1, 1), \\ 2. f(0) = 0, \lim_{s \rightarrow \pm 1} f(s) = \pm \infty, \\ 3. f'(s) \geq 0, \lim_{s \rightarrow \pm 1} f'(s) = +\infty, \\ 4. f''(s) \text{sign}(s) \geq 0. \end{cases} \quad (2.5)$$

The logarithmic function f given by (1.2) satisfies these conditions.

In (2.5), the condition $f(0) = 0$ is merely a normalization: in case $f(0) \neq 0$, then by changing $f(s)$ into $f(s) - f(0)$ and w into $w - f(0)$ in system (1.1), we recover this normalization.

We assume that the (nonlinear) function g satisfies

$$g \in C^2(\mathbb{R}), \quad g'(s) \geq 0 \text{ and } \liminf_{s \rightarrow \pm \infty} g'(s) \geq \kappa_1, \quad (2.6)$$

for some $\kappa_1 > 0$. Note that we do not require $g(0) = 0$.

Remark 2.1. Let \tilde{g} be a function which belongs to $C^2([-1, 1])$. Then we can extend \tilde{g} to the whole real line to a C^2 function with compact support, also denoted \tilde{g} , and such that

$$\tilde{g}(s) = g(s) - \alpha s, \quad s \in \mathbb{R},$$

where g satisfies (2.6) and $\alpha > 0$ is chosen large enough. Thus, we recover the assumptions on the nonlinearities f and \tilde{g} which were made in [15].

We set

$$F(s) = \int_0^s f(r)dr, \quad s \in (-1, 1), \quad G(s) = \int_0^s g(r)dr, \quad s \in \mathbb{R}.$$

If $\lim_{s \rightarrow +1} F(s)$ exists, then we extend F by continuity to $s = +1$ and similarly, if $\lim_{s \rightarrow -1} F(s)$ exists, we extend F by continuity to $s = -1$. This is the case, e.g. with the logarithmic function f (1.2). Moreover, we set $F(s) = +\infty$ outside the effective domain of F ,

$$\text{dom}(F) = \{s \in \mathbb{R}, F(s) < +\infty\} \subset [-1, 1].$$

Then, identifying f and g with maximal monotone graphs in $\mathbb{R} \times \mathbb{R}$, we have $f = \partial F$ and $g = \partial G$, ∂ representing the *subdifferential* of convex analysis (here in \mathbb{R}) [2, 3, 7].

Next, we define the functional

$$J : \mathcal{H} \rightarrow \mathbb{R} \cup \{+\infty\}, \quad J(v, \varphi) := \int_{\Omega} F(v)dx + \int_{\Gamma} G(\varphi)d\sigma,$$

where it is understood that one of, or both, the integrals in the expression of J may take the value $+\infty$. We denote by ∂J the subdifferential of J in the space \mathcal{H} , namely, for $(u, \psi), (\xi, \zeta) \in \mathcal{H}$, we have

$$(\xi, \zeta) \in \partial J(u, \psi) \stackrel{\text{def}}{\iff} J(v, \varphi) \geq J(u, \psi) + ((\xi, \zeta), (v, \varphi) - (u, \psi))_{\mathcal{H}} \quad \forall (v, \varphi) \in \mathcal{H}.$$

It is well known (cf, e.g., [3, Prop. 2.8 p. 67]) that the above condition is equivalent to

$$\xi = f(u) \text{ a.e. in } \Omega \quad \text{and} \quad \zeta = g(\psi) \text{ a.e. on } \Gamma \quad (2.7)$$

(in particular, the function u then takes values in $(-1, 1)$ a.e. in Ω).

We will also need a relaxation of the functional J . Thus, we introduce the restriction $J_{\mathcal{V}}$ of J to the space \mathcal{V} and its subdifferential $\partial_{\mathcal{V}, \mathcal{V}'} J_{\mathcal{V}}$ in the \mathcal{V}' - \mathcal{V} duality. This, in view of the identification $\mathcal{H} \sim \mathcal{H}'$, has to be understood as a maximal monotone operator in $\mathcal{V} \times \mathcal{V}'$, namely, for $U \in \mathcal{V}$ and $\xi \in \mathcal{V}'$, we have

$$\xi \in \partial_{\mathcal{V}, \mathcal{V}'} J_{\mathcal{V}}(U) \stackrel{\text{def}}{\iff} J_{\mathcal{V}}(\tilde{U}) \geq J_{\mathcal{V}}(U) + \langle \xi, \tilde{U} - U \rangle_{\mathcal{V}} \quad \forall \tilde{U} \in \mathcal{V}. \quad (2.8)$$

A precise characterization of $\partial_{\mathcal{V}, \mathcal{V}'} J$ in the spirit of (2.7) is not immediate to be given. In particular, it is reasonable to expect that $\partial_{\mathcal{V}, \mathcal{V}'} J$ may be *multivalued* due to the bounded domain of f (see, e.g., [37]).

2.2. Existence and uniqueness of energy solutions. Our assumptions on the initial data are

$$U_0 := (u_0, \psi_0) \in \mathcal{V} \text{ with } J_{\mathcal{V}}(U_0) < +\infty \text{ and } w_0 \in H. \quad (2.9)$$

Definition 2.2. Let assumption (2.5)-(2.6) hold. Given (U_0, w_0) which satisfies (2.9), we say that a pair (U, w) with $U = (u, \psi)$ is an *energy solution* of problem (1.1) originating from (u_0, ψ_0, w_0) if

- $U(0) = U_0$ in \mathcal{H} and $w(0) = w_0$ in H ;
- $U \in C^0([0, +\infty); \mathcal{H}) \cap L^\infty(0, T; \mathcal{V})$ for any $T > 0$;
- $\partial_t U \in L^2(0, T; \mathcal{H})$ for any $T > 0$;
- $w \in C^0([0, +\infty); H) \cap L^2(0, T; V)$ for any $T > 0$;
- $\partial_t w \in L^2(0, T; V')$ for any $T > 0$;

and the following relations hold for a.e. t in $(0, +\infty)$:

$$\partial_t w(t) + \partial_t u(t) + Aw(t) = 0, \quad \text{in } V', \quad (2.10)$$

$$\partial_t U(t) + \mathcal{A}U(t) + \xi(t) = (w(t), 0) + (\lambda u(t), \alpha \psi(t)), \quad \text{in } \mathcal{V}', \quad (2.11)$$

$$\xi(t) \in \partial_{\mathcal{V}, \mathcal{V}'} J_{\mathcal{V}}(U(t)), \quad \text{in } \mathcal{V}'. \quad (2.12)$$

We have:

Lemma 2.3. *For two energy solutions (U^i, w^i) departing from (U_0^i, w_0^i) , $i = 1, 2$, we have the following estimate on the difference $(\tilde{U}, \tilde{w}) = (U^1 - U^2, w^2 - w^1)$ in terms of the initial datum $(\tilde{U}_0, \tilde{w}_0) := (U_0^1 - U_0^2, w_0^1 - w_0^2)$:*

$$\begin{aligned} & \|\tilde{U}(t)\|_{\mathcal{H}}^2 + \|\tilde{w}(t)\|_{V'}^2 + \int_0^t \left(\langle \mathcal{A}\tilde{U}(s), \tilde{U}(s) \rangle_{\mathcal{V}} + \|\tilde{w}(s)\|^2 \right) ds \\ & \leq \Lambda e^{\lambda' t} \left(\|\tilde{U}_0\|_{\mathcal{H}}^2 + \|\tilde{w}_0\|_{V'}^2 \right), \end{aligned} \quad (2.13)$$

where Λ is a positive constant which is independent of t and of the initial data, and $\lambda' = 2 \max\{\lambda, \alpha\} + 1$.

Proof. We write (2.10) for (U^1, w^1) and for (U^2, w^2) , we take the difference, and we integrate in time. We find that for all $t \geq 0$,

$$\tilde{w}(t) + \tilde{u}(t) + A \int_0^t \tilde{w}(s) ds = \tilde{w}_0 + \tilde{u}_0, \quad \text{in } V'. \quad (2.14)$$

Next, we write (2.11) for (U^1, w^1) and for (U^2, w^2) , and we take the difference. This yields, for a.e. $t \in (0, +\infty)$,

$$\partial_t \tilde{U}(t) + \mathcal{A}\tilde{U}(t) + \xi^1(t) - \xi^2(t) = (\tilde{w}(t), 0) + (\lambda \tilde{u}(t), \alpha \tilde{\psi}(t)), \quad \text{in } \mathcal{V}'. \quad (2.15)$$

We take the product of (2.14) by $\tilde{w}(t)$ (in the V' - V duality) and the product of (2.15) by $\tilde{U}(t)$ (in the \mathcal{V}' - \mathcal{V} duality), we add the resulting equations, and we obtain

