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Some mathematical problems related to the 2nd order optimal shape of a crystallization interface

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Abstract

We consider the problem to optimize the stationary temperature distribution and the equilibrium shape of the solid-liquid interface in a two-phase system subject to a temperature gradient. The interface satisfies the minimization principle of the free energy, while the temperature is solving the heat equation with a radiation boundary conditions at the outer wall. Under the condition that the temperature gradient is uniformly negative in the direction of crystallization, the interface is expected to have a global graph representation. We reformulate this condition as a pointwise constraint on the gradient of the state, and we derive the first order optimality system for a class of objective functionals that account for the second surface derivatives, and for the surface temperature gradient.

1 Introduction

In this paper, we consider the problem to optimize the stationary temperature distribution and the equilibrium position of the solid-liquid interface S in a two-phase system $\Omega \subset \mathbb{R}^3$ subject to a temperature gradient. In semiconductor crystal growth, there is evidence for the fact that the the curvature profile of S near the boundary of the growth container influences the incorporation of defects in the crystal [DDEN08]. The temperature gradient on the interface is the source of thermal stresses that influence the crystal quality as well. In this context the mathematical optimization has to consider the shape of the interface up to the second order geometrical properties (curvatures, convexity), and at the same time quantities like the tangential temperature gradient on the surface.

The objective to prescribe desired curvatures and other quantities on an unknown surface makes sense in the context of industrial crystal growth only because the crystallization occurs in a *privileged direction*. Mathematically speaking the interface S is expected to be the graph of a function.

The free surface S is modeled by the minimization principle of the free energy Ψ (see [Vis96], Chapter VI for a mathematically oriented introduction to the Gibbs-Thompson law), given by

$$\Psi(S,\, \theta) := \int_S \sigma(s,\, \nu)\, dS + \int_{\partial\Omega} \kappa\, \chi_S\, dH - \int_\Omega \lambda(\theta)\, \chi_S\, dx\,. \tag{1}$$

Here $\sigma = \sigma(x, z, q)$ ($(x, z) \in \Omega$, $q \in \mathbb{R}^3$) is a given, positive one-homogeneous function in the q variable. The unit normal to the interface pointing into the solid phase is denoted ν. The functions $\kappa :\, \partial\Omega \to \mathbb{R}$ and $\lambda :\, \mathbb{R}^+ \to \mathbb{R}$ are given, and θ denotes the absolute temperature in Ω. The phase-function χ_S associated with S takes the value 1 in the solid, and -1 in the liquid.

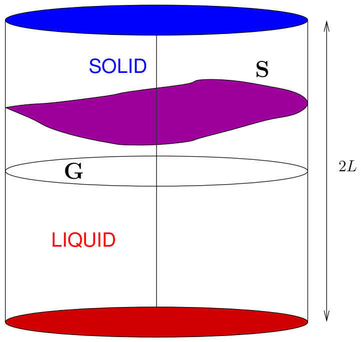

Figure 1: A model configuration Ω: 'Hot' bottom (red), and 'cold' top (blue)

Throughout the paper, the privileged growth direction is taken to be the $z-$ axis. According to the assumption that the interface S is a graph, we consider $\Omega = G\times]-L, L[$ with a bounded domain $G \subset \mathbb{R}^2$, and $L > 0$. It is well known that the Euler-Lagrange equation for nonparametric variations of the free energy leads to a boundary-value problem for the minimizer $\psi : G \to]-L, L[$. For the case that the functions σ and κ do not depend on the $z-$variable, this boundary value problem has the form

$$\operatorname{div} \sigma_q(x, -\nabla\psi, 1) = \lambda(\theta(x, \psi)) \text{ in } G\,, \tag{2}$$

$$\sigma_q(x, -\nabla\psi, 1) \cdot n = \kappa(x) \qquad \text{on } \partial G\,, \tag{3}$$

where n is the outward unit normal to ∂G. We assume that heat mainly propagates in Ω by conduction, the heat transfer in Ω can be modeled by the heat equation

$$-\operatorname{div}(k_S\, \nabla\theta) = f \qquad \text{in } \Omega \setminus S, \tag{4}$$

$$[\theta] = 0, \quad [-k_S\, \nabla\theta \cdot \nu] = 0 \qquad \text{on } S \tag{5}$$

$$-k_S\, \nabla\theta \cdot n = \beta\, (\theta^4 - \theta_{\text{Ext}}^4) \text{ on } \partial\Omega\,. \tag{6}$$

