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Second-order analysis of a boundary control problem for the viscous Cahn–Hilliard equation with dynamic boundary condition

Dedicated to the memory of Prof. Dr. Viorel Arnăutu

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Abstract

In this paper we establish second-order sufficient optimality conditions for a boundary control problem that has been introduced and studied by three of the authors in the preprint arXiv:1407.3916. This control problem regards the viscous Cahn–Hilliard equation with possibly singular potentials and dynamic boundary conditions.

1 Introduction

This paper deals with second-order optimality conditions of a special boundary control problem for the viscous Cahn–Hilliard equation with dynamic boundary conditions. It continues the work [2] by three of the present authors in which the first-order necessary conditions of optimality were derived. For the work of other authors concerning the optimal control of Cahn–Hilliard systems, we refer the reader to the references given in [2].

Crucial contributions in [2] were the derivation of the adjoint problem, whose form turned out to be nonstandard, and an existence result for its solutions. As is well known, first-order conditions are in the case of nonlinear equations usually not sufficient for optimality. Also, second-order sufficient optimality conditions for nonlinear optimal control problems are essential both in the numerical analysis and for the construction of reliable optimization algorithms. For instance, the strong convergence of optimal controls and states for numerical discretizations of the problem rests heavily on the availability of second-order sufficient optimality conditions; furthermore, one can show that numerical algorithms such as SQP methods are locally convergent if second-order sufficient optimality conditions hold true. For a general discussion of second-order sufficient conditions for elliptic and parabolic control problems we refer to [6] and references therein; for the case of control problems involving phase field models we refer to, e. g., [3, 5].

In this paper, we aim to establish second-order sufficient optimality conditions for the boundary control problem studied in [2]. To this end, we assume that an open, bounded and connected set $\Omega \subset \mathbb{R}^3$, with smooth boundary Γ and unit outward normal $\mathbf{n}$, and some final time $T > 0$ are given, and we set $Q := \Omega \times (0,T)$ and $\Sigma := \Gamma \times (0,T)$. Moreover, we denote by Δ_Γ, ∇_Γ, $\partial_{\mathbf{n}}$, the Laplace–Beltrami operator, the surface gradient, and the outward normal derivative on Γ, in this order. We make the following general assumptions:

(A1) There are given nonnegative constants $b_Q, b_\Sigma, b_\Omega, b_\Gamma, b_0$, which do not all vanish, functions $z_Q \in L^2(Q)$, $z_\Sigma \in L^2(\Sigma)$, $z_\Omega \in L^2(\Omega)$, $z_\Gamma \in L^2(\Gamma)$, as well as a constant $M_0 > 0$ and functions $u_{\Gamma,\min} \in L^\infty(\Sigma)$ and $u_{\Gamma,\max} \in L^\infty(\Sigma)$ with $u_{\Gamma,\min} \le u_{\Gamma,\max}$ a. e. in Σ.

(A2) There are given constants $-\infty \le r_- < 0 < r_+ \le +\infty$ and two functions $f, f_\Gamma : (r_-, r_+) \to [0, +\infty)$ such that the following holds:

$$f, f_\Gamma \in C^4(r_-, r_+), \quad f(0) = f_\Gamma(0) = 0, \tag{1.1}$$

$$f'' \text{ and } f''_\Gamma \text{ are bounded from below,} \tag{1.2}$$

$$\lim_{r \searrow r_-} f'(r) = \lim_{r \searrow r_-} f'_\Gamma(r) = -\infty \quad \text{and} \quad \lim_{r \nearrow r_+} f'(r) = \lim_{r \nearrow r_+} f'_\Gamma(r) = +\infty\,, \tag{1.3}$$

$$|f'(r)| \le \eta\, |f'_\Gamma(r)| + C \quad \text{for some } \eta,\ C > 0 \text{ and every } r \in (r_-, r_+). \tag{1.4}$$

In fact, (1.1) is fully used only in the last part of the paper and many of our results hold under a weaker assumption. We also note that the conditions (1.1)–(1.4) allow for the possibility of splitting f' in (1.3) in the form $f' = \beta + \pi$, where β is a monotone function that diverges at $r_\pm$ and π is a perturbation with a bounded derivative. Since the same is true for f_Γ, the general assumptions of [1] are satisfied. Typical and important examples for f and f_Γ are the classical regular potential $f_{\rm reg}$ and the logarithmic double-well potential $f_{\log}$ given by

$$f_{\rm reg}(r) = \frac{1}{4}(r^2-1)^2\,, \quad r \in \mathbb{R} \tag{1.5}$$

$$f_{\log}(r) = ((1+r)\ln(1+r) + (1-r)\ln(1-r)) - cr^2\,, \quad r \in (-1,1), \tag{1.6}$$

where in the latter case we assume that $c > 0$ is so large that $f_{\log}$ is nonconvex.

With the above assumptions, we consider the following tracking type optimal boundary control problem:

(**CP**) Minimize

$$\begin{aligned} \mathcal{J}(y, y_\Gamma, u_\Gamma) \;\; := & \frac{b_Q}{2}\,\|y - z_Q\|^2_{L^2(Q)} + \frac{b_\Sigma}{2}\,\|y_\Gamma - z_\Sigma\|^2_{L^2(\Sigma)} + \frac{b_\Omega}{2}\,\|y(T) - z_\Omega\|^2_{L^2(\Omega)} \\ & + \frac{b_\Gamma}{2}\,\|y_\Gamma(T) - z_\Gamma\|^2_{L^2(\Gamma)} + \frac{b_0}{2}\,\|u_\Gamma\|^2_{L^2(\Sigma)} \end{aligned} \tag{1.7}$$

subject to the control constraint

$$\begin{aligned} u_\Gamma \in \mathcal{U}_{ad} := \;\; & \big\{v_\Gamma \in H^1(0,T;L^2(\Gamma)) \cap L^\infty(\Sigma) : \\ & u_{\Gamma,\min} \le v_\Gamma \le u_{\Gamma,\max} \text{ a.e. on } \Sigma,\; \|\partial_t v_\Gamma\|_2 \le M_0\big\} \end{aligned} \tag{1.8}$$

and to the Cahn–Hilliard equation with nonlinear dynamic boundary conditions as the state system,

$$\partial_t y - \Delta w = 0 \quad \text{in } Q, \tag{1.9}$$

$$w = \partial_t y - \Delta y + f'(y) \quad \text{in } Q, \tag{1.10}$$

$$\partial_{\mathbf{n}} w = 0 \quad \text{on } \Sigma, \tag{1.11}$$

$$y_\Gamma = y_{|\Gamma} \quad \text{on } \Sigma, \tag{1.12}$$

$$\partial_t y_\Gamma + \partial_{\mathbf{n}} y - \Delta_\Gamma y_\Gamma + f_\Gamma'(y_\Gamma) = u_\Gamma \quad \text{on } \Sigma, \tag{1.13}$$

$$y(\cdot,0) = y_0 \quad \text{in } \Omega, \quad y_\Gamma(\cdot,0) = y_{0_\Gamma} \quad \text{on } \Gamma. \tag{1.14}$$

Here, and throughout this paper, we generally assume that the admissible set $\mathcal{U}_{ad}$ is nonempty. Moreover, we postulate:

(A3) $y_0 \in H^2(\Omega)$, $y_{0_\Gamma} := y_{0|\Gamma} \in H^2(\Gamma)$, and it holds (notice that $y_0 \in C^0(\overline{\Omega})$)

$$r_- < y_0 < r_+ \quad \text{in } \overline{\Omega}. \tag{1.15}$$

We remark at this place that in [1] the additional assumption $\partial_{\mathbf{n}} y_0 = 0$ was made; this postulate is however unnecessary for the results of [1] to hold, since it is nowhere used in the proofs.

The system (1.9)–(1.14) is an initial-boundary value problem with nonlinear dynamic boundary condition for a Cahn–Hilliard equation. In this connection, the unknown y usually stands for the order parameter of an isothermal phase transition, and w denotes the chemical potential of the system.

Our paper is organized as follows: in Section 2, we provide and collect some results proved in [2, 1] concerning the state system, and we study a certain linear counterpart thereof that will be employed repeatedly in the later analysis. In Section 3, the existence of the second-order Fréchet derivative of the control-to-state mapping will be shown. Section 4 then brings the derivation of the second-order sufficient condition of optimality.

In order to simplify notation, we will in the following write y_Γ for the trace $y_{|\Gamma}$ of a function $y \in H^1(\Omega)$ on Γ, and we introduce the abbreviations

$$\begin{aligned} &V := H^1(\Omega), \quad H := L^2(\Omega), \quad V_\Gamma := H^1(\Gamma), \quad H_\Gamma := L^2(\Gamma), \quad \mathcal{H} := H \times H_\Gamma, \\ &\mathcal{V} := \{(v, v_\Gamma) \in V \times V_\Gamma : \, v_\Gamma = v_{|\Gamma}\}, \quad \mathcal{G} := H^2(\Omega) \times H^2(\Gamma), \\ &\mathcal{X} := H^1(0,T;H_\Gamma) \cap L^\infty(\Sigma), \quad \mathcal{Y} := H^1(0,T;\mathcal{H}) \cap L^\infty(0,T;\mathcal{V}), \end{aligned} \tag{1.16}$$

and endow these spaces with their natural norms. Moreover, for the generic Banach space X we denote by X^* its dual space and by $\|\cdot\|_X$ its norm. Furthermore, the symbol $\langle\,\cdot\,,\,\cdot\,\rangle$ stands for the duality pairing between the spaces V^* and V, where it is understood that H is embedded in V^* in the usual way, i. e., such that we have $\langle u, v\rangle = (u, v)$ for every $u \in H$ and $v \in V$ with the standard inner product $(\,\cdot\,,\,\cdot\,)$ of H. Finally, for $u \in V^*$ and $v \in L^1(0,T;V^*)$ we define their generalized mean values $u^\Omega \in \mathbb{R}$ and $v^\Omega \in L^1(0,T)$, respectively, by setting

$$u^\Omega := \frac{1}{|\Omega|}\langle u, 1\rangle \quad \text{and} \quad v^\Omega(t) := (v(t))^\Omega \quad \text{for a. e. } t \in (0,T), \tag{1.17}$$

where $|\Omega|$ stands for the Lebesgue measure of Ω.

During the course of our analysis, we will make repeated use of the elementary Young's inequality

$$ab \le \delta a^2 + \frac{1}{4\delta}\, b^2 \quad \text{for every } a, b \ge 0 \text{ and } \delta > 0, \tag{1.18}$$

of Hölder's inequality, and of Poincaré's inequality

$$\|v\|_V^2 \le \widehat{C}\big(\|\nabla v\|_H^2 + |v^\Omega|^2\big) \quad \text{for every } v \in V, \tag{1.19}$$

where $\widehat{C} > 0$ depends only on Ω.

Next, we recall a tool that is commonly used in the context of problems related to the Cahn–Hilliard equations. We define

$$\operatorname{dom}\mathcal{N} := \{v_* \in V^* : \, v_*^\Omega = 0\} \quad \text{and} \quad \mathcal{N} : \operatorname{dom}\mathcal{N} \to \{v \in V : \, v^\Omega = 0\} \tag{1.20}$$

by setting, for $v_* \in \operatorname{dom}\mathcal{N}$,

$$\mathcal{N}v_* \in V, \quad (\mathcal{N}v_*)^\Omega = 0, \quad \text{and} \quad \int_\Omega \nabla\mathcal{N}v_* \cdot \nabla z \, dx = \langle v_*, z\rangle \quad \text{for every } z \in V\,. \tag{1.21}$$

That is, $\mathcal{N}v_*$ is the unique solution v to the generalized Neumann problem for $-\Delta$ with datum v_* that satisfies $v^\Omega = 0$. Indeed, if $v_* \in H$, then the above variational equation means that $-\Delta\mathcal{N}v_* = v_*$ in Ω and $\partial_{\mathbf{n}}\mathcal{N}v_* = 0$ on Γ. Moreover, we have

$$\langle u_*, \mathcal{N}v_*\rangle = \langle v_*, \mathcal{N}u_*\rangle = \int_\Omega (\nabla\mathcal{N}u_*) \cdot (\nabla\mathcal{N}v_*) \, dx \quad \text{for all } u_*, v_* \in \operatorname{dom}\mathcal{N}, \tag{1.22}$$

whence also

$$2\langle \partial_t v_*(t), \mathcal{N}v_*(t)\rangle = \frac{d}{dt}\int_\Omega |\nabla\mathcal{N}v_*(t)|^2 \, dx = \frac{d}{dt}\|v_*(t)\|_*^2 \quad \text{for a.a. } t \in (0,T) \tag{1.23}$$

for every $v_* \in H^1(0,T;V^*)$ satisfying $(v_*)^\Omega = 0$ a.e. in $(0,T)$.