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \left\| \int_0^t \nabla \tilde{w}(s) ds \right\|^2 + \frac{1}{2} \frac{d}{dt} \|\tilde{U}(t)\|_{\mathcal{H}}^2 + \|\tilde{w}(t)\|^2 + \langle \mathcal{A}\tilde{U}(t), \tilde{U}(t) \rangle_{\mathcal{V}} \\ & + \langle \xi^1(t) - \xi^2(t), \tilde{U}(t) \rangle_{\mathcal{V}} = \lambda \|\tilde{u}\|^2 + \alpha \|\tilde{\psi}(t)\|_{\Gamma}^2 + (\tilde{w}_0, \tilde{w}(t)) + (\tilde{u}_0, \tilde{w}(t)), \end{aligned}$$

for a.e. $t \in (0, +\infty)$. We used here that the term $(\tilde{u}(t), \tilde{w}(t))$ cancels. We write

$$\begin{aligned} (\tilde{w}_0, \tilde{w}(t)) &= (\tilde{w}_0, \tilde{w}(t) - \langle \tilde{w}(t) \rangle) + (\langle \tilde{w}_0 \rangle, \tilde{w}(t)) \\ &= \frac{1}{2} \frac{d}{dt} \left(2\tilde{w}_0, \int_0^t \tilde{w}(s) - \langle \tilde{w}(s) \rangle ds \right) + (\langle \tilde{w}_0 \rangle, \tilde{w}(t)). \end{aligned}$$

Using the monotonicity of $\partial_{\mathcal{V}, \mathcal{V}'} J_{\mathcal{V}}$ and Young's inequality, we find

$$\frac{d}{dt} \mathcal{Y}(t) + \langle \mathcal{A}\tilde{U}(t), \tilde{U}(t) \rangle_{\mathcal{V}} + \|\tilde{w}(t)\|^2 \leq 2 \max\{\lambda, \alpha\} \mathcal{Y}(t) + 2\|\langle \tilde{w}_0 \rangle\|^2 + 2\|\tilde{u}_0\|^2, \quad (2.16)$$

where

$$\mathcal{Y}(t) = \left\| \int_0^t \nabla \tilde{w}(s) ds \right\|^2 - \left(2\tilde{w}_0, \int_0^t \tilde{w}(s) - \langle \tilde{w}(s) \rangle ds \right) + c \|\tilde{w}_0\|_{V'}^2 + \|\tilde{U}(t)\|_{\mathcal{H}}^2.$$

Here, $c > 0$ is chosen large enough so that

$$\mathcal{Y}(t) \geq c_0 \left(\left\| \int_0^t \nabla \tilde{w}(s) ds \right\|^2 + \|\tilde{w}_0\|_{V'}^2 + \|\tilde{U}(t)\|_{\mathcal{H}}^2 \right) \quad (2.17)$$

for some $c_0 > 0$ (use (2.4) and Young's inequality). By (2.2), we have

$$\|\langle \tilde{w}_0 \rangle\|^2 \leq c'_\Omega \|\tilde{w}_0\|_{V'}^2. \quad (2.18)$$

Using (2.18) in (2.16) and applying Gronwall's lemma to the resulting differential inequality, we obtain

$$\mathcal{Y}(t) \leq C e^{\lambda' t} \left(\|\tilde{U}_0\|_{\mathcal{H}}^2 + \|\tilde{w}_0\|_{V'}^2 \right), \quad t \geq 0, \quad (2.19)$$

with $\lambda' = 2 \max\{\lambda, \alpha\} + 1$. Using (2.14) and (2.1), we see that

$$\|\tilde{w}(t)\|_{V'}^2 \leq C' \left(\left\| \int_0^t \nabla \tilde{w}(s) ds \right\|^2 + \|\tilde{w}_0\|_{V'}^2 + \|\tilde{u}(t)\|^2 + \|\tilde{u}_0\|^2 \right). \quad (2.20)$$

Estimate (2.13) follows from (2.19), (2.17) and (2.20). \square

Theorem 2.4. *For every initial datum (u_0, ψ_0, w_0) which satisfies (2.9), problem (1.1) possesses a unique energy solution (U, w) in the sense of Definition 2.2.*

Proof. Uniqueness follows from Lemma 2.3. Existence is a consequence of Theorem 3.4. \square

By using a regularization argument, we obtain the following result.

Theorem 2.5. *Let (u_0, ψ_0, w_0) satisfy (2.9). Then the energy solution to problem (1.1) is also a variational solution (in the sense defined in [15, Definition 4.1]).*

Proof. We first note [15, Theorem 4.3] that problem (1.1) possesses a unique variational solution for any initial condition which satisfies

$$(u_0, \psi_0, w_0) \in L^\infty(\Omega) \times L^\infty(\Gamma) \times L^2(\Omega) \text{ and } \|u_0\|_{L^\infty(\Omega)} \leq 1, \|\psi_0\|_{L^\infty(\Gamma)} \leq 1.$$

This is a weaker requirement than (2.9). We approximate the initial datum (u_0, ψ_0, w_0) which satisfies (2.9) by a sequence (u_0^k, ψ_0^k, w_0^k) such that for each k , (u_0^k, ψ_0^k, w_0^k) is regular enough, satisfies (2.9), and

$$\|u_0^k - u_0\| + \|\psi_0^k - \psi_0\|_\Gamma + \|w_0^k - w_0\| \rightarrow 0, \quad \text{as } k \rightarrow +\infty.$$

We also introduce a C^1 regularization f_N of the nonlinearity f , as in [15]. Since f_N is regular, the (unique) solution (u_N^k, ψ_N^k, w_N^k) to (1.1) where f is replaced by f_N and where the initial condition is (u_0^k, ψ_0^k, w_0^k) , is regular. Now, we let first N tend to $+\infty$, and then k tend to $+\infty$. The proof of Theorem 4.3 in [15] shows that the limit (u, ψ, w) that we obtain is the variational solution to problem (1.1). On the other hand, the theory of maximal monotone operators [2, 3, 7] shows that for each k , (u_N^k, ψ_N^k, w_N^k) tends to the energy solution (u^k, ψ^k, w^k) of (1.1) with initial condition (u_0^k, ψ_0^k, w_0^k) , as N tends to $+\infty$. Lemma 2.3 implies that, as k tends to $+\infty$, (u^k, ψ^k, w^k) tends to the energy solution of (1.1) which, by uniqueness of the limit, is (u, ψ, w) . \square

From [15, Proposition 1], we deduce:

Corollary 2.6. *We assume that either $\lim_{s \rightarrow \pm 1} F(s) = +\infty$ or*

$$g(-1) + \alpha < 0 < g(1) - \alpha. \quad (2.21)$$

Then the energy solution satisfies $-1 < u(x, t) < 1$ for a.e. $(x, t) \in \Omega \times \mathbb{R}_+$ and for a.e. $(x, t) \in \Gamma \times \mathbb{R}_+$; for all $t_0 > 0$ and for $t \geq t_0$, this solution solves (1.1) in the usual sense.

Condition (2.21) is known as the *sign condition*. For the logarithmic function f (1.2), we have $\lim_{s \rightarrow \pm 1} F(s) < +\infty$, and this sign condition is needed to guarantee that every solution to problem (1.1) is classical.

3. THE TIME SEMI-DISCRETE SCHEME

Let $\delta t > 0$ denote an arbitrary (fixed) time step. In a formal way (that is, assuming that the solution is regular enough), our time semi-discretization of (1.1) reads: let $(u^0, \psi^0, w^0) = (u_0, \psi_0, w_0)$ be given and for $n = 0, 1, 2 \dots$, let $(u^{n+1}, \psi^{n+1}, w^{n+1})$ solve

$$\begin{cases} (i) (u^{n+1} - u^n)/\delta t - \Delta u^{n+1} + f(u^{n+1}) = \lambda u^n + w^n & \text{in } \Omega, \\ (ii) (\psi^{n+1} - \psi^n)/\delta t - \Delta_\Gamma \psi^{n+1} + g(\psi^{n+1}) + \partial_n u^{n+1} = \alpha \psi^n & \text{on } \Gamma, \\ (iii) u^{n+1}|_\Gamma = \psi^{n+1}, \\ (iv) (w^{n+1} - w^n)/\delta t - \Delta w^{n+1} = -(u^{n+1} - u^n)/\delta t & \text{in } \Omega, \\ (v) \partial_n w^{n+1}|_\Gamma = 0. \end{cases} \quad (3.1)$$

This scheme is based on two types of splitting: a *splitting in time*, since we first solve the system (i)-(ii)-(iii) of (3.1), which gives us (u^{n+1}, ψ^{n+1}) , and secondly we solve (iv)-(v), which gives us w^{n+1} . We also use a *convex splitting* of the energy in (i)-(ii)-(iii), which ensures an unconditional unique solvability: the nonlinear (contractive) terms are treated implicitly, whereas the (expansive) terms λu and $\alpha \psi$ are treated explicitly.

