OPTIMAL CONTROL OF A SEMIDISCRETE CAHN-HILLIARD-NAVIER-STOKES SYSTEM WITH NON-MATCHED FLUID DENSITIES *

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Abstract. This paper is concerned with the distributed optimal control of a time-discrete Cahn–Hilliard/Navier–Stokes system with variable densities. It focuses on the double-obstacle potential which yields an optimal control problem for a family of coupled systems in each time instance of a variational inequality of fourth order and the Navier–Stokes equation. By proposing a suitable time-discretization, energy estimates are proved and the existence of solutions to the primal system and of optimal controls is established for the original problem as well as for a family of regularized problems. The latter correspond to Moreau–Yosida type approximations of the double-obstacle potential. The consistency of these approximations is shown and first order optimality conditions for the regularized problems are derived. Through a limit process, a stationarity system for the original problem is established which is related to a function space version of C-stationarity.

Key words. Cahn-Hilliard, limiting C-stationarity, mathematical programming with equilibrium constraints, Navier-Stokes, non-matched densities, non-smooth potentials, optimal control, semidiscretization in time, Yosida regularization.

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1. Introduction. In this paper we are concerned with the optimal control of two (or more) immiscible fluids with non-matched densities. For the mathematical formulation of the fluid phases, we use phase field models which have recently been used successfully in applications involving, e.g., phase separation phenomena (see, e.g., [4, 14, 30]). Some of the strengths of phase field approaches are due to their ability to overcome both, analytical difficulties of topological changes, such as, e.g., droplet break-ups or the coalescence of interfaces, and numerical challenges in capturing the interface dynamics. In this context, a so-called order parameter depicts the concentration of the fluids, attaining extreme values at the pure phases and intermediate values within a thin (diffuse) interface layer, and it is associated with decreasing/minimizing a suitably chosen energy.

A renowned diffuse interface model is the Cahn-Hilliard system which was first introduced by Cahn and Hilliard in [9]. In the presence of hydrodynamic effects, the system has to be enhanced by an equation which captures the behavior of the fluid. In [28], Hohenberg and Halperin published a first basic model for immiscible, viscous two-phase flows. Their so-called 'model H' combines the Cahn-Hilliard system with the Navier-Stokes equation. It is however restricted to the case where the two fluids possess nearly identical densities, i.e., matched densities. Recently, Abels, Garcke and Grün [2] obtained the following diffuse interface model for two-phase flows with

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non-matched densities:

$$(1.1a) \qquad \partial_t \varphi + v \nabla \varphi - \operatorname{div}(m(\varphi) \nabla \mu) = 0,$$

$$(1.1b) \qquad -\Delta \varphi + \partial \Psi_0(\varphi) - \mu - \kappa \varphi = 0,$$

$$\partial_t(\rho(\varphi)v) + \operatorname{div}(v \otimes \rho(\varphi)v) - \operatorname{div}(2\eta(\varphi)\epsilon(v)) + \nabla p$$

$$(1.1c) \qquad + \operatorname{div}(v \otimes J) - \mu \nabla \varphi = 0,$$

$$(1.1d) \qquad \operatorname{div} v = 0,$$

$$(1.1e) \qquad v_{|\partial\Omega} = 0,$$

$$(1.1f) \qquad \partial_n \varphi_{|\partial\Omega} = \partial_n \mu_{|\partial\Omega} = 0,$$

$$(1.1g) \qquad (v, \varphi)_{|t=0} = (v_a, \varphi_a),$$

which is supposed to hold in the space-time cylinder $\Omega \times (0, \infty)$, where $\partial\Omega$ denotes the boundary of Ω. This system is thermodynamically consistent in the sense that it allows for the derivation of local entropy or free energy inequalities.

In the above model, v represents the velocity of the fluid and p describes the fluid pressure. The symmetric gradient of v is defined by $\epsilon(v) := \frac{1}{2}(\nabla v + \nabla v^\top)$. The density ρ of the mixture of the fluids depends on the order parameter φ which reflects the mass concentration of the fluid phases. More precisely,

$$(1.2) \qquad \rho(\varphi) = \frac{\rho_1 + \rho_2}{2} + \frac{\rho_2 - \rho_1}{2}\varphi,$$

where φ ranges in the interval $[-1, 1]$, and $0 < \rho_1 \le \rho_2$ are the given densities of the two fluids under consideration. This is one of the main distinctions compared to the model with matched densities, where ρ is a fixed constant. The quantity μ denotes the chemical potential in the Cahn-Hilliard system and helps to split the fourth-order in space differential operator into two second-order operators. Another important difference between (1.1) and model 'H' is the presence of a relative flux $J := -\frac{\rho_2 - \rho_1}{2}m(\varphi)\nabla\mu$ which corresponds to the diffusion of the two phases and additionally complicates the analytical situation. The viscosity and mobility coefficients of the system, η and m, depend on the actual concentration of the two fluids at each point in time and space. The initial states are given by v_a and φ_a, and $\kappa > 0$ is a positive constant. Furthermore, Ψ_0 represents the convex part of the homogeneous free energy density contained in the Ginzburg-Landau energy model which is associated with the Cahn-Hilliard part of (1.1). Usually, the homogeneous free energy density serves the purpose of restricting the order parameter φ to the physically meaningful range $[-1, 1]$ and to capture the spinodal decomposition of the phases. For this reason, it is typically non-convex and maintains two local minima near or at -1 and 1.

Depending on the underlying applications, different choices have been investigated in the literature. In their original paper [9], Cahn and Hilliard considered the logarithmic form $\Psi(\varphi) = (1 + \varphi)\ln(1 + \varphi) + (1 - \varphi)\ln(1 - \varphi) - \frac{\kappa}{2}\varphi^2$ which also plays an important role in the Flory-Huggins solution theory of the thermodynamics of polymer solutions. Another possible choice is the smooth double-well potential $\Psi(\varphi) = \frac{\kappa}{2}(1 - \varphi^2)^2$, see e.g. [12, 16]. It permits pure phases but fails to restrict the order parameter to $[-1, 1]$. Therefore, it is perhaps a less relevant choice in material science. In [35], Oono and Puri found that in the case of deep quenches of, e.g. binary alloys, the double-obstacle potential, is better suited than the other free energy models mentioned above. A similar observation appears to be true in the case of polymeric membrane formation under rapid wall hardening. The double-obstacle

potential $\Psi(\varphi) = I_{[-1,1]}(\varphi) - \frac{\kappa}{2}\varphi^2$, with $I_{[-1,1]}$ denoting the indicator function of the interval $[-1,1]$ in $\mathbb{R}$, combines the advantage of the existence of pure phases and the exclusiveness of the interval $[-1,1]$ at the cost of losing differentiability (when compared, e.g., to the double-well potential). As a consequence, (1.1b) becomes a variational inequality which complicates the analytical and numerical treatment of the overall model.

In this paper we study the optimal control of a time discrete coupled Cahn-Hilliard-Navier-Stokes (CHNS) system with the double-obstacle potential. For this purpose, we introduce a distributed control u which enters the Navier-Stokes equation (1.1c) on the right-hand side and aims to minimize an objective functional $\mathcal{J}$ subject to the control-version CHNS(u) of the Cahn-Hilliard-Navier-Stokes system:

$$\text{minimize } \mathcal{J}(\varphi, \mu, v, u) \text{ over } (\varphi, \mu, v, u)$$
$$\text{subject to (s.t.) } u \in U_{ad}, \; (\varphi, \mu, v, u) \text{ satisfies CHNS}(u),$$

where U_{ad} is a given set of admissible controls.

Regarding physical applications, we point out that the CHNS system is used to model a variety of situations. These range from the aforementioned solidification process of liquid metal alloys, cf. [14], or the simulation of bubble dynamics, as in Taylor flows [4], or pinch-offs of liquid-liquid jets [29], to the formation of polymeric membranes [45] or proteins crystallization, see e.g. [30] and references within. Furthermore, the model can be easily adapted to include the effects of surfactants such as colloid particles at fluid-fluid interfaces in gels and emulsions used in food, pharmaceutical, cosmetic, or petroleum industries [5, 37]. In many of these situations an optimal control context is desirable where the system is influenced in such a way that a prescribed system behavior needs to be guaranteed.

In the literature, the classical case of two-phase flows of liquids with matched densities is well investigated, see e.g. [28]. When it comes to the modeling of fluids with different densities, then the literature presents various approaches, ranging from quasi-incompressible models with non-divergence free velocity fields, see e.g. [32], to possibly thermodynamically inconsistent models with solenoidal fluid velocities, cf. [13]. We refer to [7, 8, 18] for additional analytical and numerical results for some of these models. In [1], Abels, Depner and Garcke derived an existence result for the given system (1.1) with a logarithmic potential, and in the recent preprint [19] system (1.1) with smooth potentials (thus excluding the double-obstacle homogeneous free energy density) is considered in a fully discrete and an alternative semi-discrete in time setting including numerical simulations.

The optimal control problem associated to the Cahn-Hilliard-Navier-Stokes system with matched densities and a non-smooth homogeneous free energy density (double-obstacle potential) has been previously studied by the first and last author of this work in [27]. We also mention the recent preprint [17] which treats the control of a nonlocal Cahn-Hilliard-Navier-Stokes system in two dimensions. Apart from these contributions the literature on the optimal control of the coupled CHNS-system with non-matched densities is - to the best of our knowledge - essentially void. Nevertheless, we mention that there are numerous publications concerning the optimal control of the phase separation process itself, i.e. the distinct Cahn-Hilliard system, see e.g. [10, 11, 21, 25, 43, 44].

We point out that the presence of a non-smooth homogeneous free energy density associated with the underlying Ginzburg-Landau energy in the Cahn-Hilliard system gives rise to an optimal control problem for the Navier-Stokes system coupled to

the Cahn-Hilliard variational inequality. In particular, due to the presence of the variational inequality constraint, classical constraint qualifications (see, e.g., [46]) fail which prevents the application of Karush-Kuhn-Tucker (KKT) theory in Banach space for the first-order characterization of an optimal solution by (Lagrange) multipliers. In fact, it is known [22, 27] that the resulting problem falls into the realm of mathematical programs with equilibrium constraints (MPECs) in function space. Even in finite dimensions, this problem class is well-known for its constraint degeneracy [33, 36]. As a result, stationarity conditions for this problem class are no longer unique (in contrast to KKT conditions); compare [22, 23] in function space and, e.g., [39] in finite dimensions. They rather depend on the underlying problem structure and/or on the chosen analytical approach. In this work, we utilize a Yosida regularization technique with a subsequent passage to the limit with the Yosida parameter in order to derive conditions of C-stationarity type. This technique is reminiscent of the one pioneered by Barbu in [6], but for different problem classes.

The remainder of the paper is organized as follows. In section 2 we introduce the semi-discrete Cahn-Hilliard-Navier-Stokes system and assign it to the corresponding optimal control problem. In section 3 we show the existence of feasible points to the original optimal control problem, as well as to regularized problems. Section 4 is concerned with the existence of globally optimal solutions, and section 5 deals with the consistency of the chosen regularization technique. In section 6 we derive first-order optimality conditions for the regularized problems using a classical result from non-linear optimization theory. Then a limiting process leads to a stationarity system for the original problem. The latter is the content of section 7.

2. The semi-discrete CHNS-system and the optimal control problem. As a first step towards the numerical treatment of the underlying Cahn-Hilliard-Navier-Stokes system, we study a semi-discrete (in time) variant. For our subsequent analysis we start by fixing the associated function spaces and by invoking our working assumptions.

For this purpose, let $\Omega \subset \mathbb{R}^N, N = 2, 3$, be a bounded domain with smooth boundary $\partial \Omega \in C^2(\Omega)$. In particular, Ω satisfies the cone condition, cf. [3, Chapter IV, 4.3].

For $k \in \mathbb{N}$ and $1 \leq p \leq \infty$ we introduce the following Sobolev spaces:

$$H_{0,\sigma}^k(\Omega; \mathbb{R}^N) = \left\{ f \in H^k(\Omega; \mathbb{R}^N) \cap H_0^1(\Omega; \mathbb{R}^N) : \mathrm{div} f = 0, \text{ a.e. on } \Omega \right\},$$

$$\overline{W}^{k,p}(\Omega) = \left\{ f \in W^{k,p}(\Omega) : \int_\Omega f dx = 0 \right\},$$

$$\overline{W}_{\partial_n}^{k,p}(\Omega) = \left\{ f \in \overline{W}^{k,p}(\Omega) : \partial_n f_{|\partial\Omega} = 0 \text{ on } \partial\Omega \right\},$$

where 'a.e.' stands for 'almost everywhere'. Here, $W^{k,p}(\Omega)$ and $W_0^{k,p}(\Omega)$ denote the usual Sobolev space, see [3]. For $p = 2$, we also write $H^k(\Omega)$ respectively $H_0^k(\Omega)$ instead. Unless otherwise noted, $(\cdot, \cdot)$ represents the L^2-inner product, $\|\cdot\|$ the induced norm, and $\langle \cdot, \cdot \rangle := \langle \cdot, \cdot \rangle_{\overline{H}^{-1}, \overline{H}^1}$ the duality pairing between $\overline{H}^1(\Omega)$ and $\overline{H}^{-1}(\Omega)$. For a Banach space W, we denote by W^* its topological dual, and $\mathcal{L}(W, W^*)$ defines the space of all linear and continuous operators from W to W^*. In our notation for norms, we do not distinguish between scalar- or vector-valued functions. The inner product of vectors is denoted by '$\cdot$', the vector product is represented be '$\otimes$' and the tensor product for matrices is written as '$:$'.

REMARK 2.1. *Before we present the semi-discrete system and assuming integrability in time, from (1.1a) we get*

$$\int_\Omega \partial_t \varphi dx = -\int_\Omega v \nabla \varphi dx + \int_\Omega \operatorname{div}(m(\varphi)\nabla\mu)dx = 0,$$

Hence utilizing (1.1g) the integral mean of φ satisfies

$$\frac{1}{|\Omega|}\int_\Omega \varphi dx \equiv \frac{1}{|\Omega|}\int_\Omega \varphi_a dx =: \overline{\varphi_a},$$

i.e., it is constant in time. By assuming $\overline{\varphi_a} \in (-1,1)$, we exclude the uninteresting case $|\overline{\varphi_a}| = 1$. This can be achieved by considering the shifted system (1.1), where φ is replaced by its projection onto $\overline{L}^2(\Omega)$. Consequently, we need to work with shifted variables such as, e.g. $m(y + \overline{\varphi_a})$, which we again denote by $m(y)$ in a slight misuse of notation.

Motivated by physics, we assume throughout that the mobility and viscosity coefficients are strictly positive as specified in Assumption 2.2 below. Furthermore, we extend the connection (1.2) between φ and ρ to all of $\mathbb{R}$, as our studies include certain double-well type potentials which allow for values of φ outside the physically relevant interval $[-1, 1]$.

ASSUMPTION 2.2.
1. *The coefficient functions $m, \eta \in C^2(\mathbb{R})$ in (1.1c) and (1.1a) as well as their derivatives up to second order are bounded, i.e. there exist constants $0 < b_1 \le b_2$ such that for every $x \in \mathbb{R}$, it holds that $b_1 \le \min\{m(x), \eta(x)\}$ and*

$$\max\{m(x), \eta(x), |m'(x)|, |\eta'(x)|, |m''(x)|, |\eta''(x)|\} \le b_2.$$

2. *The initial state satisfies $(v_a, \varphi_a) \in H^2_{0,\sigma}(\Omega; \mathbb{R}^N) \times \left(\overline{H}^2_{\partial_n}(\Omega) \cap \mathbb{K}\right)$ where*

$$\mathbb{K} := \left\{ v \in \overline{H}^1(\Omega) : \psi_1 \le v \le \psi_2 \text{ a.e. in } \Omega \right\},$$

with $-1 - \overline{\varphi_a} =: \psi_1 < 0 < \psi_2 := 1 - \overline{\varphi_a}$.
3. *The density ρ depends on the order parameter φ via*

$$\rho(\varphi) = \max\left\{ \frac{\rho_1 + \rho_2}{2} + \frac{\rho_2 - \rho_1}{2}(\varphi + \overline{\varphi_a}), 0 \right\} \ge 0.$$

We note that by Remark 2.1 the pure phases are attained at x when $\varphi(x) = \psi_1$ or $\varphi(x) = \psi_2$, and the *max*-operator in Assumption 2.2.3 ensures that the density remains always non-negative. The latter is necessary to derive appropriate energy estimates.

With these assumptions we now state the semi-discrete Cahn-Hilliard-Navier-Stokes system. For the sake of generality, we additionally introduce a distributed force on the right-hand side of the Navier-Stokes equation, which will later serve the purpose of a distributed control. Below and throughout the paper, $\tau > 0$ denotes the time step-size and $M \in \mathbb{N}$ the total number of time instances in the semi-discrete setting.

DEFINITION 2.1 (Semi-discrete CHNS-system). *Let $\Psi_0 : \overline{H}^1(\Omega) \to \mathbb{R}$ be a convex functional with subdifferential $\partial\Psi_0$. Fixing $(\varphi_{-1}, v_0) = (\varphi_a, v_a)$ we say that a triple*

$$(\varphi, \mu, v) = ((\varphi_i)_{i=0}^{M-1}, (\mu_i)_{i=0}^{M-1}, (v_i)_{i=1}^{M-1})$$

in $\overline{H}_{\partial_n}^2(\Omega)^M \times \overline{H}_{\partial_n}^2(\Omega)^M \times H_{0,\sigma}^1(\Omega;\mathbb{R}^N)^{M-1}$ solves the semi-discrete CHNS system with respect to a given control $u = (u_i)_{i=1}^{M-1} \in L^2(\Omega;\mathbb{R}^N)^{M-1}$, denoted as $(\varphi,\mu,v) \in S_\Psi(u)$, if it holds for all $\phi \in \overline{H}^1(\Omega)$ and $\psi \in H_{0,\sigma}^1(\Omega;\mathbb{R}^N)$ that

(2.1) $\quad \left\langle \dfrac{\varphi_{i+1} - \varphi_i}{\tau}, \phi \right\rangle + \langle v_{i+1}\nabla\varphi_i, \phi \rangle - \langle \operatorname{div}(m(\varphi_i)\nabla\mu_{i+1}), \phi \rangle = 0,$

(2.2) $\quad \langle -\Delta\varphi_{i+1}, \phi \rangle + \langle \partial\Psi_0(\varphi_{i+1}), \phi \rangle - \langle \mu_{i+1}, \phi \rangle - \langle \kappa\varphi_i, \phi \rangle = 0,$

$$\left\langle \dfrac{\rho(\varphi_i)v_{i+1} - \rho(\varphi_{i-1})v_i}{\tau}, \psi \right\rangle_{H_{0,\sigma}^{-1}, H_{0,\sigma}^1} + \langle \operatorname{div}(v_{i+1} \otimes \rho(\varphi_{i-1})v_i), \psi \rangle_{H_{0,\sigma}^{-1}, H_{0,\sigma}^1}$$

$$- \left\langle \operatorname{div}\left(v_{i+1} \otimes \dfrac{\rho_2 - \rho_1}{2} m(\varphi_{i-1})\nabla\mu_i\right), \psi \right\rangle_{H_{0,\sigma}^{-1}, H_{0,\sigma}^1} + (2\eta(\varphi_i)\epsilon(v_{i+1}), \epsilon(\psi))$$

(2.3) $$- \langle \mu_{i+1}\nabla\varphi_i, \psi \rangle_{H_{0,\sigma}^{-1}, H_{0,\sigma}^1} = \langle u_{i+1}, \psi \rangle_{H_{0,\sigma}^{-1}, H_{0,\sigma}^1}.$$

The first two equations are supposed to hold for every $0 \leq i+1 \leq M-1$ and the last equation holds for every $1 \leq i+1 \leq M-1$.

REMARK 2.3. *In general, the subdifferential of a convex function Ψ_0 can be a set-valued mapping, see, e.g., [15]. In this case, by equation (2.2) there exists $\beta \in \partial\Psi_0(\varphi_{i+1})$ such that*

$$\langle -\Delta\varphi_{i+1}, \phi \rangle + \langle \beta, \phi \rangle - \langle \mu_{i+1}, \phi \rangle - \langle \kappa\varphi_i, \phi \rangle = 0, \ \forall\phi \in \overline{H}^1(\Omega).$$

We note that in the above system the boundary conditions specified in (1.1) are included in the respective function spaces.

It is interesting to note that our semi-discretization of (1.1) in time involves three time instances $(i-1, i, i+1)$. Equations (2.1) and (2.2), however, do not involve the velocity at the "old" time instance $i-1$. As a consequence, (φ_0, μ_0) are characterized by the (decoupled) Cahn-Hilliard system only. At the final time instance, however, the coupling of the Cahn-Hilliard and the Navier-Stokes system is maintained; otherwise, we have little hope to derive some energy estimates for the system.