2 The state equation

At first, we specify our notion of solution to the state system (1.9)–(1.14).

Definition 2.1. Suppose that the general assumptions **(A1)**–**(A3)** are fulfilled, and let $u_\Gamma \in \mathcal{X}$ be given. By a *solution* to (1.9)–(1.14) we mean a triple (y, y_Γ, w) that satisfies

$$y \in W^{1,\infty}(0,T;H) \cap H^1(0,T;V) \cap L^\infty(0,T;H^2(\Omega)), \tag{2.1}$$

$$y_\Gamma \in W^{1,\infty}(0,T;H_\Gamma) \cap H^1(0,T;V_\Gamma) \cap L^\infty(0,T;H^2(\Gamma)), \tag{2.2}$$

$$y_\Gamma(t) = y(t)_{|\Gamma} \quad \text{for a. a. } t \in (0,T), \tag{2.3}$$

$$r_- < \inf_Q \operatorname{ess} y \le \sup_Q \operatorname{ess} y < r_+ \,, \quad r_- < \inf_\Sigma \operatorname{ess} y_\Gamma \le \sup_\Sigma \operatorname{ess} y_\Gamma < r_+ \,, \tag{2.4}$$

$$w \in L^\infty(0,T;H^2(\Omega)), \tag{2.5}$$

as well as, for almost every $t \in (0,T)$, the variational equations

$$\int_\Omega \partial_t y(t)\, v \, dx + \int_\Omega \nabla w(t) \cdot \nabla v \, dx = 0, \tag{2.6}$$

$$\int_\Omega w(t)\, v\, dx = \int_\Omega \partial_t y(t)\, v\, dx + \int_\Gamma \partial_t y_\Gamma(t)\, v_\Gamma \, d\Gamma + \int_\Omega \nabla y(t) \cdot \nabla v \, dx$$
$$+ \int_\Gamma \nabla_\Gamma y_\Gamma(t) \cdot \nabla_\Gamma v_\Gamma \, d\Gamma + \int_\Omega f'(y(t))\, v\, dx + \int_\Gamma \big(f_\Gamma'(y_\Gamma(t)) - u_\Gamma(t) \big)\, v_\Gamma \, d\Gamma,$$

for every $v \in V$ and every $(v, v_\Gamma) \in \mathcal{V}$, respectively, and the Cauchy condition

$$y(0) = y_0 \,, \quad y_\Gamma(0) = y_{0_\Gamma} \,. \tag{2.7}$$

Remark 2.2. It is worth noting that (recall the notation (1.17))

$$(\partial_t y(t))^\Omega = 0 \quad \text{for a. a. } t \in (0,T) \quad \text{and } y(t)^\Omega = m_0 \quad \text{for every } t \in [0,T],$$
$$\text{where } m_0 = (y_0)^\Omega \text{ is the mean value of } y_0, \tag{2.8}$$

as usual for the Cahn–Hilliard equation.

Now recall that $\mathcal{U}_{ad}$ is a convex, closed, and bounded subset of the Banach space $\mathcal{X}$ and thus contained in some bounded open ball in $\mathcal{X}$. For convenience, we fix such a ball once and for all, noting that any other such ball could be used instead. The next assumption is thus rather a denotation:

(A4) The set $\mathcal{U}$ is some open ball in $\mathcal{X}$ that contains $\mathcal{U}_{ad}$ and satisfies

$$\|u_\Gamma\|_{H^1(0,T;L^2(\Gamma))} + \|u_\Gamma\|_{L^\infty(\Sigma)} \le R \quad \forall\, u_\Gamma \in \mathcal{U}, \tag{2.9}$$

where $R > 0$ is a fixed given constant.

Concerning the well-posedness of the state sytem, we have the following result.

Theorem 2.3. *Suppose that the general hypotheses* **(A1)**–**(A4)** *are fulfilled. Then the state system* (1.9)–(1.14) *has for any* $u_\Gamma \in \mathcal{U}$ *a unique solution* (y, y_Γ, w) *in the sense of Definition 2.1. Moreover, there are constants* $K_1^* > 0$, $K_2^* > 0$, *and* $\widetilde{r}_-, \widetilde{r}_+ \in (r_-, r_+)$, *which only depend on* Ω, T, *the shape of the nonlinearities* f *and* f_Γ, *the initial datum* y_0, *and the constant* R, *such that the following holds:*
(i) *Whenever* (y, y_Γ, w) *is the solution to* (1.9)–(1.14) *associated with some* $u_\Gamma \in \mathcal{U}$ *then*

$$\|(y, y_\Gamma)\|_{W^{1,\infty}(0,T;\mathcal{H}) \cap H^1(0,T;\mathcal{V}) \cap L^\infty(0,T;\mathcal{G})} + \|w\|_{L^\infty(0,T;H^2(\Omega))} \le K_1^* \,, \tag{2.10}$$

$$\widetilde{r}_- \le y \le \widetilde{r}_+ \quad a.e. \ in \ Q, \qquad \widetilde{r}_- \le y_\Gamma \le \widetilde{r}_+ \quad a.e. \ on \ \Sigma. \tag{2.11}$$

(ii) *Whenever* $(y_i, y_{i,\Gamma}, w_i)$, $i = 1, 2$, *are the solutions to* (1.9)–(1.14) *associated with* $u_{i,\Gamma} \in \mathcal{U}$, $i = 1, 2$, *then*

$$\|(y_1, y_{1,\Gamma}) - (y_2, y_{2,\Gamma})\|_{H^1(0,T;\mathcal{H})\cap L^\infty(0,T;\mathcal{V})} \le K_2^* \|u_{1,\Gamma} - u_{2,\Gamma}\|_{L^2(\Sigma)} . \tag{2.12}$$

Proof. We may apply Theorems 2.2, 2.3, 2.4, 2.6 and Corollary 2.7 of [1] (where $\mathcal{V}$ has a slightly different meaning with respect to the present paper) to deduce that (i) holds true. Moreover, assertion (ii) is a consequence of [2, Lemma 4.1]. □

Remark 2.4. It follows from Theorem 2.3 that the control-to-state operator

$$\mathcal{S} : \mathcal{U} \to W^{1,\infty}(0, T; \mathcal{H}) \cap H^1(0, T; \mathcal{V}) \cap L^\infty(0, T; \mathcal{G}), \quad u_\Gamma \mapsto (y, y_\Gamma) , \tag{2.13}$$

is well defined and Lipschitz continuous from $\mathcal{U}$, viewed as a subset of $L^2(\Sigma)$, into $\mathcal{Y}$. Moreover, in view of (2.10) and (2.11) we may assume (by possibly choosing a larger K_1^*) that for any $u_\Gamma \in \mathcal{U}$ the corresponding state $(y, y_\Gamma) = \mathcal{S}(u_\Gamma)$ satisfies

$$\max_{1\le i\le 4} \Big(\|f^{(i)}(y)\|_{L^\infty(Q)} + \|f_\Gamma^{(i)}(y_\Gamma)\|_{L^\infty(\Sigma)} \Big) \le K_1^* . \tag{2.14}$$

Next, in order to ensure the solvability of a number of linearized systems later in this paper, we introduce the linear initial-boundary value problem

$$\partial_t \mathcal{X} - \Delta \mu = 0 \quad \text{in } Q, \tag{2.15}$$

$$\mu = \partial_t \mathcal{X} - \Delta \mathcal{X} + \lambda\, \mathcal{X} + g \quad \text{in } Q, \tag{2.16}$$

$$\partial_{\mathbf{n}} \mu = 0 \quad \text{on } \Sigma, \tag{2.17}$$

$$\mathcal{X}_\Gamma = \mathcal{X}_{|_\Gamma} \quad \text{on } \Sigma, \tag{2.18}$$

$$\partial_t \mathcal{X}_\Gamma + \partial_{\mathbf{n}} \mathcal{X} - \Delta_\Gamma \mathcal{X}_\Gamma + \lambda_\Gamma\, \mathcal{X}_\Gamma = g_\Gamma \quad \text{on } \Sigma, \tag{2.19}$$

$$\mathcal{X}(0) = \mathcal{X}_0 \quad \text{in } \Omega, \quad \mathcal{X}_\Gamma(0) = \mathcal{X}_{0_\Gamma} := \mathcal{X}_{0|\Gamma} \quad \text{on } \Gamma, \tag{2.20}$$

and its variational counterpart, namely, for almost every $t \in (0, T)$,

$$\int_\Omega \partial_t \mathcal{X}(t)\, v\, dx + \int_\Omega \nabla\mu(t) \cdot \nabla v\, dx = 0 \quad \text{for every } v \in V, \tag{2.21}$$

$$\begin{aligned} \int_\Omega \mu(t) v\, dx = \int_\Omega \partial_t \mathcal{X}(t)\, v\, dx + \int_\Gamma \partial_t \mathcal{X}_\Gamma(t)\, v_\Gamma\, d\Gamma + \int_\Omega \nabla \mathcal{X}(t) \cdot \nabla v\, dx \\ + \int_\Gamma \nabla_\Gamma \mathcal{X}_\Gamma(t) \cdot \nabla_\Gamma v_\Gamma\, d\Gamma + \int_\Omega \big(\lambda(t)\, \mathcal{X}(t) + g(t)\big)\, v\, dx + \int_\Gamma \big(\lambda_\Gamma(t)\, \mathcal{X}_\Gamma(t) - g_\Gamma(t)\big)\, v_\Gamma\, d\Gamma \\ \text{for every } (v, v_\Gamma) \in \mathcal{V}, \end{aligned} \tag{2.22}$$

together with the Cauchy condition

$$\mathcal{X}(0) = \mathcal{X}_0, \quad \mathcal{X}_\Gamma(0) = \mathcal{X}_{0_\Gamma}. \tag{2.23}$$

We have the following result.