3.1. Unconditional unique solvability and energy estimate. The rigorous version of (3.1) reads as follows. Assume that $(U^0, w^0) = (U_0, w_0)$ which satisfies (2.9) is given and for $n = 0, 1, 2, \dots$ let $(U^{n+1}, w^{n+1}) \in \mathcal{V} \times V$ with $U^{n+1} = (u^{n+1}, \psi^{n+1})$ be defined by

$$U^{n+1} \text{ minimizes } \bar{U} \mapsto \mathcal{E}_n(\bar{U}) \text{ in } \mathcal{V}, \quad (3.2)$$

where

$$\begin{aligned} \mathcal{E}_n(\bar{U}) &:= \frac{1}{2\delta t} \|\bar{U} - U^n\|_{\mathcal{H}}^2 + \frac{1}{2} \langle \mathcal{A}\bar{U}, \bar{U} \rangle_{\mathcal{V}} + J_{\mathcal{V}}(\bar{U}) \\ &\quad - \lambda(u^n, \bar{u}) - (w^n, \bar{u}) - \alpha(\psi^n, \bar{\psi})_{\Gamma} \end{aligned} \quad (3.3)$$

with $\bar{U} = (\bar{u}, \bar{\psi})$, and (once U^{n+1} is computed) $w^{n+1} \in V$ solves

$$(w^{n+1} - w^n)/\delta t + Aw^{n+1} = -(u^{n+1} - u^n)/\delta t, \quad \text{in } V'. \quad (3.4)$$

We have:

Proposition 3.1 (Unique solvability for all δt). *Assume that $(U^0, w^0) = (U_0, w_0)$ which satisfies (2.9) is given. Then there exists a unique sequence $(U^n, w^n)_{n \in \mathbb{N}}$ in $(\mathcal{V} \times H)^{\mathbb{N}}$ generated by the scheme (3.2)-(3.4). Moreover, for all $n \in \mathbb{N}$, we have $J_{\mathcal{V}}(U^n) < +\infty$.*

Proof. Assume that (U^n, w^n) satisfies $U^n \in \mathcal{V}$ and $w^n \in H$ for some $n \in \mathbb{N}$. Since $J_{\mathcal{V}}$ is convex on \mathcal{V} , the function \mathcal{E}_n , which is the sum of $J_{\mathcal{V}}$, of a continuous coercive quadratic form on \mathcal{V} and of a continuous linear form on \mathcal{V} , is strictly convex on \mathcal{V} and lower semi-continuous. Moreover, by (2.5), we have $F(s) \geq 0$ for all $s \in \text{dom}(F)$ and by (2.6), we also have

$$G(s) \geq \frac{\kappa_1}{4} s^2 - \kappa_2, \quad s \in \mathbb{R},$$

for some $\kappa_2 \geq 0$. Since the linear terms in \mathcal{E}_n are dominated by the quadratic terms, we have

$$\mathcal{E}_n(\bar{U}) \geq c_0 \|\bar{U}\|_{\mathcal{V}}^2 - c_1, \quad \bar{U} \in V,$$

for some $c_0 > 0$ small enough and some $c_1 \geq 0$. Thus, $\mathcal{E}_n(\bar{U}) \rightarrow +\infty$ as $\|\bar{U}\|_{\mathcal{V}} \rightarrow +\infty$ and so \mathcal{E}_n has a unique minimizer U^{n+1} in the Hilbert space \mathcal{V} (see, e.g., [22]). Moreover, $\mathcal{E}_n(U^{n+1}) \leq \mathcal{E}_n(U^n) < +\infty$, so $J_{\mathcal{V}}(U^{n+1}) < +\infty$ as well. Finally, the Lax-Milgram theorem shows that problem (3.4) has a unique solution $w^{n+1} \in V$. \square

We define the energy associated to U through

$$\mathcal{E}(\bar{U}) := \frac{1}{2} \langle \mathcal{A}\bar{U}, \bar{U} \rangle_{\mathcal{V}} + J_{\mathcal{V}}(\bar{U}) - \frac{\lambda}{2} \|\bar{u}\|^2 - \frac{\alpha}{2} \|\bar{\psi}\|_{\Gamma}^2, \quad \bar{U} = (\bar{u}, \bar{\psi}) \in \mathcal{V}. \quad (3.5)$$

Lemma 3.2 (Energy estimate for small δt). *Assume that $\delta t \leq 1/2$ and let $(U^n, w^n) \in \mathcal{V} \times H$ such that $J_{\mathcal{V}}(U^n) < +\infty$. Then the solution (U^{n+1}, w^{n+1}) of (3.2)-(3.4) satisfies*

$$\mathcal{E}(U^{n+1}) + \frac{1}{2} \|w^{n+1}\|^2 + \frac{1}{4\delta t} \|U^{n+1} - U^n\|_{\mathcal{H}}^2 + \delta t \|\nabla w^{n+1}\|^2 \leq \mathcal{E}(U^n) + \frac{1}{2} \|w^n\|^2. \quad (3.6)$$

Proof. By (3.2), we have $\mathcal{E}_n(U^{n+1}) \leq \mathcal{E}_n(U^n)$, which reads

$$\begin{aligned} & \frac{1}{2\delta t} \|U^{n+1} - U^n\|_{\mathcal{H}}^2 + \frac{1}{2} \langle \mathcal{A}U^{n+1}, U^{n+1} \rangle_{\mathcal{V}} + J_{\mathcal{V}}(U^{n+1}) \\ & + \lambda(u^n, u^n - u^{n+1}) + \alpha(\psi^n, \psi^n - \psi^{n+1})_{\Gamma} - (w^n, u^{n+1} - u^n) \\ & \leq \frac{1}{2} \langle \mathcal{A}U^n, U^n \rangle_{\mathcal{V}} + J_{\mathcal{V}}(U^n), \end{aligned}$$

where $U^n = (u^n, \psi^n)$. Using the well-known identity

$$(a, a - b) = \frac{1}{2} \|a\|^2 - \frac{1}{2} \|b\|^2 + \frac{1}{2} \|a - b\|^2 \quad (3.7)$$

(and similarly for the scalar product in H_{Γ}) in the terms involving λ and α , we find

$$\begin{aligned} & \frac{1}{2\delta t} \|U^{n+1} - U^n\|_{\mathcal{H}}^2 + \frac{1}{2} \langle \mathcal{A}U^{n+1}, U^{n+1} \rangle_{\mathcal{V}} + J_{\mathcal{V}}(U^{n+1}) - (w^n, u^{n+1} - u^n) \\ & - \frac{\lambda}{2} \|u^{n+1}\|^2 + \frac{\lambda}{2} \|u^{n+1} - u^n\|^2 - \frac{\alpha}{2} \|\psi^{n+1}\|_{\Gamma}^2 + \frac{\alpha}{2} \|\psi^{n+1} - \psi^n\|_{\Gamma}^2 \\ & \leq \frac{1}{2} \langle \mathcal{A}U^n, U^n \rangle_{\mathcal{V}} + J_{\mathcal{V}}(U^n) - \frac{\lambda}{2} \|u^n\|^2 - \frac{\alpha}{2} \|\psi^n\|_{\Gamma}^2. \end{aligned} \quad (3.8)$$

Next, we write

$$\begin{aligned} -(w^n, u^{n+1} - u^n) &= -(w^{n+1}, u^{n+1} - u^n) + (w^{n+1} - w^n, u^{n+1} - u^n) \\ &= (w^{n+1}, w^{n+1} - w^n) + \delta t \|\nabla w^{n+1}\|^2 + (w^{n+1} - w^n, u^{n+1} - u^n) \\ &= \frac{1}{2} \|w^{n+1}\|^2 - \frac{1}{2} \|w^n\|^2 + \frac{1}{2} \|w^{n+1} - w^n\|^2 \\ &\quad + \delta t \|\nabla w^{n+1}\|^2 + (w^{n+1} - w^n, u^{n+1} - u^n) \end{aligned}$$

where, in the second line, we used (3.4) and in the third line, we used (3.7). By the Cauchy-Schwarz inequality and Young's inequality, we have

$$|(w^{n+1} - w^n, u^{n+1} - u^n)| \leq \frac{1}{4\delta t} \|u^{n+1} - u^n\|^2 + \delta t \|w^{n+1} - w^n\|^2,$$

and so (3.8) implies

$$\begin{aligned} & \frac{1}{4\delta t} \|U^{n+1} - U^n\|_{\mathcal{H}}^2 + \mathcal{E}(U^{n+1}) + \frac{1}{2} \|w^{n+1}\|^2 + \delta t \|\nabla w^{n+1}\|^2 \\ & + \left(\frac{1}{2} - \delta t\right) \|w^{n+1} - w^n\|^2 \leq \mathcal{E}(U^n) + \frac{1}{2} \|w^n\|^2. \end{aligned} \quad (3.9)$$

Since $\delta t \leq 1/2$, this yields (3.6). \square

Remark 3.3. The energy estimate (3.6) is a discrete version of (1.3).

3.2. Convergence as $\delta t \rightarrow 0$. For a time step $\delta t > 0$, let $(U^n, w^n)_{n \geq 0}$ be a sequence generated by the time semi-discrete scheme (3.2)-(3.4). We define the following functions from \mathbb{R}_+ into \mathcal{V} :

$$\begin{aligned} U_{\delta t}(t) &= ((n+1) - t/\delta t)U^n + (t/\delta t - n)U^{n+1}, \quad t \in [n\delta t, (n+1)\delta t) \quad (n \in \mathbb{N}), \\ \bar{U}_{\delta t}(t) &= U^{n+1}, \quad t \in [n\delta t, (n+1)\delta t) \quad (n \in \mathbb{N}), \\ \underline{U}_{\delta t}(t) &= U^n, \quad t \in [n\delta t, (n+1)\delta t) \quad (n \in \mathbb{N}). \end{aligned}$$

We define similarly the functions $w_{\delta t}$, $\bar{w}_{\delta t}$ and $\underline{w}_{\delta t}$ from \mathbb{R}_+ to H associated to the sequence $(w^n)_{n \geq 0}$. Note that

$$\partial_t U_{\delta t} = \frac{U^{n+1} - U^n}{\delta t} \text{ in } \mathcal{D}'((0, +\infty); \mathcal{V}) \quad (3.10)$$

and

$$\partial_t w_{\delta t} = \frac{w^{n+1} - w^n}{\delta t} \text{ in } \mathcal{D}'((0, +\infty); H). \quad (3.11)$$

Here, as usual, the notation \mathcal{D}' means that the equality holds in the sense of distributions (see, e.g., [32]).