Finally, we present the optimal control problem for the semi-discrete CHNS system. For its formulation, let $U_{ad} \subset L^2(\Omega;\mathbb{R}^N)^{M-1}$ and $\mathcal{J}: \mathcal{X} \to \mathbb{R}$ be a Fréchet differentiable function, with

$$\mathcal{X} := \overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H_{0,\sigma}^1(\Omega;\mathbb{R}^N)^{M-1} \times L^2(\Omega;\mathbb{R}^N)^{M-1}.$$

Further requirements on U_{ad} and $\mathcal{J}$ are made explicit in connection with the existence result, Theorem 4.1, below.

DEFINITION 2.2. *The optimal control problem is given by*

(P_Ψ) $\qquad$ $\min \mathcal{J}(\varphi, \mu, v, u)$ over $(\varphi, \mu, v, u) \in \mathcal{X}$

$\qquad\qquad$ s.t. $u \in U_{ad}, \ (\varphi, \mu, v) \in S_\Psi(u).$

In many applications, $\mathcal{J}$ is given by a tracking-type functional and U_{ad} by unilateral or bilateral box constraints.

3. Existence of feasible points. In this section, we prove the existence of feasible points for the optimization problem (P_Ψ). As stated earlier, for deriving stationarity conditions we will later on approximate the double-obstacle potential by a sequence of smooth potentials of double-well type. Therefore, we consider here the following two types of free energy densities.

ASSUMPTION 3.1. *The functional* $\Psi_0 : \overline{H}^1(\Omega) \to \mathbb{R}$ *is convex, proper and lower-semicontinuous. It has one of the two subsequent properties:*

1. *Either it is given by* $\Psi_0(\varphi) := \int_\Omega \psi_0(\varphi(x))dx$ *where* $\psi_0 : \mathbb{R} \to \overline{\mathbb{R}} := \mathbb{R} \cup \{+\infty\}$ *represents the double-obstacle potential,*

$$\psi_0(z) := \begin{cases} +\infty & if\ z < \psi_1, \\ 0 & if\ \psi_1 \leq z \leq \psi_2, \\ +\infty & if\ z > \psi_2. \end{cases}$$

2. *Or it originates from a double-well type potential and satisfies:*
   (a) Ψ_0 *is Fréchet differentiable with* $\{\Psi_0'(\varphi)\} = \partial\Psi_0(\varphi) \subset L^2(\Omega)$ *for every* $\varphi \in \overline{H}^1(\Omega)$;
   (b) *There exists* $B_u \in \mathbb{R}$ *such that* $\Psi_0(\varphi) \leq B_u$ *for every* $\varphi \in \mathbb{K}$.

Additionally, we assume that the functional $\Psi(\varphi) := \Psi_0(\varphi) - \int_\Omega \frac{\kappa}{2}\varphi(x)^2dx, \kappa > 0$, *is bounded from below by a constant* $B_l \in \mathbb{R}$.

We start by studying the semi-discrete CHNS system for a single time step. For this purpose, assume that the pair $(\tilde{\varphi}, \tilde{v}) \in \overline{H}^1(\Omega) \times H_{0,\sigma}^1(\Omega; \mathbb{R}^N)$ is given. We then show the existence of a point (φ, μ, v) which solves a slightly modified system. Theorem 3.5 collects the results for all time steps via an induction argument. Finally, Theorem 3.7 shows that the modified system equals the original CHNS system under suitable assumptions.

The starting point for our considerations is an energy estimate for the generalized system. This estimate will be useful to establish the boundedness of the feasible set. We note that in what follows, C, C_1 and C_2 denote generic constants which may take different values at different occasions.

LEMMA 3.1 (Energy estimate for a single time step). *Let* $\tilde{\varphi} \in \overline{H}^1(\Omega)$, $\tilde{v} \in H_{0,\sigma}^1(\Omega; \mathbb{R}^N)$, $\Theta_v \in (H_{0,\sigma}^1(\Omega; \mathbb{R}^N))^*$, $\Theta_\mu, \Theta_\varphi \in \overline{H}^{-1}(\Omega)$, $\nu \in H^1(\Omega; \mathbb{R}^N)$, $f_0, f_{-1} \in L^2(\Omega)$, $f_0, f_{-1} \geq 0$ *be given such that*

$$(3.1) \qquad \frac{f_0 - f_{-1}}{\tau} + \mathrm{div}\nu = 0\ a.e.\ on\ \Omega.$$

In case of the double-obstacle potential suppose additionally that $\tilde{\varphi} \in \mathbb{K}$.

Then, if $(\varphi, \mu, v) \in \overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H_{0,\sigma}^1(\Omega; \mathbb{R}^N)$ *solves the system*

$$(3.2) \qquad \left\langle \frac{\varphi - \tilde{\varphi}}{\tau}, \phi \right\rangle + \langle v\nabla\tilde{\varphi}, \phi \rangle - \langle \mathrm{div}(m(\tilde{\varphi})\nabla\mu), \phi \rangle = \langle \Theta_\mu, \phi \rangle, \ \forall \phi \in \overline{H}^1(\Omega),$$

$$(3.3) \qquad -\langle \mu, \phi \rangle - \langle \kappa\tilde{\varphi}, \phi \rangle + \langle -\Delta\varphi, \phi \rangle + \langle \partial\Psi_0(\varphi), \phi \rangle = \langle \Theta_\varphi, \phi \rangle, \ \forall \phi \in \overline{H}^1(\Omega),$$

$$\left\langle \frac{f_0 v - f_{-1}\tilde{v}}{\tau}, \psi \right\rangle_{H_{0,\sigma}^{-1}, H_{0,\sigma}^1} + \langle \mathrm{div}(v \otimes \nu), \psi \rangle_{H_{0,\sigma}^{-1}, H_{0,\sigma}^1} + (2\eta(\tilde{\varphi})\epsilon(v), \epsilon(\psi))$$

$$(3.4) \qquad - \langle \mu\nabla\tilde{\varphi}, \psi \rangle_{H_{0,\sigma}^{-1}, H_{0,\sigma}^1} = \langle \Theta_v, \psi \rangle_{H_{0,\sigma}^{-1}, H_{0,\sigma}^1}, \ \forall \psi \in H_{0,\sigma}^1(\Omega; \mathbb{R}^N),$$

the following energy estimate holds true:

$$\int_\Omega \frac{f_0\,|v|^2}{2}dx + \int_\Omega \frac{|\nabla\varphi|^2}{2}dx + \Psi(\varphi) + \int_\Omega f_{-1}\frac{|v-\tilde{v}|^2}{2}dx + \int_\Omega \frac{|\nabla\varphi - \nabla\tilde{\varphi}|^2}{2}dx$$

$$+\,\tau \int_\Omega 2\eta(\tilde{\varphi})\,|\epsilon(v)|^2\,dx + \tau \int_\Omega m(\tilde{\varphi})\,|\nabla\mu|^2\,dx + \int_\Omega \kappa\frac{(\varphi-\tilde{\varphi})^2}{2}$$

(3.5)
$$\leq \int_\Omega \frac{f_{-1}\,|\tilde{v}|^2}{2}dx + \int_\Omega \frac{|\nabla\tilde{\varphi}|^2}{2}dx + \Psi(\tilde{\varphi}) + g(\varphi,\mu,v),$$

where g is defined as

(3.6)
$$g(\varphi,\mu,v) := \langle\Theta_\mu,\mu\rangle + \left\langle\Theta_\varphi, \frac{\varphi-\tilde{\varphi}}{\tau}\right\rangle + \langle\Theta_v,v\rangle_{H_{0,\sigma}^{-1},H_{0,\sigma}^{1}}.$$

Proof. First, we observe that

$$(\mathrm{div}(v\otimes\nu),v) = ((\mathrm{div}\nu)v + (\nu\cdot\nabla)v,v)$$

$$= \int_\Omega ((\mathrm{div}\nu)\frac{v}{2} + (\nu\cdot\nabla)v)v\,dx + \int_\Omega (\mathrm{div}\nu)\frac{v}{2}v\,dx$$

(3.7)
$$= \int_\Omega \mathrm{div}\left(\nu\frac{|v|^2}{2}\right) + (\mathrm{div}\nu)\frac{|v|^2}{2}dx = \int_\Omega (\mathrm{div}\nu)\frac{|v|^2}{2}dx.$$

Next, one verifies

$$(f_0 v - f_{-1}\tilde{v}, v) = \int_\Omega \frac{f_0\,|v|^2}{2}dx - \int_\Omega \frac{f_{-1}\,|\tilde{v}|^2}{2}dx$$

(3.8)
$$+ \int_\Omega \frac{(f_0 - f_{-1})\,|v|^2}{2}dx + \int_\Omega \frac{f_{-1}\,|v-\tilde{v}|^2}{2}dx.$$

Testing (3.2),(3.3) and (3.4) with μ, $\frac{\varphi-\tilde{\varphi}}{\tau}$ and v, respectively, summing up and integrating by parts, we obtain

$$0 = \int_\Omega \frac{f_0\,|v|^2 - f_{-1}\,|\tilde{v}|^2}{2\tau}dx + \int_\Omega f_{-1}\frac{|v-\tilde{v}|^2}{2\tau}dx + \int_\Omega \frac{(f_0 - f_{-1})\,|v|^2}{2\tau}dx$$

$$+ \int_\Omega (\mathrm{div}\nu)\frac{|v|^2}{2}dx + \int_\Omega 2\eta(\tilde{\varphi})\,|\epsilon(v)|^2\,dx + \int_\Omega m(\tilde{\varphi})\,|\nabla\mu|^2\,dx$$

$$+ \frac{1}{\tau}\langle\partial\Psi_0(\varphi),\varphi-\tilde{\varphi}\rangle_{\overline{H}^{-1},\overline{H}^1} - \kappa\int_\Omega \tilde{\varphi}\frac{\varphi-\tilde{\varphi}}{\tau}dx$$

(3.9)
$$+ \frac{1}{\tau}\int_\Omega \nabla\varphi(\nabla\varphi - \nabla\tilde{\varphi})dx - g(\varphi,\mu,v),$$

where we also use the previous equations (3.7) and (3.8). From the definition of the subdifferential we infer

(3.10)
$$\langle\partial\Psi_0(\varphi),\varphi-\tilde{\varphi}\rangle \geq \Psi(\varphi) - \Psi(\tilde{\varphi}) + \frac{\kappa}{2}\int_\Omega \varphi^2 - \tilde{\varphi}^2 dx.$$

Inserting (3.1),(3.10) into (3.9) and using $2a(a-b) = a^2 - b^2 + (a-b)^2$ once for $(a,b) = (\nabla\varphi, \nabla\tilde{\varphi})$ and then for $(a,b) = (\tilde{\varphi}, \varphi)$ we obtain the assertion. $\square$

REMARK 3.2. *Note that the system (3.2)-(3.4) corresponds to the system (2.1)-(2.3) for one time step only when choosing*

$$\tilde{v} = v_i, \ \tilde{\varphi} = \varphi_i, \ f_0 = \rho(\varphi_i), \ f_{-1} = \rho(\varphi_{i-1}),$$
$$\nu = \rho(\varphi_{i-1})v_i - \frac{\rho_2 - \rho_1}{2}m(\varphi_{i-1})\nabla\mu_i,$$
$$\Theta_v = u, \ \Theta_\varphi = \Theta_\mu = 0.$$

Now we prove the existence of solutions to the system (3.2)-(3.4). The proof mainly relies on the application of Schaefer's fixed point theorem, also called the Leray-Schauder principle, and combines arguments from [1, Lemma 4.3] and monotone operator theory.

THEOREM 3.2 (Existence of solutions to the CHNS system for a single time step). *Let the assumptions of Lemma 3.1 be satisfied. Then the system (3.2)-(3.4) has a solution $(\varphi, \mu, v) \in \overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)$.*

Proof. We start by defining

$$(3.11) \qquad X := \overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N),$$

$$(3.12) \qquad Y := \overline{H}^{-1}(\Omega) \times \overline{H}^{-1}(\Omega) \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^*,$$

and the operators $\mathcal{G}_1 : \overline{H}^1(\Omega) \to \overline{H}^{-1}(\Omega), \mathcal{G}_2 : \overline{H}^1(\Omega) \rightrightarrows \overline{H}^{-1}(\Omega), \mathcal{G}_3 : H^1_{0,\sigma}(\Omega; \mathbb{R}^N) \to H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^*, \mathcal{G} : X \rightrightarrows Y$ and $\mathcal{F} : X \to Y$ (here and below '$\rightrightarrows$' indicates a set-valued mapping) via

$$\mathcal{G}_1(\mu) := -\text{div}(m(\tilde{\varphi})\nabla\mu) - \Theta_\mu, \ \mathcal{G}_2(\varphi) := -\Delta\varphi + \partial\Psi_0(\varphi) - \Theta_\varphi,$$
$$\mathcal{G}_3(v) := -\text{div}(2\eta(\tilde{\varphi})\epsilon(v)) - \Theta_v,$$
$$\mathcal{G}(\varphi, \mu, v) := (\mathcal{G}_1(\mu), \mathcal{G}_2(\varphi), \mathcal{G}_3(v))^\top, \ \mathcal{F}(\varphi, \mu, v) := (\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3)^\top,$$

with

$$\mathcal{F}_1(\varphi, \mu, v) := -\frac{\varphi - \tilde{\varphi}}{\tau} - v\nabla\tilde{\varphi}, \ \mathcal{F}_2(\varphi, \mu, v) := \mu + \kappa\tilde{\varphi},$$
$$\mathcal{F}_3(\varphi, \mu, v) := -\frac{f_0 v - f_{-1}\tilde{v}}{\tau} - \text{div}(v \otimes \nu) + \mu\nabla\tilde{\varphi}.$$

Using this notation, the system (3.2)-(3.4) can be stated as

$$(3.13) \qquad 0 \in \mathcal{G}(\varphi, \mu, v) - \mathcal{F}(\varphi, \mu, v) \subset Y.$$

By standard arguments, the mappings $\mathcal{G}_1$ and $\mathcal{G}_3$ are invertible and the respective inverse mapping is continuous. Since the Laplace operator is invertible from $\overline{H}^1(\Omega)$ to $\overline{H}^{-1}(\Omega)$ and the subdifferential $\partial\Psi_0$ is maximal monotone (cf. [38, Theorem A]), $\mathcal{G}_2$ is invertible, as well. Concerning the continuity of $\mathcal{G}_2^{-1}$, let $\xi_1, \xi_2 \in \overline{H}^{-1}(\Omega)$ and $\varphi_1, \varphi_2 \in \overline{H}^1(\Omega)$ satisfy $\varphi_j = \mathcal{G}_2^{-1}(\xi_j)$ for $j = 1, 2$. Using Poincaré's inequality and the monotonicity of $\partial\Psi_0$, we immediately obtain

$$\|\varphi_2 - \varphi_1\|^2_{H^1} \le C(\langle -\Delta(\varphi_2 - \varphi_1), \varphi_2 - \varphi_1\rangle + \langle\partial\Psi_0(\varphi_2) - \partial\Psi_0(\varphi_1), \varphi_2 - \varphi_1\rangle)$$
$$= C\langle\xi_2 - \xi_1, \varphi_2 - \varphi_1\rangle \le C\|\xi_2 - \xi_1\|_{H^{-1}}\|\varphi_2 - \varphi_1\|_{H^1},$$

showing the continuity of $\mathcal{G}_2^{-1}$.

Due to the compact embedding of the space $\overline{Y} := L^{\frac{3}{2}}(\Omega) \times L^{\frac{3}{2}}(\Omega) \times L^{\frac{3}{2}}(\Omega; \mathbb{R}^N)$, into Y, the inverse of $\mathcal{G}$ is a compact operator from $\overline{Y}$ to X. Further, $\mathcal{F} : X \to \overline{Y}$ is continuous. Hence, the operator $\mathcal{F} \circ \mathcal{G}^{-1} : \overline{Y} \to \overline{Y}$ is compact.

In what follows, we show the existence of a solution δ^* to the fixed point equation

$$(3.14) \qquad \delta^* - \mathcal{F} \circ \mathcal{G}^{-1}(\delta^*) = 0 \in \overline{Y}.$$

Then it immediately follows that $\mathcal{G}^{-1}(\delta^*)$ solves the system (3.2)-(3.4). In order to apply Schaefer's theorem with respect to the operator $\mathcal{F} \circ \mathcal{G}^{-1}$ we verify the condition that the set $D := \bigcup_{0 \leq \lambda \leq 1} \left\{ \delta \in \overline{Y} | \delta = \lambda \mathcal{F} \circ \mathcal{G}^{-1}(\delta) \right\}$ is bounded. For this purpose, assume that $\delta \in \overline{Y}$ and $\lambda \in [0, 1]$ satisfy

$$(3.15) \qquad \delta = \lambda \mathcal{F} \circ \mathcal{G}^{-1}(\delta),$$

and define $(\varphi, \mu, v) := \mathcal{G}^{-1}(\delta) \in X$. Thus, (3.15) can be rewritten as

$$(3.16) \qquad \mathcal{G}(\varphi, \mu, v) - \lambda \mathcal{F}(\varphi, \mu, v) = 0$$

which is equivalent to the following system of equations

$$\left\langle \lambda \frac{\varphi - \tilde{\varphi}}{\tau}, \phi \right\rangle + \langle \lambda v \nabla \tilde{\varphi}, \phi \rangle = \langle \operatorname{div}(m(\tilde{\varphi}) \nabla \mu), \phi \rangle + \langle \Theta_\mu, \phi \rangle, \ \forall \phi \in \overline{H}^1(\Omega),$$

$$\langle \lambda \mu, \phi \rangle + \langle \lambda \kappa \tilde{\varphi}, \phi \rangle = \langle -\Delta \varphi, \phi \rangle + \langle \partial \Psi_0(\varphi)), \phi \rangle - \langle \Theta_\varphi, \phi \rangle, \ \forall \phi \in \overline{H}^1(\Omega),$$

$$\lambda \left\langle \frac{f_0 v - f_{-1} \tilde{v}}{\tau}, \psi \right\rangle_{H_{0,\sigma}^{-1}, H_{0,\sigma}^1} + \lambda \langle \operatorname{div}(v \otimes \nu), \psi \rangle_{H_{0,\sigma}^{-1}, H_{0,\sigma}^1} + (2\eta(\tilde{\varphi})\epsilon(v), \epsilon(\psi))$$

$$= \lambda \langle \mu \nabla \tilde{\varphi}, \psi \rangle_{H_{0,\sigma}^{-1}, H_{0,\sigma}^1} + \langle \Theta_v, \psi \rangle_{H_{0,\sigma}^{-1}, H_{0,\sigma}^1}, \ \forall \psi \in H_{0,\sigma}^1(\Omega; \mathbb{R}^N).$$

Analogously to the proof of Lemma 3.1, we test this system by μ, $\frac{\varphi - \tilde{\varphi}}{\tau}$ and v, respectively, sum up the resulting equations and integrate by parts to derive

$$0 = \lambda \int_\Omega \frac{f_0 |v|^2 - f_{-1} |\tilde{v}|^2}{2\tau} dx + \lambda \int_\Omega f_{-1} \frac{|v - \tilde{v}|^2}{2\tau} dx + \int_\Omega 2\eta(\tilde{\varphi}) |\epsilon(v)|^2 dx$$

$$+ \int_\Omega m(\tilde{\varphi}) |\nabla \mu|^2 dx + \frac{1}{\tau} \int_\Omega \partial \Psi_0(\varphi)(\varphi - \tilde{\varphi}) dx - \lambda \kappa \int_\Omega \tilde{\varphi} \frac{\varphi - \tilde{\varphi}}{\tau} dx$$

$$(3.17) \qquad + \frac{1}{\tau} \int_\Omega \nabla \varphi (\nabla \varphi - \nabla \tilde{\varphi}) dx - g(\varphi, \mu, v),$$

which leads to

$$\int_\Omega 2\eta(\tilde{\varphi}) |\epsilon(v)|^2 dx + \int_\Omega m(\tilde{\varphi}) |\nabla \mu|^2 dx + \frac{1}{\tau} \Psi(\varphi) + \frac{1}{\tau} \int_\Omega |\nabla \varphi|^2 dx - g(\varphi, \mu, v)$$

$$(3.18) \qquad\qquad\qquad \leq \lambda \int_\Omega \frac{f_{-1} |\tilde{v}|^2}{2\tau} dx + \frac{1}{\tau} \int_\Omega |\nabla \tilde{\varphi}|^2 dx + \frac{1}{\tau} \Psi(\tilde{\varphi}).$$

Note that for obtaining (3.17) we also make use of (3.1). The right-hand side of (3.18) can be bounded by a constant $C := C(N, \Omega, \tau, f_{-1}, \tilde{v}, \tilde{\varphi}) > 0$ which is independent of λ. Since Ψ is bounded from below, this leads to

$$(3.19) \qquad \int_\Omega 2\eta(\tilde{\varphi}) |\epsilon(v)|^2 dx + \int_\Omega m(\tilde{\varphi}) |\nabla \mu|^2 dx + \frac{1}{\tau} \int_\Omega |\nabla \varphi|^2 dx \leq C + g(\varphi, \mu, v).$$

Due to Korn's inequality, Poincaré's inequality and from the boundedness of $\eta(\cdot)$ and $m(\cdot)$, we infer

$$\|v\|_{H^1}^2 + \|\mu\|_{H^1}^2 + \|\varphi\|_{H^1}^2 \leq C + g(\varphi, \mu, v)$$

(3.20)
$$\leq C_1 + C_2(\|v\|_{H^1} + \|\mu\|_{H^1} + \|\varphi\|_{H^1}),$$

where $C_2 > 0$ depends only on Θ_μ, Θ_φ and Θ_v. The last inequality yields the boundedness of (φ, μ, v) in X. Next, we derive bounds for $\mathcal{F}$. In fact, we have

$$\|\mathcal{F}_1(\varphi, \mu, v)\|_{L^{3/2}} \leq C(\|\varphi\| + \|\tilde{\varphi}\| + \|v\|_{H^1}\|\tilde{\varphi}\|_{H^1}),$$
$$\|\mathcal{F}_2(\varphi, \mu, v)\|_{L^{3/2}} \leq C(\|\mu\| + \|\tilde{\varphi}\|),$$
$$\|\mathcal{F}_3(\varphi, \mu, v)\|_{L^{3/2}} \leq C(\|v\|_{H^1} + \|v\|_{H^1}\|\nu\|_{H^1} + \|\mu\|\|\tilde{\varphi}\|_{H^1} + \|\tilde{v}\|_{H^1}).$$

Since $\tilde{\varphi}$, $\tilde{v}$ and ν are fixed, D is bounded in $\overline{Y}$. Hence Schaefer's theorem is applicable implying that equation (3.14) admits a fixed point $\delta^* \in \overline{Y}$. Then $\mathcal{G}^{-1}(\delta^*)$ solves the system (3.2)-(3.4). □

In our setting, the right-hand sides of the system (3.2)-(3.4) are square integrable functions. This enables the derivation of higher regularity properties for the solutions obtained in Theorem 3.2.