In the equation (4), the heat conductivity k_S is defined in $\overline{\Omega} \setminus S$. In general it depends on the solution S to the geometric equation (2) (dependence on the phase), and additionally on the temperature. The conditions (5) are the usual Stefan conditions at equilibrium. In this paper where the focus is on optimal control, we only treat the special case that the heat-conductivities of the solid and the liquid phase are equal at the interface, that is

$$\exists\, k \in C^1(\overline{\Omega};\, \mathbb{R}^{3\times3}) \;:\; k_S = k \text{ in } \Omega\,. \tag{7}$$

The equations (2) and (4) then decouple, which provides a major simplification for the mathematical analysis of the forward problem. In accordance with the equation (2), anisotropy affects only in the $x-$direction, that is

$$k = \begin{pmatrix} \tilde{k} & 0 \\ 0 & 1 \end{pmatrix}, \quad \tilde{k} \in C^1(\overline{\Omega};\, \mathbb{R}^{2\times2})\,. \tag{8}$$

The function f is a given heat source density. In the condition (6), β is a positive constant, and θ_{Ext} is the given external temperature that is applying a temperature-gradient to the system. The nonlinear Stefan-Boltzmann radiation condition is here considered instead of more classical linear boundary conditions due the high-temperatures characteristic of semiconductor crystal growth.

We denote (P) the forward problem of finding ψ subject to (2), (3), and θ satisfying (4), (5), (6) with $k_S = k$.

For the optimal control, we will consider the problem of controlling the external temperature of the system in the condition (6). For a given control u, we denote $(P(u))$ the problem of solving (P) for $\theta_{\text{Ext}} = u$.

We are in general interested in objective functionals $J = J(\psi,\, \theta)$ on the space $C^2(\overline{G}) \times C^1(\overline{\Omega})$: The reason for this is the wish to control the surface up to second order, and the temperature up to its surface gradient. Convenient to handle are integral functionals

$$J(\psi,\, \theta) = \int_G j_1(x,\, \psi,\, D\psi,\, D^2\psi) dx + \int_S j_2(s,\, \theta,\, \nabla_S \theta)\, dS\,. \tag{9}$$

with suitable functions $j_1,\, j_2$. A typical quadratic example is given by

$$J(\psi,\, \theta) := \frac{1}{2}\, \|\psi - \psi_d\|^2_{W^{2,2}(G)} + \frac{1}{2}\, \|\theta - \theta_d\|^2_{W^{1,2}(S)}\,, \tag{10}$$

where ψ_d is a desired interface, and θ_d a desired temperature profile on the surface.

Moreover we have to incorporate pointwise state-constraints in the optimal control problem. The temperature has to remain in a certain range to prevent melting of the growth container, and the interface should not approach too near the set $G \times \{-L,\, L\}$ (top and bottom of the container). We require that

$$\theta_{\text{min}} \;\leq\; \theta \;\leq\; \theta_{\text{max}} \quad \text{in}\, \Omega, \quad -L' \;\leq\; \psi \;\leq\; L' \quad \text{in}\, G\,, \tag{11}$$

where $\theta_{\text{min}} < \theta_{\text{max}}$ and $L' < L$ are positive real numbers.

We cannot expect for general temperature profiles that the solution of the minization problem for the interface energy Ψ is a smooth graph. The $z-$direction is a privileged growth direction for the crystal only *if the decreasing temperature gradient shows in that direction*. The mathematical expression for this constraint is $\partial_z\theta \leq 0$ in Ω, which turns out to be a pointwise constraint on the gradient of the state. For reason inherent in the analysis of the problem, we consider the stronger constraint

$$\partial_z\theta \;\leq\; \gamma \quad \text{in}\, \Omega\,, \tag{12}$$

where $\gamma < 0$ is a parameter. We denote (P_{opt}) the problem of finding the optimal control $u = \theta_{\text{Ext}}$ in order to minimize the objective functional $J = J(\psi,\, \theta)$ (cf. (9), (10)), where $\psi,\, \theta$ are subject to the boundary-value problem $(P(u))$ and to the state constraints (11), (12).