Theorem 3.4. *Let $(U^0, w^0) = (U_0, w_0)$ such that (2.9) holds. Then the solution $(U_{\delta t}, w_{\delta t})$ associated to scheme (3.2)-(3.4) tends to the energy solution (U, w) of problem (1.1) in the following sense, as $\delta t \rightarrow 0$:*

$$\begin{aligned} U_{\delta t} &\rightarrow U && \text{weakly-} \star \text{ in } L^\infty(0, +\infty; \mathcal{V}), \\ U_{\delta t} &\rightarrow U && \text{strongly in } C^0([0, T]; \mathcal{H}), \text{ for any } T > 0, \\ \partial_t U_{\delta t} &\rightarrow \partial_t U && \text{weakly in } L^2(0, +\infty; \mathcal{H}), \\ w_{\delta t} &\rightarrow w && \text{weakly-} \star \text{ in } L^\infty(0, +\infty; H), \\ w_{\delta t} &\rightarrow w && \text{strongly in } C^0([0, T]), \text{ for any } T > 0, \\ \partial_t w_{\delta t} &\rightarrow \partial_t w && \text{weakly in } L^2(0, T; V'), \text{ for any } T > 0. \end{aligned}$$

Proof. By Proposition 3.1, for all n we have $J_{\mathcal{V}}(U^n) < +\infty$, so that

$$-1 \leq u^n \leq 1 \text{ for a.e. } x \in \Omega \text{ and } -1 \leq \psi^n \leq 1 \text{ for a.e. } x \in \Gamma. \quad (3.12)$$

By induction, estimate (3.6) yields

$$\mathcal{E}(U^n) + \frac{1}{2} \|w^n\|^2 + \frac{1}{4\delta t} \sum_{k=0}^{n-1} \|U^{k+1} - U^k\|_{\mathcal{H}}^2 + \delta t \sum_{k=0}^{n-1} \|\nabla w^{k+1}\|^2 \leq \mathcal{E}(U^0) + \frac{1}{2} \|w^0\|^2,$$

for all $n \geq 1$. Using (3.12) and the definition (3.5) of \mathcal{E} , this yields

$$\begin{aligned} & \frac{1}{2} \langle \mathcal{A}U^n, U^n \rangle + J_{\mathcal{V}}(U^n) + \frac{1}{2} \|w^n\|^2 + \frac{1}{4\delta t} \sum_{k=0}^{n-1} \|U^{k+1} - U^k\|_{\mathcal{H}}^2 \\ & + \delta t \sum_{k=0}^{n-1} \|\nabla w^{k+1}\|^2 \leq \mathcal{E}(U^0) + \frac{1}{2} \|w^0\|^2 + \frac{\lambda}{2} |\Omega|^{1/2} + \frac{\alpha}{2} |\Gamma|^{1/2}, \end{aligned} \quad (3.13)$$

for all $n \geq 1$. Since the right-hand side above is finite by assumption, this shows that $(U^n)_n$ is bounded in \mathcal{V} and $(w^n)_n$ is bounded in H . Thus, $(U_{\delta t})$, $(\bar{U}_{\delta t})$, $(\underline{U}_{\delta t})$ are bounded in $L^\infty(0, +\infty; \mathcal{V})$ and $(w_{\delta t})$, $(\bar{w}_{\delta t})$, $(\underline{w}_{\delta t})$ are bounded in $L^\infty(0, +\infty; H)$. By letting n tend to $+\infty$ in (3.13), we see that

$$\frac{1}{4\delta t} \sum_{k=0}^{+\infty} \|U^{k+1} - U^k\|_{\mathcal{H}}^2 + \delta t \sum_{k=0}^{+\infty} \|\nabla w^{k+1}\|^2 \leq C, \quad (3.14)$$

where $C < +\infty$ is the right-hand side of (3.13). Thanks to (3.10), this can be rewritten

$$\frac{1}{4} \int_0^{+\infty} \|\partial_t U_{\delta t}\|_{\mathcal{H}}^2 dt + \int_0^{+\infty} \|\nabla \bar{w}_{\delta t}\|^2 dt \leq C, \quad (3.15)$$

which shows that $(\partial_t U_{\delta t})$ is bounded in $L^2(0, +\infty; \mathcal{H})$ and $(\nabla \bar{w}_{\delta t})$ is bounded in $L^2(0, +\infty; H^d)$ (with $d = 2$ if $\Omega \subset \mathbb{R}^2$ and $d = 3$ if $\Omega \subset \mathbb{R}^3$). Moreover,

$$\delta t \sum_{k=0}^{+\infty} \|U^{k+1} - U^k\|_{\mathcal{H}}^2 = \int_0^{+\infty} \|\bar{U}_{\delta t} - \underline{U}_{\delta t}\|_{\mathcal{H}}^2 dt \leq 4\delta t^2 C, \quad (3.16)$$

and similarly,

$$\int_0^{+\infty} \|\bar{U}_{\delta t} - U_{\delta t}\|_{\mathcal{H}}^2 dt \leq 4\delta t^2 C \quad (3.17)$$

From the estimates above, we deduce that, up to a subsequence, $(U_{\delta t})$, $(\bar{U}_{\delta t})$ and $(\underline{U}_{\delta t})$ converge weakly- \star in $L^\infty(0, +\infty; \mathcal{V})$ to the same limit U , as δt tends to 0. The limit U is the same in $L^2(0, +\infty; \mathcal{H})$ by (3.16)-(3.17), and therefore also in $\mathcal{D}'(0, +\infty; \mathcal{H})$. Moreover, $\partial_t U \in L^2(0, +\infty; \mathcal{H})$ by (3.15). By a well-known result [38], for any $T > 0$, the space $\{\tilde{U} \in L^\infty(0, T; \mathcal{V}), \partial_t \tilde{U} \in L^2(0, T; \mathcal{H})\}$ is compactly imbedded in the space $C^0([0, T]; \mathcal{H})$. Thus, $(U_{\delta t})$ converges to U strongly in $C^0([0, T]; \mathcal{H})$, for any $T > 0$. In particular, the initial condition $U(0) = U_0$ is satisfied.

Using (3.4) and (2.1), we have

$$\|w^{n+1} - w^n\|_{V'} \leq \delta t \|\nabla w^{n+1}\| + \|u^{n+1} - u^n\|_H.$$

Thus,

$$\delta t \sum_{n=0}^{+\infty} \|w^{n+1} - w^n\|_{V'}^2 \leq 2\delta t^3 \sum_{n=0}^{+\infty} \|\nabla w^{n+1}\|^2 + 2\delta t \sum_{n=0}^{+\infty} \|u^{n+1} - u^n\|_H^2. \quad (3.18)$$

Using the estimates above, we see that

$$\int_0^{+\infty} \|\bar{w}_{\delta t} - w_{\delta t}\|_{V'}^2 dt \leq \int_0^{+\infty} \|\bar{w}_{\delta t} - \underline{w}_{\delta t}\|_{V'}^2 dt \leq 8C\delta t^2.$$

From these estimates, we deduce that, up to a subsequence, $(w_{\delta t})$, $(\bar{w}_{\delta t})$, and $(\underline{w}_{\delta t})$ converge weakly- \star in $L^\infty(0, +\infty; H)$ and weakly in $L^2(0, T; V)$ for any $T > 0$ to the same limit w .

It remains to prove that the limit, which has been denoted (U, w) for notational convenience, is indeed the energy solution to problem (1.1).

First, owing to (3.10)-(3.11), equation (3.4) can be written

$$\partial_t w_{\delta t} = -A\bar{w}_{\delta t} - \partial_t u_{\delta t} \text{ in } L^2(0, T; V'), \text{ for any } T > 0. \quad (3.19)$$

Thus, $(\partial_t w_{\delta t})$ is bounded in $L^2(0, T; V')$ for any $T > 0$ and letting δt tend to 0 in this (linear) equation, we find that

$$\partial_t w = -Aw - \partial_t u \text{ in } L^2(0, T; V'), \text{ for any } T > 0. \quad (3.20)$$

Since, for any $T > 0$, the space $\{\tilde{w} \in L^2(0, T; V), \partial_t \tilde{w} \in L^2(0, T; V')\}$ is compactly imbedded in the space $C^0([0, T]; H)$ [38], we also obtain that $(w_{\delta t})$ converges strongly to w in $C^0([0, T]; H)$, for any $T > 0$. In particular, the initial condition $w(0) = w_0$ is satisfied.