LEMMA 3.3 (Regularity of solutions). *Let the assumptions of Lemma 3.1 be satisfied, and suppose additionally that $\Theta_\mu, \Theta_\varphi \in L^2(\Omega)$, as well as $f_0, f_{-1} \in L^3(\Omega)$ and $\tilde{\varphi} \in H^2(\Omega)$.*

Then it holds that $\varphi, \mu \in \overline{H}_{\partial_n}^2(\Omega)$ and $v \in H^2(\Omega; \mathbb{R}^N)$, provided that $(\varphi, \mu, v) \in \overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H_{0,\sigma}^1(\Omega; \mathbb{R}^N)$ satisfies the system (3.2)-(3.4). Moreover, there exists a constant $C = C(N, \Omega, b_1, b_2, \tau, \kappa) > 0$ such that

$$\|\varphi\|_{H^2} + \|\mu\|_{H^2} + \|v\|_{H^2}$$

(3.21)
$$\leq C(\|\varphi\| + \|\mu\| + \|\tilde{\varphi}\| + \|\Theta_\varphi\| + \|\Theta_\mu\| + \|v\|_{H^1}\|\tilde{\varphi}\|_{H^2} + \|\Psi_0'(\varphi)\|).$$

In case of the double-obstacle potential, it also holds that $\varphi \in \mathbb{K}$ and the term $\|\Psi_0'(\varphi)\|$ in the above inequality is dropped.

Proof. Equation (3.3) is equivalent to

(3.22)
$$\Delta\varphi + g_1 \in \partial\Psi_0(\varphi) \text{ in } \overline{H}^{-1}(\Omega)$$

with $g_1 := \mu + \kappa\tilde{\varphi} + \Theta_\varphi$. By Sobolev's embedding theorem g_1 is in $L^2(\Omega)$. In case of the double-well type potential, Assumption 3.1.2 (a) then implies $g_2 := -g_1 + \Psi_0'(\varphi) \in L^2(\Omega)$ and $\Delta\varphi = g_2$. Applying [34, Theorem 2.3.6] and [34, Remark 2.3.7], we deduce that $\varphi \in \overline{H}^2(\Omega)$ is the unique solution of the Neumann problem

$$\Delta\varphi = g_2 \text{ in } \Omega, \ \partial_n\varphi_{|\partial\Omega} = 0 \text{ on } \partial\Omega.$$

Furthermore, [34, Theorem 2.3.1] yields the existence of a constant $C := C(N, \Omega)$ such that

(3.23)
$$\|\varphi\|_{H^2} \leq C(\|\varphi\| + \|g_2\|) \leq C(\|\varphi\| + \|\mu\| + \kappa\|\tilde{\varphi}\| + \|\Theta_\varphi\| + \|\Psi_0'(\varphi)\|).$$

In case of the double-obstacle potential, (3.22) is equivalent to the variational inequality problem:

(3.24)
$$\text{Find } \varphi \in \mathbb{K}: \ \langle -\Delta\varphi - g_1, \phi - \varphi \rangle \geq 0, \ \forall\phi \in \mathbb{K}.$$

Then the assertion follows from the subsequent lemma.

LEMMA 3.4. *If* $\varphi \in \mathbb{K}$ *solves the variational inequality problem (3.24) with* $g_1 \in L^2(\Omega)$, *then* $\varphi \in \overline{H}^2_{\partial_n}(\Omega)$ *and there exists a constant* $C = C(N, \Omega) > 0$ *such that* $\|\varphi\|_{H^2} \le C \|g_1\|$.

For the sake of completeness we provide a proof in the appendix. It closely follows the lines of argumentation of [31, Chapter IV].

Regarding μ, we argue similarly. Indeed, first note that by Sobolev's embedding theorem and Hölder's inequality $g_3 := \frac{\varphi - \tilde{\varphi}}{\tau} + v \nabla \tilde{\varphi} - \Theta_\mu - \mu$ is an element of $L^2(\Omega)$. Furthermore, the coefficient function $m(\tilde{\varphi})$ is contained in $H^2(\Omega)$ and $W^{1,6}(\Omega)$, respectively (cf. [31, II, Lemma A.3]). Equation (3.2) is equivalent to

$$(3.25) \qquad m(\tilde{\varphi})\Delta\mu + \nabla(m(\tilde{\varphi}))\nabla\mu - \mu = g_3 \text{ in } \overline{H}^{-1}(\Omega).$$

Again by [34, Theorem 2.3.5] and [34, Theorem 2.3.1] $\mu \in \overline{H}^2_{\partial_n}(\Omega)$ and it holds that

$$(3.26) \quad \|\mu\|_{H^2} \le C(\|\mu\| + \|g_3\|) \le C(\|\mu\| + \|\varphi\| + \|\tilde{\varphi}\| + \|v\|_{H^1}\|\tilde{\varphi}\|_{H^2} + \|\Theta_\mu\|),$$

where $C > 0$ depends only on $N, \Omega, b_1, b_2, \tau$.

Finally, we show the desired regularity of v. Since $\text{div}(\epsilon(v)) = \frac{1}{2}(\Delta v + \nabla(\text{div } v))$, it holds that

$$\text{div}(2\eta(\tilde{\varphi})\epsilon(v)) = 2\eta'(\tilde{\varphi})\epsilon(v)\nabla\tilde{\varphi} + \eta(\tilde{\varphi})\Delta v,$$

and therefore by equation (3.4) that

$$(3.27) \quad \Delta v = \eta(\tilde{\varphi})^{-1}\left[\text{div}(v \otimes \nu) - 2\eta'(\tilde{\varphi})\epsilon(v)\nabla\tilde{\varphi} + \frac{1}{\tau}(f_0 v - f_{-1}\tilde{v}) - \mu\nabla\tilde{\varphi} - \Theta_v\right]$$

Moreover, $\text{div}(v \otimes \nu) = (Dv)\nu + v \, \text{div } \nu$. By the assumptions all summands in the second line of (3.27) belong to $L^2(\Omega; \mathbb{R}^N)$ and $\nu \in H^1(\Omega; \mathbb{R}^N)$. Hence, we have

$$(3.28) \qquad \Delta v = \eta(\tilde{\varphi})^{-1}\left[(Dv)\nu + v \, \text{div } \nu - 2\eta'(\tilde{\varphi})\epsilon(v)\nabla\tilde{\varphi} + f\right],$$

with $\|f\| \le C(z)$ for a constant $C(z) > 0$ depending only on

$$z = (N, \Omega, \eta, \tau, \|\varphi\|_{H^2}, \|\tilde{\varphi}\|_{H^2}, \|\mu\|_{H^2}, \|\Theta_v\|).$$

In order to show $v \in H^2(\Omega; \mathbb{R}^N)$, we apply a bootstrap argument and well-known regularity results for the stationary Stokes' equation, cf. [41].

1. Since $v \in H^1_{0,\sigma}(\Omega; \mathbb{R}^N)$, we have that $(Dv)\nu$, $\epsilon(v)\nabla\tilde{\varphi}$ and $v \, \text{div } \nu$ belong to $L^{3/2}(\Omega; \mathbb{R}^N)$. Therefore, [41, Prop. 2.3, p. 35] and (3.28) show that $v \in W^{2,3/2}(\Omega; \mathbb{R}^N)$ and that $\|v\|_{W^{2,3/2}} \le C(z)$ for a constant C depending only on z.

2. Next, $v \in W^{2,3/2}(\Omega; \mathbb{R}^N)$ and the continuous embedding of $W^{1,3/2}(\Omega)$ into $L^3(\Omega)$ (which we denote by $W^{1,3/2}(\Omega) \hookrightarrow L^3(\Omega)$) imply that $(Dv)\nu$ and $\epsilon(v)\nabla\tilde{\varphi}$ belong to $L^2(\Omega; \mathbb{R}^N)$. Moreover, $W^{2,3/2}(\Omega) \hookrightarrow L^p(\Omega)$ for every $p < \infty$. Hence $v \, \text{div } \nu \in L^{2-\varepsilon}(\Omega; \mathbb{R}^N)$ for every $\varepsilon > 0$. Applying [41, Prop. 2.3, p. 35] again yields $v \in W^{2,2-\varepsilon}(\Omega; \mathbb{R}^N)$ for all $\varepsilon > 0$ and $\|v\|_{W^{2,2-\varepsilon}} \le C(\varepsilon, z)$.

3. Finally, having $v \in W^{2,2-\varepsilon}(\Omega; \mathbb{R}^N)$ and since $W^{2,2-\varepsilon}(\Omega) \hookrightarrow L^\infty(\Omega)$ for ε sufficiently small, it follows that also $v \, \text{div } \nu$ belongs to $L^2(\Omega; \mathbb{R}^N)$. Thus, we arrive at $v \in H^2(\Omega; \mathbb{R}^N)$ and $\|v\|_{H^2} \le C(z)$.

This completes the proof. $\square$

Our aim is to prove the existence of a solution to the semi-discrete CHNS system with the help of Theorem 3.2. This result, however, is not directly applicable with the setting of Remark 3.2, as f_0, f_{-1} and ν need not satisfy equation (3.1). This is due to the nonsmoothness of the density function and the fact that φ may attain values in $\mathbb{R}$ (rather than $[\psi_1, \psi_2]$) for a double-well-type potential. We overcome this difficulty by applying Theorem 3.2 with the setting

(3.29)
$$\tilde{v} := v_i, \ \tilde{\varphi} := \varphi_i, \ f_0 := \rho(\varphi_i), \ f_{-1} := \rho(\varphi_{i-1}),$$
$$\nu := \overline{\nu}(v_i, \varphi_i, \varphi_{i-1}, \mu_i), \ \Theta_v := u_{i+1}, \ \Theta_\varphi := \Theta_\mu := 0,$$

where $\overline{\nu} : H^1_{0,\sigma}(\Omega; \mathbb{R}^N) \times \overline{H}^2(\Omega)^3 \to H^1(\Omega; \mathbb{R}^N)$ is given by

(3.30) $$\overline{\nu}(v, \varphi, \tilde{\varphi}, \mu) := \begin{cases} \rho(\tilde{\varphi})v - \frac{\rho_2 - \rho_1}{2} m(\tilde{\varphi}) \nabla \mu & \text{if } \rho(\varphi), \rho(\tilde{\varphi}) > 0 \text{ a.e. in } \Omega, \\ G(\frac{\rho(\varphi) - \rho(\tilde{\varphi})}{\tau}) & \text{else.} \end{cases}$$

Here $G : L^2(\Omega) \to H^1(\Omega; \mathbb{R}^N), \delta \longmapsto \zeta$, is a solution operator to

(3.31) $$-\text{div}\zeta = \delta \text{ a.e. on } \Omega.$$

A specific realization of G is obtained by first solving $-\Delta \xi = \delta$ in $L^2(\Omega)$ with $\xi = 0$ on $\partial\Omega$, yielding $\xi \in H^2(\Omega) \cap H^1_0(\Omega)$, and then setting $\zeta := \nabla \xi \in H^1(\Omega, \mathbb{R}^N)$. We next prove that there always exists a solution to the system (2.1),(2.2),(3.32) where the semi-discrete Navier-Stokes equation (2.3) is replaced by

$$\left\langle \frac{\rho(\varphi_i)v_{i+1} - \rho(\varphi_{i-1})v_i}{\tau}, \psi \right\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} + (2\eta(\varphi_i)\epsilon(v_{i+1}), \epsilon(\psi))$$

$$+ \langle \text{div}(v_{i+1} \otimes \overline{\nu}(v_i, \varphi_i, \varphi_{i-1}, \mu_i)), \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} - \langle \mu_{i+1} \nabla \varphi_i, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}}$$

(3.32) $$= \langle u_{i+1}, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}}, \ \forall \psi \in H^1_{0,\sigma}(\Omega; \mathbb{R}^N).$$

We point out that (3.32) coincides with (2.3) if

(3.33) $$\min\{\rho(\varphi_i), \rho(\varphi_{i-1})\} > 0 \text{ a.e. on } \Omega.$$

For the double-obstacle potential this always holds true, since φ_i is contained in the interval $[\psi_1, \psi_2]$. Hence in this case $\rho(\varphi_i) \geq \rho(\psi_1) = \rho_1 > 0$.

In Theorem 3.7 we show that for the double-well type potentials under consideration φ remains in a close neighborhood of $[\psi_1, \psi_2]$ and therefore condition (3.33) is satisfied as well.

PROPOSITION 3.5 (Existence of solution to a modified state system). *Let* $\overline{\nu} : H^1_{0,\sigma}(\Omega; \mathbb{R}^N) \times \overline{H}^1(\Omega)^3 \to H^1(\Omega; \mathbb{R}^N)$ *be defined by (3.30). Then for every* $u \in L^2(\Omega; \mathbb{R}^N)^{M-1}$ *there exists a point* $(\varphi, \mu, v) \in \overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^{M-1}$ *which solves the semi-discrete system (2.1),(2.2),(3.32). Moreover, every solution* (φ, μ, v) *satisfies* $(\varphi, \mu, v) \in \overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^{M-1}$.

Proof. Standard arguments guarantee the existence of $(\varphi_0, \mu_0) \in \overline{H}^1(\Omega) \times \overline{H}^1(\Omega)$ such that (2.1)-(2.2) is satisfied for $i = -1$. Lemma 3.3 yields $(\varphi_0, \mu_0) \in \overline{H}^2_{\partial_n}(\Omega) \times \overline{H}^2_{\partial_n}(\Omega)$.

If condition (3.33) holds true, then Assumption 2.2.3 and (2.1) imply

$$\text{div}\overline{\nu}(v_i, \varphi_i, \varphi_{i-1}, \mu_i) = \frac{\rho_2 - \rho_1}{2}(\nabla\varphi_{i-1}v_i - \text{div}(m(\varphi_{i-1})\nabla\mu_i))$$

$$= -\frac{\rho_2 - \rho_1}{2}(\frac{\varphi_i - \varphi_{i-1}}{\tau}) = -\frac{\rho(\varphi_i) - \rho(\varphi_{i-1})}{\tau}.$$

Consequently, if (φ_i, μ_i, v_i) satisfies (2.1), then assumption (3.1) is always satisfied by the definition of $\overline{\nu}$ in the sense that

$$(3.34) \qquad \frac{\rho(\varphi_i) - \rho(\varphi_{i-1})}{\tau} + \operatorname{div}\overline{\nu}(v_i, \varphi_i, \varphi_{i-1}, \mu_i) = 0 \text{ a.e. on } \Omega.$$

Therefore, we can apply Theorem 3.2 with the setting (3.29) for $i = 0$ to guarantee the existence of $(\varphi_1, \mu_1, v_1) \in \overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H_{0,\sigma}^1(\Omega; \mathbb{R}^N)$ such that the system (2.1),(2.2),(3.32) is satisfied.

Now Lemma 3.3 yields $(\varphi_1, \mu_1, v_1) \in \overline{H}_{\partial_n}^2(\Omega) \times \overline{H}_{\partial_n}^2(\Omega) \times H_{0,\sigma}^1(\Omega; \mathbb{R}^N)$. In the case of the double-obstacle potential it additionally follows that $\varphi_1 \in \mathbb{K}$.

Repeated applications of Theorem 3.2 and Lemma 3.3 for each time step $i = 1, .., M - 2$ prove the assertion.□

As discussed above, this theorem directly guarantees the existence of a solution to the semi-discrete CHNS system for the double-obstacle potential. Next we address the boundedness of the solutions which is needed later on to ensure the existence of optimal points for (P_Ψ). For this purpose, we apply the energy estimate of Lemma 3.1 at each time step.

LEMMA 3.6 (Boundedness of the state). *There exists a positive constant $C = C(N, \Omega, b_1, b_2, \tau, \kappa, v_a, \varphi_a, u) > 0$ such that for every solution $(\varphi, \mu, v) \in \overline{H}_{\partial_n}^2(\Omega)^M \times \overline{H}_{\partial_n}^2(\Omega)^M \times H_{0,\sigma}^1(\Omega; \mathbb{R}^N)^{M-1}$ of Theorem 3.5 it holds that*

$$(3.35) \qquad \|v\|_{(H^2)^M}^2 + \|\mu\|_{(H^2)^M}^2 + \|\varphi\|_{(H^2)^{M+1}}^2 \le C.$$

Furthermore, the operator $L^2(\Omega, \mathbb{R}^N)^{M-1} \ni u \longmapsto C(N, \Omega, b_1, b_2, \tau, \kappa, v_a, \varphi_a, u) \in \mathbb{R}$ is bounded.

Proof. We define the functional $E : \overline{H}_{0,\sigma}^1(\Omega) \times \overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \to \mathbb{R}$ as follows:

$$(3.36) \qquad E(v, \varphi, \phi) := \int_\Omega \frac{\rho(\phi) |v|^2}{2} dx + \int_\Omega \frac{|\nabla\varphi|^2}{2} dx + \Psi(\varphi).$$

Let $j \in \{1, .., M - 2\}$ be arbitrarily fixed. Then by repeatedly applying Lemma 3.1 with the setting (3.29) for $i = j, j - 1, .., 0$, we conclude that

$$
\begin{aligned}
&E(v_{j+1}, \varphi_{j+1}, \varphi_j) + \tau \int_\Omega 2\eta(\varphi_j) |\epsilon(v_{j+1})|^2 dx + \tau \int_\Omega m(\varphi_j) |\nabla\mu_{j+1}|^2 dx \\
&\le E(v_j, \varphi_j, \varphi_{j-1}) + (u_{j+1}, v_{j+1}) \\
&\le E(v_{j-1}, \varphi_{j-1}, \varphi_{j-2}) + (u_j, v_j) + (u_{j+1}, v_{j+1}) \\
&\vdots \\
&\le E(v_0, \varphi_0, \varphi_{-1}) + \sum_{i=1}^{j+1} (u_i, v_i).
\end{aligned}
$$

By Assumptions 2.2 and 3.1 this yields

$$
\int_\Omega \frac{|\nabla\varphi_{j+1}|^2}{2} dx + \Psi(\varphi_{j+1}) + 2\tau b_1 \int_\Omega |\epsilon(v_{j+1})|^2 dx + \tau b_1 \int_\Omega |\nabla\mu_{j+1}|^2 dx
$$

$$(3.37) \qquad \le E(v_0, \varphi_0, \varphi_{-1}) + \sum_{i=1}^{M-1} \|u_i\| \|v_i\| \le C_1 + C_2 \|u\|_{(L^2)^{M-1}} \|v\|_{(H^1)^M},$$

where C_1 depends only on the initial data $(N, \Omega, B_l, B_u, v_a, \varphi_a)$. Due to Korn's inequality and Poincaré's inequality, this ensures

$$\|v_{j+1}\|_{H^1}^2 + \|\mu_{j+1}\|_{H^1}^2 + \|\varphi_{j+1}\|_{H^1}^2 \leq C_1 + C_2 \|u\|_{(L^2)^{M-1}} \|v\|_{(H^1)^M}.$$

Since $j \in \{1, .., M-1\}$ is arbitrarily chosen, we infer

$$(3.38) \quad \|v\|_{(H^1)^M}^2 + \|\mu\|_{(H^1)^M}^2 + \|\varphi\|_{(H^1)^{M+1}}^2 \leq C_1 + C_2 \left(\|u\|_{(L^2)^{M-1}} \|v\|_{(H^1)^M} \right).$$

Hence (φ, μ, v) is bounded in $\overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H_{0,\sigma}^1(\Omega; \mathbb{R}^N)^{M-1}$. Then the boundedness in the respective H^2-spaces follows directly by applying Lemma 3.3 for each time step.□

Next we address the case of the double-well potential and show that for appropriate double-well type potentials the order parameter of a solution to the system (2.1),(2.2),(3.32) is always greater than $\psi_1 - \varepsilon$ for some small $\varepsilon > 0$.