Notations and main assumptions on the data Throughout the paper, the domain $G \subset \mathbb{R}^2$ is of class $\mathcal{C}^{2,\alpha}$ for a fixed $\alpha \in]0,1]$. The potential $\sigma : \overline{G} \times \mathbb{R}^3 \to \mathbb{R}$ appearing in (2) is assumed to satisfy

$$\sigma \in C^{3,\alpha}(\overline{G} \times \mathbb{R}^3 \setminus \{0\})\, (\alpha > 0)\,. \tag{13}$$

We assume that there exist positive constants ν_j ($j = 0, 2$) and μ_i ($i = 0, \ldots, 4$) such that for all $(x,\, q) \in \overline{G} \times \mathbb{R}^{n+1}$

$$\nu_0\, |q| \leq \sigma(x,\, q) \leq \mu_0\, |q| \tag{14a}$$

$$|\sigma_q(x,\, q)| \leq \mu_1 \tag{14b}$$

$$\frac{\nu_2}{|q|}\, |\xi|^2 \leq \sum_{i,j=1}^{3} \sigma_{q_i,q_j}(x,\, q)\, \xi_i\, \xi_j \leq \frac{\mu_2}{|q|}\, |\xi|^2 \quad \text{for all } \xi \in \mathbb{R}^3 \text{ such that } \xi \cdot q = 0 \tag{14c}$$

$$\sum_{i=j}^{3} \sigma_{q_i,q_j}(x,\, q)\, q_j = 0 \quad \text{for } i = 1, \ldots, n+1 \tag{14d}$$

$$|\sigma_{q,x}(x,\, q)| \le \mu_3\,, \quad |\sigma_{q,x,x}(x,\, q)| \le \mu_4\,. \tag{14e}$$

Note that the hypotheses (14a), (14b), (14c) and (14d) are completely natural and in particular satisfied if σ is positively homogeneous of degree one in the q variable (cf. [Ura71] a.o. for a proof). A well known example is $\sigma(x,\, q) = \sigma(x)\,|q|$ ($\sigma =$ isotropic surface tension coefficient): The problem (16), (17) is nothing else but the contact angle problem for the mean-curvature equation.

Instead of σ, it is convenient to introduce a function $F:\, G \times \mathbb{R}^2 \to \mathbb{R}$

$$F(x,\, p) = \sigma(x,\, -p,\, 1), \quad (x, p) \in G \times \mathbb{R}^2\,. \tag{15}$$

The system (2), (3) then reads

$$-\operatorname{div} F_p(x,\, \nabla\psi) = \lambda(\theta(x,\, \psi)) \text{ in } G\,, \tag{16}$$

$$-F_p(x,\, \nabla\psi) \cdot n = \kappa(x) \qquad \text{on } \partial G\,, \tag{17}$$

The equation (16) has a singularity of mean-curvature type. For κ, we assume that

$$\kappa \in C^{1,\alpha}(\partial G)\ (\alpha > 0)\,, \qquad \|\kappa\|_{L^\infty(\partial G)} < \nu_0 \quad \text{on } \partial G\,, \tag{18}$$

with the constant of (14a). For the function λ, we assume that

$$\lambda \in C^{1,\alpha}(\mathbb{R}), \quad \inf_{\mathbb{R}} \lambda' > 0\,. \tag{19}$$

Moreover, λ has one zero at $\theta_{\text{eq}} \in \mathbb{R}^+$. These assumptions of course allow for the linear model $\lambda(\theta) = \lambda_0\,(\theta - \theta_{\text{eq}})$, $\lambda_0 \in \mathbb{R}^+$.

For the data of the heat equation, we assume that

$$f \in L^q(\Omega)\,(q > 3), \quad f \ge 0 \text{ almost everywhere in } \Omega\,. \tag{20}$$

Since we are interested in the interface S and in the temperature, we call *state* a pair $y = (\psi,\, \theta)$, and define for α as in (13) and (18), and for q as in (20) the state space

$$Y := C^{2,\alpha}(\overline{G}) \times W^{2,q}(\Omega)\,. \tag{21}$$

The control for the problem is the external temperature θ_{Ext}. The natural choice for a control space is the trace space $W^{1/q',q}(\partial\Omega)$. Since we can always identify elements of this space with some of their extension into Ω, we find it more convenient to choose

$$U = W^{1,q}(\Omega)\,. \tag{22}$$

The main challenges for the analysis of the optimal control problem are the second order objective functional and the pointwise constraint on the gradient in the first order analysis. Here we need the corresponding higher regularity of the state. Due to regularity results for second order elliptic equations on polyhedra [Dau92, Dau88] (cp. Lemma A.1), it is worth noticing that we do not need to assume that the domain Ω is convex or smooth. The existence of the control to state mapping in classical function spaces relies on the results of [Ura71, Ura73, Ura75, Ura82] on the solvatility of the problem (16), (17) (see [Dru11] for a recent summary and further references). The basic ideas for the derivation of first order optimality conditions in presence of pointwise constraints on the gradient of the state are to find in [CF93, HK09]. Essential differences to these investigations are the higher-order objective functional in connection with boundary control and with the nonlinearity (6). Moreover, we consider a nonlinear system with mean-curvature type singsularity that neither fits into the single equation setting of [CF93], nor into the abstract linear differential setting of [HK09].