Lemma 2.5. *Suppose that* $(g, g_\Gamma) \in H^1(0,T;\mathcal{H}) \cap (L^\infty(Q) \times L^\infty(\Sigma))$ *and* $(\lambda, \lambda_\Gamma) \in W^{1,\infty}(0,T;\mathcal{H}) \cap (L^\infty(Q) \times L^\infty(\Sigma))$ *are given, and let* $\chi_0 \in H^2(\Omega)$ *be such that* $\chi_{0_\Gamma} := \chi_{0|\Gamma} \in H^2(\Gamma)$. *Then the problem* (2.15)–(2.20) *has a unique solution in the sense that there is a unique triple* (χ, χ_Γ, μ) *that fulfills* (2.21)–(2.23) *and whose components satisfy the analogue of the regularity requirements* (2.1), (2.2), *and* (2.5), *respectively. Moreover, there exists a constant* $K_3^* > 0$, *which only depends on* Ω, T, $\|\lambda\|_{L^\infty(Q)}$, *and* $\|\lambda_\Gamma\|_{L^\infty(\Sigma)}$, *such that the following holds: whenever* $\chi_0 = 0$ *then*

$$\|(\chi, \chi_\Gamma)\|_{H^1(0,T;\mathcal{H}) \cap L^\infty(0,T;\mathcal{V})} \le K_3^* \,\|(g, g_\Gamma)\|_{L^2(0,T;\mathcal{H})} . \tag{2.24}$$

Proof. In the following, we denote by C_i, $i \in \mathbb{N}$, positive constants that only depend on the quantities mentioned in the assertion. First, we observe that the results concerning existence, uniqueness, and regularity follow from a direct application of [1, Cor. 2.5]. Now assume that $\chi_0 = 0$. Then we have $\chi^\Omega(t) = 0$ for almost every $t \in (0,T)$. We thus may choose in (2.21) $v = \mathcal{N}(\chi(t))$, and in (2.22) $v = -\chi(t)$. Adding the resulting equalities, then adding two additional terms on both sides for convenience, and integrating with respect to time, we arrive at the identity

$$\frac{1}{2}\left(\|\chi(t)\|_*^2 + \|\chi(t)\|_H^2 + \|\chi_\Gamma(t)\|_{H_\Gamma}^2\right) + \int_0^t\!\!\int_\Omega |\nabla \chi|^2 \, dx\, ds + \int_0^t\!\!\int_\Gamma |\nabla_\Gamma \chi_\Gamma|^2 \, d\Gamma\, ds$$
$$= \int_0^t\!\!\int_\Omega \big(g - \lambda\, \chi\big)\, \chi \, dx\, ds + \int_0^t\!\!\int_\Gamma \big(g_\Gamma - \lambda_\Gamma\, \chi_\Gamma\big)\, \chi_\Gamma \, d\Gamma\, ds$$

for all $t \in [0,T]$. Estimating the right-hand side with the help of Young's and Poincaré's inequalities, and applying Gronwall's lemma, we have that

$$\|(\chi, \chi_\Gamma)\|_{L^\infty(0,T;\mathcal{H}) \cap L^2(0,T;\mathcal{V})} \le C_1 \,\|(g, g_\Gamma)\|_{L^2(0,T;\mathcal{H})}. \tag{2.25}$$

Moreover, we may insert $v = \mathcal{N}(\partial_t \chi(t))$ in (2.21) and $v = -\partial_t \chi(t)$ in (2.22). Adding the resulting equations, integrating with respect to time, and using (1.21), we obtain the identity

$$\int_0^t \|\partial_t \chi(s)\|_*^2 \, ds + \int_0^t\!\!\int_\Omega |\partial_t \chi|^2 \, dx\, ds + \int_0^t\!\!\int_\Gamma |\partial_t \chi_\Gamma|^2 \, d\Gamma\, ds$$
$$+ \frac{1}{2}\left(\|\nabla \chi(t)\|_H^2 + \|\nabla_\Gamma \chi_\Gamma(t)\|_{H_\Gamma}^2\right)$$
$$= \int_0^t\!\!\int_\Omega (g - \lambda\, \chi)\, \partial_t \chi \, dx\, ds + \int_0^t\!\!\int_\Gamma (g_\Gamma - \lambda_\Gamma\, \chi_\Gamma)\, \partial_t \chi_\Gamma \, d\Gamma\, ds . \tag{2.26}$$

Invoking Young's inequality, we can easily infer from (2.25) and (2.26) the estimate

$$\|(\chi, \chi_\Gamma)\|_{H^1(0,T;\mathcal{H}) \cap L^\infty(0,T;\mathcal{V})} \le C_2 \,\|(g, g_\Gamma)\|_{L^2(0,T;\mathcal{H})}, \tag{2.27}$$

whence the assertion follows. □

3 Differentiability properties of the control-to-state mapping

The main objective in this section is to prove that the control-to-state mapping is twice continuously differentiable. We begin our analysis with the following result.

Theorem 3.1. *Suppose that* **(A1)**–**(A4)** *are fulfilled. Then the following holds true:*

(i) *The control-to-state mapping* $\mathcal{S}$ *is Fréchet differentiable in* $\mathcal{U}$ *as a mapping from* $\mathcal{U} \subset \mathcal{X}$ *to* $\mathcal{Y}$.

(ii) *For every $u_\Gamma \in \mathcal{U}$, the Fréchet derivative $D\mathcal{S}(u_\Gamma) \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$ is given as follows: for any $h_\Gamma \in \mathcal{X}$ it holds $D\mathcal{S}(u_\Gamma)h_\Gamma = (\xi, \xi_\Gamma)$, where (ξ, ξ_Γ, ζ) with*

$$\xi \in W^{1,\infty}(0,T;H) \cap H^1(0,T;V) \cap L^\infty(0,T;H^2(\Omega)), \tag{3.1}$$

$$\xi_\Gamma \in W^{1,\infty}(0,T;H_\Gamma) \cap H^1(0,T;V_\Gamma) \cap L^\infty(0,T;H^2(\Gamma)), \tag{3.2}$$

$$\zeta \in L^\infty(0,T;H^2(\Omega)), \tag{3.3}$$

is the unique solution to the linearized system

$$\partial_t \xi - \Delta\zeta = 0 \quad \textit{in } Q, \tag{3.4}$$

$$\zeta = \partial_t \xi - \Delta \xi + f''(y)\,\xi \quad \textit{in } Q, \tag{3.5}$$

$$\partial_{\mathbf{n}} \zeta = 0 \quad \textit{on } \Sigma, \tag{3.6}$$

$$\xi_\Gamma = \xi_{|\Gamma} \quad \textit{on } \Sigma, \tag{3.7}$$

$$\partial_t \xi_\Gamma + \partial_{\mathbf{n}} \xi_\Gamma - \Delta_\Gamma \xi_\Gamma + f_\Gamma''(y_\Gamma)\,\xi_\Gamma = h_\Gamma \quad \textit{on } \Sigma, \tag{3.8}$$

$$\xi(0) = 0 \quad \textit{in } \Omega, \quad \xi_\Gamma(0) = 0 \quad \textit{on } \Gamma. \tag{3.9}$$

(iii) *The mapping $D\mathcal{S} : \mathcal{U} \to \mathcal{L}(\mathcal{X}, \mathcal{Y})$, $u_\Gamma \mapsto D\mathcal{S}(u_\Gamma)$, is Lipschitz continuous on $\mathcal{U}$ in the following sense: there is a constant $K_4^* > 0$, which only depends on the data and the constant R, such that for all $u_{1,\Gamma}, u_{2,\Gamma} \in \mathcal{U}$ and all $h_\Gamma \in \mathcal{X}$ it holds*

$$\|(D\mathcal{S}(u_{1,\Gamma}) - D\mathcal{S}(u_{2,\Gamma}))h_\Gamma\|_{\mathcal{Y}} \,\le\, K_4^* \,\|u_{1,\Gamma} - u_{2,\Gamma}\|_{L^2(\Sigma)}\,\|h_\Gamma\|_{L^2(\Sigma)}. \tag{3.10}$$

Proof. At first, observe that the system (3.4)–(3.9) is of form (2.15)–(2.20), where with $(\chi, \chi_\Gamma, \mu) := (\xi, \xi_\Gamma, \zeta)$, $g \equiv 0$, $g_\Gamma := h_\Gamma$, and $(\lambda, \lambda_\Gamma) := (f''(y), f_\Gamma''(y_\Gamma))$, the assumptions of Lemma 2.5 are fulfilled. Consequently, for every $h_\Gamma \in \mathcal{X}$, there is a unique triple (ξ, ξ_Γ, ζ) that satisfies the corresponding variational system (2.21)–(2.23) and whose components have the regularity properties in (3.1), (3.2) and (3.3). We may therefore apply [2, Thm. 4.2] to conclude the validity of the assertions (i) and (ii).

It remains to show (iii). To this end, let $u_\Gamma \in \mathcal{U}$ be arbitrary and let $k_\Gamma \in \mathcal{X}$ be such that $u_\Gamma + k_\Gamma \in \mathcal{U}$. We denote $(y^k, y_\Gamma^k) = \mathcal{S}(u_\Gamma + k_\Gamma)$ and $(y, y_\Gamma) = \mathcal{S}(u_\Gamma)$, and we assume that any $h_\Gamma \in \mathcal{X}$ with $\|h_\Gamma\|_{\mathcal{X}} = 1$ is given. It then suffices to show that there is some $L > 0$, independent of h_Γ, u_Γ and k_Γ, such that

$$\|(\xi^k, \xi_\Gamma^k) - (\xi, \xi_\Gamma)\|_{\mathcal{Y}} \,\le\, L\,\|k_\Gamma\|_{L^2(\Sigma)}\,, \tag{3.11}$$

where $(\xi^k, \xi_\Gamma^k) = D\mathcal{S}(u_\Gamma + k_\Gamma)h_\Gamma$ and $(\xi, \xi_\Gamma) = D\mathcal{S}(u_\Gamma)h_\Gamma$. For this purpose, in the following we denote by C_i, $i \in \mathbb{N}$, positive constants that neither depend on u_Γ, k_Γ, nor on the special choice of $h_\Gamma \in \mathcal{X}$ with $\|h_\Gamma\|_{\mathcal{X}} = 1$. To begin with, observe that the triple $(\widehat{\xi}, \widehat{\xi}_\Gamma, \widehat{\zeta}) := (\xi^k, \xi_\Gamma^k, \zeta^k) - (\xi, \xi_\Gamma, \zeta)$ is the unique solution to the variational analogue of the initial-boundary value problem

$$\partial_t \widehat{\xi} - \Delta \widehat{\zeta} = 0 \quad \text{in } Q, \tag{3.12}$$

$$\widehat{\zeta} = \partial_t \widehat{\xi} - \Delta \widehat{\xi} + f''(y)\,\widehat{\xi} + \xi^k (f''(y^k) - f''(y)) \quad \text{in } Q, \tag{3.13}$$

$$\partial_{\mathbf{n}} \widehat{\zeta} = 0 \quad \text{on } \Sigma, \tag{3.14}$$

$$\widehat{\xi}_\Gamma = \widehat{\xi}_{|\Gamma} \quad \text{on } \Sigma, \tag{3.15}$$

$$\partial_t \widehat{\xi}_\Gamma + \partial_{\mathbf{n}} \widehat{\xi} - \Delta_\Gamma \widehat{\xi}_\Gamma + f_\Gamma''(y_\Gamma)\,\widehat{\xi}_\Gamma = -\xi_\Gamma^k (f_\Gamma''(y_\Gamma^k) - f_\Gamma''(y_\Gamma)) \quad \text{on } \Sigma, \tag{3.16}$$

$$\widehat{\xi}(0) = 0 \quad \text{in } \Omega, \quad \widehat{\xi}_\Gamma(0) = 0 \quad \text{on } \Gamma. \tag{3.17}$$

Moreover, the components of $(\widehat{\xi}, \widehat{\xi}_\Gamma, \widehat{\zeta})$ enjoy the regularity properties indicated in (2.1), (2.2), and (2.5), respectively.