THEOREM 3.7. *Let* $u \in L^2(\Omega; \mathbb{R}^N)^{M-1}$ *be given and* $\left\{ \Psi_0^{(k)} \right\}_{k \in \mathbb{N}}$ *a sequence of functions which satisfies the following two conditions:*

1. *For every* $k \in \mathbb{N}$ $\Psi_0^{(k)}$ *fulfills Assumption 3.1.*

2. *If* $\{\hat{\varphi}^{(k)}\}_{k \in \mathbb{N}}$ *is a sequence in* $\overline{H}^1(\Omega)$ *such that there exists* $C > 0$ *with* $\Psi_0^{(k)}(\hat{\varphi}^{(k)}) \leq C$ *for* $k \in \mathbb{N}$, *then*

$$\left\| \max(-\hat{\varphi}^{(k)} + \psi_1, 0) \right\|_{L^1} \to 0, \ as \ k \to \infty.$$

Furthermore, let $\left\{ (\varphi^{(k)}, \mu^{(k)}, v^{(k)}) \right\}_{k \in \mathbb{N}}$ *be a sequence of solutions to the systems* (2.1),(2.2),(3.32) *with* $\Psi_0 = \Psi_0^{(k)}$. *Then*

$$\left\| \max(-\varphi^{(k)} + \psi_1, 0) \right\|_{L^\infty} \to 0, \ as \ k \to \infty.$$

Proof. Employing Lemma 3.6, in particular inequality (3.37) from its proof, then we see that for every $i \in \{-1, .., M-1\}$ and $k \in \mathbb{N}$ it holds that $\Psi^{(k)}(\varphi_i^{(k)}) \leq C_1$. Hence, we conclude

$$\Psi_0^{(k)} \left(\varphi_i^{(k)} \right) \leq C_1 + \frac{\kappa}{2} \left\| \varphi_i^{(k)} \right\|_{L^2}^2 \leq C_2.$$

By assumption, this yields

$$(3.39) \qquad \left\| \max(-\varphi_i^{(k)} + \psi_1, 0) \right\|_{L^1} \to 0 \text{ for } k \to \infty.$$

Next, we use the technique of [24, Proposition 2.4] and [24, Remark 2.5] to derive that $\left\| \max(-\varphi_i^{(k)} + \psi_1, 0) \right\|_{L^\infty} \to 0$ for $k \to \infty$. We stay brief here and refer to [24] for details on the technique. By Lemma 3.6 the sequence $\{\varphi^{(k)}\}_{k \in \mathbb{N}}$ is bounded in $\overline{H}^2(\Omega)$, and due to Sobolev's embedding theorem it is also bounded in $W^{1,6}(\Omega)$ and $C^{0,\beta}(\overline{\Omega})$, $\beta \leq \frac{1}{2}$, respectively. Thus, there exists a constant C_β such that for every $k \in \mathbb{N}$ we have $\left\| \varphi^{(k)} \right\|_{C^{0,\beta}} \leq C_\beta$.

For fix $k \in \mathbb{N}$ assume that $\left\|\max(-\varphi_i^{(k)} + \psi_1, 0)\right\|_{L^\infty} > 0$ and define the set $\mathbb{G} :=$
$\left\{\omega \in \overline{\Omega} : \varphi_i^{(k)}(\omega) \leq \psi_1 < 0\right\}$. Then let $\omega_{max} \in \mathbb{G}$ satisfy

$$-\varphi_i^{(k)}(\omega_{max}) + \psi_1 = \left\|-\varphi_i^{(k)} + \psi_1\right\|_{L^\infty(\mathbb{G})} = \left\|\max(-\varphi_i^{(k)} + \psi_1, 0)\right\|_{L^\infty(\Omega)}.$$

Due to the Hölder continuity of $\varphi_i^{(k)}$, for every $x \in \Omega$ which satisfies $|x - \omega_{max}|_{\mathbb{R}^N} \leq$
$\left(\frac{-\varphi_i^{(k)}(\omega_{max}) + \psi_1}{2C_\beta}\right)^{\frac{1}{\beta}}$ it holds that

$$-\varphi_i^{(k)}(x) + \psi_1 \geq -\varphi_i^{(k)}(\omega_{max}) + \psi_1 - \left\|\varphi_i^{(k)}\right\|_{C^{(0,\beta)}(\Omega)} |\omega_{max} - x|_{\mathbb{R}^N}^\beta$$

$$\geq \frac{-\varphi_i^{(k)}(\omega_{max}) + \psi_1}{2} > 0.$$

As Ω satisfies the cone condition, there exists a finite cone $K_r(\omega_{max}) := K(\omega_{max}) \cap B(\omega_{max}, r)$ of radius r and with vertex ω_{max} such that $K_r(\omega_{max}) \subset \Omega$. Hence the cone $K_R(\omega_{max})$ with $R := \min\left(r, \left(\frac{-\varphi_i^{(k)}(\omega_{max}) + \psi_1}{2C_\beta}\right)^{\frac{1}{\beta}}\right)$ is contained in $\mathbb{G}$. Consequently, we find

$$\left\|\max(-\varphi_i^{(k)} + \psi_1, 0)\right\|_{L^1(\Omega)} \geq \int_{K_R(\omega_{max})} -\varphi_i^{(k)} + \psi_1 dx$$

$$\geq \int_{K_R(\omega_{max})} \frac{\left(-\varphi_i^{(k)}(\omega_{max}) + \psi_1\right)}{2} dx$$

$$\geq \frac{|K_R(0)|}{2} \left\|\max(-\varphi_i^{(k)} + \psi_1, 0)\right\|_{L^\infty(\Omega)}$$

In combination with (3.39) this proves the assertion. $\blacksquare$

We define $\varphi^- \in \mathbb{R}$ as

(3.40)
$$\varphi^- := \inf\{\varphi \in \mathbb{R} : \rho(\varphi) > 0\} < \psi_1.$$

Let $u \in L^2(\Omega; \mathbb{R}^N)^{M-1}$ be given and let $\left\{\Psi_0^{(k)}\right\}_{k \in \mathbb{N}}$ be a sequence of double-well type potentials which approximates the double-obstacle potential in a certain sense, i.e., it satisfies condition 2 of Theorem 3.7. Then Theorem 3.7 ensures that there exists $k^* \in \mathbb{N}$ such that for every $k \geq k^*$ the solutions $(\varphi^{(k)}, \mu^{(k)}, v^{(k)})$ to the corresponding systems (2.1),(2.2),(3.32) with $\Psi_0 = \Psi_0^{(k)}$ satisfy

(3.41)
$$\varphi_i^{(k)} > \varphi^-, \ \forall i = -1, .., M - 1.$$

Hence $\rho(\varphi_i^{(k)}) > 0$ for every $i = -1, .., M - 1$ and $k \geq k^*$. Thus, (3.32) coincides with (2.3), which leads to the subsequent theorem.

THEOREM 3.8 (Existence of feasible points). *Let* $u \in L^2(\Omega; \mathbb{R}^N)^{M-1}$. *Let* $\overline{\Psi}_0$ *be the double-obstacle potential defined in Assumption 3.1.1 and let* $\left\{\Psi_0^{(k)}\right\}_{k \in \mathbb{N}}$ *be a sequence which satisfies the conditions of Theorem 3.7.*

Then there exists $k^* \in \mathbb{N}$ such that the system (2.1)-(2.3) admits a solution (φ, μ, v) *for every* $\Psi_0 \in \{\overline{\Psi}_0\} \cup \left\{\Psi_0^{(k)}\right\}_{k \geq k^*}$. *For this solution* (φ, μ, v) *the result of Lemma 3.6 remains true.*

In other words, the semi-discrete CHNS system (2.1)-(2.3) has a solution if the double-well type potential under consideration is close enough to the double-obstacle potential. In the following sections we always assume that this is the case. In Definition 7.1 below, we propose a specific regularization which satisfies the conditions of Theorem 3.7.

4. Existence of globally optimal points. The previous section guarantees the existence of feasible points for the optimal control problem (P_Ψ). Next we investigate the existence of a solution to (P_Ψ). For this purpose, we need to impose additional assumptions on the objective functional and the constraint set U_{ad}.

THEOREM 4.1 (Existence of global solutions). *Suppose that* $\mathcal{J} : \overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^{M-1} \times L^2(\Omega; \mathbb{R}^N)^{M-1} \to \mathbb{R}$ *is convex and weakly lower-semi-continuous and U_{ad} is non-empty, closed and convex. Assume that either U_{ad} is bounded or $\mathcal{J}$ is partially coercive, i.e. for every sequence* $\left\{(\varphi^{(k)}, \mu^{(k)}, v^{(k)}, u^{(k)})\right\}_{k \in \mathbb{N}}$ *with* $\lim_{k \to \infty} \|u^{(k)}\| = \infty$ *it holds that* $\lim_{k \to \infty} \mathcal{J}(\varphi^{(k)}, \mu^{(k)}, v^{(k)}, u^{(k)}) = \infty$. *Then the optimization problem (P_Ψ) admits a global solution.*

Proof. By Theorem 3.5 the feasible set of the problem (P_Ψ) is non-empty and contained in $\overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^{M-1} \times U_{ad}$.

Let $\left\{(\varphi^{(k)}, \mu^{(k)}, v^{(k)}, u^{(k)})\right\}_{k \in \mathbb{N}}$ be an infimizing sequence of $\mathcal{J}$ in $\overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^{M-1} \times U_{ad}$ with $(\varphi^{(k)}, \mu^{(k)}, v^{(k)}) \in S_\Psi(u^{(k)})$ such that

$$(4.1) \qquad \lim_{k \to \infty} \mathcal{J}(\varphi^{(k)}, \mu^{(k)}, v^{(k)}, u^{(k)}) = \inf_{u \in U_{ad}, (\varphi, \mu, v) \in S_\Psi(u)} \mathcal{J}(\varphi, \mu, v, u).$$

Note that the infimum on the right-hand side may be $-\infty$. The sequence $\left\{u^{(k)}\right\}_{k \in \mathbb{N}}$ is bounded in the reflexive Banach space $L^2(\Omega; \mathbb{R}^N)^{M-1}$. This follows either directly from the boundedness of the set U_{ad} or from the partial coercivity of $\mathcal{J}$. Then by Lemma 3.6 the sequence $(\varphi^{(k)}, \mu^{(k)}, v^{(k)})$ is bounded in $\overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^{M-1}$. Setting $\left\{w^{(k)}\right\}_{k \in \mathbb{N}} := \left\{(\varphi^{(k)}, \mu^{(k)}, v^{(k)}, u^{(k)})\right\}_{k \in \mathbb{N}}$, there exists a weakly convergent subsequence $\left\{w^{(k_l)}\right\}_{l \in \mathbb{N}}$ with limit point $w^* := (\varphi^*, \mu^*, v^*, u^*) \in \overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^{M-1}$. Using the weak lower-semicontinuity of $\mathcal{J}$, this implies

$$-\infty < \mathcal{J}(w^*) \leq \liminf_{l \to \infty} \mathcal{J}(w^{(k_l)}) = \inf_{u \in U_{ad}, (\varphi, \mu, v) \in S_\Psi(u)} \mathcal{J}(\varphi, \mu, v, u)$$

where the last equality holds due to (4.1). Since U_{ad} is weakly closed, u^* belongs to U_{ad}.

It remains to show that $(\varphi^*, \mu^*, v^*) \in S_\Psi(u^*)$. For this purpose, we write l instead of k_l, and we start by considering the limit of $\left\langle -\text{div}(v_{i+1}^{(l)} \otimes \frac{\rho_2 - \rho_1}{2} m(\varphi_{i-1}^{(l)}) \nabla \mu_i^{(l)}), \psi \right\rangle$ for arbitrary $i \in \{0, .., M-2\}$ and $\psi \in H^1(\Omega; \mathbb{R}^N)$. Using the triangle and Hölder's

inequality we derive

$$
\left\| m(\varphi_{i-1}^{(l)})\nabla\mu_i^{(l)} \cdot \nabla\psi - m(\varphi_{i-1}^*)\nabla\mu_i^* \cdot \nabla\psi \right\|_{L^{4/3}}
$$
$$
\leq \left\| m(\varphi_{i-1}^{(l)})(\nabla\mu_i^{(l)} - \nabla\mu_i^*) \cdot \nabla\psi \right\|_{L^{4/3}} + \left\| (m(\varphi_{i-1}^{(l)}) - m(\varphi_{i-1}^*))\nabla\mu_i^* \cdot \nabla\psi \right\|_{L^{4/3}}
$$
$$
\leq \left\| m(\varphi_{i-1}^{(l)}) \right\|_{L^\infty} \left\| \nabla\mu_i^{(l)} - \nabla\mu_i^* \right\|_{L^4} \|\nabla\psi\|_{L^2} + \left\| m(\varphi_{i-1}^{(l)}) - m(\varphi_{i-1}^*) \right\|_{L^\infty} \|\nabla\mu_i^*\|_{L^4} \|\nabla\psi\|_{L^2}.
$$

Since $\nabla\mu_i^{(l)}$ converges weakly to $\nabla\mu_i^*$ in $H^1(\Omega)$ and $H^1(\Omega)$ is compactly embedded into $L^4(\Omega)$, $\left\| \nabla\mu_i^{(l)} - \nabla\mu_i^* \right\|_{L^4}$ tends to zero for $l \to \infty$. Due to the compact embedding of $H^2(\Omega)$ into $W^{1,4}(\Omega)$, we have $\varphi_{i-1}^{(l)} \to \varphi_{i-1}^*$ strongly in $W^{1,4}(\Omega)$. Due to Assumption 2.2.1, m is Lipschitz continuous. Since $W^{1,4}(\Omega)$ can be embedded into $L^\infty(\Omega)$, we infer $\left\| m(\varphi_{i-1}^{(l)}) - m(\varphi_{i-1}^*) \right\|_{L^\infty} \to 0$.

Consequently, the sequence $\frac{\rho_2-\rho_1}{2} m(\varphi_{i-1}^{(l)})\nabla\mu_i^{(l)} \cdot \nabla\psi$ converges strongly in $L^{4/3}(\Omega)$ to $\frac{\rho_2-\rho_1}{2} m(\varphi_{i-1}^*)\nabla\mu_i^* \cdot \nabla\psi$. By Sobolev's embedding theorem and the weak continuity of the embedding operator, $v_{i+1}^{(l)}$ converges weakly in $L^4(\Omega)$ to v_{i+1}^*. Hence $\left\langle \mathrm{div}(v_{i+1}^{(l)} \otimes \frac{\rho_2-\rho_1}{2} m(\varphi_{i-1}^{(l)})\nabla\mu_i^{(l)}), \psi \right\rangle$ converges to $\left\langle \mathrm{div}(v_{i+1}^* \otimes \frac{\rho_2-\rho_1}{2} m(\varphi_{i-1}^*)\nabla\mu_i^*), \psi \right\rangle$ as $l \to \infty$.

One proceeds analogously for the remaining terms in the system (2.1)-(2.3) which do not depend on the subdifferential of Ψ_0.

In this way we also show that $\Delta\varphi_{i+1}^{(l)} + \mu_{i+1}^{(l)} + \kappa\varphi_i^{(l)}$ converges strongly in $\overline{H}^{-1}(\Omega)$ to $\Delta\varphi_{i+1}^* + \mu_{i+1}^* + \kappa\varphi_i^*$ for every $i = -1, .., M-2$. Furthermore, $\varphi_{i+1}^{(l)} \to \varphi_{i+1}^*$ in $\overline{H}^1(\Omega)$, and for every $l \in \mathbb{N}$ it holds that $\Delta\varphi_{i+1}^{(l)} + \mu_{i+1}^{(l)} + \kappa\varphi_i^{(l)} \in \partial\Psi_0(\varphi_{i+1}^{(l)})$. Due to the maximal monotonicity of $\partial\Psi_0$, this implies

$$
(4.2) \qquad \Delta\varphi_{i+1}^* + \mu_{i+1}^* + \kappa\varphi_i^* \in \partial\Psi_0(\varphi_{i+1}^*)
$$

for every $i = -1, .., M-2$. In summary, we have shown $(\varphi^*, \mu^*, v^*) \in S_\Psi(u^*)$. Hence the w^* is contained in the feasible set of the problem (P_Ψ) and therefore solves the problem. $\square$

5. Convergence of minimizers. Now we turn our focus to the consistency of the regularization, i.e. the convergence of a sequence of solutions to $(P_{\Psi^{(k)}})$ with $\Psi^{(k)}$ a double-well potential approaching the double-obstacle potential in the limit as $k \to \infty$, to a solution of (P_Ψ) with Ψ the double-obstacle potential. For this purpose, we consider a sequence of functionals $\left\{ \Psi^{(k)} \right\}_{k \in \mathbb{N}}$ satisfying Assumption 3.1.2 and a corresponding limit functional $\overline{\Psi}$.

The following theorem provides conditions under which a sequence of globally optimal solutions to $(P_{\Psi^{(k)}})$ converge to a global solution of $(P_{\overline{\Psi}})$, as $k \to \infty$.

THEOREM 5.1 (Consistency of the regularization). *Let the assumptions of Theorem 4.1 be fulfilled. The objective $\mathcal{J} : \overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H_{0,\sigma}^1(\Omega;\mathbb{R}^N)^{M-1} \times L^2(\Omega;\mathbb{R}^N)^{M-1} \to \mathbb{R}$ is supposed to be upper-semicontinuous, and let $\left\{ \Psi^{(k)} \right\}_{k \in \mathbb{N}}$ be a sequence of potentials satisfying Assumption 3.1.2. Assume further that $\overline{\Psi}$ is given such that for every sequence $\left\{ (x^{(k)}, y^{(k)}) \right\}_{k \in \mathbb{N}} \subset \overline{H}^1(\Omega) \times \overline{H}^{-1}(\Omega)$ with $y^{(k)} = {\Psi^{(k)}}'(x^{(k)})$ and $(x^{(k)}, y^{(k)}) \to (x^{(\infty)}, y^{(\infty)})$ strongly in $\overline{H}^1(\Omega) \times \overline{H}^{-1}(\Omega)$ it holds that $y^{(\infty)} \in \partial\overline{\Psi}(x^{(\infty)})$.*

Then a sequence $\{(\varphi^{(k)},\mu^{(k)},v^{(k)},u^{(k)})\}_{k\in\mathbb{N}}$ of global solutions to $(P_{\Psi^{(k)}})$ in $\overline{H}^2(\Omega)^M \times \overline{H}^2(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times U_{ad}$ converges to a global solution of $(P_{\overline{\Psi}})$, provided that $\{\mathcal{J}(\varphi^{(k)},\mu^{(k)},v^{(k)},u^{(k)})\}_{k\in\mathbb{N}}$ is assumed bounded, whenever U_{ad} is unbounded.

Proof. First note that the sequence $\{u^{(k)}\}_{k\in\mathbb{N}}$ is bounded in the reflexive Banach space $L^2(\Omega;\mathbb{R}^N)^{M-1}$. This follows either from the boundedness of the set U_{ad} or from the partial coercivity of $\mathcal{J}$ and the boundedness of $\{\mathcal{J}(\varphi^{(k)},\mu^{(k)},v^{(k)},u^{(k)})\}_{k\in\mathbb{N}}$. By Lemma 3.6, the sequence $\{(\varphi^{(k)},\mu^{(k)},v^{(k)})\}_{k\in\mathbb{N}}$ is bounded in $\overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}$. Hence there exists a weakly convergent sequence $\{w^{(k_l)}\}_{l\in\mathbb{N}} := \{(\varphi^{(k_l)},\mu^{(k_l)},v^{(k_l)},u^{(k_l)})\}_{l\in\mathbb{N}}$ with limit point $\overline{w}:=(\overline{\varphi},\overline{\mu},\overline{v},\overline{u})\in\overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}$. Moreover, since U_{ad} is weakly closed, $\overline{u}$ belongs to U_{ad}.