The structure of the paper is as follows. In the section 2, we prove the existence of the control to state mapping $\mathcal{S}$. For reasons inherent in the analysis of the problem (16), (17), the natural solution mapping cannot be introduced on the entire control space U, and has to be extended. We study the differentiability of $\mathcal{S}$ in the section 3. In the section 4, we prove the existence of local solutions to the optimal control problem, and we derive the first order optimality system for a class of objective functionals having the application-relevant properties. In the final section 5, we illustrate our analysis at the example of the functional (10). In the appendix we have collected a few auxiliary propositions. To our knowledge, the Lemma A.1 on higher regularity for the nonhomogeneous Neumann problem of the heat equation also deserves some attention.

2 Control to state mapping

The first ingredient is the solution operator to the heat equation (4).

Proposition 2.1. *Assume that $\Omega = G\times]-L,\,L[$, with $G \subset \mathbb{R}^2$ a bounded domain of class $\mathcal{C}^{2,\alpha}$. Assume that* (20) *is valid for f, that k satisfies* (8)*, and let $u \in U$ (cp.* (22)*), $u \geq 0$ in Ω. Then, there is a unique $\theta \in W^{2,q}(\Omega)$ that satisfies the equation* (4) *and the boundary condition* (6) *with $\theta_{Ext} = u$. Moreover $\theta \geq \inf_{\partial\Omega} u$ in $\overline{\Omega}$.*

Proof. Consider the weak solution space $V^{2,5}(\Omega) := \{\theta \in W^{1,2}(\Omega) \,:\, \mathrm{trace}(\theta) \in L^5(\partial\Omega)\}$. Due to standard results about monotone operators, we easily prove the existence of a unique $\theta \in V^{2,5}(\Omega)$ such that

$$\int_\Omega k\nabla\theta\cdot\nabla\phi + \int_{\partial\Omega} \beta\left(|\theta|^3\,\theta - |u|^3\,u\right)\phi = \int_\Omega f\,\phi, \quad \forall \phi \in V^{2,5}(\Omega)\,. \tag{23}$$

This was for the first time proved in [DPZ87]. Since f is nonnegative, the usual weak maximum principle helps proving that $\theta \geq \inf_{\partial\Omega} u \geq 0$. Therefore, we can replace $|\theta|^3\,\theta$ by θ^4 in (23), proving the existence of a weak solution.

Using standard regularity arguments (Stampacchia's Lemma, cf. for instance [Tro87], Th. 2.7), there is $C = C(\Omega, q) > 0$ such that

$$\sup_\Omega \theta \leq \sup_{\partial\Omega} u + C\,\|f\|_{L^{q/2}(\Omega)}\,.$$

Using that $W^{1,q}(\Omega)$ is continuously embedded in $C(\overline{\Omega})$, the latest implies that $\theta^4 - u^4 \in L^\infty(\Omega)$. Clearly, the functional

$$F(\phi) := -\int_{\partial\Omega} \beta\,(\theta^4 - u^4)\,\phi + \int_\Omega f\,\phi\,, \tag{24}$$

extends by density to a continuous element of $[W^{1,1}(\Omega)]^*$. By the arguments of [Dau92], Th. 3.2, we obtain the estimate

$$\|\nabla\theta\|_{L^q(\Omega)} \leq C\,\|F\|_{W^{1,q'}(\Omega)}\,. \tag{25}$$

Using that the embedding $W^{1,q}(\Omega) \hookrightarrow C(\overline{\Omega})$ is continuous for $q > 3$ and the chain rule for Sobolev functions, one now sees that $\theta^4 \in W^{1,q}(\Omega)$. Due to the trace theorem, it follows that $\theta^4 \in W^{1/q',q}(\partial\Omega)$. Thus, defining $Q := \beta\,(\theta^4 - u^4)$ and using that $u \in U$, we see that $Q \in W^{1/q',q}(\partial\Omega)$. Thus, the problem (4), (6) has the required structure to apply Lemma A.1. The claim follows. ☐

We define $S_{\text{heat}} \,:\, U^+ \longrightarrow W^{2,q}(\Omega)$ the solution mapping to the problem (4), (6) according to Lemma 2.1. (Here $U^+ = \{u \in U \,:\, u \geq 0\}$).