Now observe that it follows from Theorem 2.3, from part (i) of this proof, and from (2.14), that $(g, g_\Gamma) := (\xi^k\,(f''(y^k) - f''(y)), -\xi_\Gamma^k\,(f''(y_\Gamma^k) - f''(y_\Gamma)))$ belongs to $H^1(0,T;\mathcal{H}) \cap (L^\infty(Q) \times L^\infty(\Sigma))$, while $(\lambda, \lambda_\Gamma) := (f''(y), f_\Gamma''(y_\Gamma))$ belongs to $W^{1,\infty}(0,T;\mathcal{H}) \cap (L^\infty(Q) \times L^\infty(\Sigma))$. Moreover, (2.14) also implies that for every $u_\Gamma \in \mathcal{U}$ we have for $(y, y_\Gamma) = \mathcal{S}(u_\Gamma)$ the estimate

$$\|f''(y)\|_{L^\infty(Q)} \,+\, \|f_\Gamma''(y_\Gamma)\|_{L^\infty(\Sigma)} \,\le\, K_1^*\,.$$

Hence, it follows from estimate (2.24) in Lemma 2.5 that

$$\|(\widehat{\xi}, \widehat{\xi}_\Gamma)\|_{\mathcal{Y}} \,\le\, C_1\,\left(\|\xi^k\,(f''(y^k) - f''(y))\|_{L^2(Q)} \,+\, \|\xi_\Gamma^k\,(f_\Gamma''(y_\Gamma^k) - f_\Gamma''(y_\Gamma))\|_{L^2(\Sigma)}\right)\,. \tag{3.18}$$

Now, by the mean value theorem and (2.14), there exists a positive constant C_2 such that almost everywhere in Q (on Σ, respectively)

$$|f''(y^k) - f''(y)| \,\le\, C_2\,|y^k - y| \quad \text{and} \quad |f_\Gamma''(y_\Gamma^k) - f_\Gamma''(y_\Gamma)| \,\le\, C_2\,|y_\Gamma^k - y_\Gamma|\,. \tag{3.19}$$

At this point, we recall that $\mathcal{U}$ is a bounded subset of $\mathcal{X}$. Since $u_\Gamma + k_\Gamma \in \mathcal{U}$ and $\|h_\Gamma\|_{\mathcal{X}} = 1$, we thus can infer from (2.14) and from the estimate (2.24) in Lemma 2.5 that (ξ^k, ξ_Γ^k) is bounded in $\mathcal{Y}$ independently of k_Γ, u_Γ, and the choice of $h_\Gamma \in \mathcal{X}$ with $\|h_\Gamma\|_{\mathcal{X}} = 1$. Using the embedding $V \subset L^4(\Omega)$ and the stability estimate proved in Theorem 2.3, we therefore have

$$\begin{aligned}
&\|\xi^k\,(f''(y^k) - f''(y))\|^2_{L^2(Q)} \,\le\, C_2 \int_0^T\!\!\int_\Omega \left(|\xi^k|^2\,|y^k - y|^2\right)\,dx\,dt \\
&\le\, C_2 \int_0^T \left(\|\xi^k(t)\|^2_{L^4(\Omega)}\,\|y^k(t) - y(t)\|^2_{L^4(\Omega)}\right)dt \\
&\le\, C_3\,\|(y^k, y_\Gamma^k) - (y, y_\Gamma)\|^2_{\mathcal{Y}} \,\le\, C_4\,\|k_\Gamma\|^2_{L^2(\Sigma)}\,.
\end{aligned} \tag{3.20}$$

Since an analogous estimate holds for the second summand in the bracket on the right-hand side of (3.18), the assertion follows. $\square$

With the Lipschitz estimate (3.10) we are now in the position to show the existence of the second-order Fréchet derivative. We have the following result.

Theorem 3.2. *Assume that* **(A1)–(A4)** *are fulfilled. Then the following holds true:*

(i) *The control-to-state operator $\mathcal{S}$ is twice Fréchet differentiable in $\mathcal{U}$ as a mapping from $\mathcal{U} \subset \mathcal{X}$ to $\mathcal{Y}$.*

(ii) *For every $u_\Gamma \in \mathcal{U}$ the second Fréchet derivative $D^2\mathcal{S}(u_\Gamma) \in \mathcal{L}(\mathcal{X}, \mathcal{L}(\mathcal{X}, \mathcal{Y}))$ is defined as follows: if $h_\Gamma, k_\Gamma \in \mathcal{X}$ are arbitrary then $D^2\mathcal{S}(u_\Gamma)[h_\Gamma, k_\Gamma] =: (\eta, \eta_\Gamma)$ is the unique solution to the initial-boundary value problem*

$$\partial_t \eta - \Delta \vartheta = 0 \quad \text{in } Q, \tag{3.21}$$

$$\vartheta = \partial_t \eta - \Delta \eta + f''(y)\,\eta + f^{(3)}(y)\,\varphi\,\psi \quad \text{in } Q, \tag{3.22}$$

$$\partial_{\mathbf{n}} \vartheta = 0 \quad \text{on } \Sigma, \tag{3.23}$$

$$\eta_\Gamma = \eta_{|\Gamma} \quad \text{on } \Sigma, \tag{3.24}$$

$$\partial_t \eta_\Gamma + \partial_{\mathbf{n}} \eta - \Delta_\Gamma \eta_\Gamma + f_\Gamma''(y_\Gamma)\,\eta_\Gamma = -f_\Gamma^{(3)}(y_\Gamma)\,\varphi_\Gamma\,\psi_\Gamma \quad \text{on } \Sigma, \tag{3.25}$$

$$\eta(0) = 0 \quad \text{in } \Omega, \quad \eta_\Gamma(0) = 0 \quad \text{on } \Gamma, \tag{3.26}$$

where we have put

$$(y, y_\Gamma) = \mathcal{S}(u_\Gamma), \quad (\varphi, \varphi_\Gamma) = D\mathcal{S}(u_\Gamma)h_\Gamma, \quad (\psi, \psi_\Gamma) = D\mathcal{S}(u_\Gamma)k_\Gamma \,. \tag{3.27}$$

(iii) *The mapping* $D^2\mathcal{S} : \mathcal{U} \to \mathcal{L}(\mathcal{X}, \mathcal{L}(\mathcal{X}, \mathcal{Y}))$, $u_\Gamma \mapsto D^2\mathcal{S}(u_\Gamma)$, *is Lipschitz continuous on* $\mathcal{U}$ *in the following sense: there exists a constant* $K_5^* > 0$, *which only depends on the data and on the constant* R, *such that for every* $u_{1,\Gamma}, u_{2,\Gamma} \in \mathcal{U}$ *and all* $h_\Gamma, k_\Gamma \in \mathcal{X}$ *it holds*

$$\|(D^2\mathcal{S}(u_{1,\Gamma}) - D^2\mathcal{S}(u_{2,\Gamma}))[h_\Gamma \,,\, k_\Gamma]\|_{\mathcal{Y}} \;\le\; K_5^* \, \|u_{1,\Gamma} - u_{2,\Gamma}\|_{L^2(\Sigma)} \, \|h_\Gamma\|_{L^2(\Sigma)} \, \|k_\Gamma\|_{L^2(\Sigma)} . \tag{3.28}$$

Proof. At first, it is easily verified that the pair $(g, g_\Gamma) := (f^{(3)}(y)\, \varphi\, \psi, -f_\Gamma^{(3)}(y_\Gamma)\, \varphi_\Gamma\, \psi_\Gamma)$ belongs to $H^1(0,T;\mathcal{H}) \cap (L^\infty(Q) \times L^\infty(\Sigma))$. We thus can argue as in the proof of Theorem 3.1 to deduce from Lemma 2.5 that the system (3.21)–(3.26) is uniquely solvable in the sense that its variational counterpart has a unique solution $(\eta, \eta_\Gamma, \vartheta)$ whose components enjoy the regularity indicated in (2.1), (2.2), and (2.5), respectively. Moreover, by (2.24) we have the estimate

$$\|(\eta, \eta_\Gamma)\|_{\mathcal{Y}} \;\le\; C_1 \left(\left\| f^{(3)}(y)\, \varphi\, \psi \right\|_{L^2(Q)} \,+\, \left\| f_\Gamma^{(3)}(y_\Gamma)\, \varphi_\Gamma\, \psi_\Gamma \right\|_{L^2(\Sigma)} \right) . \tag{3.29}$$

Here, and in the remainder of the proof of parts (i), (ii), we denote by C_i, $i \in \mathbb{N}$, positive constants that do not depend on the quantities h_Γ, k_Γ, and u_Γ. Using (2.14), and invoking the embedding $V \subset L^4(\Omega)$, we find that

$$\begin{aligned} &\left\| f^{(3)}(y)\, \varphi\, \psi \right\|_{L^2(Q)}^2 \;\le\; C_2 \int_0^T \!\! \int_\Omega |\varphi|^2 \, |\psi|^2 \, dx\, dt \;\le\; C_2 \int_0^T \|\varphi(t)\|_{L^4(\Omega)}^2 \, \|\psi(t)\|_{L^4(\Omega)}^2 \, dt \\ &\le\; C_3 \, \|\varphi\|_{L^\infty(0,T;V)}^2 \, \|\psi\|_{L^\infty(0,T;V)}^2 \;\le\; C_4 \, \|h_\Gamma\|_{L^2(\Sigma)}^2 \, \|k_\Gamma\|_{L^2(\Sigma)}^2 \,, \end{aligned} \tag{3.30}$$

where the validity of the last inequality can be seen as follows: by definition (recall (3.27)), $(\varphi, \varphi_\Gamma)$ is the unique solution to the linear problem (3.4)–(3.9). We can therefore infer from (2.24) that $\|(\varphi, \varphi_\Gamma)\|_{\mathcal{Y}} \;\le\; C_5 \, \|h_\Gamma\|_{L^2(\Sigma)}$. By the same token, we conclude that $\|(\psi, \psi_\Gamma)\|_{\mathcal{Y}} \;\le\; C_6 \, \|k_\Gamma\|_{L^2(\Sigma)}$. The asserted inequality therefore follows from the definition of the norm of the space $\mathcal{Y}$, and we obtain from similar reasoning that also

$$\left\| f_\Gamma^{(3)}(y_\Gamma)\, \varphi_\Gamma\, \psi_\Gamma \right\|_{L^2(\Sigma)} \;\le\; C_7 \, \|h_\Gamma\|_{L^2(\Sigma)} \, \|k_\Gamma\|_{L^2(\Sigma)} \,.$$

Hence, we get

$$\|(\eta, \eta_\Gamma)\|_{\mathcal{Y}} \;\le\; C_8 \, \|h_\Gamma\|_{L^2(\Sigma)} \, \|k_\Gamma\|_{L^2(\Sigma)} \,. \tag{3.31}$$

In particular, it follows that the bilinear mapping $\mathcal{X} \times \mathcal{X} \mapsto \mathcal{Y}$, $[k_\Gamma, h_\Gamma] \mapsto (\eta, \eta_\Gamma)$, is continuous.

Now we prove the assertions concerning existence and form of the second Fréchet derivative. Since $\mathcal{U}$ is open, there is some $\Lambda > 0$ such that $u_\Gamma + k_\Gamma \in \mathcal{U}$ whenever $\|k_\Gamma\|_{\mathcal{X}} \;\le\; \Lambda$. In the following, we only consider such perturbations $k_\Gamma \in \mathcal{X}$. We observe that for $(y, y_\Gamma) = \mathcal{S}(u_\Gamma)$ and for $(y^k, y_\Gamma^k) = \mathcal{S}(u_\Gamma + k_\Gamma)$ the global estimates (2.10)–(2.12) and (2.14) are satisfied.

After these preparations, we notice that it suffices to show that

$$\begin{aligned} &\left\| D\mathcal{S}(u_\Gamma + k_\Gamma) - D\mathcal{S}(u_\Gamma) - D^2\mathcal{S}(u_\Gamma)k_\Gamma \right\|_{\mathcal{L}(\mathcal{X},\mathcal{Y})} \\ &= \sup_{\|h_\Gamma\|_{\mathcal{X}}=1} \left\| \left(D\mathcal{S}(u_\Gamma + k_\Gamma) - D\mathcal{S}(u_\Gamma) - D^2\mathcal{S}(u_\Gamma)k_\Gamma \right) h_\Gamma \right\|_{\mathcal{Y}} \\ &\le\; \overline{C} \, \|k_\Gamma\|_{L^2(\Sigma)}^2 \end{aligned} \tag{3.32}$$

with a constant $\overline{C}$ independent of k_Γ.