Secondly, owing to the definition (2.8) of $\partial_{\mathcal{V}, \mathcal{V}'} J_{\mathcal{V}}$, the Euler-Lagrange equation of the minimization problem (3.2)-(3.3) reads

$$\frac{1}{\delta t}(U^{n+1} - U^n) + \mathcal{A}U^{n+1} + \xi^{n+1} = (\lambda u^n, \alpha \psi^n) + (w^n, 0) \text{ in } \mathcal{V}',$$

with $\xi^{n+1} \in \partial_{\mathcal{V}, \mathcal{V}'} J_{\mathcal{V}}(U^{n+1})$. This can be rewritten

$$\partial_t U_{\delta t} + \mathcal{A}\bar{U}_{\delta t} + \bar{\xi}_{\delta t} = (\lambda \underline{u}_{\delta t}, \alpha \underline{\psi}_{\delta t}) + (\underline{w}_{\delta t}, 0) \text{ in } L^2(0, T; \mathcal{V}'), \quad (3.21)$$

for any $T > 0$, where

$$\bar{\xi}_{\delta t}(t) \stackrel{\text{def}}{=} \xi^{n+1} \in \partial_{\mathcal{V}, \mathcal{V}'} J_{\mathcal{V}}(\bar{U}_{\delta t}(t)) \text{ for all } t \in [n\delta t, (n+1)\delta t) \quad (n \in \mathbb{N}). \quad (3.22)$$

We set $T > 0$ and we introduce the maximal monotone operator \mathcal{B}_T in $L^2(0, T; \mathcal{V}) \times L^2(0, T; \mathcal{V}')$ defined for all $(U, \xi) \in L^2(0, T; \mathcal{V}) \times L^2(0, T; \mathcal{V}')$ by [7, Exemple 2.3.3. p.25]

$$\xi \in \mathcal{B}_T(U) \iff \xi(t) \in \mathcal{B}_T U(t) \text{ for a.e. } t \in (0, T).$$

Since \mathcal{B}_T is a maximal monotone operator [7, p.22], for all $(U, \xi) \in L^2(0, T; \mathcal{V}) \times L^2(0, T; \mathcal{V}')$, we have

$$\xi \in \mathcal{B}_T(U) \iff \int_0^T \langle \xi(t) - \tilde{\xi}(t), U(t) - \tilde{U}(t) \rangle_{\mathcal{V}} dt \geq 0 \quad (3.23)$$

for all $(\tilde{U}, \tilde{\xi}) \in L^2(0, T; \mathcal{V}) \times L^2(0, T; \mathcal{V}')$ such that $\tilde{\xi} \in \mathcal{B}_T(\tilde{U})$.

Let $(\tilde{U}, \tilde{\xi}) \in L^2(0, T; \mathcal{V}) \times L^2(0, T; \mathcal{V}')$ such that $\tilde{\xi} \in \mathcal{B}_T(\tilde{U})$. From (3.22)-(3.23), we deduce that

$$I_{\delta t} \stackrel{\text{def}}{=} \int_0^T \langle \bar{\xi}_{\delta t} - \tilde{\xi}, \bar{U}_{\delta t} - \tilde{U} \rangle_{\mathcal{V}} dt \geq 0. \quad (3.24)$$

Equation (3.21) yields

$$I_{\delta t} = \int_0^T \langle -\partial_t U_{\delta t} - \mathcal{A}\bar{U}_{\delta t} + (\lambda \underline{u}_{\delta t}, \alpha \underline{\psi}_{\delta t}) + (\underline{w}_{\delta t}, 0) - \tilde{\xi}, \bar{U}_{\delta t} - \tilde{U} \rangle_{\mathcal{V}} dt.$$

We write $I_{\delta t} = I_{\delta t}^1 + I_{\delta t}^2 + I_{\delta t}^3$ where

$$\begin{aligned} I_{\delta t}^1 &= - \int_0^T \langle \partial_t U_{\delta t}, \bar{U}_{\delta t} - \tilde{U} \rangle_{\mathcal{V}} dt, \\ I_{\delta t}^2 &= - \int_0^T \langle \mathcal{A} \bar{U}_{\delta t}, \bar{U}_{\delta t} - \tilde{U} \rangle_{\mathcal{V}} dt, \\ I_{\delta t}^3 &= \int_0^T \langle (\lambda \underline{u}_{\delta t}, \alpha \underline{\psi}_{\delta t}) + (\underline{w}_{\delta t}, 0) - \tilde{\xi}, \bar{U}_{\delta t} - \tilde{U} \rangle_{\mathcal{V}} dt. \end{aligned}$$

Arguing as in (3.17), we see that

$$\int_0^T \|U_{\delta t} - \underline{U}_{\delta t}\|_{\mathcal{H}}^2 dt \leq 4\delta t^2 C.$$

Using that $(U_{\delta t})$ converges strongly to U in $C^0([0, T]; \mathcal{H})$, we obtain that $(\underline{U}_{\delta t})$ converges strongly to U in $L^2(0, T; \mathcal{H})$. Thus, $((\lambda \underline{u}_{\delta t}, \alpha \underline{\psi}_{\delta t}))$ converges strongly to $(\lambda u, \alpha \psi)$ in $L^2(0, T; \mathcal{V}')$. Similarly, $(\underline{w}_{\delta t})$ converges strongly to w in $L^2(0, T; H)$. This shows that

$$I_{\delta t}^3 \rightarrow \int_0^T \langle (\lambda u, \alpha \psi) + (w, 0) - \tilde{\xi}, U - \tilde{U} \rangle_{\mathcal{V}} dt, \quad (3.25)$$

as $\delta t \rightarrow 0$.

Next, we write

$$I_{\delta t}^1 = - \int_0^T \langle \partial_t U_{\delta t}, U_{\delta t} \rangle_{\mathcal{V}} dt - \int_0^T \langle \partial_t U_{\delta t}, \bar{U}_{\delta t} - U_{\delta t} \rangle_{\mathcal{V}} dt + \int_0^T \langle \partial_t U_{\delta t}, \tilde{U} \rangle_{\mathcal{V}} dt.$$

In the right-hand side above, the last integral tends to $\int_0^T \langle \partial_t U, \tilde{U} \rangle_{\mathcal{V}} dt$ and the second integral tends to 0 thanks to the Cauchy-Schwarz inequality and the estimates (3.15) and (3.17). The first integral reads (see, e.g. [39, Lemma 1.2, Ch. III])

$$\int_0^T \langle \partial_t U_{\delta t}, U_{\delta t} \rangle_{\mathcal{V}} dt = \frac{1}{2} \|U_{\delta t}(T)\|_{\mathcal{H}}^2 - \frac{1}{2} \|U_{\delta t}(0)\|_{\mathcal{H}}^2,$$

and this tends to

$$\frac{1}{2} \|U(T)\|_{\mathcal{H}}^2 - \frac{1}{2} \|U(0)\|_{\mathcal{H}}^2 = \int_0^T \langle \partial_t U, U \rangle_{\mathcal{V}} dt,$$

owing to the strong convergence of $(U_{\delta t})$ in $C^0([0, T], \mathcal{H})$. Thus,

$$I_{\delta t}^1 \rightarrow - \int_0^T \langle \partial_t U, U - \tilde{U} \rangle_{\mathcal{V}} dt, \quad (3.26)$$

as $\delta t \rightarrow 0$.

The term $I_{\delta t}^2$ reads

$$I_{\delta t}^2 = - \int_0^T \langle \mathcal{A} U_{\delta t}, U_{\delta t} \rangle_{\mathcal{V}} dt + \int_0^T \langle \mathcal{A} U_{\delta t}, U \rangle_{\mathcal{V}} dt.$$

The second integral in the right-hand side above tends to $\int_0^T \langle \mathcal{A} U, U \rangle_{\mathcal{V}} dt$, and by lower semi-continuity of the semi-norm in the Hilbert space $L^2(0, T; \mathcal{V})$, we have

$$\int_0^T \langle \mathcal{A} U, U \rangle_{\mathcal{V}} dt \leq \liminf_{\delta t \rightarrow 0} \int_0^T \langle \mathcal{A} U_{\delta t}, U_{\delta t} \rangle_{\mathcal{V}} dt.$$

Thus,

$$-\int_0^T \langle \mathcal{A}U, U - \tilde{U} \rangle_{\mathcal{V}} dt \geq \limsup_{\delta t \rightarrow 0} I_{\delta t}^2. \quad (3.27)$$

Summing up (3.24)-(3.27), we have proved that

$$\int_0^T \langle -\partial_t U - \mathcal{A}U + (\lambda u, \alpha \psi) + (w, 0) - \tilde{\xi}, U - \tilde{U} \rangle_{\mathcal{V}} dt \geq 0.$$

From (3.23), we deduce that $\xi \in \mathcal{B}_T(U)$ where

$$\xi = -\partial_t U - \mathcal{A}U + (\lambda u, \alpha \psi) + (w, 0) \text{ in } L^2(0, T; \mathcal{V}').$$

Recalling the definition of \mathcal{B}_T , this reads

$$\partial_t U(t) + \mathcal{A}U(t) + \xi(t) = (\lambda u(t), \alpha \psi(t)) + (w(t), 0) \text{ in } \mathcal{V}',$$

with $\xi(t) \in \partial_{\mathcal{V}, \mathcal{V}'} J(U(t))$, for a.e. $t \in (0, T)$. This relation is valid for any $T > 0$. It shows that (U, w) is the energy solution to problem (1.1). By uniqueness of the energy solution, the whole sequence $(U_{\delta t}, w_{\delta t})$ tends to (U, w) . The proof is complete. \square

4. ANALYSIS AND NUMERICAL APPROACH FOR A SINGULAR 1D STATIONARY CASE

In this section, we focus on the following boundary value problem in $(-L, L)$ ($0 < L < +\infty$): for a given $K \geq 0$, find the function y which solves

$$\begin{cases} -y'' + f(y) = 0 & \text{in } (-L, L), \\ y'(-L) = K, \quad y'(L) = K, \end{cases} \quad (4.1)$$

where f is the (singular) logarithmic potential

$$f(s) = \ln \left(\frac{1+s}{1-s} \right), \quad s \in (-1, 1). \quad (4.2)$$

This problem was pointed out as a counter-example in [34]. It can be seen as a stationary case of the Caginalp system (1.1) for $\Omega = (-L, L)$ by choosing $w = 0$, $y = u$, $\lambda = \alpha = 0$ and $g(s) = -K$ if $x = +L$, $g(s) = +K$ if $x = -L$ (since Ω is an interval, the Laplace-Beltrami operator does not appear in this case).