At second, we need the solution operator to the mean-curvature-type equation (16) with contact-angle condition (17). In the following statement, we somewhat abuse notation, defining $C^{1,\alpha}(\overline{G}\times\mathbb{R}) := \{\theta \in C(\overline{G}\times\mathbb{R}) \,:\, \nabla\theta \in C^\alpha(\overline{G}\times\mathbb{R})\}$. Note that this space is not complete.

Proposition 2.2. *Let $G \subset \mathbb{R}^2$ be a bounded domain of class $\mathcal{C}^{2,\alpha}$, $\alpha \in]0,1]$. Assume that* (13), (14) *are valid for σ, and let $\kappa \in C^{1,\alpha}(\partial G)$ satisfy* (18). *Let λ satisfy* (19). *Assume moreover that $\theta \in C^{1,\alpha}(\overline{G}\times\mathbb{R})$ satisfies the monotonicity condition*

$$\gamma_0 := \sup_{G\times\mathbb{R}} \theta_z < 0 \text{ in } G\times\mathbb{R}\,. \tag{26}$$

Then there is a unique $\psi \in C^{2,\alpha}(\overline{G})$ solution to (16), (17).

Moreover, there is a number M independent on θ except for γ_0 and $\|\theta\|_{L^\infty(G\times\{0\})}$ such that $-M \leq \psi(x) \leq M$ for all $x \in G$. There further exists a constant C depending on the domain G on the number $\nu_0 - \|\kappa\|_{L^\infty(\partial G)}$, on γ_0, $\inf_{\mathbb{R}}\lambda'$ and on $\|\nabla\theta\|_{L^\infty(G\times[-M,M])}$ so that

$$\|D^2\psi\|_{C^\alpha(\overline{G})} \leq C\left(\|\lambda(\theta)\|_{C^\alpha(\overline{S})} + \|\kappa\|_{C^{1,\alpha}(\partial S)}\right).$$

Proof. The unique solvability of contact-angle problems (capilarity problems) for generalized equations of mean-curvature type under the condition (26) was first proved in papers by Uraltseva (cf. [Ura71], [Ura73], [Ura75], [Ura82]). A unified presentation can also be found in the survey paper [Dru11]. Due to the assumption (19), note that

$$\partial_z\lambda(\theta) = \lambda'(\theta)\,\theta_z \leq \gamma_0\,\inf_{\mathbb{R}}\lambda' < 0 \quad \text{in } G\times\mathbb{R}\,,$$

which garanties the applicability of these results. The L^∞ estimate and the higher-order estimates on ψ are proved in the same references. ☐

We define $S_{\text{curv}} : C^{1,\alpha}(\overline{G} \times \mathbb{R}) \to C^{2,\alpha}(\overline{G})$ as the solution mapping to the problem (16), (17) according to Proposition 2.2.

Remark 2.3. *Despite the Propositions 2.1 and 2.2, it is still not completely straightforward to introduce the solution operator to the problem (P), due to the following two reasons:*

(1) The solution θ to (4), (6) *does not necessarily satisfy the assumption* (26)*;*

(2) The heat-transfer problem detemines θ only in the cylinder $G\times]-L, L[$. To apply Proposition 2.2, we would at least need that the temperature is defined in $G\times]-M, M[$, $M > L$ being possible.

To solve the difficulties raised by the Remark 2.3 we go for a practical way to indroduce a control to state mapping. To this aim we formulate a technical assumption about the existence of a suitbable extension and monotonization operator. We refer to Lemma B.1 for a justification.

Assumption 2.4. *Let $\gamma < 0$, and $0 < L' < L$. Then, there is a continuously differentiable operator $E = E_{\gamma, L'} : W^{2,q}(\Omega) \to C^{1,\alpha}(\overline{G} \times \mathbb{R})$ such that*

$$\sup_{G\times\mathbb{R}} \partial_z E(\theta) < 0 \text{ for all } \theta \in W^{2,q}(\Omega)\,. \tag{27}$$

Moreover, $E(\theta) = \theta$ in $\Omega_{L'}$ for all $\theta \in W^{2,q}(\Omega)$ such that $\sup_{\Omega} \partial_z\theta \leq \gamma$.