To this end, let $h_\Gamma \in \mathcal{X}$ be arbitrary with $\|h_\Gamma\|_{\mathcal{X}} = 1$. We put $(\rho, \rho_\Gamma) = D\mathcal{S}(u_\Gamma + k_\Gamma)h_\Gamma$, define the pairs $(\varphi, \varphi_\Gamma), (\psi, \psi_\Gamma)$ as in (3.27), and define

$$(\nu, \nu_\Gamma) := (\rho, \rho_\Gamma) - (\varphi, \varphi_\Gamma) - (\eta, \eta_\Gamma).$$

Observe that the components of (ν, ν_Γ) have the regularity properties indicated in (2.1) and (2.2), respectively. Moreover, in view of (3.32), we need to show that

$$\|(\nu, \nu_\Gamma)\|_{\mathcal{Y}} \le \overline{C}\, \|k_\Gamma\|^2_{L^2(\Sigma)} . \tag{3.33}$$

Now, invoking the explicit expressions for the quantities defined above, it is easily seen that the triple (ν, ν_Γ, π) (where π is defined below) is the unique solution to the variational counterpart of the linear initial-boundary value problem

$$\partial_t \nu - \Delta \pi = 0 \quad \text{in } Q, \tag{3.34}$$

$$\pi = \partial_t \nu - \Delta \nu + f''(y)\, \nu + \sigma \quad \text{in } Q, \tag{3.35}$$

$$\partial_{\mathbf{n}} \pi = 0 \quad \text{on } \Sigma, \tag{3.36}$$

$$\nu_\Gamma = \nu_{|\Gamma} \quad \text{and} \quad \partial_t \nu_\Gamma + \partial_{\mathbf{n}} \nu - \Delta_\Gamma \nu_\Gamma + f_\Gamma''(y_\Gamma)\, \nu_\Gamma = \sigma_\Gamma \quad \text{on } \Sigma, \tag{3.37}$$

$$\nu(0) = 0 \quad \text{in } \Omega, \quad \nu_\Gamma(0) = 0 \quad \text{on } \Gamma, \tag{3.38}$$

where we have put

$$\begin{aligned} &\sigma := \rho \left(f''(y^k) - f''(y) \right) \; - \; f^{(3)}(y)\, \varphi\, \psi, \\ &\sigma_\Gamma := -\rho_\Gamma \left(f_\Gamma''(y_\Gamma^k) - f_\Gamma''(y_\Gamma) \right) \; + \; f_\Gamma^{(3)}(y_\Gamma)\, \varphi_\Gamma\, \psi_\Gamma \,. \end{aligned} \tag{3.39}$$

In view of (2.14), and since it is easily checked that (σ, σ_Γ) belongs to the space $H^1(0,T;\mathcal{H}) \cap (L^\infty(Q)) \times L^\infty(\Sigma))$, we may again invoke the estimate (2.24) in Lemma 2.5 to conclude that (3.33) is satisfied if only

$$\|(\sigma, \sigma_\Gamma)\|_{L^2(0,T;\mathcal{H})} \le \overline{C}\, \|k_\Gamma\|^2_{L^2(\Sigma)} . \tag{3.40}$$

Applying Taylor's theorem to f'', and recalling (3.27), we readily see that there is a function $\omega_f \in L^\infty(Q)$ such that

$$f''(y^k) - f''(y) = f^{(3)}(y)\,(y^k - y - \psi) \; + \; f^{(3)}(y)\, \psi \; + \; \omega_f\, (y^k - y)^2 \quad \text{a.e. in } Q\,. \tag{3.41}$$

Hence, we have that

$$\sigma \; = \rho\, f^{(3)}(y)\,(y^k - y - \psi) \; + \; \psi\, f^{(3)}(y)\,(\rho - \varphi) \; + \; \rho\, \omega_f\, (y^k - y)^2 \,. \tag{3.42}$$

Now observe that from the proof of Fréchet differentiability (see inequality (4.5) in the proof of [2, Thm. 4.2]) and from (3.10) we can conclude the estimates

$$\begin{aligned} &\|(y^k, y_\Gamma^k) - (y, y_\Gamma) - (\psi, \psi_\Gamma)\|_{\mathcal{Y}} \le C_9\, \|k_\Gamma\|^2_{L^2(\Sigma)} \,, \\ &\|(\rho, \rho_\Gamma) - (\varphi, \varphi_\Gamma)\|_{\mathcal{Y}} \le C_{10}\, \|k_\Gamma\|_{L^2(\Sigma)} \,. \end{aligned} \tag{3.43}$$

Moreover, we can infer from inequality (2.12) in Theorem 2.3 that

$$\|(y^k, y_\Gamma^k) - (y, y_\Gamma)\|_{\mathcal{Y}} \le K_2^*\, \|k_\Gamma\|_{L^2(\Sigma)} \,, \tag{3.44}$$

and it follows from Lemma 2.5 that (ρ, ρ_Γ) is bounded in $\mathcal{Y}$ by a positive constant that is independent of $k_\Gamma, h_\Gamma \in \mathcal{X}$ with $\|k_\Gamma\|_{\mathcal{X}} \le \Lambda$ and $\|h_\Gamma\|_{\mathcal{X}} = 1$.

Finally, we conclude from Lemma 2.5 (ii) that with a suitable constant $C_{11} > 0$ it holds

$$\|(\psi, \psi_\Gamma)\|_{\mathcal{Y}} \le C_{11} \|k_\Gamma\|_{L^2(\Sigma)} . \tag{3.45}$$

After these preparations, and invoking Hölder's inequality and the continuity of the embeddings $V \subset L^4(\Omega)$ and $V \subset L^6(\Omega)$, we can estimate as follows:

$$\begin{aligned}
\|\sigma\|^2_{L^2(Q)} &\le C_{12} \int_0^T \!\! \int_\Omega \big(|\rho|^2 \, |y^k - y - \psi|^2 \, + \, |\psi|^2 \, |\rho - \varphi|^2 \, + \, |\rho|^2 \, |y^k - y|^4 \big) \, dx \, dt \\
&\le C_{12} \int_0^T \Big(\|\rho(t)\|^2_{L^4(\Omega)} \|(y^k - y - \psi)(t)\|^2_{L^4(\Omega)} \, + \, \|\psi(t)\|^2_{L^4(\Omega)} \|\rho(t) - \varphi(t)\|^2_{L^4(\Omega)} \Big) \, dt \\
&\quad + C_{12} \int_0^T \Big(\|\rho(t)\|^2_{L^6(\Omega)} \, \|y^k(t) - y(t)\|^4_{L^6(\Omega)} \Big) \, dt \\
&\le C_{13} \sup_{t \in (0,T)} \big(\|\rho(t)\|^2_V \, \|(y^k - y - \psi)(t)\|^2_V \, + \, \|\psi(t)\|^2_V \, \|\rho(t) - \varphi(t)\|^2_V \\
&\qquad\qquad + \, \|\rho(t)\|^2_V \, \|y^k(t) - y(t)\|^4_V \big) \\
&\le C_{14} \|k_\Gamma\|^4_{L^2(\Sigma)} .
\end{aligned} \tag{3.46}$$

By the same reasoning, a similar estimate can be derived for $\|\sigma_\Gamma\|_{L^2(\Sigma)}$, which concludes the proof of the assertions (i) and (ii).

Next, we prove the assertion (iii). To this end, suppose that $u_\Gamma \in \mathcal{U}$ and that h_Γ and k_Γ are arbitrarily chosen in $\mathcal{X}$, and let $\delta_\Gamma \in \mathcal{X}$ be arbitrary with $u_\Gamma + \delta_\Gamma \in \mathcal{U}$. In the following, we will denote by C_i, $i \in \mathbb{N}$, positive constants that do not depend on any of these quantities. We put

$$\begin{aligned}
&(y, y_\Gamma) = \mathcal{S}(u_\Gamma), \quad (y^\delta, y^\delta_\Gamma) = \mathcal{S}(u_\Gamma + \delta_\Gamma), \\
&(\varphi, \varphi_\Gamma) = D\mathcal{S}(u_\Gamma) h_\Gamma, \quad (\varphi^\delta, \varphi^\delta_\Gamma) = D\mathcal{S}(u_\Gamma + \delta_\Gamma) h_\Gamma, \\
&(\psi, \psi_\Gamma) = D\mathcal{S}(u_\Gamma) k_\Gamma, \quad (\psi^\delta, \psi^\delta_\Gamma) = D\mathcal{S}(u_\Gamma + \delta_\Gamma) k_\Gamma, \\
&(\eta, \eta_\Gamma) = D^2\mathcal{S}(u_\Gamma)[h_\Gamma, k_\Gamma], \quad (\eta^\delta, \eta^\delta_\Gamma) = D^2\mathcal{S}(u_\Gamma + \delta_\Gamma)[h_\Gamma, k_\Gamma] .
\end{aligned}$$

From the previous results, in particular, (2.12) and (3.10), we can infer that there is a constant $C_1 > 0$ such that

$$\begin{aligned}
&\|(\varphi, \varphi_\Gamma)\|_{\mathcal{Y}} + \|(\varphi^\delta, \varphi^\delta_\Gamma)\|_{\mathcal{Y}} \le C_1 \|h_\Gamma\|_{L^2(\Sigma)}, \\
&\|(\psi, \psi_\Gamma)\|_{\mathcal{Y}} + \|(\psi^\delta, \psi^\delta_\Gamma)\|_{\mathcal{Y}} \le C_1 \|k_\Gamma\|_{L^2(\Sigma)}, \\
&\|(\eta, \eta_\Gamma)\|_{\mathcal{Y}} + \|(\eta^\delta, \eta^\delta_\Gamma)\|_{\mathcal{Y}} \le C_1 \|h_\Gamma\|_{L^2(\Sigma)} \|k_\Gamma\|_{L^2(\Sigma)}, \\
&\|(y^\delta, y^\delta_\Gamma) - (y, y_\Gamma)\|_{\mathcal{Y}} \le C_1 \|\delta_\Gamma\|_{L^2(\Sigma)}, \\
&\|(\varphi^\delta, \varphi^\delta_\Gamma) - (\varphi, \varphi_\Gamma)\|_{\mathcal{Y}} \le C_1 \|\delta_\Gamma\|_{L^2(\Sigma)} \|h_\Gamma\|_{L^2(\Sigma)}, \\
&\|(\psi^\delta, \psi^\delta_\Gamma) - (\psi, \psi_\Gamma)\|_{\mathcal{Y}} \le C_1 \|\delta_\Gamma\|_{L^2(\Sigma)} \|k_\Gamma\|_{L^2(\Sigma)} .
\end{aligned} \tag{3.47}$$

Now observe that $(\tilde\eta, \tilde\eta_\Gamma) = (\eta^\delta, \eta^\delta_\Gamma) - (\eta, \eta_\Gamma)$ and $\tilde\vartheta = \vartheta^\delta - \vartheta$ (where ϑ^δ and ϑ have their obvious meaning corresponding to (3.22)) satisfy the linear initial-boundary value problem

$$\partial_t \tilde\eta - \Delta\tilde\vartheta = 0 \quad \text{in } Q, \tag{3.48}$$

$$\tilde\vartheta = \partial_t\tilde\eta - \Delta\tilde\eta + f''(y)\,\tilde\eta + \sigma \quad \text{in } Q, \tag{3.49}$$

$$\partial_{\mathbf n}\tilde\vartheta = 0 \quad \text{on } \Sigma, \tag{3.50}$$

$$\tilde\eta_\Gamma = \tilde\eta_{|\Gamma} \quad \text{and} \quad \partial_t\tilde\eta_\Gamma + \partial_{\mathbf n}\tilde\eta - \Delta_\Gamma\tilde\eta_\Gamma + f''_\Gamma(y_\Gamma)\,\tilde\eta_\Gamma = \sigma_\Gamma \quad \text{on } \Sigma, \tag{3.51}$$

$$\tilde\eta(0) = 0 \quad \text{in } \Omega, \quad \tilde\eta_\Gamma(0) = 0 \quad \text{on } \Gamma, \tag{3.52}$$

where we have put

$$\sigma = \eta^\delta(f''(y^\delta) - f''(y)) + (f^{(3)}(y^\delta)\,\varphi^\delta\,\psi^\delta - f^{(3)}(y)\,\varphi\,\psi)\,,$$
$$\sigma_\Gamma = -\eta^\delta_\Gamma(f''_\Gamma(y^\delta_\Gamma) - f''_\Gamma(y_\Gamma)) - (f^{(3)}_\Gamma(y^\delta_\Gamma)\,\varphi^\delta_\Gamma\,\psi^\delta_\Gamma - f^{(3)}_\Gamma(y_\Gamma)\,\varphi_\Gamma\,\psi_\Gamma)\,. \tag{3.53}$$

The system (3.48)–(3.52) is again of the form (2.15)–(2.20), and since it is readily verified that (σ,σ_Γ) belongs to the space $H^1(0,T;\mathcal H)\cap(L^\infty(Q)\times L^\infty(\Sigma))$, we may employ Lemma 2.5 once more to conclude that

$$\|(\tilde\eta,\tilde\eta_\Gamma)\|_{\mathcal Y} \,\le\, C_2\,\|(\sigma,\sigma_\Gamma)\|_{L^2(0,T;\mathcal H)}\,, \tag{3.54}$$

so that it remains to show an estimate of the form

$$\|(\sigma,\sigma_\Gamma)\|_{L^2(0,T;\mathcal H)} \,\le\, C_3\,\|\delta_\Gamma\|_{L^2(\Sigma)}\,\|h_\Gamma\|_{L^2(\Sigma)}\,\|k_\Gamma\|_{L^2(\Sigma)}\,. \tag{3.55}$$