As in the proof of Theorem 4.1, it can be shown that the limit point satisfies $(\overline{\varphi},\overline{\mu},\overline{v}) \in S_{\overline{\Psi}}(\overline{u})$. The only difference is that inclusion (4.2) follows from the above assumption instead of the maximal monotonicity.

Next, we prove that $\overline{w}$ is an optimal point of $(P_{\overline{\Psi}})$. For this purpose, let $(\widehat{\varphi},\widehat{\mu},\widehat{v},\widehat{u})$ be an optimal solution of $(P_{\overline{\Psi}})$. We consider a sequence $(\widehat{\varphi}^{(k)},\widehat{\mu}^{(k)}) \in \overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M$ such that

$$\left\langle \frac{\widehat{\varphi}^{(k)}_{i+1}-\widehat{\varphi}^{(k)}_i}{\tau},\phi\right\rangle + \left\langle \widehat{v}_{i+1}\nabla\widehat{\varphi}^{(k)}_i,\phi\right\rangle - \left\langle \mathrm{div}(m(\widehat{\varphi}^{(k)}_i)\nabla\widehat{\mu}^{(k)}_{i+1}),\phi\right\rangle = 0,$$

$$\left\langle -\Delta\widehat{\varphi}^{(k)}_{i+1},\phi\right\rangle + \left\langle \left(\Psi^{(k)}_0\right)'(\widehat{\varphi}^{(k)}_{i+1}),\phi\right\rangle - \left\langle \widehat{\mu}^{(k)}_{i+1},\phi\right\rangle - \left\langle \kappa\widehat{\varphi}^{(k)}_i,\phi\right\rangle = 0,$$

for every $\phi \in \overline{H}^1(\Omega)$ and $i \in \{-1,..,M-2\}$, where $\widehat{v}$ corresponds to the previously specified solution of $(P_{\overline{\Psi}})$. Note that the operator $L^{(k)}_a : \overline{H}^1(\Omega)\times\overline{H}^1(\Omega) \to \overline{H}^{-1}(\Omega)\times\overline{H}^{-1}(\Omega)$ defined by

$$(5.1)\qquad L^{(k)}_a(\varphi,\mu) := \left(-\Delta\varphi + \left(\Psi^{(k)}_0\right)'(\varphi) - \mu, \varphi - \mathrm{div}(a\nabla\mu)\right)$$

is monotone, coercive and continuous, if $a \in H^2(\Omega)$ satisfies $0 < \tau b_1 \le a(x) \le \tau b_2$ almost everywhere on Ω. Hence for fixed $k \in \mathbb{N}$, the pair $(\widehat{\varphi}^{(k)}_{i+1},\widehat{\mu}^{(k)}_{i+1})$ of each subsequent time step is uniquely determined as the solution to

$$(5.2)\qquad L^{(k)}_{m(\widehat{\varphi}^{(k)}_i)\tau}(\widehat{\varphi}^{(k)}_{i+1},\widehat{\mu}^{(k)}_{i+1}) = (\kappa\widehat{\varphi}^{(k)}_i, \widehat{\varphi}^{(k)}_i - \tau\widehat{v}_{i+1}\nabla\widehat{\varphi}^{(k)}_i)$$

where $0 < \tau b_1 \le a := m(\widehat{\varphi}^{(k)}_i)h \le \tau b_2$ almost everywhere on Ω (cf. [40, Chapter II, Theorem 2.2]. Then, by Lemma 3.3 the sequence $(\widehat{\varphi}^{(k)},\widehat{\mu}^{(k)},\widehat{v})_{k\in\mathbb{N}}$ is bounded in $\overline{H}^2(\Omega)^M \times \overline{H}^2(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}$. Consequently, there exists a subsequence (denoted the same) which converges weakly in the associated product space to a limit point $(\widehat{\varphi}^*,\widehat{\mu}^*,\widehat{v})$. In accordance with the above observations, $(\widehat{\varphi}^*_{i+1},\widehat{\mu}^*_{i+1})$ is the unique solution to

$$\left\langle \frac{\widehat{\varphi}^*_{i+1}-\widehat{\varphi}^*_i}{\tau},\phi\right\rangle + \langle\widehat{v}_{i+1}\nabla\widehat{\varphi}^*_i,\phi\rangle - \langle\mathrm{div}(m(\widehat{\varphi}^*_i)\nabla\widehat{\mu}^*_{i+1}),\phi\rangle = 0,\ \forall\phi\in\overline{H}^1(\Omega),$$

$$\langle-\Delta\widehat{\varphi}^*_{i+1},\phi\rangle + \langle\partial\Psi^*_0(\widehat{\varphi}^*_{i+1}),\phi\rangle - \langle\widehat{\mu}^*_{i+1},\phi\rangle - \langle\kappa\widehat{\varphi}^*_i,\phi\rangle = 0,\ \forall\phi\in\overline{H}^1(\Omega)$$

for every $i \in \{-1, .., M-2\}$. Note that here we also use the prerequisite that $y_{i+1}^* \in \partial \Psi_0^*(\widehat{\varphi}_{i+1}^*)$ when $(y_{i+1}^{(k)}, \widehat{\varphi}_{i+1}^{(k)}) \to (y_{i+1}^*, \widehat{\varphi}_{i+1}^*)$ with $y^{(k)})_{i+1} = \Psi_0^{(k)'}(\widehat{\varphi}_{i+1}^{(k)})$. Since the feasibility of $(\widehat{\varphi}, \widehat{\mu}, \widehat{v}, \widehat{u})$ implies $(\widehat{\varphi}, \widehat{\mu}, \widehat{v}) \in S_{\overline{\Psi}}(\widehat{u})$, this yields $\widehat{\varphi}^* = \widehat{\varphi}$ and $\widehat{\mu}^* = \widehat{\mu}$.

Now we show that $\widehat{\mu}^{(k)}$ converges strongly in $(\overline{H}_{\partial_n}^2(\Omega))^M$ to $\widehat{\mu}^*$. For this purpose, fix $i \in \{-1, .., M-2\}$ and define

$$(5.3) \qquad g_i^{(k)} := \frac{\widehat{\varphi}_{i+1}^{(k)} - \widehat{\varphi}_i^{(k)}}{\tau} + \widehat{v}_{i+1} \nabla \widehat{\varphi}_i^{(k)}, \quad g_i^* := \frac{\widehat{\varphi}_{i+1}^* - \widehat{\varphi}_i^*}{\tau} + \widehat{v}_{i+1} \nabla \widehat{\varphi}_i^*.$$

By the Rellich-Kondrachov theorem $g_i^{(k)}$ converges strongly in $L^2(\Omega)$ to g_i^*. It further holds that $g_i^{(k)} - g_i^* = \mathrm{div}(m(\widehat{\varphi}_i^{(k)}) \nabla \widehat{\mu}_{i+1}^{(k)}) - \mathrm{div}(m(\widehat{\varphi}_i^*) \nabla \widehat{\mu}_{i+1}^*)$. Hence, we have

$$\mathrm{div}(m(\widehat{\varphi}_i^*) \nabla(\widehat{\mu}_{i+1}^{(k)} - \widehat{\mu}_{i+1}^*)) = g_i^{(k)} - g_i^* - \mathrm{div}((m(\widehat{\varphi}_i^{(k)}) - m(\widehat{\varphi}_i^*)) \nabla \widehat{\mu}_{i+1}^{(k)}) =: \delta_i^{(k)}.$$

Again by the Rellich-Kondrachov theorem $m(\widehat{\varphi}_i^{(k)})$ converges strongly to $m(\widehat{\varphi}_i^*)$ in $W^{1,5}(\Omega)$. Furthermore, $\nabla \widehat{\mu}_{i+1}^{(k)}$ is bounded in $H^1(\Omega)$. As a consequence, $\delta_i^{(k)} \to 0$ strongly in $L^2(\Omega)$. Applying [34, Theorem 2.3.1], we conclude

$$\left\| \widehat{\mu}_{i+1}^{(k)} - \widehat{\mu}_{i+1}^* \right\|_{H^2} \leq C \left\| \delta_i^{(k)} \right\| \to 0.$$

Next, we define $\widehat{u}_{i+1}^{(k)} \in L^2(\Omega; \mathbb{R}^N)$ for all $i \in \{0, .., M-2\}$ by

$$\begin{aligned}
\widehat{u}_{i+1}^{(k)} := & \frac{\rho(\widehat{\varphi}_i^{(k)}) \widehat{v}_{i+1} - \rho(\widehat{\varphi}_{i-1}^{(k)}) \widehat{v}_i}{\tau} + \mathrm{div}(\widehat{v}_{i+1} \otimes \rho(\widehat{\varphi}_{i-1}^{(k)}) \widehat{v}_i) \\
& - \mathrm{div}(\widehat{v}_{i+1} \otimes \frac{\rho_2 - \rho_1}{2} m(\widehat{\varphi}_{i-1}^{(k)}) \nabla \widehat{\mu}_i^{(k)}) \\
& - \mathrm{div}(2\eta(\widehat{\varphi}_i^{(k)}) \epsilon(\widehat{v}_{i+1})) - \widehat{\mu}_{i+1}^{(k)} \nabla \widehat{\varphi}_i^{(k)}.
\end{aligned}$$

Similarly to the proof of Theorem 4.1, it can be shown that $\widehat{u}^{(k)}$ converges strongly in $L^2(\Omega; \mathbb{R}^N)^{M-1}$ to $\widehat{u}$.

Summarizing, the sequence $\left\{ (\widehat{\varphi}^{(k)}, \widehat{\mu}^{(k)}, \widehat{v}, \widehat{u}^{(k)}) \right\}_{k \in \mathbb{N}}$ converges towards $(\widehat{\varphi}, \widehat{\mu}, \widehat{v}, \widehat{u})$ strongly in $\overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H_{0,\sigma}^1(\Omega; \mathbb{R}^N)^{M-1} \times L^2(\Omega; \mathbb{R}^N)^{M-1}$. Employing the continuity properties of the objective functional $\mathcal{J}$, this yields

$$\begin{aligned}
\mathcal{J}(\overline{\varphi}, \overline{\mu}, \overline{v}, \overline{u}) &\leq \lim_{k \to \infty} \mathcal{J}(\varphi^{(k)}, \mu^{(k)}, v^{(k)}, u^{(k)}) \leq \lim_{k \to \infty} \mathcal{J}(\widehat{\varphi}^{(k)}, \widehat{\mu}^{(k)}, \widehat{v}, \widehat{u}^{(k)}) \\
(5.4) \qquad &\leq \mathcal{J}(\widehat{\varphi}, \widehat{\mu}, \widehat{v}, \widehat{u}).
\end{aligned}$$

Since $(\widehat{\varphi}, \widehat{\mu}, \widehat{v}, \widehat{u})$ is optimal, the assertion holds true. $\square$

In summary, the optimal control problems under consideration are well-posed and admit globally optimal solutions. Furthermore, the chosen regularization approach is consistent in the sense of Theorem 5.1.

6. Stationarity conditions. Now we turn our attention to the derivation of stationarity conditions for the optimal control problem. For smooth potentials Ψ_0 stationarity or first-order optimality conditions for the problem (P_Ψ) can be derived by applying classical results concerning the existence of Lagrange multipliers. The latter approach is employed in the following theorem.

THEOREM 6.1 (First-order optimality conditions for smooth potentials). *Let $\mathcal{J}$: $\overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times L^2(\Omega;\mathbb{R}^N)^{M-1} \to \mathbb{R}$ be Fréchet differentiable and let Ψ_0 satisfy Assumption 3.1.2 such that Ψ'_0 maps $\overline{H}^2_{\partial_n}(\Omega)$ continuously Frèchet-differentiably into $L^2(\Omega)$. Further, let $\overline{z} := (\overline{\varphi}, \overline{\mu}, \overline{v}, \overline{u})$ be a minimizer of (P_Ψ). Then there exist $(p, r, q) \in \overline{L}^2(\Omega)^M \times \overline{L}^2(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}$, $p = (p_{-1}, ... p_{M-2})$, $r = (r_{-1}, ... r_{M-2})$, $q = (q_0, ... q_{M-2})$, such that*

$$-\frac{1}{\tau}(p_i - p_{i-1}) + a(m'(\varphi_i), \mu_{i+1}, p_i) - \mathrm{div}(p_i v_{i+1}) - \Delta^t r_{i-1}$$

$$+ \Psi''_0(\varphi_i)^* r_{i-1} - \kappa r_{i+1} - \frac{1}{\tau}\rho'(\varphi_i)v_{i+1} \cdot (q_{i+1} - q_i)$$

$$- (\rho'(\varphi_i)v_{i+1} - \frac{\rho_2 - \rho_1}{2}m'(\varphi_i)\nabla\mu_{i+1})(Dq_{i+1})^\top v_{i+2}$$

(6.1)
$$+ 2\eta'(\varphi_i)\epsilon(v_{i+1}) : Dq_i + \mathrm{div}(\mu_{i+1}q_i) = \frac{\partial\mathcal{J}}{\partial\varphi_i}(\overline{z}),$$

$$- r_{i-1} + b(m(\varphi_{i-1}), p_{i-1}) - \mathrm{div}(\frac{\rho_2 - \rho_1}{2}m(\varphi_{i-1})(Dq_i)^\top v_{i+1})$$

(6.2)
$$- q_{i-1} \cdot \nabla\varphi_{i-1} = \frac{\partial\mathcal{J}}{\partial\mu_i}(\overline{z}),$$

$$-\frac{1}{\tau}\rho(\varphi_{j-1})(q_j - q_{j-1}) - \rho(\varphi_{j-1})(Dq_j)^\top v_{j+1}$$

$$- (Dq_{j-1})(\rho(\varphi_{j-2})v_{j-1} - \frac{\rho_2 - \rho_1}{2}m(\varphi_{j-2})\nabla\mu_{j-1})$$

(6.3)
$$- \mathrm{div}(2\eta(\varphi_{j-1})\epsilon(q_{j-1})) + p_{j-1}\nabla\varphi_{j-1} = \frac{\partial\mathcal{J}}{\partial v_j}(\overline{z}),$$

(6.4)
$$\left(\frac{\partial\mathcal{J}}{\partial u_k}(\overline{z}) - q_{k-1}\right)_{k=1}^{M-1} \in \left[\mathbb{R}_+(U_{ad} - \overline{u})\right]^+,$$

for all $i = 0, ..., M - 1$ and $j = 1, ..., M - 1$. Here, $\left[\mathbb{R}_+(U_{ad} - \overline{u})\right]^+$ denotes the polar cone of the set $\{r(w - u)|w \in U_{ad} \wedge r \in \mathbb{R}^+\}$. Furthermore, we use the convention that p_i, r_i, q_i are equal to 0 for $i \geq M - 1$ along with q_{-1} and φ_i, μ_i, v_i for $i \geq M$. Moreover, $a(\hat{f}, \hat{w}, \hat{p}), b(\hat{m}, \hat{p}), \Delta^t(\hat{r}) \in \overline{H}^2_{\partial_n}(\Omega)^*$ are defined by $\langle\Delta^t\hat{r}, \hat{z}\rangle := \int_\Omega \hat{r}\Delta\hat{z}dx$, $\langle a(\hat{f}, \hat{w}, \hat{p}), \hat{z}\rangle := \int_\Omega -\hat{p}\,\mathrm{div}(\hat{f}\hat{z}\nabla\hat{w})dx$, $\langle b(\hat{m}, \hat{p}), \hat{z}\rangle := \int_\Omega -\hat{p}\,\mathrm{div}(\hat{m}\nabla\hat{z})dx$, for functions $\hat{f}, \hat{m} \in C^1(\overline{\Omega}), \hat{w} \in H^1(\Omega), \hat{r}, \hat{p} \in L^2(\Omega)$ and $\hat{z} \in \overline{H}^2_{\partial_n}(\Omega)$.

Proof. Utilizing the spaces X and Y and the set C given by

$$X := \overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times L^2(\Omega;\mathbb{R}^N)^{M-1},$$

$$C := \overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times U_{ad},$$

$$Y := (\overline{L}^2(\Omega))^{*M} \times (\overline{L}^2(\Omega))^{*M} \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{*M-1},$$

for $\varphi = (\varphi_0, ..., \varphi_{M-1})$, $\mu = (\mu_0, ..., \mu_{M-1})$, $v = (v_1, ..., v_{M-1})$, $u = (u_1, ..., u_{M-1})$ we define a mapping $g : X \to Y$ by

$$g(\varphi, \mu, v, u)$$
$$:= \begin{pmatrix} \left(\ \frac{1}{\tau}(\varphi_{i+1} - \varphi_i) - \mathrm{div}(m(\varphi_i)\nabla\mu_{i+1}) + v_{i+1} \cdot \nabla\varphi_i \ \right)_{i=-1}^{M-2} \\ \left(\ -\mu_{i+1} - \Delta\varphi_{i+1} + \Psi_0'(\varphi_{i+1}) - \kappa\varphi_i \ \right)_{i=-1}^{M-2} \\ \begin{pmatrix} \frac{1}{\tau}(\rho(\varphi_i)v_{i+1} - \rho(\varphi_{i-1})v_i) - \mathrm{div}(2\eta(\varphi_i)\epsilon(v_{i+1})) \\ + \mathrm{div}(v_{i+1} \otimes (\rho(\varphi_{i-1})v_i - \frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})\nabla\mu_i)) - \mu_{i+1}\nabla\varphi_i - u_{i+1} \end{pmatrix}_{i=0}^{M-2} \end{pmatrix}.$$

Then, (P_Ψ) can be stated as $\min\{\mathcal{J}(\varphi, \mu, v, u) : (\varphi, \mu, v, u) \in C, \ g(\varphi, \mu, v, u) = 0\}$, with $\overline{z} = (\overline{\varphi}, \overline{\mu}, \overline{v}, \overline{u})$ an associated minimizer. The mapping g is continuously Frèchet differentiable from X into Y. To see this, let us exemplarily consider the term $\mathrm{div}(m(\varphi_i)\nabla\mu_{i+1})$. The other terms can be treated analogously. First note that $\mathrm{div}(m(\varphi_i)\nabla\mu_{i+1})$ equals $\nabla m(\varphi_i) \cdot \nabla\mu_{i+1} + m(\varphi_i)\Delta\mu_{i+1}$ where $m(\varphi_i)$ is given by $m(\varphi_i)$. Hence $\nabla m(\varphi_i) = m'(\varphi_i)\nabla\varphi_i$. Assumption 2.2 implies that both superposition operators $\widetilde{\varphi} \mapsto m(\widetilde{\varphi})$, $\widetilde{\varphi} \mapsto m'(\widetilde{\varphi})$ are continuously Frèchet differentiable from $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ into $L^\infty(\Omega)$ (cf. [42]). Therefore, the mappings $(\widetilde{\varphi}, \widetilde{\mu}) \to m'(\widetilde{\varphi})\nabla\widetilde{\varphi} \cdot \nabla\widetilde{\mu} : H^2(\Omega) \times H^2(\Omega) \to L^3(\Omega)$ and $(\widetilde{\varphi}, \widetilde{\mu}) \to m(\widetilde{\varphi})\Delta\widetilde{\mu} : H^2(\Omega) \times H^2(\Omega) \to L^2(\Omega)$, are continuously Frèchet differentiable. This shows the continuous Frèchet differentiability of $\mathrm{div}(m(\varphi_i)\nabla\mu_{i+1})$. The Frèchet derivative of g in (φ, μ, v, u) applied to $(\varphi^\delta, \mu^\delta, v^\delta, u^\delta) \in X$ is given by

$$g'(\varphi, \mu, v, u)(\varphi^\delta, \mu^\delta, v^\delta, u^\delta)$$
$$= \begin{pmatrix} \begin{pmatrix} \frac{1}{\tau}(\varphi_{i+1}^\delta - \varphi_i^\delta) - \mathrm{div}(m'(\varphi_i)\varphi_i^\delta\nabla\mu_{i+1}) - \mathrm{div}(m(\varphi_i)\nabla\mu_{i+1}^\delta) \\ + v_{i+1} \cdot \nabla\varphi_i^\delta + v_{i+1}^\delta \cdot \nabla\varphi_i \end{pmatrix}_{i=-1}^{M-2} \\ \left(\ -\mu_{i+1}^\delta - \Delta\varphi_{i+1}^\delta + \Psi_0''(\varphi_{i+1}; \varphi_{i+1}^\delta) - \kappa\varphi_i^\delta \ \right)_{i=-1}^{M-2} \\ \begin{pmatrix} \frac{1}{\tau}(\rho'(\varphi_i)\varphi_i^\delta v_{i+1} - \rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i) + \frac{1}{\tau}(\rho(\varphi_i)v_{i+1}^\delta - \rho(\varphi_{i-1})v_i^\delta) \\ + \mathrm{div}(v_{i+1} \otimes (\rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i + \rho(\varphi_{i-1})v_i^\delta)) \\ - \mathrm{div}(v_{i+1} \otimes (\frac{\rho_2-\rho_1}{2}m'(\varphi_{i-1})\varphi_{i-1}^\delta\nabla\mu_i - \frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})\nabla\mu_i^\delta)) \\ + \mathrm{div}(v_{i+1}^\delta \otimes (\rho(\varphi_{i-1})v_i - \frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})\nabla\mu_i)) \\ - \mathrm{div}(2\eta'(\varphi_i)\varphi_i^\delta\epsilon(v_{i+1})) - \mathrm{div}(2\eta(\varphi_i)\epsilon(v_{i+1}^\delta)) \\ -\mu_{i+1}\nabla\varphi_i^\delta - \mu_{i+1}^\delta\nabla\varphi_i - u_{i+1}^\delta \end{pmatrix}_{i=0}^{M-2} \end{pmatrix}.$$