Presently we are interested in the following direct consequence.

Corollary 2.5. *Under the Assumption 2.4, there is a for every $u \in U^+$ a unique pair $(\psi,\, \theta) \in C^{2,\alpha}(\overline{G}) \times W^{2,q}(\Omega)$ such that θ satisfies* (4), (6)*, and such that ψ satisfies*

$$-\operatorname{div} F_p(x,\, \nabla\psi) = \lambda(E(\theta)(x,\, \psi)) \text{ in } G\,, \tag{28}$$

$$-F_p(x,\, \nabla\psi)\cdot n = \kappa(x) \qquad \text{on } \partial G\,, \tag{29}$$

Proof. For $u \in U^+$, let $\theta := S_{\text{heat}}(u)$. Due to Lemma 2.1, θ belongs to $W^{2,q}(\Omega)$. Choose E according to the Assumption 2.4. Obviously, $E(\theta)$ satisfies the assumptions of Proposition 2.2. There is a unique $\psi \in C^{2,\alpha}(\overline{G})$ such that (28) and (29) are valid. ☐

Definition 2.6. *We denote $\mathcal{S} = \mathcal{S}_E : U^+ \to Y = C^{2,\alpha}(\overline{G}) \times W^{2,q}(\Omega)$ the (extended) mapping $u \mapsto (\psi,\, \theta)$ according to Corollary 2.5. We call it the control-to-state mapping associated with (P).*

The construction of the mapping $\mathcal{S}$ includes some obvious arbitrariness, since the choice of the extension operator E is by no means unique. However, the next Remark 2.7 shows that this procedure does not affect the core of the optimal control problem.

Remark 2.7. *Call feasible the controls $u \in U^+$ such that the solution $(\psi,\, \theta)$ to $(P(u))$ satisfies the state constraints* (11) *and* (12)*. If u is feasible and if $E_1,\, E_2$ both satisfy the Assumption 2.4, then $\mathcal{S}_{E_1}(u) = \mathcal{S}_{E_2}(u)$.*

3 Differentiability

In this section, we study the continuous differentiability of the mapping $\mathcal{S}$. We recall that the state space is given by

$$Y := \{(\psi, \theta) \,:\, \psi \in C^{2,\alpha}(\overline{G}),\, \theta \in W^{2,q}(\Omega)\}\,. \tag{30}$$

We prove the differentiability of $\mathcal{S}$ by means of the implicit function theorem. To this aim it is convenient to put the PDE problem in its operator setting.

Denote A_1 the second order nonlinear differential operator associtated with the equation (16), that is

$$A_1(\psi,\, \theta) := -\sum_{i=1}^{2} \frac{d}{dx_i} F_{p_i}(x,\, \nabla\psi) - \lambda(E(\theta)(x,\, \psi))\,. \tag{31}$$

The operator A_1 obviously maps Y into $C^{\alpha}(\overline{G})$. Denote B_1 the boundary differential operator associated with the condition (17). Since we want to consider B_1 on Y as well, we define

$$B_1(\psi,\, \theta) = B_1(\psi) := n \cdot F_p(x,\, \nabla\psi) - \kappa(x)\,. \tag{32}$$

Then, $B_1 \,:\, Y \to C^{1,\alpha}(\partial G)$. We denote A_2 the affine differential operator associated with the heat equation

$$A_2(\psi,\, \theta) = A_2(\theta) := -\operatorname{div}(k\nabla\theta) - f\,, \tag{33}$$

which maps Y into $L^q(\Omega)$. In order to deal with the boundary condition (6), we introduce

$$B_2(\psi,\, \theta,\, u) = B_2(\theta,\, u) := -k\nabla\theta \cdot n - \beta\,(\theta^4 - u^4)\,. \tag{34}$$

Obviously, $B_2 \,:\, Y \times U \to W^{1/q',q}(\partial\Omega)$. The vector valued operator

$$T(y,\, u) := (A_1(y),\, B_1(y),\, A_2(y),\, B_2(y, u)) \quad y \in Y,\, u \in U\,, \tag{35}$$

maps the space $Y \times U$ into the image space

$$Z = C^{\alpha}(\overline{G}) \times C^{1,\alpha}(\partial G) \times L^q(\Omega) \times W^{1/q',q}(\partial\Omega)\,. \tag{36}$$

For $u \in U$, observe that $T(y,\, u) = 0$ if and only if $y = \mathcal{S}(u)$. For $y = (\psi,\, \theta) \in Y$ are equivalent:

$$y \text{ is a solution to } (P(u)) \Longleftrightarrow T(y, u) = 0\,. \tag{37}$$

Moreover the following Lemma is a straightforward exercise.