Since

$$f^{(3)}(y^\delta)\,\varphi^\delta\,\psi^\delta - f^{(3)}(y)\,\varphi\,\psi$$
$$= \varphi^\delta\,\psi\,(f^{(3)}(y^\delta) - f^{(3)}(y)) + f^{(3)}(y^\delta)\,\varphi^\delta\,(\psi^\delta-\psi) + f^{(3)}(y)\,\psi\,(\varphi^\delta-\varphi)\,, \tag{3.56}$$

we can infer from (2.14) that, almost everywhere in Q,

$$|\sigma| \,\le\, C_4\,(|\eta^\delta|\,|y^\delta-y| \,+\, |\varphi^\delta|\,|\psi|\,|y^\delta-y| \,+\, |\varphi^\delta|\,|\psi^\delta-\psi| \,+\, |\psi|\,|\varphi^\delta-\varphi|)\,. \tag{3.57}$$

Using (3.47), Hölder's inequality, and the continuity of the embedding $V\subset L^4(\Omega)$, we find

$$\int_0^T\!\!\int_\Omega \big(|\eta^\delta|^2\,|y^\delta-y|^2\big)\,dx\,dt \,\le\, \int_0^T \Big(\|\eta^\delta(t)\|^2_{L^4(\Omega)}\,\|(y^\delta-y)(t)\|^2_{L^4(\Omega)}\Big)\,dt$$
$$\le\, C_5\,\|\eta^\delta\|^2_{L^\infty(0,T;V)}\,\|y^\delta-y\|^2_{L^\infty(0,T;V)} \,\le\, C_6\,\|\delta_\Gamma\|^2_{L^2(\Sigma)}\,\|h_\Gamma\|^2_{L^2(\Sigma)}\,\|k_\Gamma\|^2_{L^2(\Sigma)}\,. \tag{3.58}$$

Similar reasoning yields

$$\|\varphi^\delta(\psi^\delta-\psi)\|^2_{L^2(Q)} \,+\, \|\psi(\varphi^\delta-\varphi)\|^2_{L^2(Q)} \,\le\, C_7\,\|\delta_\Gamma\|^2_{L^2(\Sigma)}\,\|h_\Gamma\|^2_{L^2(\Sigma)}\,\|k_\Gamma\|^2_{L^2(\Sigma)}\,. \tag{3.59}$$

Moreover, once again invoking (3.47), Hölder's inequality, and the continuity of the embedding $V\subset L^6(\Omega)$, we conclude that

$$\int_0^T\!\!\int_\Omega \big(|\varphi^\delta|^2\,|\psi|^2\,|y^\delta-y|^2\big)\,dx\,dt \,\le\, \int_0^T\Big(\|(y^\delta-y)(t)\|^2_{L^6(\Omega)}\,\|\varphi^\delta(t)\|^2_{L^6(\Omega)}\,\|\psi(t)\|^2_{L^6(\Omega)}\Big)\,dt$$
$$\le\, C_8\,\|\varphi^\delta\|^2_{L^\infty(0,T;V)}\,\|\psi\|^2_{L^\infty(0,T;V)}\,\|y^\delta-y\|^2_{L^\infty(0,T;V)}$$
$$\le\, C_9\,\|\delta_\Gamma\|^2_{L^2(\Sigma)}\,\|h_\Gamma\|^2_{L^2(\Sigma)}\,\|k_\Gamma\|^2_{L^2(\Sigma)}\,. \tag{3.60}$$

Finally, we can estimate $\|\sigma_\Gamma\|_{L^2(\Sigma)}$, deriving estimates similar to (3.57)–(3.60), which entails the validity of the required estimate (3.55). With this, the assertion is completely proved. ☐

4 Optimality conditions

Now that the second-order Fréchet-derivative of the control-to-state operator for problem **(CP)** is obtained, we can address the matter of deriving second-order sufficient optimality conditions. As a preparation of the corresponding theorem, we provide the adjoint system and the first-order necessary optimality conditions. Since these were already established in [2], we only present the results without proofs.

At first, it is easily shown (cf. [2, Thm. 2.2]) that **(CP)** has a solution. For the remainder of this paper, let us assume that $\bar{u}_\Gamma \in \mathcal{U}_{ad}$ is any such minimizer and that $(\bar{y}, \bar{y}_\Gamma, \bar{w})$, where $(\bar{y}, \bar{y}_\Gamma) = \mathcal{S}(\bar{u}_\Gamma)$, is the associated solution to the state system. Recall that $(\bar{y}, \bar{y}_\Gamma, \bar{w})$ has the regularity properties (2.1), (2.2), and (2.5), respectively, and that (2.14) is satisfied for $(y, y_\Gamma) = (\bar{y}, \bar{y}_\Gamma)$.

The adjoint system to the problem **(CP)** is formally given by

$$q + \Delta p = 0 \quad \text{in } Q, \tag{4.1}$$

$$-\partial_t(p+q) - \Delta q + f''(\bar{y})\, q = b_Q(\bar{y} - z_Q) \quad \text{in } Q, \tag{4.2}$$

$$\partial_{\mathbf{n}} p = 0 \quad \text{on } \Sigma, \tag{4.3}$$

$$q_\Gamma = q_{|\Gamma} \quad \text{and} \quad -\partial_t q_\Gamma + \partial_{\mathbf{n}} q - \Delta_\Gamma q_\Gamma + f''_\Gamma(\bar{y}_\Gamma)\, q_\Gamma = b_\Sigma(\bar{y}_\Gamma - z_\Sigma) \quad \text{on } \Sigma, \tag{4.4}$$

$$(p+q)(T) = b_\Omega(\bar{y}(T) - z_\Omega) \quad \text{in } \Omega, \tag{4.5}$$

$$q_\Gamma(T) = b_\Gamma(\bar{y}_\Gamma(T) - z_\Gamma) \quad \text{on } \Gamma, \tag{4.6}$$

and was derived in [2] under the additional compatibility assumption

$$b_\Omega = b_\Gamma = 0. \tag{4.7}$$

In order to keep the technicalities at a reasonable level, we will from now on always assume that (4.7) is fulfilled; we remark that in [2, Remark 5.6] it has been pointed out that this assumption is dispensable at the expense of less regularity of the adjoint state variables.

The following result was proved in [2, Thm. 2.4].

Theorem 4.1. *Let* **(A1)–(A4)** *and* (4.7) *be fulfilled. Then the adjoint system* (4.1)–(4.6) *has a unique solution in the following sense: there is a unique triple* (p, q, q_Γ) *with the regularity properties*

$$p \in H^1(0,T; H^2(\Omega)) \cap L^2(0,T; H^4(\Omega)), \tag{4.8}$$
$$q \in H^1(0,T; H) \cap L^2(0,T; H^2(\Omega)), \tag{4.9}$$
$$q_\Gamma \in H^1(0,T; H_\Gamma) \cap L^2(0,T; H^2(\Gamma)), \tag{4.10}$$
$$q_\Gamma(t) = q(t)_{|\Gamma} \quad \textit{for a.a. } t \in (0,T), \tag{4.11}$$

that solves for a.a. $t \in (0,T)$ *the variational equations*

$$\int_\Omega q(t)\, v\, dx = \int_\Omega \nabla p(t) \cdot \nabla v\, dx \quad \forall\, v \in V, \tag{4.12}$$

$$\begin{aligned} &- \int_\Omega \partial_t\big(p(t) + q(t)\big)\, v\, dx + \int_\Omega \nabla q(t) \cdot \nabla v\, dx + \int_\Omega f''(\bar{y}(t))\, q(t)\, v\, dx \\ &\quad - \int_\Gamma \partial_t q_\Gamma(t)\, v_\Gamma\, d\Gamma + \int_\Gamma \nabla_\Gamma q_\Gamma(t) \cdot \nabla_\Gamma v_\Gamma\, d\Gamma + \int_\Gamma f''_\Gamma(\bar{y}_\Gamma(t))\, q_\Gamma(t)\, v_\Gamma\, d\Gamma \\ &= \int_\Omega b_Q\big(\bar{y}(t) - z_Q(t)\big) v\, dx + \int_\Gamma b_\Sigma\big(\bar{y}_\Gamma(t) - z_\Sigma(t)\big) v_\Gamma\, d\Gamma \\ &\quad \textit{for all } (v, v_\Gamma) \in \mathcal{V}, \end{aligned} \tag{4.13}$$

and the final condition

$$\int_\Omega (p+q)(T)\, v\, dx + \int_\Gamma q_\Gamma(T)\, v_\Gamma\, d\Gamma = 0 \quad \forall (v, v_\Gamma) \in \mathcal{V}\,. \tag{4.14}$$

Now, let us introduce the "reduced cost functional" $\widetilde{\mathcal{J}} : \mathcal{U} \to \mathbb{R}$ by

$$\widetilde{\mathcal{J}}(u_\Gamma) := \mathcal{J}(y, y_\Gamma, u_\Gamma), \quad \text{where} \quad (y, y_\Gamma) = \mathcal{S}(u_\Gamma). \tag{4.15}$$

Since $\bar{u}_\Gamma$ is an optimal control with associated optimal state $(\bar{y}, \bar{y}_\Gamma) = \mathcal{S}(\bar{u}_\Gamma)$, the necessary condition for optimality is

$$D\widetilde{\mathcal{J}}(\bar{u}_\Gamma)(v_\Gamma - \bar{u}_\Gamma) \ \geq 0, \quad \text{for every } v_\Gamma \in \mathcal{U}_{ad}, \tag{4.16}$$

or, written explicitly (recall that $b_\Omega = b_\Gamma = 0$),

$$b_Q \int_0^T \!\! \int_\Omega (\bar{y} - z_Q)\, \xi\, dx\, dt \ + \ b_\Sigma \int_0^T \!\! \int_\Gamma (\bar{y}_\Gamma - z_\Sigma)\, \xi_\Gamma\, d\Gamma\, dt \ + \ b_0 \int_0^T \!\! \int_\Gamma \bar{u}_\Gamma\, (v_\Gamma - \bar{u}_\Gamma)\, d\Gamma\, dt \ \geq \ 0$$
$$\text{for every } \ v_\Gamma \in \mathcal{U}_{ad}, \tag{4.17}$$

where, for any given $v_\Gamma \in \mathcal{U}_{ad}$, the functions ξ, ξ_Γ are the first two components of the solution triple (ξ, ξ_Γ, ζ) to the linearized problem (3.4)–(3.9) associated with $h_\Gamma = v_\Gamma - \bar{u}_\Gamma$. Moreover, since the adjoint variables have been constructed in such a way that

$$b_Q \int_0^T \!\! \int_\Omega (\bar{y} - z_Q)\, \xi\, dx\, dt \ + \ b_\Sigma \int_0^T \!\! \int_\Gamma (\bar{y}_\Gamma - z_\Sigma)\, \xi_\Gamma\, d\Gamma\, dt \ = \ \int_0^T \!\! \int_\Gamma q_\Gamma\, (v_\Gamma - \bar{u}_\Gamma)\, d\Gamma\, dt, \tag{4.18}$$

we can rewrite (4.17) in the form (see also [2, Thm. 2.5])

$$\int_0^T \!\! \int_\Gamma (q_\Gamma + b_0\, \bar{u}_\Gamma)(v_\Gamma - \bar{u}_\Gamma)\, d\Gamma\, dt \ \geq \ 0 \quad \text{for every } v_\Gamma \in \mathcal{U}_{ad}. \tag{4.19}$$

In particular, if $b_0 > 0$, $\bar{u}_\Gamma$ is the orthogonal projection of $-q_\Gamma/b_0$ onto $\mathcal{U}_{ad}$ with respect to the standard scalar product in $L^2(\Sigma)$.