Due to our convention for φ_{-1} and v_0, we require that $\varphi_{-1}^\delta = 0$ and $v_0^\delta = 0$. For the application of a result due to Zowe and Kurcyusz [46] concerning the existence of Lagrange multipliers, we show that $g'(\overline{z})$ maps $\mathbb{R}_+(C - \overline{z}) \subset X$ onto Y. For this purpose, let $(\Theta_i^c, \Theta_i^w, \Theta_i^v) \in Y$ be arbitrarily fixed. We have to show that there exists

a tuple $(\varphi^\delta, \mu^\delta, v^\delta, u^\delta) \in \mathbb{R}_+(C - \overline{z})$ such that

$$\frac{1}{\tau}(\varphi_{i+1}^\delta - \varphi_i^\delta) - \operatorname{div}(m'(\varphi_i)\varphi_i^\delta \nabla \mu_{i+1}) - \operatorname{div}(m(\varphi_i)\nabla \mu_{i+1}^\delta)$$

$$(6.5) \qquad\qquad\qquad\qquad + v_{i+1} \cdot \nabla \varphi_i^\delta + v_{i+1}^\delta \cdot \nabla \varphi_i = \Theta_i^w,$$

$$(6.6) \qquad\qquad -\mu_{i+1}^\delta - \Delta \varphi_{i+1}^\delta - \kappa \varphi_i^\delta + \Psi_0''(\varphi_{i+1}; \varphi_{i+1}^\delta) = \Theta_i^c,$$

$$\frac{1}{\tau}(\rho'(\varphi_i)\varphi_i^\delta v_{i+1} - \rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i) + \frac{1}{\tau}(\rho(\varphi_i)v_{i+1}^\delta - \rho(\varphi_{i-1})v_i^\delta)$$

$$+ \operatorname{div}(v_{i+1} \otimes (\rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i + \rho(\varphi_{i-1})v_i^\delta))$$

$$- \operatorname{div}(v_{i+1} \otimes (\frac{\rho_2 - \rho_1}{2}m'(\varphi_{i-1})\varphi_{i-1}^\delta \nabla \mu_i - \frac{\rho_2 - \rho_1}{2}m(\varphi_{i-1})\nabla \mu_i^\delta))$$

$$+ \operatorname{div}(v_{i+1}^\delta \otimes (\rho(\varphi_{i-1})v_i - \frac{\rho_2 - \rho_1}{2}m(\varphi_{i-1})\nabla \mu_i))$$

$$- \operatorname{div}(2\eta'(\varphi_i)\varphi_i^\delta \epsilon(v_{i+1})) - \operatorname{div}(2\eta(\varphi_i)\epsilon(v_{i+1}^\delta))$$

$$(6.7) \qquad\qquad -\mu_{i+1}\nabla \varphi_i^\delta - \mu_{i+1}^\delta \nabla \varphi_i - u_{i+1}^\delta = \Theta_i^v,$$

where (6.5) and (6.6) hold for $i = -1, ..., M - 2$ and (6.7) for all $i = 0, ..., M - 1$. As in Theorem 3.2, standard arguments show the existence of $(\varphi_0^\delta, \mu_0^\delta) \in \overline{H}_{\partial_n}^2(\Omega) \times \overline{H}_{\partial_n}^2(\Omega)$ such that (6.5) and (6.6) are fulfilled for $i = -1$. Now we apply induction over i. Therefore, let us assume that (6.5)–(6.7) hold for $i < M - 1$. In order to show the existence of a solution to this system for $i + 1$, we note that it can be written as

$$\frac{1}{\tau}(\varphi_{i+2}^\delta - \varphi_{i+1}^\delta) - \operatorname{div}(m(\varphi_{i+1})\nabla \mu_{i+2}^\delta) + v_{i+2}^\delta \cdot \nabla \varphi_{i+1} = \Theta_\mu,$$

$$-\mu_{i+2}^\delta - \Delta \varphi_{i+2}^\delta - \kappa \varphi_{i+1}^\delta + \Psi_0''(\varphi_{i+2}; \varphi_{i+2}^\delta) = \Theta_\varphi,$$

$$\frac{1}{\tau}(\rho(\varphi_{i+1})v_{i+2}^\delta - \rho(\varphi_i)v_{i+1}^\delta) + \operatorname{div}(v_{i+2}^\delta \otimes (\rho(\varphi_i)v_{i+1} - \frac{\rho_2 - \rho_1}{2}m(\varphi_i)\nabla \mu_{i+1}))$$

$$- \operatorname{div}(2\eta(\varphi_{i+1})\epsilon(v_{i+2}^\delta)) - \mu_{i+2}^\delta \nabla \varphi_{i+1} - u_{i+2}^\delta = \Theta_v,$$

for a triple $(\Theta_\varphi, \Theta_\mu, \Theta_v) \in (\overline{L}^2(\Omega))^* \times (\overline{L}^2(\Omega))^* \times H_{0,\sigma}^1(\Omega; \mathbb{R}^N)^*$ that only depends on (φ, μ, v), on $\varphi_i^\delta, \mu_i^\delta$ and v_i^δ for $i < M - 1$ and on $(\Theta_{i+1}^c, \Theta_{i+1}^w, \Theta_{i+1}^v)$. But now the existence of a solution follows readily from Theorem 3.2 and from Lemma 3.3 when choosing $\nu = \rho(\varphi_i)v_{i+1} - \frac{\rho_2 - \rho_1}{2}m(\varphi_i)\nabla \mu_{i+1}$ as well as $f_0 = \rho(\varphi_{i+1})$, $f_{-1} = \rho(\varphi_i)$ and $u_{i+2}^\delta = 0$. Notice, here the functions $\rho(\varphi_{i+1}), m(\varphi_{i+1}), \eta(\varphi_{i+1})$ do not depend on the unknown φ_{i+2}^δ. Further observe that we can always find a convex, affine functional $\psi : \overline{H}_{\partial_n}^2(\Omega) \mapsto \mathbb{R}$ with $(D\psi)z = \Psi_0''(\varphi_{i+2}; z)$ for all $z \in \overline{H}_{\partial_n}^2(\Omega)$. Hence we deduce the existence of a Lagrange multiplier $(p, r, q) \in Y^*$ such that

$$\mathcal{J}'(\bar{\varphi}, \bar{\mu}, \bar{v}, \bar{u})(\varphi^\delta, \mu^\delta, v^\delta, u^\delta) = \langle g'(\bar{\varphi}, \bar{\mu}, \bar{v}, \bar{u})(\varphi^\delta, \mu^\delta, v^\delta, u^\delta), (p, r, q)\rangle$$

$$(6.8) \qquad\qquad = \langle g'(\bar{\varphi}, \bar{\mu}, \bar{v}, \bar{u})^*(p, r, q), (\varphi^\delta, \mu^\delta, v^\delta, u^\delta)\rangle$$

for all $(\varphi^\delta, \mu^\delta, v^\delta, u^\delta) \in \overline{H}_{\partial_n}^2(\Omega)^M \times \overline{H}_{\partial_n}^2(\Omega)^M \times H_{0,\sigma}^1(\Omega; \mathbb{R}^N)^{M-1} \times \mathbb{R}_+(U_{ad} - \bar{u})$. In order to derive the desired system for (p, r, q) from this variational equation, the adjoint of $g'(\bar{\varphi}, \bar{\mu}, \bar{v}, \bar{u})$ has to be calculated. Exemplarily, we show this calculation for two terms. First, consider the term $\operatorname{div}(v_{i+1} \otimes (\rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i))$ which gets tested by

q_i. Notice that for vector fields $z^{(1)}, z^{(2)}, z^{(3)}$ in $H^1(\Omega; \mathbb{R}^N)$ and with $z^{(2)}|_{\partial\Omega} = 0$ we have

$$(6.9) \qquad \int_\Omega z^{(3)} \cdot \operatorname{div}(z^{(2)} \otimes z^{(1)}) = -\int_\Omega z^{(2)} \cdot (Dz^{(3)})z^{(1)},$$

by Gauß' theorem. Hence we get

$$\langle \operatorname{div}(v_{i+1} \otimes \rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i), q_i \rangle = -\int_\Omega v_{i+1} \cdot (Dq_i)(\rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i)dx$$

$$= -\int_\Omega \rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i \cdot (Dq_i)^\top v_{i+1}dx.$$

Secondly, the term $\operatorname{div}(v_{i+1} \otimes -\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})\nabla\mu_i^\delta)$ gets tested by q_i. This yields

$$\langle \operatorname{div}(v_{i+1} \otimes -\frac{\rho_2 - \rho_1}{2}m(\varphi_{i-1})\nabla\mu_i^\delta), q_i \rangle = \int_\Omega v_{i+1} \cdot (Dq_i)(\frac{\rho_2 - \rho_1}{2}m(\varphi_{i-1})\nabla\mu_i^\delta)dx$$

$$= \int_\Omega \frac{\rho_2 - \rho_1}{2}m(\varphi_{i-1})\nabla\mu_i^\delta \cdot (Dq_i)^\top v_{i+1}dx$$

$$= \int_\Omega \mu_i^\delta \operatorname{div}(-\frac{\rho_2 - \rho_1}{2}m(\varphi_{i-1})(Dq_i)^\top v_{i+1})dx$$

since $v_{i+1}|_{\partial\Omega} = 0$. The other terms can be treated similarly. After collecting all terms which contain φ_i^δ, μ_i^δ and v_i^δ, respectively, it follows that

$$g'(\bar\varphi, \bar\mu, \bar v, \bar u)^*(p, r, q)$$

$$= \begin{pmatrix} \begin{pmatrix} -\frac{1}{\tau}(p_i - p_{i-1}) + a(m'(\varphi_i), \mu_{i+1}, p_i) - \operatorname{div}(p_i v_{i+1}) - \Delta^t r_{i-1} \\ +\Psi_0''(\varphi_i)^* r_{i-1} - \kappa r_{i+1} - \rho'(\varphi_i)v_{i+1} \cdot \frac{1}{\tau}(q_{i+1} - q_i) \\ -(\rho'(\varphi_i)v_{i+1} - \frac{\rho_2-\rho_1}{2}m'(\varphi_i)\nabla\mu_{i+1})(Dq_{i+1})^\top v_{i+2} \\ +2\eta'(\varphi_i)\epsilon(v_{i+1}) : Dq_i + \operatorname{div}(\mu_{i+1}q_i) \end{pmatrix}_{i=0}^{M-1} \\ \begin{pmatrix} -r_{i-1} + b(m(\varphi_{i-1}), p_{i-1}) - \operatorname{div}(\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})(Dq_i)^\top v_{i+1}) \\ -q_{i-1} \cdot \nabla\varphi_{i-1} \end{pmatrix}_{i=1}^{M-1} \\ \begin{pmatrix} -\rho(\varphi_{i-1})\frac{1}{\tau}(q_i - q_{i-1}) - \rho(\varphi_{i-1})(Dq_i)^\top v_{i+1} \\ -(Dq_{i-1})(\rho(\varphi_{i-2})v_{i-1} - \frac{\rho_2-\rho_1}{2}m(\varphi_{i-2})\nabla\mu_{i-1}) \\ -\operatorname{div}(2\eta(\varphi_{i-1})\epsilon(q_{i-1})) + p_{i-1}\nabla\varphi_{i-1} \end{pmatrix}_{i=1}^{M-1} \\ \begin{pmatrix} -q_{i-1} \end{pmatrix}_{i=1}^{M-1} \end{pmatrix}.$$

Plugging this into (6.8) and using the fact that $(\varphi^\delta, \mu^\delta, v^\delta, u^\delta)$ can be chosen arbitrarily in $\overline{H}_{\partial_n}^2(\Omega)^M \times \overline{H}_{\partial_n}^2(\Omega)^M \times H_{0,\sigma}^1(\Omega; \mathbb{R}^N)^{M-1} \times \mathbb{R}_+(U_{ad} - \bar u)$, we obtain the desired system for (p, r, q). □

The preceding theorem states first-order optimality conditions for problem (P_Ψ) in the case of smooth double-well type potentials. In the following, we derive stationarity conditions for a nonsmooth potential via a limit process; compare section 7. For this purpose, the boundedness of the adjoint states is crucial. In order to guarantee this, further regularity conditions on $\mathcal{J}$ are required.

LEMMA 6.2. *Suppose that the assumptions of Theorem 6.1 are fulfilled. Then*

$(p, r) \in \overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^{M-1}$ *and it holds that*

$$
\begin{aligned}
a(m'(\varphi_i), \mu_{i+1}, p_i) &= m'(\varphi_i)\nabla\mu_{i+1} \cdot \nabla p_i && \in \overline{H}^1(\Omega)^*, \\
b(m(\varphi_{i-1}), p_{i-1}) &= -\operatorname{div}(m(\varphi_{i-1})\nabla p_{i-1}) && \in \overline{H}^1(\Omega)^*, \\
-\Delta^t r_{i-1} &= -\Delta r_{i-1} && \in \overline{H}^1(\Omega)^*.
\end{aligned}
$$

Proof. We prove the claim by backward induction over i. For $i = M - 1$ we have $p_{M-1} = r_{M-1} = 0$ by convention. Now, we take the induction step from i to $i - 1$ assuming that $p_i, r_i \in \overline{H}^1(\Omega)$. This higher regularity implies for $\hat{z} \in \overline{H}^2_{\partial_n}(\Omega)$ that

$$
\begin{aligned}
\langle a(m'(\varphi_i), \mu_{i+1}, p_i), \hat{z} \rangle &= -\int_\Omega p_i \operatorname{div}(m'(\varphi_i)\hat{z}\nabla\mu_{i+1})dx \\
&= \int_\Omega m'(\varphi_i)\hat{z}\nabla\mu_{i+1} \cdot \nabla p_i dx \\
&\le C\|m'(\varphi_i)\|_{L^\infty}\|\nabla\mu_{i+1}\|_{L^4}\|\nabla p_i\|_{L^2}\|\hat{z}\|_{L^4} \\
&\le C\|m'(\varphi_i)\|_{L^\infty}\|\mu_{i+1}\|_{H^2}\|p_i\|_{H^1}\|\hat{z}\|_{H^1}
\end{aligned}
$$

because of $\nabla\mu_{i+1} \cdot \vec{n} = 0$ on $\partial\Omega$. Consequently, $a(m'(\varphi_i), \mu_{i+1}, p_i) \in \overline{H}^1(\Omega)^*$. Equations (6.1) and (6.2) and the assumption yield that $\Delta^t r_{i-1}$, $b(m(\varphi_{i-1}), p_{i-1}) \in \overline{H}^1(\Omega)^*$. By standard regularity arguments one shows that r_{i-1} and p_{i-1} are indeed elements of $\overline{H}^1(\Omega)$ and the desired relations for $b(m(\varphi_{i-1}), p_{i-1})$ and $\Delta^t r_{i-1}$ follow at once. $\square$

The next lemma is used in the subsequent theorem in order to prove the boundedness of the adjoint state.

LEMMA 6.3. *Let $\alpha > 0$ be given and M_1 and M_2 be bounded subsets of $\overline{H}^1(\Omega)^*$ and $H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^*$, respectively. Let $\mathcal{M}$ be the set of all tuples $(\hat{p}, \hat{r}, \hat{q}; \hat{A}; h_p, h_r, h_q; \hat{c}, \hat{u}; \hat{m}, \hat{\eta}, \hat{\rho})$ with*

$$
\begin{aligned}
(\hat{p}, \hat{r}, \hat{q}) &\in \overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N), \\
\hat{A} &\in \mathcal{L}(\overline{H}^1(\Omega); \overline{H}^1(\Omega)^*) \text{ be monotone}, \\
(h_r, h_p, h_q) &\in M_1 \times M_1 \times M_2, \\
(\hat{c}, \hat{u}) &\in \overline{H}^1(\Omega) \times H^1(\Omega; \mathbb{R}^N), \\
\hat{m}, \hat{\eta}, \hat{\rho} &\in L^\infty(\Omega) \text{ with } 1/\alpha \ge \hat{m}, \hat{\eta} \ge \alpha \text{ and } \hat{\rho} \ge 0 \text{ a.e. on } \Omega,
\end{aligned}
$$

for which the following system is satisfied:

$$
\frac{1}{\tau}\hat{p} - \Delta\hat{r} + \hat{A}\hat{r} = h_r, \tag{6.10}
$$

$$
-\hat{r} - \operatorname{div}(\hat{m}\nabla\hat{p}) - \hat{q} \cdot \nabla\hat{c} = h_p, \tag{6.11}
$$

$$
\frac{1}{\tau}\hat{\rho}\hat{q} - \operatorname{div}(2\hat{\eta}\epsilon(\hat{q})) - (D\hat{q})\hat{u} + \hat{p}\nabla\hat{c} = h_q, \tag{6.12}
$$

$$
\frac{1}{\tau}\int_\Omega \hat{\rho}|\hat{q}|^2 - \langle(D\hat{q})\hat{u}, \hat{q}\rangle \ge 0. \tag{6.13}
$$

Then the set $\{(\hat{p}, \hat{r}, \hat{q}) : (\hat{p}, \hat{r}, \hat{q}; \hat{A}; h_p, h_r, h_q; \hat{c}, \hat{u}; \hat{m}, \hat{\eta}, \hat{\rho}) \in \mathcal{M}\}$ is bounded in $\overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)$.

In order to keep the flow of the presentation, we defer the proof to the appendix.

Employing the preceding results, we finally perform the limit process with respect to the first-order optimality conditions of Theorem 6.1.

THEOREM 6.4 (Stationarity conditions). *Suppose that the following assumptions are satisfied.*

1. *$\mathcal{J}'$ is a bounded mapping from $\overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times U_{ad}$ into the space $(\overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times L^2(\Omega;\mathbb{R}^N)^{M-1})^*$ and $\frac{\partial \mathcal{J}}{\partial u}$ satisfies the following weak lower-semicontinuity property*

$$\left\langle \frac{\partial \mathcal{J}}{\partial u}(\hat{z}), \hat{u} \right\rangle \leq \liminf_{n \to \infty} \left\langle \frac{\partial \mathcal{J}}{\partial u}(\hat{z}^{(n)}), \hat{u}^{(n)} \right\rangle$$

for $\hat{z}^{(n)} = (\hat{\varphi}^{(n)}, \hat{\mu}^{(n)}, \hat{v}^{(n)}, \hat{u}^{(n)})$ converging weakly in $\overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times U_{ad}$ to $\hat{z} = (\hat{\varphi}, \hat{\mu}, \hat{v}, \hat{u})$.