Lemma 3.1. *For all $y \in Y$, the mapping $T \,:\, Y \times U \to Z$ is Fréchet-differentiable. For $u^*,\, u \in U$ it holds*

$$\partial_u T(y,\, u^*)\, u = (0,\, 0,\, 0,\, 4\,\beta\,(u^*)^3\, u) \in Z\,. \tag{38}$$

We now prove the solvability of the linearized problem.

Lemma 3.2. *Let $u^* \in U^+$, and denote $(\psi^*, \theta^*) = y^* = \mathcal{S}(u^*)$. Let $F \in Z$ arbitrary. Then, the equation $\partial_y T(y^*, u^*)\, y = F$ has a unique solution $y = (\psi, \theta) \in Y$ such that*

$$-\frac{d}{dx_i}(F_{p_i,p_j}(x, \nabla\psi^*)\,\partial_{x_j}\psi) - \lambda'(E(\theta^*)(x, \psi^*))\,\partial_z E(\theta^*)(x, \psi^*)\,\psi$$
$$= \lambda'(E(\theta^*)(x, \psi^*))\,E'(\theta^*)\,\theta(x, \psi^*) + F_1 \quad \text{in } G\,, \tag{39}$$
$$-n_i\,F_{p_i,p_j}(x, \nabla\psi^*)\,\partial_{x_j}\psi = F_2 \quad \text{on } \partial G\,, \tag{40}$$
$$-\operatorname{div}(k\nabla\theta) = F_3 \quad \text{in } \Omega, \tag{41}$$
$$-k\nabla\theta\cdot n = 4\,\beta\,(\theta^*)^3\theta + F_4 \quad \text{on } \partial\Omega\,. \tag{42}$$

Proof. Since T is differentiable, we easily show that $\partial_y T(y^*, u^*)\, y = F \in Z$ if and only if the system (39), (40), (41), (42) is valid.

The equation (41) with the boundary condition (42) can be solved independently. As in the proof of Lemma 2.1, we first obtain the regularity $\theta \in W^{1,q}(\Omega)$. Then $Q := 4\,\beta\,(\theta^*)^3\,\theta + F_4 \in W^{1/q',q}(\partial\Omega)$. We obtain the higher regularity $\theta \in W^{2,q}(\Omega)$ from Lemma A.1.

Due to the choice of E, $\sup_{G\times\mathbb{R}} \partial_z E(\theta^*) < 0$. Moreover, since $\psi^* \in C^{2,\alpha}(\overline{G})$, the matrix $\{F_{p_i,p_j}(x, \nabla\psi^*)\}$ is uniformly elliptic and belongs to $C^{1,\alpha}(\overline{G})$. Since G is of class $\mathcal{C}^{2,\alpha}$, the vector $n_i\,F_{p_i,p_j}(x, \nabla\psi^*)$ belongs to $C^{1,\alpha}(\partial G)$. Standard results on the classical solvability of elliptic second order problems (among others [Tro87], Theorems 3.23 and 3.28) imply that (39), (40) admits a unique solution $\psi \in C^{2,\alpha}(\overline{G})$. This proves the claim. ☐

We are now ready to prove a differentiability property of $\mathcal{S}$.

Corollary 3.3. *The control-to-state mapping $\mathcal{S} : U \to Y$ is continuously differentiable. Its derivative at $u^* \in U^+$ in arbitrary direction $u \in U$ is given by*

$$\mathcal{S}'(u^*)\,u = [\partial_y T(\mathcal{S}(u^*), u^*)]^{-1}\,(0, 0, 0, -4\,\beta\,(u^*)^3\,u)\,. \tag{43}$$

Proof. The derivative $\partial_y T(\mathcal{S}(u^*), u^*)$ is an isomorphism from Y into Z according to Lemma 3.2. Since $T(\mathcal{S}(u), u) = 0$ for all $u \in U$, the claim follows from the implicit function theorem in Banach spaces [GT01], Theorem 17.6. The formula (43) follows from the (38). ☐