After these preparations, we now derive sufficient conditions for optimality. But, since the control-to-state operator $\mathcal{S}$ is not Fréchet differentiable on $L^2(\Sigma)$ but only on $\mathcal{U} \subset \mathcal{X}$, we are faced with the so-called "two-norm discrepancy", which makes it impossible to establish second-order sufficient optimality conditions by means of the same simple arguments as in the finite-dimensional case or, e. g., in the proof of [6, Thm. 4.23, p. 231]. It will thus be necessary to tailor the conditions in such a way as to overcome the two-norm discrepancy. At the same time, for practical purposes the conditions should not be overly restrictive. For such an approach, we follow the lines of Chapter 5 in [6], here. Since many of the arguments developed here are rather similar to those employed in [6], we can afford to be sketchy and refer the reader to [6] for full details.

To begin with, the quadratic cost functional $\mathcal{J}$, viewed as a map from $C^0([0,T];\mathcal{H}) \times \mathcal{U}$ into $\mathbb{R}$, is obviously twice continuously Fréchet differentiable on $C^0([0,T];\mathcal{H}) \times \mathcal{U}$ and thus, in particular, at $((\bar{y}, \bar{y}_\Gamma), \bar{u}_\Gamma)$. Moreover, since $b_\Omega = b_\Gamma = 0$, we have for any $((y, y_\Gamma), u_\Gamma) \in C^0([0,T];\mathcal{H}) \times \mathcal{U}$ and any $((v, v_\Gamma), h_\Gamma), ((\omega, \omega_\Gamma), k_\Gamma) \in C^0([0,T];\mathcal{H}) \times \mathcal{X}$ that

$$D^2\mathcal{J}((y, y_\Gamma), u_\Gamma)[((v, v_\Gamma), h_\Gamma), ((\omega, \omega_\Gamma), k_\Gamma)]$$
$$= b_Q \int_0^T \!\! \int_\Omega v\, \omega\, dx\, dt \ + \ b_\Sigma \int_0^T \!\! \int_\Gamma v_\Gamma\, \omega_\Gamma\, d\Gamma\, dt \ + \ b_0 \int_0^T \!\! \int_\Gamma h_\Gamma\, k_\Gamma\, d\Gamma\, dt\,. \tag{4.20}$$

It then follows from Theorem 3.2 and from the chain rule that the reduced cost functional $\tilde{\mathcal{J}}$ is also twice continuously Fréchet differentiable on $\mathcal{U}$. Now let $h_\Gamma, k_\Gamma \in \mathcal{X}$ be arbitrary. In accordance with our previous notation, we put

$$(\varphi,\varphi_\Gamma) = D\mathcal{S}(\bar u_\Gamma)h_\Gamma, \quad (\psi,\psi_\Gamma) = D\mathcal{S}(\bar u_\Gamma)k_\Gamma, \quad (\eta,\eta_\Gamma) = D^2\mathcal{S}(\bar u_\Gamma)[h_\Gamma,k_\Gamma]\,.$$

Then a straightforward calculation resembling that carried out on page 241 in [6], using the chain rule as main tool, yields the equality

$$\begin{aligned} D^2\tilde{\mathcal{J}}(\bar u_\Gamma)[h_\Gamma,k_\Gamma] \;&=\; D_{(y,y_\Gamma)}\mathcal{J}((\bar y,\bar y_\Gamma),\bar u_\Gamma)(\eta,\eta_\Gamma) \\ &\quad + D^2\mathcal{J}((\bar y,\bar y_\Gamma),\bar u_\Gamma)[((\varphi,\varphi_\Gamma),h_\Gamma)\,,\,((\psi,\psi_\Gamma),k_\Gamma)]\,. \end{aligned} \tag{4.21}$$

For the first summand on the right-hand side of (4.21) we have

$$D_{(y,y_\Gamma)}\mathcal{J}((\bar y,\bar y_\Gamma),\bar u_\Gamma)(\eta,\eta_\Gamma) \;=\; b_Q\int_0^T\!\!\int_\Omega (\bar y - z_Q)\,\eta\,dx\,dt + b_\Sigma\int_0^T\!\!\int_\Gamma (\bar y_\Gamma - z_\Sigma)\,\eta_\Gamma\,d\Gamma\,dt\,, \tag{4.22}$$

where (η,η_Γ) solves the system (3.21)–(3.26). We now claim that

$$\begin{aligned} & b_Q\int_0^T\!\!\int_\Omega (\bar y - z_Q)\,\eta\,dx\,dt \;+\; b_\Sigma\int_0^T\!\!\int_\Gamma (\bar y_\Gamma - z_\Sigma)\,\eta_\Gamma\,d\Gamma\,dt \\ &\quad = -\int_0^T\!\!\int_\Omega f^{(3)}(\bar y)\,\varphi\,\psi\,q\,dx\,dt \;-\; \int_0^T\!\!\int_\Gamma f_\Gamma^{(3)}(\bar y_\Gamma)\,\varphi_\Gamma\,\psi_\Gamma\,q_\Gamma\,d\Gamma\,dt\,. \end{aligned} \tag{4.23}$$

To prove this claim, we test (3.21) by p, insert $v = \vartheta$ in (4.12), and add the resulting equations to obtain

$$0 \;=\; \int_0^T\!\!\int_\Omega (\partial_t\eta\,p \;+\; q\,\vartheta)\,dx\,dt\,. \tag{4.24}$$

Next, we test (3.22) by q. Since $q_{|\Gamma} = q_\Gamma$, we find the identity

$$\begin{aligned} &\int_0^T\!\!\int_\Omega q\,\vartheta\,dx\,dt \;=\; \int_0^T\!\!\int_\Omega \partial_t\eta\,q\,dx\,dt \;+\; \int_0^T\!\!\int_\Omega \nabla\eta\cdot\nabla q\,dx\,dt \;+\; \int_0^T\!\!\int_\Gamma \partial_t\eta_\Gamma\,q_\Gamma\,d\Gamma\,dt \\ &+ \int_0^T\!\!\int_\Gamma \nabla_\Gamma\eta_\Gamma\cdot\nabla_\Gamma q_\Gamma\,d\Gamma\,dt \;+\; \int_0^T\!\!\int_\Omega f''(\bar y)\,\eta\,q\,dx\,dt \;+\; \int_0^T\!\!\int_\Omega f^{(3)}(\bar y)\,\varphi\,\psi\,q\,dx\,dt \\ &+ \int_0^T\!\!\int_\Gamma f_\Gamma''(\bar y_\Gamma)\,\eta_\Gamma\,q_\Gamma\,d\Gamma\,dt \;+\; \int_0^T\!\!\int_\Gamma f_\Gamma^{(3)}(\bar y_\Gamma)\,\varphi_\Gamma\,\psi_\Gamma\,q_\Gamma\,d\Gamma\,dt\,. \end{aligned} \tag{4.25}$$

Now observe that the initial condition $\eta(0) = \eta_\Gamma(0) = 0$ and the final condition (4.14) imply, using integration by parts with respect to time, that

$$\begin{aligned} &\int_0^T\!\!\int_\Omega \partial_t\eta\,(p+q)\,dx\,dt \;+\; \int_0^T\!\!\int_\Gamma \partial_t\eta_\Gamma\,q_\Gamma\,d\Gamma\,dt \\ &\quad = -\int_0^T\!\!\int_\Omega \partial_t(p+q)\,\eta\,dx\,dt \;-\; \int_0^T\!\!\int_\Gamma \eta_\Gamma\,\partial_t q_\Gamma\,d\Gamma\,dt\,. \end{aligned}$$

Hence, by adding (4.24) and (4.25) to each other, we obtain the identity

$$\begin{aligned} 0 = &-\int_0^T\!\!\int_\Omega \partial_t(p+q)\,\eta\,dx\,dt \;-\; \int_0^T\!\!\int_\Gamma \eta_\Gamma\,\partial_t q_\Gamma\,d\Gamma\,dt \;+\; \int_0^T\!\!\int_\Omega \nabla\eta\cdot\nabla q\,dx\,dt \\ &+ \int_0^T\!\!\int_\Gamma \nabla_\Gamma\eta_\Gamma\cdot\nabla_\Gamma q_\Gamma\,d\Gamma\,dt \;+\; \int_0^T\!\!\int_\Omega f''(\bar y)\,\eta\,q\,dx\,dt \;+\; \int_0^T\!\!\int_\Omega f^{(3)}(\bar y)\,\varphi\,\psi\,q\,dx\,dt \\ &+ \int_0^T\!\!\int_\Gamma f_\Gamma''(\bar y_\Gamma)\,\eta_\Gamma\,q_\Gamma\,d\Gamma\,dt \;+\; \int_0^T\!\!\int_\Gamma f_\Gamma^{(3)}(\bar y_\Gamma)\,\varphi_\Gamma\,\psi_\Gamma\,q_\Gamma\,d\Gamma\,dt\,. \end{aligned} \tag{4.26}$$

Inserting $(v, v_\Gamma) = (\eta, \eta_\Gamma)$ in (4.13), we finally obtain

$$0 = \int_0^T \int_\Omega \big(b_Q(\bar{y} - z_Q)\, \eta \,+\, f^{(3)}(\bar{y})\, \varphi\, \psi\, q \big)\, dx\, dt \\ + \int_0^T \int_\Gamma \Big(b_\Sigma(\bar{y}_\Gamma - z_\Sigma)\, \eta_\Gamma \,+\, f_\Gamma^{(3)}(\bar{y}_\Gamma)\, \varphi_\Gamma\, \psi_\Gamma\, q_\Gamma \Big)\, d\Gamma\, dt,$$

by comparison. From this the claim (4.23) follows.

Now we can recall (4.20)–(4.23) in order to find the representation formula

$$D^2\tilde{\mathfrak{J}}(\bar{u}_\Gamma)[h_\Gamma, h_\Gamma] = b_0\, \|h_\Gamma\|^2_{L^2(\Sigma)} + \int_0^T \int_\Omega \big(b_Q - q\, f^{(3)}(\bar{y}) \big)\, |\varphi|^2\, dx\, dt \\ + \int_0^T \int_\Gamma \Big(b_\Sigma - q_\Gamma\, f_\Gamma^{(3)}(\bar{y}_\Gamma) \Big)\, |\varphi_\Gamma|^2\, d\Gamma\, dt\ . \tag{4.27}$$

Equality (4.27) gives rise to hope that, under appropriate conditions, $D^2\tilde{\mathfrak{J}}(\bar{u}_\Gamma)$ might be a positive definite operator on a suitable subset of the space $L^2(\Sigma)$. To formulate such a condition, we introduce for fixed $\tau > 0$ the *set of strongly active constraints for* $\bar{u}_\Gamma$ by

$$A_\tau(\bar{u}_\Gamma) \;:=\; \{(x,t) \in \Sigma :\; |q_\Gamma(x,t) + b_0\, \bar{u}_\Gamma(x,t)| > \tau\}\,, \tag{4.28}$$

and we define the $\tau-$*critical cone* $C_\tau(\bar{u}_\Gamma)$ to be the set of all $h_\Gamma \in \mathcal{X}_{M_0} := \{h_\Gamma \in \mathcal{X} : \|\partial_t h_\Gamma\|_{L^2(\Sigma)} \le M_0\}$ such that

$$h_\Gamma(x,t) \begin{cases} = 0 & \text{if} \quad (x,t) \in A_\tau(\bar{u}_\Gamma) \\ \ge 0 & \text{if} \quad \bar{u}_\Gamma(x,t) = u_{\Gamma,\min} \text{ and } (x,t) \notin A_\tau(\bar{u}_\Gamma) \\ \le 0 & \text{if} \quad \bar{u}_\Gamma(x,t) = u_{\Gamma,\max} \text{ and } (x,t) \notin A_\tau(\bar{u}_\Gamma) \end{cases} . \tag{4.29}$$

After these preparations, we can formulate the second-order sufficient optimality condition (SSC) as follows:

there exist constants $\delta > 0$ and $\tau > 0$ such that

$$D^2\tilde{\mathfrak{J}}(\bar{u}_\Gamma)\,[h_\Gamma, h_\Gamma] \;\ge\; \delta\, \|h_\Gamma\|^2_{L^2(\Sigma)} \quad \forall\, h_\Gamma \in C_\tau(\bar{u}_\Gamma)\,,$$

where $D^2\tilde{\mathfrak{J}}(\bar{u}_\Gamma)\,[h_\Gamma, h_\Gamma]$ is given by (4.27) with $(\bar{y}, \bar{y}_\Gamma) = \mathcal{S}(\bar{u}_\Gamma)$, $(\varphi, \varphi_\Gamma) = D\mathcal{S}(\bar{u}_\Gamma) h_\Gamma$ and the associated adjoint state (p, q, q_Γ). (4.30)

The following result resembles Theorem 5.17 in [6].