2. *For every $n \in \mathbb{N}$ let $\Psi_0^{(n)} : \overline{H}^2_{\partial_n}(\Omega) \to \overline{\mathbb{R}}$ be a convex, lower-semicontinuous and proper functional satisfying the assumptions of Theorem 6.1.*

3. *Let $(\varphi^{(n)}, \mu^{(n)}, v^{(n)}, u^{(n)}) \in \overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times U_{ad}$ be a minimizer for $(P_{\Psi^{(n)}})$ and let $(p^{(n)}, r^{(n)}, q^{(n)}) \in \overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}$ be given as in Theorem 6.1 and Lemma 6.2.*

Then there exists an element $(\varphi, \mu, v, u, p, r, q)$ and a subsequence denoted by $\{(\varphi^{(m)}, \mu^{(m)}, v^{(m)}, u^{(m)}, p^{(m)}, r^{(m)}, q^{(m)})\}_{m \in \mathbb{N}}$ with

$$\varphi^{(m)} \to \varphi \text{ weakly in } \overline{H}^2_{\partial_n}(\Omega)^M, \; \mu^{(m)} \to \mu \text{ weakly in } \overline{H}^2_{\partial_n}(\Omega)^{M-1},$$

$$v^{(m)} \to v \text{ weakly in } H^2(\Omega;\mathbb{R}^N)^{M-1}, \; u^{(m)} \to u \text{ weakly in } L^2(\Omega;\mathbb{R}^N)^{M-1},$$

$$p^{(m)} \to p \text{ weakly in } \overline{H}^1(\Omega)^M, \; r^{(m)} \to r \text{ weakly in } \overline{H}^1(\Omega)^{M-1},$$

$$q^{(m)} \to q \text{ weakly in } H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}, \; \Psi_0^{(m)''}(\varphi_{i+1}^{(m)})^* r_i^{(n)} \to \lambda_i \text{ weakly in } \overline{H}^1(\Omega)^*,$$

for all $i = -1, ..., M - 2$ such that for $z = (\varphi, \mu, v, u)$ and $\tilde{q}_k := q_{k-1}$ it holds that

$$-\frac{1}{\tau}(p_i - p_{i-1}) + m(\varphi_i)' \nabla \mu_{i+1} \cdot p_i - \text{div}(p_i v_{i+1}) - \Delta r_{i-1}$$

$$+ \lambda_{i-1} - \kappa r_{i+1} - \frac{1}{\tau}\rho(\varphi_i)' v_{i+1} \cdot (q_{i+1} - q_i)$$

$$- (\rho(\varphi_i)' v_{i+1} - \frac{\rho_2 - \rho_1}{2} m'(\varphi_i) \nabla \mu_{i+1})(Dq_{i+1})^\top v_{i+2}$$

(6.14) $$+ 2\eta(\varphi_i)' \epsilon(v_{i+1}) : Dq_i + \text{div}(\mu_{i+1} q_i) = \frac{\partial \mathcal{J}}{\partial \varphi_i}(z),$$

$$- r_{i-1} - \text{div}(m(\varphi_{i-1}) \nabla p_{i-1}) - \text{div}(\frac{\rho_2 - \rho_1}{2} m(\varphi_{i-1})(Dq_i)^\top v_{i+1})$$

(6.15) $$- q_{i-1} \cdot \nabla \varphi_{i-1} = \frac{\partial \mathcal{J}}{\partial \mu_i}(z),$$

$$- \frac{1}{\tau}\rho(\varphi_{j-1})(q_j - q_{j-1}) - \rho(\varphi_{j-1})(Dq_j)^\top v_{j+1}$$

$$- (Dq_{j-1})(\rho(\varphi_{j-2}) v_{j-1} - \frac{\rho_2 - \rho_1}{2} m(\varphi_{j-2}) \nabla \mu_{j-1})$$

(6.16) $$- \text{div}(2\eta(\varphi_{j-1}) \epsilon(q_{j-1})) + p_{j-1} \nabla \varphi_{j-1} = \frac{\partial \mathcal{J}}{\partial v_j}(z),$$

(6.17) $$\frac{\partial \mathcal{J}}{\partial u}(z) - \tilde{q} \in \left[\mathbb{R}_+(U_{ad} - u)\right]^+.$$

Proof. 1. In the first step, we show the boundedness of $\{(p^{(n)}, r^{(n)}, q^{(n)})\}_{n\in\mathbb{N}}$ in $\overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}$. Moreover, the boundedness of the sequence $\{(\varphi^{(n)}, \mu^{(n)}, v^{(n)}, u^{(n)})\}_{n\in\mathbb{N}}$ in $\overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^2_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times L^2(\Omega;\mathbb{R}^N)^{M-1}$ follows from Lemma 3.6. For $i = 0, ..., M-1$, $j = 1, ..., M-1$ and $n \in \mathbb{N}$ the adjoint system for $(\mathrm{P}_{\Psi^{(n)}})$ corresponding to (6.1)–(6.4) can be rewritten as

(6.18)
$$\frac{1}{\tau}p^{(n)}_{i-1} - \Delta r^{(n)}_{i-1} + \Psi^{(n)''}_0(\varphi^{(n)}_i)^* r^{(n)}_{i-1} = \Theta^{(n)}_{r,i-1},$$

$$-r^{(n)}_{j-1} - \mathrm{div}(m(\varphi^{(n)}_{j-1})\nabla p^{(n)}_{j-1}) - q^{(n)}_{j-1} \cdot \nabla\varphi^{(n)}_{j-1} = \Theta^{(n)}_{p,j-1},$$

$$\frac{1}{\tau}\rho(\varphi^{(n)}_{j-1})q^{(n)}_{j-1} - \mathrm{div}(2\eta(\varphi^{(n)}_{j-1})\epsilon(q^{(n)}_{j-1})) + p^{(n)}_{j-1}\nabla\varphi^{(n)}_{j-1}$$
$$-(Dq_{j-1})(\rho(\varphi^{(n)}_{j-2})v^{(n)}_{j-1} - \frac{\rho_2-\rho_1}{2}m(\varphi^{(n)}_{j-2})\nabla\mu^{(n)}_{j-1}) = \Theta^{(n)}_{q,j-1},$$

where the functionals $\Theta^{(n)}_r$, $\Theta^{(n)}_p$ and $\Theta^{(n)}_q$ are given by

$$\Theta^{(n)}_{r,i-1} = \frac{\partial\mathcal{J}}{\partial\varphi_i}(z^{(n)}) + \frac{1}{\tau}p^{(n)}_i - \left[m'(\varphi^{(n)}_i)\nabla\mu^{(n)}_{i+1} \cdot p^{(n)}_i - \mathrm{div}(p^{(n)}_i v^{(n)}_{i+1}) - \kappa r^{(n)}_{i+1}\right.$$
$$-\frac{1}{\tau}\rho(\varphi^{(n)}_i)' v^{(n)}_{i+1} \cdot (q^{(n)}_{i+1} - q^{(n)}_i) + 2\eta(\varphi^{(n)}_i)'\epsilon(v^{(n)}_{i+1}) : Dq^{(n)}_i + \mathrm{div}(\mu^{(n)}_{i+1}q^{(n)}_i)$$
$$\left.- (\rho(\varphi^{(n)}_i)'v^{(n)}_{i+1} - \frac{\rho_2-\rho_1}{2}m'(\varphi^{(n)}_i)\nabla\mu^{(n)}_{i+1})(Dq^{(n)}_{i+1})^\top v^{(n)}_{i+2}\right],$$

$$\Theta^{(n)}_{p,i-1} = \frac{\partial\mathcal{J}}{\partial\mu_i}(z^{(n)}) + \mathrm{div}(\frac{\rho_2-\rho_1}{2}m(\varphi^{(n)}_{i-1})(Dq^{(n)}_i)^\top v^{(n)}_{i+1}),$$

$$\Theta^{(n)}_{q,i-1} = \frac{\partial\mathcal{J}}{\partial v_i}(z^{(n)}) + \frac{1}{\tau}\rho(\varphi^{(n)}_{i-1})q^{(n)}_i - \rho(\varphi^{(n)}_{i-1})(Dq^{(n)}_i)^\top v^{(n)}_{i+1}.$$

Here, $z^{(n)}$ denotes the tuple $(\varphi^{(n)}, \mu^{(n)}, v^{(n)}, u^{(n)})$. We prove the boundedness of $\{(p^{(n)}, r^{(n)}, q^{(n)})\}_{n\in\mathbb{N}}$ in $\overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}$ by backward induction over i. If $i \geq M-1$, then $(p^{(n)}_i, r^{(n)}_i, q^{(n)}_i) = 0$ by convention. In the induction step assume that for $i \in \{0, ..., M-1\}$ and for $j \geq i$ the sequence $\left\{(p^{(n)}_j, r^{(n)}_j, q^{(n)}_j)\right\}_{n\in\mathbb{N}}$ is bounded in $\overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$. This and the assumption on $\mathcal{J}$ imply that $\left\{(\Theta^{(n)}_{p,i-1}, \Theta^{(n)}_{r,i-1}, \Theta^{(n)}_{q,i-1})\right\}_{n\in\mathbb{N}}$ is bounded in $(\overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N))^*$. To see this, we exemplarily consider first $2\eta(\varphi^{(n)}_i)'\epsilon(v^{(n)}_{i+1}):Dq^{(n)}_i$, which is bounded by

$$\|2\eta(\varphi^{(n)}_i)'\epsilon(v^{(n)}_{i+1}) : Dq^{(n)}_i\|_{L^{6/5}} \leq C\|\eta(\varphi^{(n)}_i)'\|_{L^\infty}\|\epsilon(v^{(n)}_{i+1})\|_{L^3}\|Dq^{(n)}_i\|_{L^2}$$
$$\leq C\|\eta(\varphi^{(n)}_i)'\|_{L^\infty}\|v^{(n)}_{i+1}\|_{H^2}\|q^{(n)}_i\|_{H^1}$$

and secondly $-\frac{\rho_2-\rho_1}{2}m'(\varphi^{(n)}_i)\nabla\mu^{(n)}_{i+1}(Dq^{(n)}_{i+1})^\top v^{(n)}_{i+2}$, which we bounded using

$$\| - \frac{\rho_2 - \rho_1}{2}m'(\varphi^{(n)}_i)\nabla\mu^{(n)}_{i+1}(Dq^{(n)}_{i+1})^\top v^{(n)}_{i+2}\|_{L^{6/5}}$$
$$\leq C\| - \frac{\rho_2 - \rho_1}{2}m'(\varphi^{(n)}_i)\|_{L^\infty}\|\nabla\mu^{(n)}_{i+1}\|_{L^6}\|Dq^{(n)}_{i+1}\|_{L^2}\|v^{(n)}_{i+2}\|_{L^6}$$
$$\leq C\| - \frac{\rho_2 - \rho_1}{2}m'(\varphi^{(n)}_i)\|_{L^\infty}\|\mu^{(n)}_{i+1}\|_{H^2}\|q^{(n)}_{i+1}\|_{H^1}\|v^{(n)}_{i+2}\|_{H^2}.$$

Consequently, these terms define continuous linear functionals on $\overline{H}^1(\Omega)$, that are bounded independently of n. The other summands can be estimated similarly.

In case of $i > 0$ we apply Lemma 6.3 to

$$(\hat{p}, \hat{r}, \hat{q}; \hat{A}; h_p, h_r, h_q; \hat{c}, \hat{u}; \hat{m}, \hat{\eta}, \hat{\rho})$$
$$:= (p_{i-1}^{(n)}, r_{i-1}^{(n)}, q_{i-1}^{(n)}; \Psi_0^{(n)''}(\varphi_i^{(n)})^*; \Theta_{p,i-1}^{(n)}, \Theta_{r,i-1}^{(n)}, \Theta_{q,i-1}^{(n)};$$
$$\varphi_{i-1}^{(n)}, \rho(\varphi_{i-2}^{(n)})v_{i-1}^{(n)} - \frac{\rho_2 - \rho_1}{2}m(\varphi_{i-2}^{(n)})\nabla\mu_{i-1}^{(n)}; -\frac{\rho_2 - \rho_1}{2}m(\varphi_{i-1}^{(n)}), \eta(\varphi_{i-1}^{(n)}), \rho(\varphi_{i-1}^{(n)})).$$

Note that due to $\mathrm{div}v_{i-1}^{(n)} = 0$ we have

$$\mathrm{div}\,\hat{u} = \rho(\varphi_{i-2}^{(n)})' v_{i-1}^{(n)} \cdot \nabla\varphi_{i-1}^{(n)} - \mathrm{div}(\frac{\rho_2 - \rho_1}{2}m(\varphi_{i-2}^{(n)})\nabla\mu_{i-1}^{(n)})$$
$$= \frac{\rho_2 - \rho_1}{2}\left[v_{i-1}^{(n)} \cdot \nabla\varphi_{i-1}^{(n)} - \mathrm{div}(m(\varphi_{i-2}^{(n)})\nabla\mu_{i-1}^{(n)})\right]$$
$$= \frac{1}{\tau}\frac{\rho_2 - \rho_1}{2}(\varphi_{i-1}^{(n)} - \varphi_{i-2}^{(n)}) \;\; = \;\; -\frac{1}{\tau}(\rho(\varphi_{i-1}^{(n)}) - \rho(\varphi_{i-2}^{(n)})).$$

With the help of $\int_\Omega \langle (D\hat{q})\hat{u}, \hat{q}\rangle = -\int_\Omega \hat{q} \cdot \mathrm{div}(\hat{q} \otimes \hat{u})$ (cf. (6.9)), (3.7) yields

$$\frac{1}{\tau}\int_\Omega \hat{\rho}|\hat{q}|^2 dx - \langle(D\hat{q})\hat{u}, \hat{q}\rangle = \frac{1}{\tau}\int_\Omega \rho(\varphi_{i-1}^{(n)})|q_{i-1}^{(n)}|^2 - \frac{1}{2}(\rho(\varphi_{i-1}^{(n)}) - \rho(\varphi_{i-2}^{(n)}))|q_{i-1}^{(n)}|^2 dx$$
$$= \frac{1}{2\tau}\int_\Omega (\rho(\varphi_{i-2}^{(n)}) + \rho(\varphi_{i-1}^{(n)}))|q_{i-1}^{(n)}|^2 dx \;\; \geq \;\; 0,$$

because of $\rho(\varphi_{i-2}^{(n)}) \geq 0$ and $\rho(\varphi_{i-1}^{(n)}) \geq 0$ almost everywhere. Hence Lemma 6.3 implies the boundedness of $(p_{i-1}^{(n)}, r_{i-1}^{(n)}, q_{i-1}^{(n)})$ in $\overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H_{0,\sigma}^1(\Omega; \mathbb{R}^N)$.

The case $i = 0$ needs some modifications in order to be treated by Lemma 6.3 since (6.3) is not defined for $i = 0$. In this case we set $(\hat{q}, h_q, \hat{c}, \hat{u}, \hat{\eta}) = (0, 0, 0, 0, \eta(\varphi_i^{(n)}))$ together with the definition of the remaining quantities as in the case $i > 0$. Now, by Lemma 6.3 we conclude the boundedness of $(p_{i-1}^{(n)}, r_{i-1}^{(n)})$ in $\overline{H}^1(\Omega) \times \overline{H}^1(\Omega)$. Moreover, from (6.18) it follows that also $(\Psi_0^{(n)''}(\varphi_i^{(n)})^* r_{i-1}^{(n)})$ remains bounded in $\overline{H}^1(\Omega)^*$.

2. With the bounds derived in step 1 and with the usual compact embeddings of Sobolev spaces, we can pass to a subsequence with the desired convergence properties.

3. Now we pass to the limit in the the adjoint systems corresponding to (6.1)–(6.4) for $(P_{\Psi^{(n)}})$. The limits for the equations (6.1) and (6.2) are considered in $\overline{H}^1(\Omega)^*$ and the limit for (6.3) in $H_{0,\sigma}^1(\Omega; \mathbb{R}^N)^*$. In the linear terms we can pass to the limit at once. For $m'(\varphi_i^{(n)})\nabla\mu_{i+1}^{(n)} \cdot p_i^{(n)}$ we have that $m'(\varphi_i^{(n)})$ converges strongly in $L^\infty(\Omega)$ to $m'(\varphi_i)$, $\nabla\mu_{i+1}^{(n)}$ strongly in $L^{6-\varepsilon}(\Omega)$ to $\nabla\mu_{i+1}$ and $p_i^{(n)}$ weakly in $L^6(\Omega)$ to p_i. Hence, $m'(\varphi_i^{(n)})\nabla\mu_{i+1}^{(n)} \cdot p_i^{(n)}$ converges weakly in $\overline{H}^1(\Omega)^*$ to $m'(\varphi_i)\nabla\mu_{i+1} \cdot p_i$. For $\frac{\rho_2 - \rho_1}{2}m'(\varphi_i^{(n)})\nabla\mu_{i+1}^{(n)}(Dq_{i+1}^{(n)})^\top v_{i+2}^{(n)}$ we note that $\frac{\rho_2 - \rho_1}{2}m'(\varphi_i^{(n)})$ and $v_{i+2}^{(n)}$ converge strongly in $L^\infty(\Omega)$ to $\frac{\rho_2 - \rho_1}{2}m'(\varphi_i)$ respectively v_{i+2}, $\nabla\mu_{i+1}^{(n)}$ strongly in $L^{6-\varepsilon}(\Omega)$ to $\nabla\mu_{i+1}$ and $Dq_i^{(n)}$ weakly in $L^2(\Omega)$ to Dq_i. Therefore $\frac{\rho_2 - \rho_1}{2}m'(\varphi_i^{(n)})\nabla\mu_{i+1}^{(n)}(Dq_{i+1}^{(n)})^\top v_{i+2}^{(n)}$ converges weakly in $\overline{H}^1(\Omega)^*$ to $\frac{\rho_2 - \rho_1}{2}m'(\varphi_i)\nabla\mu_{i+1}(Dq_{i+1})^\top v_{i+2}$.

For $\mathrm{div}(\frac{\rho_2 - \rho_1}{2}m(\varphi_{i-1}^{(n)})(Dq_i^{(n)})^\top v_{i+1}^{(n)})$ we use that $\frac{\rho_2 - \rho_1}{2}m(\varphi_{i-1}^{(n)})$ and $v_{i+1}^{(n)}$ converge strongly in $L^\infty(\Omega)$ to $\frac{\rho_2 - \rho_1}{2}m(\varphi_{i-1})$ respectively v_{i+1}, and $q_i^{(n)}$ weakly in $L^6(\Omega)$ to

q_i. As a consequence, $\operatorname{div}(\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1}^{(n)})(Dq_i^{(n)})^\top v_{i+1}^{(n)})$ converges weakly in $\overline{H}^1(\Omega)^*$ to $\operatorname{div}(\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})(Dq_i)^\top v_{i+1})$. For the convergence of $\operatorname{div}(2\eta(\varphi_{i-1}^{(n)})\epsilon(q_{i-1}^{(n)}))$ note that $\eta(\varphi_{i-1}^{(n)})$ converges strongly in $L^\infty(\Omega)$ to $\eta(\varphi_{i-1})$ and $\epsilon(q_{i-1}^{(n)})$ weakly in $L^2(\Omega)$ to $\epsilon(q_{i-1})$. Hence, $\operatorname{div}(2\eta(\varphi_{i-1}^{(n)})\epsilon(q_{i-1}^{(n)}))$ converges weakly in $H_{0,\sigma}^1(\Omega;\mathbb{R}^N)^*$ to the limit $\operatorname{div}(2\eta(\varphi_{i-1})\epsilon(q_{i-1}))$. Apart from $\Psi_0^{(n)''}(\varphi_i^{(n)})^* r_{i-1}^{(n)}$, all remaining terms appearing on the left hand sides can be treated similarly. Moreover, our assumptions on $\mathcal{J}$ imply that $\mathcal{J}'(\varphi^{(n)},\mu^{(n)},v^{(n)},u^{(n)})$ converges weakly to $\mathcal{J}'(\varphi,\mu,v,u)$ in $(\overline{H}_{\partial_n}^2(\Omega)^M \times \overline{H}_{\partial_n}^2(\Omega)^M \times H_{0,\sigma}^1(\Omega;\mathbb{R}^N)^{M-1} \times L^2(\Omega;\mathbb{R}^N)^{M-1})^*$.

Consequently, by (6.1) also $\Psi_0''(\varphi_i^{(n)})^* r_{i-1}^{(n)}$ converges weakly in $(\overline{H}^1(\Omega)^*)^M$ to some λ_{i-1}. Therefore, we arrive at the system (6.14)–(6.16). Finally, notice that for all $y \in U_{ad}$ and with $z^{(n)} := (\varphi^{(n)},\mu^{(n)},v^{(n)},u^{(n)})$ and $\tilde{q}_k^{(n)} := q_{k-1}^{(n)}$ by the weak lower-semicontinuity of $\frac{\partial\mathcal{J}}{\partial u}$ and the weak and strong convergence of the sequences involved we deduce that

$$
\begin{aligned}
\langle \tfrac{\partial\mathcal{J}}{\partial u}(z) - \tilde{q}, y - u\rangle &= \langle \tfrac{\partial\mathcal{J}}{\partial u}(z),y\rangle - \langle \tfrac{\partial\mathcal{J}}{\partial u}(z),u\rangle - \langle\tilde{q},y-u\rangle \\
&\geq \liminf_{n\to\infty}\left(\langle \tfrac{\partial\mathcal{J}}{\partial u}(z^{(n)}),y\rangle - \langle \tfrac{\partial\mathcal{J}}{\partial u}(z^{(n)}),u^{(n)}\rangle - \langle\tilde{q}^{(n)},y-u^{(n)}\rangle\right) \\
&= \liminf_{n\to\infty}\left(\tfrac{\partial\mathcal{J}}{\partial u}(z^{(n)}) - \tilde{q}^{(n)}, y - u^{(n)}\rangle\right) \\
&\geq 0,
\end{aligned}
$$

due to the optimality of $z^{(n)}$ for $(P_{\Psi^{(n)}})$. This shows (6.17) and finishes the proof. $\square$

REMARK 6.1. *We point out that a tracking-type functional, like, e.g.,*

$$
\mathcal{J}(\varphi,\mu,v,u) := \frac{1}{2}\|\varphi_{M-1} - \varphi_d\|^2 + \frac{\xi}{2}\|u\|_{(L^2)^{(M-1)}}^2, \ \xi > 0,
$$

with $\varphi_d \in L^2(\Omega)$ a desired final state, satisfies the assumptions of Theorem 6.4.