4.1. Analysis. For small K , problem (4.1) has a (unique) classical solution, but for large K , this is no longer the case (cf. Proposition 4.2) and it is necessary to introduce another notion of solution (note that for $K \leq 0$, the situation is similar since $-y$ is a solution of the ODE). In the spirit of our scheme, we consider *energy solutions*.

More precisely, assume that y is a classical solution of (4.1). Then, on multiplying the first equation by a test function φ and integrating by parts, we find that y satisfies

$$\int_{-L}^L y'(x) \varphi'(x) dx - K \varphi(+L) + K \varphi(-L) + \int_{-L}^L f(y(x)) \varphi(x) dx = 0, \quad (4.3)$$

for all $\varphi \in C^1([-1, 1])$. Thus, y is a critical point of the functional

$$\mathcal{E}_K(z) := \int_{-L}^L \frac{(z')^2}{2} + F(z) dx - Kz(+L) + Kz(-L), \quad (4.4)$$

where

$$F(s) = \int_0^s f(\sigma) d\sigma = (1+s) \ln(1+s) + (1-s) \ln(1-s), \quad s \in [-1, 1].$$

Note that F is extended by continuity on $[-1, 1]$.

Let us introduce the set

$$\mathcal{C} = \{z \in H^1(-L, L) : z(x) \in [-1, 1] \text{ for all } x \in [-L, L]\},$$

which is a closed convex subset of $H^1(-L, L)$. We have used the continuous Sobolev imbedding (see, e.g., [8])

$$H^1(-L, L) \subset C^0([-L, L]). \quad (4.5)$$

It is easily seen that \mathcal{E}_K is continuous, coercive and strictly convex on \mathcal{C} . Moreover, \mathcal{E}_K is symmetric in the sense that $\mathcal{E}_K(x \mapsto -z(-x)) = \mathcal{E}_K(z)$. Thus, we have (see, e.g. [22]):

Proposition 4.1. *The functional \mathcal{E}_K has a unique minimizer y_K on \mathcal{C} , which is odd. If $y \in C^2([-L, L])$ is a classical solution of (4.1), then $y = y_K$.*

Proof. We prove that \mathcal{E}_K is coercive, i.e. $\mathcal{E}_K(z) \rightarrow +\infty$ as $\|z\|_{H^1} \rightarrow +\infty$ with $z \in \mathcal{C}$ (the other claims are immediate). We have

$$f''(s) = \frac{2}{1-s^2} \geq 2, \quad s \in (-1, 1). \quad (4.6)$$

Thus, $f(s) \geq 2s$ for $s \in [0, 1)$ and $F(s) \geq s^2$ for $s \in [-1, 1]$. This shows that

$$\mathcal{E}_k(z) \geq \frac{1}{2} \|z\|_{H^1(-L, L)}^2 - Kz(+L) + Kz(-L).$$

The linear terms are controlled by the quadratic term thanks to the Sobolev imbedding (4.5). This proves that \mathcal{E}_K is coercive. \square

On studying the phase portrait of (4.1), the following result can be proved.

Proposition 4.2. *There exists $K_+ > 0$ such that for $0 \leq K < K_+$, problem (4.1) has a unique solution $y \in C^2([-L, L])$ and for $K > K_+$, problem (4.1) has no classical solution. For $K = K_+$ problem (4.1) has a unique solution $y_+ \in C^2((-L, L)) \cap C^1([-L, L])$ which satisfies $y_+(-L) = -1$ and $y_+(+L) = +1$.*

Proof. We have already seen that any classical solution y is equal to y_K . Conversely, we note that any odd solution satisfies $y(0) = 0$, so we consider the maximal solution of

$$-y'' + f(y) = 0 \quad (4.7)$$

with initial condition $y(0) = 0$ and $y'(0) > 0$ (the case $y'(0) < 0$ is obtained by symmetry and for $y'(0) = 0$, the solution is $y \equiv 0$ on $(-\infty, +\infty)$). By symmetry, any such solution is odd and defined on a maximal interval $(-T^+, T^+)$.

On multiplying (4.7) by y' and integrating, we find that $(y')^2/2 - F(y) = C$ for some positive constant C . Since $y'(0) > 0$, y is increasing on $[0, T^+)$ and $y' = \sqrt{2C + F(y)}$ on $[0, T^+)$. Thus, T^+ is defined by

$$\int_0^1 \frac{dz}{\sqrt{2C + F(z)}} = T^+.$$

This shows that T^+ is a continuous and (strictly) decreasing function of C , with

$$\lim_{C \rightarrow 0^+} T^+ = +\infty \quad \text{and} \quad \lim_{C \rightarrow +\infty} T^+ = 0.$$

Therefore, there exists a unique $C_L \in (0, +\infty)$ such that $T^+ = L$. This defines the solution $y_+ \in C^2((-L, L)) \cap C^1([-L, L])$ with $K_+ = y'_+(L)$ and it shows that for $0 < C < C_L$, the corresponding solution y is defined on $[0, T^+)$ which contains $[0, L]$: we have a classical solution of (4.1). For $C > C_L$, $T^+ < L$ and we have no classical solution of (4.1). \square

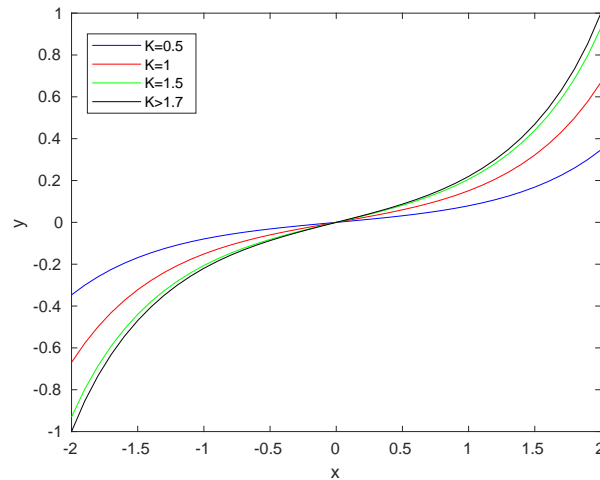


FIGURE 1. Solution y_K for different values of K

4.2. Numerical resolution. In Figure 1, we have computed numerically the solution

$$y_K = \arg \min_{z \in \mathcal{C}} \mathcal{E}_K(z)$$

whose existence is asserted by Proposition 4.1. We have used a finite difference approximation with a uniform subdivision $x_i = -L + ih$ ($i = 0, 1, \dots, 2M$) of $[-L, L]$ with step size $h = L/M$. A discrete version of the energy $\mathcal{E}_K(z)$ with the values $(z_i)_{0 \leq i \leq 2M}$ approximating $z(x_i)$ was used.

We have chosen the parameters $L = 2$, $M = 20$, and the minimization was performed with the `Matlab`[®] nonlinear programming solver `fmincon` with constraints $-1 \leq z_i \leq 1$. This solver finds the minimum of a function with inequality constraints and does not require the gradient of the function (the gradient would be singular for $z_i = \pm 1$).

We have found that the critical value K_+ in this case is approximately $K_+ = 1.7$. For $K < K_+$, the solution y_K is regular (Proposition 4.1) and for $K > K_+$, we have $y_K = y_{K_+}$ (Theorem 4.3).