Theorem 4.2. *Suppose that the conditions* **(A1)–(A4)** *and* (4.7) *are fulfilled, and assume* $\bar{u}_\Gamma \in \mathcal{U}_{ad}$, $(\bar{y}, \bar{y}_\Gamma) = \mathcal{S}(\bar{u}_\Gamma)$*, and that the triple* (p, q, q_Γ) *satisfies* (4.8)–(4.14)*. Moreover, assume that the conditions* (4.19) *and* (4.30) *are fulfilled. Then there are constants* $\varepsilon > 0$ *and* $\sigma > 0$ *such that*

$$\tilde{\mathfrak{J}}(u_\Gamma) \;\ge\; \tilde{\mathfrak{J}}(\bar{u}_\Gamma) \,+\, \sigma\, \|u_\Gamma - \bar{u}_\Gamma\|^2_{L^2(\Sigma)} \quad \textit{for all } u_\Gamma \in \mathcal{U}_{ad} \textit{ with } \|u_\Gamma - \bar{u}_\Gamma\|_{\mathcal{X}} \le \varepsilon\,. \tag{4.31}$$

In particular, $\bar{u}_\Gamma$ *is locally optimal for* **(CP)** *in the sense of* $\mathcal{X}$.

Proof. The proof closely follows that of [6, Thm. 5.17], and therefore we can refer to [6]. We only indicate one argument that needs additional explanation. To this end, let $u_\Gamma \in \mathcal{U}_{ad}$ be arbitrary. Since $\tilde{\mathcal{J}}$ is twice continuously Fréchet differentiable in $\mathcal{U}$, it follows from Taylor's theorem with integral remainder (see, e. g., [4, Thm. 8.14.3, p. 186]) that

$$\tilde{\mathcal{J}}(u_\Gamma) - \tilde{\mathcal{J}}(\bar{u}_\Gamma) = D\tilde{\mathcal{J}}(\bar{u}_\Gamma)v_\Gamma + \frac{1}{2} D^2\tilde{\mathcal{J}}(\bar{u}_\Gamma)[v_\Gamma, v_\Gamma] + R^{\tilde{\mathcal{J}}}(u_\Gamma, \bar{u}_\Gamma)\,, \tag{4.32}$$

with $v_\Gamma = u_\Gamma - \bar{u}_\Gamma$ and the remainder

$$R^{\tilde{\mathcal{J}}}(u_\Gamma, \bar{u}_\Gamma) = \int_0^1 (1-s)\left(D^2\tilde{\mathcal{J}}(\bar{u}_\Gamma + s\,v_\Gamma) - D^2\tilde{\mathcal{J}}(\bar{u}_\Gamma)\right)[v_\Gamma, v_\Gamma]\; ds. \tag{4.33}$$

Now, we estimate the integrand $(D^2\tilde{\mathcal{J}}(\bar{u}_\Gamma + s\,v_\Gamma) - D^2\tilde{\mathcal{J}}(\bar{u}_\Gamma))[v_\Gamma, v_\Gamma]$ in (4.33). To this end, we put

$$\begin{aligned}
&(y^s, y^s_\Gamma) = \mathcal{S}(\bar{u}_\Gamma + sv_\Gamma), \quad (\varphi, \varphi_\Gamma) = D\mathcal{S}(\bar{u}_\Gamma)v_\Gamma, \quad (\varphi^s, \varphi^s_\Gamma) = D\mathcal{S}(\bar{u}_\Gamma + sv_\Gamma)v_\Gamma,\\
&(\eta, \eta_\Gamma) = D^2\mathcal{S}(\bar{u}_\Gamma)[v_\Gamma, v_\Gamma], \quad (\eta^s, \eta^s_\Gamma) = D^2\mathcal{S}(\bar{u}_\Gamma + sv_\Gamma)[v_\Gamma, v_\Gamma]\,,
\end{aligned}$$

and use the representation formulas (4.20)–(4.22). We obtain

$$D_{(y,y_\Gamma)}\mathcal{J}((y^s, y^s_\Gamma), \bar{u}_\Gamma + sv_\Gamma)(\eta^s, \eta^s_\Gamma) - D_{(y,y_\Gamma)}\mathcal{J}((\bar{y}, \bar{y}_\Gamma), \bar{u}_\Gamma)(\eta, \eta_\Gamma) = I_1 + I_2, \tag{4.34}$$

with the integrals

$$\begin{aligned}
I_1 &:= b_Q \int_0^T\!\!\int_\Omega (y^s - \bar{y})\,\eta\,dx\,dt + b_\Sigma \int_0^T\!\!\int_\Gamma (y^s_\Gamma - \bar{y}_\Gamma)\,\eta_\Gamma\,d\Gamma\,dt\,,\\
I_2 &:= b_Q \int_0^T\!\!\int_\Omega (y^s - z_Q)\,(\eta^s - \eta)\,dx\,dt + b_\Sigma \int_0^T\!\!\int_\Gamma (y^s_\Gamma - z_\Sigma)\,(\eta^s_\Gamma - \eta_\Gamma)\,d\Gamma\,dt\,.
\end{aligned} \tag{4.35}$$

Moreover,

$$\begin{aligned}
&D^2\mathcal{J}((y^s, y^s_\Gamma), \bar{u}_\Gamma + sv_\Gamma)[((\varphi^s, \varphi^s_\Gamma), v_\Gamma)\,,\,((\varphi^s, \varphi^s_\Gamma), v_\Gamma)]\\
&\quad - D^2\mathcal{J}((\bar{y}, \bar{y}_\Gamma), \bar{u}_\Gamma)[((\varphi, \varphi_\Gamma), v_\Gamma)\,,\,((\varphi, \varphi_\Gamma), v_\Gamma)] = I_3, \qquad \text{where}\\
&I_3 := b_Q \int_0^T\!\!\int_\Omega (\varphi^s - \varphi)(\varphi^s + \varphi)\,dx\,dt + b_\Sigma \int_0^T\!\!\int_\Gamma (\varphi^s_\Gamma - \varphi_\Gamma)(\varphi^s_\Gamma + \varphi_\Gamma)\,d\Gamma\,dt\,.
\end{aligned} \tag{4.36}$$

We now estimate the integrals I_1, I_2, and I_3, where we denote by C_i, $i \in \mathbb{N}$, constants that neither depend on $s \in [0,1]$ nor on $u_\Gamma \in \mathcal{U}_{ad}$. At first, using the Cauchy-Schwarz inequality, we obtain

$$\begin{aligned}
|I_1| &\le \max\{b_Q, b_\Sigma\}\,\|(y^s, y^s_\Gamma) - (\bar{y}, \bar{y}_\Gamma)\|_{L^2(0,T;\mathcal{H})}\,\|(\eta, \eta_\Gamma)\|_{L^2(0,T;\mathcal{H})}\\
&\le \max\{b_Q, b_\Sigma\}\,\|(y^s, y^s_\Gamma) - (\bar{y}, \bar{y}_\Gamma)\|_{\mathcal{Y}}\;\|(\eta, \eta_\Gamma)\|_{\mathcal{Y}}\\
&\le C_1\,s\,\|v_\Gamma\|^3_{L^2(\Sigma)},
\end{aligned} \tag{4.37}$$

where in the last inequality we have employed the estimates (2.12) and (3.31). Similarly, we have

$$\begin{aligned}
|I_2| &\le \max\{b_Q, b_\Sigma\}\,\|(y^s, y^s_\Gamma) - (z_Q, z_\Sigma)\|_{L^2(0,T;\mathcal{H})}\,\|(\eta^s, \eta^s_\Gamma) - (\eta, \eta_\Gamma)\|_{L^2(0,T;\mathcal{H})}\\
&\le \max\{b_Q, b_\Sigma\}\,\|(y^s, y^s_\Gamma) - (z_Q, z_\Sigma)\|_{L^2(0,T;\mathcal{H})}\;\|(\eta^s, \eta^s_\Gamma) - (\eta, \eta_\Gamma)\|_{\mathcal{Y}}\\
&\le C_2\,s\,\|v_\Gamma\|^3_{L^2(\Sigma)},
\end{aligned} \tag{4.38}$$

where, for the last inequality, we used **(A1)** and (2.10) to estimate the first norm and (3.28) for the second one. Finally, we get

$$\begin{aligned} |I_3| &\le \max\{b_Q, b_\Sigma\} \,\|(\varphi^s, \varphi_\Gamma^s) - (\varphi, \varphi_\Gamma)\|_{L^2(0,T;\mathcal{H})} \,\|(\varphi^s, \varphi_\Gamma^s) + (\varphi, \varphi_\Gamma)\|_{L^2(0,T;\mathcal{H})} \\ &\le \max\{b_Q, b_\Sigma\} \,\|(\varphi^s, \varphi_\Gamma^s) - (\varphi, \varphi_\Gamma)\|_{\mathcal{Y}} \,\|(\varphi^s, \varphi_\Gamma^s) + (\varphi, \varphi_\Gamma)\|_{\mathcal{Y}} \\ &\le C_3 \, s \, \|v_\Gamma\|^3_{L^2(\Sigma)}. \end{aligned} \tag{4.39}$$

For the last inequality we applied (3.10) to estimate the first norm and the triangle inequality and (2.24) to estimate the second one. Combining the above estimates, we thus have finally shown that

$$\left| R^{\tilde{\mathcal{J}}}(u_\Gamma, \bar{u}_\Gamma) \right| \;\le\; C_4 \int_0^1 (1-s)\, s\, \|v_\Gamma\|^3_{L^2(\Sigma)} \, ds \;\le\; C_5 \, \|v_\Gamma\|_{\mathcal{X}} \, \|v_\Gamma\|^2_{L^2(\Sigma)} \,, \tag{4.40}$$

with global constants $C_4 > 0$ and $C_5 > 0$ that do not depend on the choice of $u_\Gamma \in \mathcal{U}_{ad}$. But this means that

$$\frac{\left| R^{\tilde{\mathcal{J}}}(u_\Gamma, \bar{u}_\Gamma) \right|}{\|u_\Gamma - \bar{u}_\Gamma\|^2_{L^2(\Sigma)}} \to 0 \quad \text{as } \|u_\Gamma - \bar{u}_\Gamma\|_{\mathcal{X}} \to 0. \tag{4.41}$$

With this information at hand, we can argue along exactly the same lines as on pages 292–294 in the proof of Theorem 5.17 in [6] to conclude the validity of the assertion. □

References

[1] P. Colli, G. Gilardi and J. Sprekels, On the Cahn–Hilliard equation with dynamic boundary conditions and a dominating boundary potential, *J. Math. Anal. Appl.* **419** (2014), pp. 972–994.

[2] P. Colli, G. Gilardi and J. Sprekels, A boundary control problem for the viscous Cahn–Hilliard equation with dynamic boundary conditions, preprint arXiv:1407.3916 [math.AP] (2014), pp. 1–27.

[3] P. Colli and J. Sprekels, Optimal control of an Allen–Cahn equation with singular potentials and dynamic boundary condition, preprint arXiv:1212.2359 [math.AP] (2012), pp. 1–24, to appear in SIAM J. Control Optim.

[4] J. Dieudonné, Foundations of Modern Analysis, Academic Press, New York, 1960.

[5] M. Heinkenschloss and F. Tröltzsch, Analysis of an SQP method for the control of a phase field equation, *Control Cybernetics* **28** (1999), pp. 177–211.

[6] F. Tröltzsch, Optimal Control of Partial Differential Equations: Theory, Methods and Applications, *Graduate Studies in Mathematics* Vol. **112**, American Mathematical Society, Providence, Rhode Island, 2010.