REMARK 6.2. *If the set U_{ad} is bounded, Theorem 6.4 holds also true for a sequence $\{(\varphi^{(n)},\mu^{(n)},v^{(n)},u^{(n)})\}_{n\in\mathbb{N}}$ of stationary points for $(P_{\Psi^{(n)}})$. If it is unbounded, then the result can still be transferred to sequences of stationary points by assuming that the sequence $\{u^{(n)}\}_{n\in\mathbb{N}}$ is bounded in $L^2(\Omega;\mathbb{R}^N)^{M-1}$.*

7. Stationarity conditions in case of the double-obstacle potential. In this section, we apply the developed theory to the initially stated optimal control problem associated to the double-obstacle potential. For this purpose, let ψ_0 be defined as in Assumption 3.1.1 and set $\gamma := \partial\psi_0 \subset \mathbb{R}\times\mathbb{R}$. Then we define the sequence of approximating double-well type potentials as follows.

DEFINITION 7.1. *Let a mollifier $\zeta \in C^1(\mathbb{R})$ with $\operatorname{supp}\zeta \subset [-1,1]$, $\int_\mathbb{R}\zeta = 1$ and $0 \leq \zeta \leq 1$ a.e. on $\mathbb{R}$, and a function $\theta:\mathbb{R}^+ \to \mathbb{R}^+$, with $\theta(\alpha) > 0$ and $\frac{\theta(\alpha)}{\alpha} \to 0$ as $\alpha \to 0$, be given. For the Yosida approximation γ_α with parameter $\alpha > 0$ of γ define*

$$
\zeta_\alpha(s) := \frac{1}{\alpha}\zeta\Big(\frac{s}{\alpha}\Big), \quad \widetilde{\gamma}_\alpha := \gamma_\alpha * \zeta_{\theta(\alpha)}, \quad \psi_{0\alpha}(s) := \int_0^s \widetilde{\gamma}_\alpha(t)\,dt,
$$

$$
\Psi_{0\alpha}(c) := \int_\Omega (\psi_{0\alpha}\circ c)(t)\,dt.
$$

Moreover, we set $\alpha_n := n^{-1}$, $\Psi_0^{(n)} := \Psi_{0\alpha_n}$.

REMARK 7.1. *We note that $\Psi_0^{(n)'}$ can be identified with the superposition operator corresponding to $\widetilde{\gamma}_{\alpha_n}$, cf. [25]. Since $\widetilde{\gamma}'_{\alpha_n}$ is bounded and since $\overline{H}^2_{\partial_n}(\Omega)$ embeds continuously into $L^{2-\delta}(\Omega)$ for $\delta > 0$, it follows that $\Psi_0^{(n)'}$ maps $\overline{H}^2_{\partial_n}(\Omega)$ continuously Fréchet-differentiably into $L^2(\Omega)$, see, e.g., [20].*

In order to obtain a stationarity condition for the optimal control problem of CHNS with the double-obstacle potential we pass to the limit (with the Yosida parameter) in a sequence of optimal control problems with approximating double-well-type potentials.

THEOREM 7.2 (Limiting ε-almost C-stationarity). *Let $\Psi_0^{(n)}$, $n \in \mathbb{N}$ be the functionals of Definition 7.1, and let the tuples $(\varphi^{(m)}, \mu^{(m)}, v^{(m)}, u^{(m)}, p^{(m)}, r^{(m)}, q^{(m)})$, $(\varphi, \mu, v, u, p, r, q)$ and $\mathcal{J}$ be as in Theorem 6.4. Moreover, let $\Lambda : \mathbb{R} \to \mathbb{R}$ be a Lipschitz function with $\Lambda(\psi_1) = \Lambda(\psi_2) = 0$. For*

$$a_i^{(m)} := \Psi_0^{(m)'}(\varphi_i^{(m)}), \quad \lambda_i^{(m)} := \Psi_0^{(m)''}(\varphi_i^{(m)})^* r_{i-1}^{(m)}$$

for $i = 0, ..., M$, and for a_i denoting the limit of $a_i^{(m)}$, it holds that

$$(a_i, \Lambda(\varphi_i))_{L^2} = 0, \qquad\qquad \langle \lambda_i, \Lambda(\varphi_i) \rangle = 0,$$

$$(a_i, r_{i-1})_{L^2} = 0, \qquad\qquad \liminf (\lambda_i^{(m)}, r_{i-1}^{(m)})_{L^2} \geq 0.$$

Moreover, for every $\varepsilon > 0$ there exist a measurable subset M_i^ε of $M_i := \{x \in \Omega : \psi_1 < \varphi_i(x) < \psi_2\}$ with $|M_i \setminus M_i^\varepsilon| < \varepsilon$ and

$$\langle \lambda_i, v \rangle = 0 \qquad \forall v \in \overline{H}^1(\Omega), \ v|_{\Omega \setminus M_i^\varepsilon} = 0.$$

Proof. 1. The subdifferential γ satisfies $y\Lambda(x) = 0$ if $(x, y) \in \gamma$. Since $(\varphi_i, a_i) \in \gamma$ a.e. on Ω and since $a_i \in L^2(\Omega)$, integration yields the complementarity condition $(a_i, \Lambda(\varphi_i))_{L^2} = 0$.

2. Now we show that $(\lambda_i, \Lambda(\varphi_i))_{L^2} = 0$. It is well-known that the superposition P_K of the metric projection p_K of $\mathbb{R}$ onto $K := [\psi_1, \psi_2]$ maps $\overline{H}^1(\Omega)$ continuously into itself. Denoting by L_Λ the Lipschitz constant of Λ, it holds that $|\Lambda(s)| \leq L_\Lambda \min(|s - \psi_1|, |s - \psi_2|)$ for $s \in \mathbb{R}$. Using $|\widetilde{\gamma}'_\alpha(s)| \leq \frac{1}{\alpha}$ for all s and $\widetilde{\gamma}'_\alpha(s) = 0$ for $\psi_1 + \theta(\alpha) \leq s \leq \psi_2 - \theta(\alpha)$ (cf. [25]) yields

$$
\begin{aligned}
|(\lambda_i^{(m)}, \Lambda(P_K(\varphi_i^{(m)})))_{L^2}|^2 &= |(r_i^{(m)}, \Psi_0^{(m)''}(\varphi_i^{(m)}) \Lambda(P_K(\varphi_i^{(m)})))_{L^2}|^2 \\
&\leq \| r_i^{(m)} \|^2_{L^2} \int_\Omega |\widetilde{\gamma}'_{\alpha_m}(\varphi_i^{(m)}) \Lambda(P_K(\varphi_i^{(m)}))|^2 \\
&\leq \left(|\Omega| \, \| r_i^{(m)} \|_{L^2} \, L_\Lambda \frac{\theta(\alpha_m)}{\alpha_m} \right)^2 \ \to\ 0
\end{aligned}
$$

as $m \to \infty$ and consequently

$$
\begin{aligned}
&\lim (\lambda_i^{(m)}, \Lambda(\varphi_i^{(m)}))_{L^2} \\
&= \lim (\lambda_i^{(m)}, \Lambda(P_K(\varphi_i^{(m)})))_{L^2} + \lim \langle \lambda_i^{(m)}, \Lambda(\varphi_i^{(m)}) - \Lambda(P_K(\varphi_i^{(m)})) \rangle_{\overline{H}^1(\Omega)} \\
&= 0,
\end{aligned}
$$

which implies $\langle \lambda_i, \Lambda(\varphi_i) \rangle = 0$ since $\varphi_i^{(m)}$ converges strongly to $\varphi_i = P_K(\varphi_i)$ in $\overline{H}^1(\Omega)$.

3. Denoting $g_m(s) := \widetilde{\gamma}_{\alpha_m}(s) - \widetilde{\gamma}'_{\alpha_m}(s)\pi(s)$ with $s - p_K(s) =: \pi(s)$ yields

$$
\begin{aligned}
(\, a_i^{(m)}, r_{i-1}^{(m)} \,)_{L^2} &= \big(\, r_{i-1}^{(m)}, \widetilde{\gamma}_{\alpha_m}(\varphi_i^{(m)}) \,\big)_{L^2} \\
&= \big(\, r_{i-1}^{(m)}, g_m(\varphi_i^{(m)}) \,\big)_{L^2} + \big(\, \lambda_i^{(m)}, \varphi_i^{(m)} - P_K(\varphi_i^{(m)}) \,\big)_{L^2}.
\end{aligned}
$$

Since $|g_m(s)| = |\widetilde{\gamma}_{\alpha_m}(s) - \widetilde{\gamma}'_{\alpha_m}(s)\pi(s)| \leq C \frac{\theta(\alpha_m)}{\alpha_m}$ for m sufficiently large (cf. Lemma 4.2 in [25]), the first term on the right-hand side converges to 0 and the second one as well because of the strong convergence of $(\varphi_i^{(m)})$ and $(P_K(\varphi_i^{(m)}))$ to φ_i in $\overline{H}^1(\Omega)$, respectively.

4. The property $\liminf(\, \lambda_i^{(m)}, r_{i-1}^{(m)} \,)_{L^2} \geq 0$ follows readily from the monotonicity of $\Psi_0^{(m)''}(\varphi_i^{(m)})$.

5. The convergence properties of $\varphi_i^{(m)}$ imply that the subset $G := \{x \in \Omega : \varphi_i^{(m)}(x) \to \varphi_i(x) \text{ as } m \to \infty\}$ of Ω has full measure (i.e. $|G| = |\Omega|$). Therefore, for every $x \in G \cap M_i$ we can find $m_0(x) \in \mathbb{N}$ with $\psi_1 + \theta(\alpha_m) < \varphi_i^{(m)}(x) < \psi_2 - \theta(\alpha_m)$ for all $m \geq m_0(x)$. Thus, $\lambda_i^{(m)}(x) = \widetilde{\gamma}'_{\alpha_m}(\varphi_i^{(m)}(x))r_i^{(m)}(x)$ converges to 0 on $G \cap M_i$. Using Egorov's theorem shows that for every $\varepsilon > 0$ there exists a subset M_i^ε of $G \cap M_i$ with $|M_i \setminus M_i^\varepsilon| < \varepsilon$ such that $\lambda_i^{(m)}$ converges uniformly to zero on M_i^ε. Hence, we obtain $\langle \lambda_i, v \rangle = \lim \langle \lambda_i^{(m)}, v \rangle = 0$ for every $v \in \overline{H}^1(\Omega)$ with $v|_{\Omega \setminus M_i^\varepsilon} = 0$. $\square$

In combination with the results from Theorem 6.4, Theorem 7.2 states stationarity conditions corresponding to a function space version of C-stationarity for MPECs, cf. [22, 23].

8. Conclusion. Our specific semi-discretization in time for the coupled CHNS system with non-matched fluid densities represents a first step towards a numerical investigation/realization of the problem. Most importantly, it preserves the strong coupling of the Cahn-Hilliard and Navier-Stokes system which, in the case of non-matched densities, is additionally enforced through the presence of the relative flux J. As a result, well-posedness of the time discrete scheme is guaranteed and energy estimates mirroring the physical fact of decreasing energies can be argued. Such an energy property is not clear for the time continuous problem at this point in time and might be the subject of further research.

Concerning the potential chosen in the Ginzburg-Landau energy, we note that while the existence of global solutions to the optimal control problem can be shown for both cases (i.e., for double-well and double obstacle potentials) simultaneously, the derivation of stationarity conditions is more delicate. In fact, the double-obstacle potential gives rise to a degenerate constraint system with the overall problem falling into the realm of mathematical programs with equilibrium constraints (MPECs). In our approach, the constraint degeneracy is handled by a Moreau-Yosida regularization approach (resulting in an approximating sequence of double-well-type potentials) and a subsequent limiting process leading to a function space version of so-called C-stationarity. For the underlying problem class, our limiting version of C-stationarity is currently the most (and, to the best of our knowledge, only) selective stationarity system available. As an alternative analytical approach, one may want to pursue set-valued analysis in order to derive stationarity conditions directly, i.e., from applying variational geometry (contingent, critical and normal cones) and generalized differentiation. This, however, is usually not possible by simple application of available tools, but rather by expanding current technology. It, thus, may serve as a subject of our future work on this problem class.

Finally, we point out that the constructive nature of our derivation of stationarity conditions facilitates a numerical implementation of the approach which can be exploited in future investigations of these problem types, both, from a numerical, as well as, from a practical point of view. In [26], this has already been effectively done for the case of matched densities.

Appendix A. Proof of Lemma 3.4.

Proof. Let $L_\varepsilon : \overline{H}^1(\Omega) \to \overline{H}^{-1}(\Omega)$ be defined by

$$\langle L_\varepsilon(\varphi), \phi \rangle := \langle -\Delta\varphi, \phi \rangle$$

(A.1)
$$- \langle g_1 + \max(-g_1, 0)\theta_\varepsilon(\varphi - \psi_1) + \min(-g_1, 0)\theta_\varepsilon(\psi_2 - \varphi), \phi \rangle$$

where $\phi \in \overline{H}^1(\Omega)$ and θ_ε is defined by

$$\theta_\varepsilon(x) := \begin{cases} 1 & \text{if } x \leq 0, \\ 1 - \frac{x}{\varepsilon} & \text{if } 0 \leq x \leq \varepsilon, \\ 0 & \text{if } x \geq \varepsilon. \end{cases}$$

Since $g_1 \in L^2(\Omega)$ and $\theta_\varepsilon(\varphi - \psi_1), \theta_\varepsilon(\psi_2 - \varphi) \in L^\infty(\Omega)$, it holds that

(A.2) $\|g_1 + \max(-g_1, 0)\theta_\varepsilon(\varphi - \psi_1) + \min(-g_1, 0)\theta_\varepsilon(\varphi - \psi_2)\| \leq \|g_1\|.$

We show that for every $0 < \varepsilon \leq \min(-\psi_1, \psi_2)$ there exists a unique $\varphi_\varepsilon \in H_m^2 \cap \mathbb{K}$ such that

(A.3) $L_\varepsilon(\varphi_\varepsilon) = 0,$

In fact, for every $w, v \in \overline{H}^1(\Omega)$, it can be seen that

$$\langle L_\varepsilon(w) - L_\varepsilon(v), w - v \rangle \geq \int_\Omega |\nabla w - \nabla v|^2 \, dx$$

where we use the monotonicity of θ_ε. By Poincaré's inequality there exists a constant $C > 0$ such that

$$\langle L_\varepsilon(w) - L_\varepsilon(v), w - v \rangle \geq \|\nabla w - \nabla v\|^2 \geq C \|w - v\|_{H^1}^2.$$

Consequently, L_ε is strongly monotone and coercive. Since L_ε is also continuous on finite dimensional subspaces of $\overline{H}^1(\Omega)$, [31, III: Corollary 1.8] is applicable which yields the existence of $\varphi_\varepsilon \in \overline{H}^1(\Omega)$ with $L_\varepsilon(\varphi_\varepsilon) = 0$.

Due to the definition of L_ε and inequality (A.2), we have $\Delta\varphi_\varepsilon \in L^2(\Omega)$. By [34, Theorem 2.3.6] and [34, Theorem 2.3.1] there exists a constant $C_1 > 0$ such that

(A.4) $\|\varphi_\varepsilon\|_{H^2} \leq C_1 \|\Delta\varphi_\varepsilon\| + \|\varphi_\varepsilon\|.$

In combination with (A.2) and Poincaré's inequality, this leads to

(A.5) $\|\varphi_\varepsilon\|_{H^2} \leq C_2 \|g_1\|.$

Now, we set $\beta_\varepsilon := \varphi_\varepsilon - \min(\varphi_\varepsilon, \psi_2) \geq 0$ and observe that

(A.6) $\|\nabla\beta_\varepsilon\|^2 = \int_{\Omega_1} \nabla(\varphi_\varepsilon - \psi_2)\nabla\beta_\varepsilon \, dx = \langle -\Delta\varphi_\varepsilon, \beta_\varepsilon \rangle$

where $\Omega_1 := \{x \in \Omega : \beta_\varepsilon(x) > 0\} = \{x \in \Omega : \varphi_\varepsilon(x) > \psi_2 \geq \psi_1 + \varepsilon\}$. By equation (A.1) and (A.3), this leads to

$$\|\nabla\beta_\varepsilon\|^2 = \int_{\Omega_1} (g_1 + \max(-g_1, 0)\theta_\varepsilon(\varphi_\varepsilon - \psi_1) + \min(-g_1, 0)\theta_\varepsilon(\psi_2 - \varphi_\varepsilon))\beta_\varepsilon dx$$

$$= \int_{\Omega_1} (g_1 + \min(-g_1, 0))\beta_\varepsilon dx \leq 0.$$

Thus, $\beta_\varepsilon = 0$ and therefore $\varphi_\varepsilon \leq \psi_2$ almost everywhere in Ω.

In a similar way, we prove that $\varphi_\varepsilon - \max(\varphi_\varepsilon, \psi_1) = 0$ and therefore $\varphi_\varepsilon \geq \psi_1$ almost everywhere on Ω. Hence φ_ε is contained in $\overline{H}^2(\Omega) \cap \mathbb{K}$. By inequality (A.5), the sequence $\{\varphi_\varepsilon\}_{\varepsilon \to 0}$ is bounded in $\overline{H}^2(\Omega)$ and there exists a weakly convergent subsequence (denoted the same) such that $\varphi_\varepsilon \rightharpoonup_{\overline{H}^2} \varphi^*$ with $\|\varphi^*\|_{H^2} \leq C_2 \|g_1\|$. Since $\mathbb{K}$ is weakly closed, it contains φ^*.

For arbitrarily small $0 < \delta \leq \min(-\psi_1, \psi_2)$, let $v \in \mathbb{K}$ be such that $\psi_1 + \delta \leq v \leq \psi_2 - \delta$ almost everywhere in Ω. Using equation (A.3) and the monotonicity of L_ε, we infer

$$0 \leq \langle L_\varepsilon(v), v - \varphi_\varepsilon \rangle = \langle -\Delta v, v - \varphi_\varepsilon \rangle - \int_\Omega (g_1 + \max(-g_1, 0)\theta_\varepsilon(v - \psi_1)$$

$$+ \min(-g_1, 0)\theta_\varepsilon(\psi_2 - v))(v - \varphi_\varepsilon)dx$$

$$= \langle -\Delta v, v - \varphi_\varepsilon \rangle - \int_\Omega g_1(v - \varphi_\varepsilon)dx$$

for every $0 < \varepsilon < \delta$. For $\varepsilon \to 0$ this leads to

$$0 \leq \langle -\Delta v, v - \varphi^* \rangle - \int_\Omega g_1(v - \varphi^*)dx.$$

Since $\delta > 0$ can be chosen arbitrarily small, the last relation holds for every $v \in \mathbb{K}$ via a limiting process. Applying [31, III: Lemma 1.5] once more, this implies

$$0 \leq \langle -\Delta\varphi^*, v - \varphi^* \rangle - \int_\Omega g_1(v - \varphi^*)dx, \ \forall v \in \mathbb{K}.$$

Due to the uniqueness of the solution for our variational inequality problem, this yields the assertion.□

Appendix B. Proof of Lemma 6.3.
Proof. Testing (6.10)–(6.12) by $\tau\hat{r}$, $\hat{p}$ and $\hat{q}$, respectively, and summing up we get

$$\tau\langle h_r, \hat{r} \rangle + \langle h_p, \hat{p} \rangle + \langle h_q, \hat{q} \rangle$$

$$= \tau\langle \nabla\hat{r}, \nabla\hat{r} \rangle + \tau\langle \hat{A}\hat{r}, \hat{r} \rangle + \langle \hat{m}\nabla\hat{p}, \nabla\hat{p} \rangle$$

$$+ \frac{1}{\tau}\langle \hat{\rho}\hat{q}, \hat{q} \rangle - \langle (D\hat{q})\hat{u}, \hat{q} \rangle + \langle 2\hat{\eta}\epsilon(\hat{q}), \epsilon(\hat{q}) \rangle$$

$$\geq \tau\|\hat{r}\|^2_{\overline{H}^1(\Omega)} + C\left(\|\hat{p}\|^2_{\overline{H}^1(\Omega)} + \|\hat{q}\|^2_{H^1_{0,\sigma}(\Omega;\mathbb{R}^N)}\right)$$

for a positive constant C depending only on α and on the constants in Korn's and Poincaré's inequalities. This estimate yields the assertion. □

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