Nonlinear solvers for the minimization of a function are known to be more efficient if a gradient is available (see, e.g., [10]). In view of the 2d computations, we have therefore computed numerically the solutions of the two regularized problems

$$y_K^\varepsilon = \arg \min_{z \in H^1(-L, L)} \mathcal{E}_K^\varepsilon(z) \quad (4.8)$$

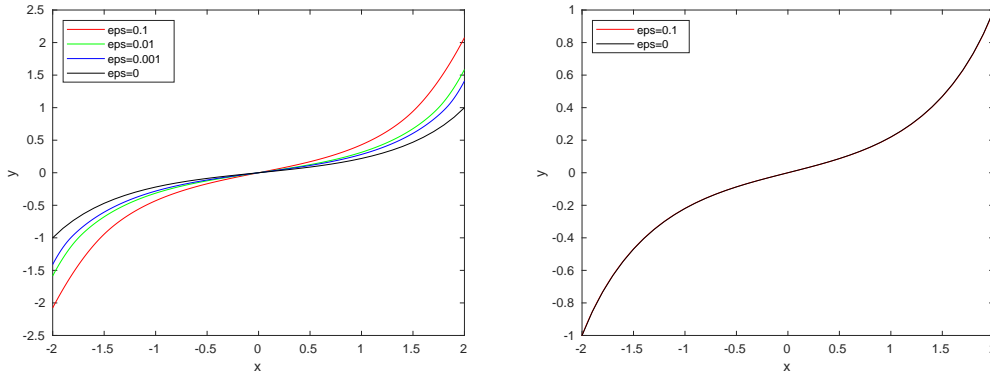


FIGURE 2. Solutions of the regularized problem without constraint (y_K^ε , left) and with constraint (\tilde{y}_K^ε , right)

and

$$\tilde{y}_K^\varepsilon = \arg \min_{z \in \mathcal{C}} \mathcal{E}_K^\varepsilon(z). \quad (4.9)$$

In this case, we replace f by the regularization

$$f^\varepsilon(s) = \begin{cases} f(s) & \text{if } |s| \leq 1 - \varepsilon, \\ f(1 - \varepsilon) & \text{if } s > 1 - \varepsilon, \\ f(-1 + \varepsilon) & \text{if } s < -1 + \varepsilon, \end{cases} \quad (4.10)$$

which is continuous and odd on \mathbb{R} . We set

$$F^\varepsilon(s) = \int_0^s f^\varepsilon(\sigma) d\sigma, \quad s \in \mathbb{R}, \quad (4.11)$$

which is of class C^1 on \mathbb{R} and even. The energy function $\mathcal{E}_K^\varepsilon$ is defined as \mathcal{E}_K (cf. (4.4)) with F replaced by F^ε . As a consequence, $\mathcal{E}_K^\varepsilon$ is of class C^1 on $H^1(-L, L)$. Moreover, $\mathcal{E}_K^\varepsilon$ is coercive and strictly convex on $H^1(-1, 1)$, so that the minimizers y_K^ε and \tilde{y}_K^ε are well-defined and unique. The function y_K^ε solves a nonconstrained convex optimization problem, whereas \tilde{y}_K^ε solves a constrained convex optimization problem.

For the numerical simulations presented in Fig. 2, we have set $K = 3$ which corresponds to a singular case for y_K (cf. Fig. 1); this singular solution y_K , which corresponds formally to the case $\varepsilon = 0$, is represented in black in Fig. 2 (left and right).

The solution y_K^ε is represented for several values of ε on the left of Fig. 2. It was computed by a finite difference approximation of problem (4.8) as previously, with a uniform subdivision of step size $h = 2L/2M$ for $M = 20$. The `Matlab`[®] minimization solver `fminunc` was used. As ε gets closer to 0, we observe that y_K^ε converges to y_K . However, the speed of convergence is slow.

In contrast, in Fig. 2 (right), we have computed the solution \tilde{y}_K^ε for a reasonable value $\varepsilon = 0.1$, and there is no visual difference between y_K^ε and y_K . In comparison with the calculation of y_K , the `fmincon` solver could be used efficiently for \tilde{y}_K^ε with a much larger number of unknowns, namely 201 (corresponding to $M = 100$), thanks to the gradient available for the regularized discrete problem.

4.3. Interpretation of the singularity. Let $K > K_+$. Formally, we have $y_K^\varepsilon \rightarrow y_K$ as $\varepsilon \rightarrow 0$. We also have $y_K = y_{K_+}$ (Theorem 4.3). This means that $(y_K^\varepsilon)'$ goes from K_+ to K on a small interval near $x = +L$, and at the limit $\varepsilon = 0$, y_K' has a discontinuity at $x = +L$, which jumps from K_+ to K . Thus, we expect that y_K'' has a Dirac measure at $x = +L$ (and also at $x = -L$, by symmetry). We make this formal argument rigorous in Corollary 4.4.

For this purpose, we use the notion of variational solution which was proposed by Miranville and Zelik [34] in the context of the Cahn-Hilliard equation. First assume that y is a classical solution of (4.1). On replacing φ by $y - \varphi$ in (4.3), we have

$$\int_{-L}^L y'(y' - \varphi')dx + \int_{-L}^L f(y)(y - \varphi)dx = K[y(+L) - \varphi(+L)] - K[y(-L) - \varphi(-L)],$$

for all $\varphi \in H^1(-L, L)$. The monotonicity of f yields

$$\int_{-L}^L f(y)(y - \varphi)dx \geq \int_{-L}^L f(\varphi)(y - \varphi)dx.$$

We also note that

$$\int_{-L}^L y'(y' - \varphi')dx \geq \int_{-L}^L \varphi'(y' - \varphi')dx.$$

Thus, if y is a regular solution of (4.1), we have

$$\int_{-L}^L \varphi'(y' - \varphi')dx + \int_{-L}^L f(\varphi)(y - \varphi)dx \leq K[y(+L) - \varphi(+L)] - K[y(-L) - \varphi(-L)], \quad (4.12)$$

for every test function φ .

We say that y is a *variational solution* to problem (4.1) if $y \in H^1(-L, L)$,

$$-1 < y(x) < 1 \text{ for all } x \in (-L, L), \quad f(y) \in L^1(-L, L)$$

and (4.12) holds for all $\varphi \in H^1(-L, L)$ such that $f(\varphi) \in L^1(-L, L)$.

From this definition, we may deduce:

Theorem 4.3. *Let K_+ and y_+ be as in Proposition 4.2. Then for $K \geq K_+$, we have $y_K = y_+$.*

Proof. Since y_+ is a regular solution of problem (4.1) for $K = K_+$, it is also a variational solution, henceforth it satisfies (4.12), that is

$$\int_{-L}^L \varphi'(y_+' - \varphi')dx + \int_{-L}^L f(\varphi)(y_+ - \varphi)dx \leq K_+[y_+(+L) - \varphi(+L)] - K_+[y_+(-L) - \varphi(-L)], \quad (4.13)$$

for all $\varphi \in H^1(-L, L)$ such that $f(\varphi) \in L^1(-L, L)$. If φ is a test function, then φ is continuous on $[-L, L]$ by (4.5) and $\varphi(x) \in [-1, 1]$ for all $x \in [-L, L]$. Thus, we have

$$[y_+(+L) - \varphi(+L)] = 1 - \varphi(+L) \geq 0$$

and

$$-[y_+(-L) - \varphi(-L)] = -[-1 - \varphi(-L)] \geq 0.$$

This shows that (4.13) also holds if we replace K_+ by any value $K \geq K_+$. In other words, y_+ is a variational solution of problem (4.1) for all $K \geq K_+$. The variational

solution is unique [15], and it can also be shown by a regularization process that the energy solution y_K is also the variational solution (see Theorem 2.5). Thus, $y_K = y_+$ for all $K \geq K_+$. \square

As a consequence, we have (compare with (4.3)):

Corollary 4.4. *Let $K \geq K_+$. Then y_K satisfies*

$$\int_{-L}^L y'_K(x)\varphi'(x)dx - K\varphi(+L) + K\varphi(-L) + \langle \mu_K, \varphi \rangle_{C^0([-L,L])} = 0,$$

for all $\varphi \in H^1(-L, L)$, where $\mu_K \in [C^0([-L, L])]'$ is the measure defined by

$$\mu_K = f(y_K) + (K - K_+)\delta_{+L} - (K - K_+)\delta_{-L}.$$

Here, $\delta_{\pm L}$ denotes the Dirac measure at $x = \pm L$. We recall that $f(y_K) \in L^1(-L, L)$.

Proof. Since $y_K = y_+$ and y_+ is a classical solution of problem (4.1), equation (4.3) shows that

$$\int_{-L}^L y'_K(x)\varphi'(x)dx - K_+\varphi(+L) + K_+\varphi(-L) + \int_{-L}^L f(y_K(x))\varphi(x)dx = 0,$$

for all $\varphi \in H^1(-L, L)$. The claim follows. \square

Remark 4.5. The apparition of a Dirac measure has been analyzed for a closely related problem in [37]. It can be related to the fact that the maximal monotone operator involved in this problem is multivalued (cf. (2.8)). Corollary 4.4 shows that for problem (4.1), the support of the singular part belongs to the boundary of the domain and corresponds to a discontinuity of the normal derivative of the solution. The latter phenomenon has been described for the evolutionary 3d Caginalp problem in terms of the variational solution of the problem in [15, Theorem 5.2].

5. 2D NUMERICAL RESULTS

We have performed numerical simulations in two space dimension for the Caginalp system (1.1) on the rectangle $\Omega = [0, L_x] \times [0, L_y]$ with $L_x = 8$ and $L_y = 4$, with periodic boundary conditions on the left/right sides and dynamic boundary conditions on the upper/lower sides (this type of domain is also known as a “slab”).

For the space discretization, we used a finite element approximation with piecewise continuous (P^1) finite elements both for the order parameter u and for the temperature w . The rectangle was divided into 6400 triangles obtained by dividing the rectangle into 3200 squares of side $h = L_x/80 = L_y/40 = 1/10$, each square being itself divided into two right-angled isosceles triangles along the south-west/north-east diagonal.

In problem (1.1), we chose the logarithmic function f defined by (1.2) and the parameters were set equal to $\lambda = 3$ and $\alpha = 0$. The function g was set equal to $g(s) = s - \beta$ where the constant β will be specified below.

For the time discretization, we used the doubly splitting scheme (3.2)-(3.4) with a continuous regularization of f , namely the approximation f^ε given by (4.10). The convex minimization problem was performed with the constraint that the solution u takes values in $[-1, 1]$, as in (4.9).

The s were made with the FreeFem++ software [29]. For the optimization problem, the Truncated Newton algorithm from the `ff-NLopt` package was used. It requires the objective function and its gradient. The algorithm was stopped when the variation of the objective function was smaller than $1e - 6$. The maximal number of evaluations of the objective function was set to 200 (but it was actually never reached).

The initial values were $w_0(x, y) = 0$ and

$$u_0(x, y) = \left(0.1 \cos\left(\frac{4\pi x}{L_x}\right) + 0.05 \sin\left(\frac{6\pi x}{L_x}\right) \right) \left(1 - \left(\frac{y}{L_y}\right)^2 \right) \text{ in } \Omega.$$

5.1. Numerical validation with a regular solution. For the numerical validation of our scheme, we used the parameter $\beta = 0.8$ in the function g , so that $g(s) = s - 0.8$. With this choice, we have $g(-1) = -1.8 < 0 < 0.2 = g(1)$ and the sign condition (cf. (2.21)) is satisfied. This guarantees that the solution is classical. We compared the solution obtained by our scheme and the solution of (1.1) computed with the linearly implicit scheme used in [15] (this scheme is implicit for the linear terms and explicit for the nonlinear terms).

m (cf. time step)	0	1	2	3	4	5
L^2 -error	0.0240	0.0124	0.0063	0.0032	0.0016	0.0008
ratio	1.94	1.97	1.97	2	2	/

TABLE 1. L^2 -error and ratio of consecutive errors vs time step

Table 1 shows the L^2 -error between the solution u_{DS} from our doubly splitting scheme and the solution u_{LI} from the linearly implicit scheme at the final time $T = 0.5$. The time step was chosen as $dt = T/(10 \times 2^m)$ with $m \in \{0, 1, \dots, 5\}$. Since both schemes are first order in time, the difference $\|u_{DS}(T) - u_{LI}(T)\|_{L^2(\Omega)}$ is expected to be first order at most. The ratio of consecutive errors between two consecutive time steps, which is very close to 2, is consistent with the first order approximation.

m (cf. time step)	0	1	2	3	4	5
LI scheme	1	2	4	8	16	32
DS scheme	165	262	305	381	511	489

TABLE 2. Normalized CPU time vs time step for the linearly implicit (LI) scheme and the doubly splitting (DS) scheme

We point out that for a regular solution, the linearly implicit scheme is much faster than our doubly splitting scheme. This is illustrated in Table 2, where the CPU computational time is represented. We used a laptop for which the computation of $u_{LI}(T)$ with the time step $dt = T/10$ takes about 6 seconds. Since the CPU time depends on the computer, in Table 2, the CPU time is normalized by comparing every computation to this case (for which the CPU time is therefore set to 1). For the linearly implicit scheme, when the time step is divided by 2, the CPU time is

multiplied by 2, as expected. For the doubly splitting scheme, the most greedy part is the minimization algorithm. The computational time could be reduced by using a second order method involving the hessian of the objective function and not only the gradient (in such a case, a C^1 regularization of f would be used, yielding a C^2 regularization of F).

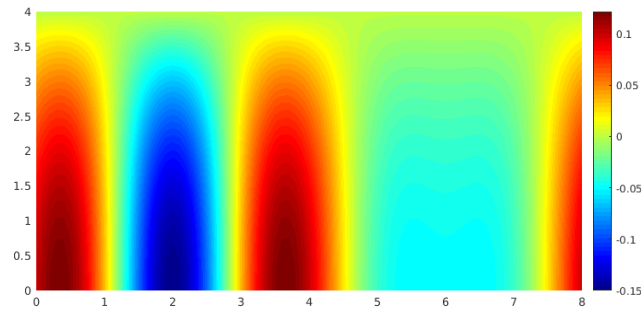


FIGURE 3. Initial condition u_0

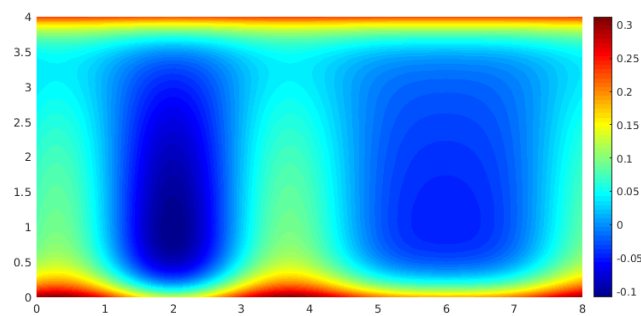


FIGURE 4. Solution $u(t)$ at time $t = 0.10$

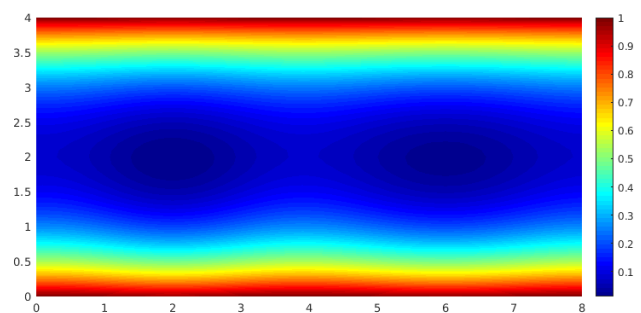
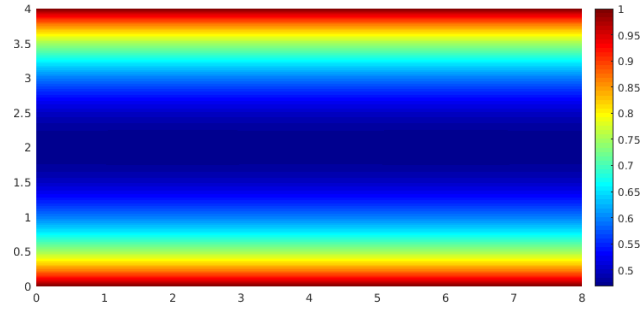
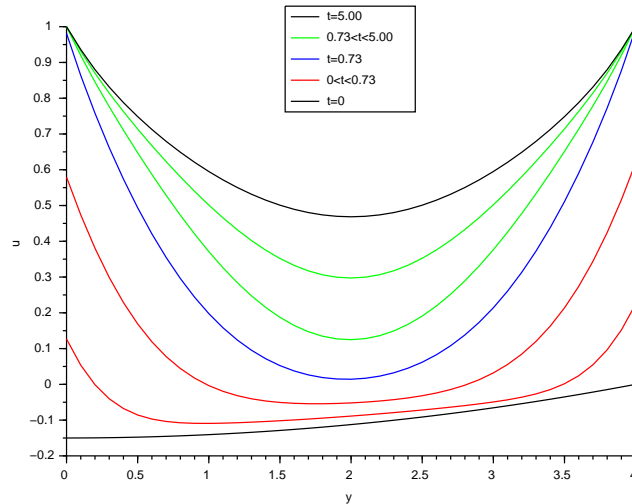


FIGURE 5. Solution $u(t)$ at singular time $t = 0.71$

5.2. Computation of a singular solution. As a test case for a singular solution, we choose the same parameters as previously except that $g(s) = s - 3$. The time

FIGURE 6. Stationary solution ($u(t)$ at time $t = 5.00$)FIGURE 7. Solution $y \mapsto u(t, x = 2, y)$ from $t = 0$ to $t = 5.00$

step is $dt = 0.01$. We have $g(-1) = -4 < g(1) = -2 < 0$ so the sign condition (2.21) is not satisfied. The solution u reaches the value $+1$ somewhere on the boundary at time $t = 0.71$ and is singular for $t \geq 0.71$. The isovalues of u are represented in Figures 3-6 at times $t = 0$, $t = 0.10$, $t = 0.71$ and $t = 5.00$ (in these Figures, the `Matlab`[®] software was used for the visualization). We observe that the solution converges to a singular steady state, which is constant along the x -direction.

In order to visualize the evolution in the y -direction, we have represented in Figure 7 the solution u on the segment $\{x = 2\} \times [0, L_y]$ as time grows. For this particular section of u , the value $+1$ is reached at time $t = 0.73$. We observe that, afterwards, u continues to evolve in the bulk, until it reaches a singular steady state.

ACKNOWLEDGEMENTS

This paper was initiated while the first author was visiting the “Laboratoire de Mathématiques et Applications” in Poitiers, whose hospitality is gratefully acknowledged. The visit of the first author was supported by the AUF (Agence Universitaire de la Francophonie) in the framework of the project “Etude des modèles mathématiques de pollution des eaux de surface et souterraines”.

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