4 The optimal control problem

For $J : Y \to \mathbb{R}^+$, we also denote $J : Y \times U \to \mathbb{R}^+$ the regularization

$$J(y, u) := J(y) + \frac{\rho}{q}\,\|u\|_U^q\,, \quad \rho > 0\,. \tag{44}$$

In order to define the set of admissible control, note that the external temperature should not violate the bounds on the temperature inside. Moreover, a meaningful control of the crystallization process must ensure that the temperature at the bottom $G \times \{-L\}$ of the container is larger than at its top $G \times \{L\}$. Recalling that $\theta_{\text{eq}} > 0$ is the only zero of the function λ, we define the set of admissible controls

$$U_{\text{ad}} := \left\{ u \in U \,:\, \begin{cases} \theta_{\min} \leq u \leq \theta_{\max} & \text{on } \partial\Omega \\ u \geq \theta_{\text{eq}} & \text{on } G \times \{-L\} \\ u \leq \theta_{\text{eq}} & \text{on } G \times \{L\} \end{cases} \right\} . \tag{45}$$

Clearly, this is a closed and convex subset of U. We investigate the problem

$$\underset{\substack{(\psi,\,\theta,\,u) \in Y \times U_{\text{ad}} \\ T(\psi,\,\theta,\,u) = 0}}{\text{minimize}} \quad J(\psi,\,\theta,\,u)\,, \tag{46}$$

subject to the state-constraints

$$-L' \;\leq\; \psi(x) \;\leq\; L' \quad \text{for } x \in G\,, \tag{47}$$

$$\theta_{\text{min}} \;\leq\; \theta(x,z) \;\leq\; \theta_{\text{max}} \text{ for } (x,z) \in \Omega\,, \tag{48}$$

$$\partial_z\theta(x,z) \;\leq \gamma \quad \text{for } x \in G,\; z \in]-L,\, L[\,. \tag{49}$$

Invoking the definition (45) and the control-to-state mapping $\mathcal{S}$, the problem (P_{opt}) can be reduced to

$$(P_{\text{opt}}) = \begin{cases} \min\limits_{(y,\,u) \in Y \times U_{\text{ad}}} f(u) := J(\mathcal{S}(u),\,u) \\ \qquad \text{subject to (47), (48), (49)}\,. \end{cases} \tag{50}$$

We call a control $u \in U_{\text{ad}}$ *feasible* if the corresponding state $y = \mathcal{S}(u)$ satisfies the state constraints (47), (48), (49).

Proposition 4.1. *Assume that the functional J is nonnegative and lower-semicontinuous in the topology of $C^2(\overline{G}) \times C^1(\overline{\Omega})$. If there is at least one a feasible control for (P_{opt}), then* (50) *admits a (possibly not unique) solution $u \in \overline{U_{ad}}$.*

Proof. Since the set of the feasible controls for (P_{opt}) is not empty, we can choose a minimal sequence $\{u_n\}$ of feasible controls. Since the Tychonov regularization of J is coercive on U, there is a constant independent on n such that $\|u_n\|_U \leq C$. Due to the fact that U is a reflexive space, we can find a subsequence (that we not relabel) and $u \in \overline{U_{\text{ad}}}$ such that $u_n \rightharpoonup u$ in U. Denote $(\psi_n,\,\theta_n) = \mathcal{S}(u_n)$. Due to the estimates in Proposition 2.1, the sequence $\{\theta_n\}$ is uniformly bounded in $W^{2,q}(\Omega)$, and $\sup_\Omega \partial_z\theta_n \leq \gamma$. Moreover, since for all $n \in \mathbb{N}$ the control u_n is feasible, we have $\|\psi_n\|_{L^\infty(G)} \leq L'$. Therefore, the Proposition 2.2 implies that the sequence $\{\psi_n\}$ is uniformly bounded in $C^{2,\alpha}(\overline{G})$. Using well-known compactness results, there are $\theta \in W^{2,q}(\Omega)$, $\psi \in C^{2,\alpha}(\overline{G})$ such that passing to a subsequence $\theta_n \to \theta$ in $C^1(\overline{\Omega})$ and $\psi_n \to \psi$ in $C^2(\overline{G})$. By assumption, the functional J is lower-semicontinuous in the topology of $C^2(\overline{G}) \times C^1(\overline{\Omega})$. Using the lower semicontinuity of $\|\cdot\|_U$, we see that $(\psi,\,\theta,\,u)$ solves the optimal control problem (50). ☐

If J is continuously differentiable on the state space, then f is continuously differentialbe and

$$f'(u^*)\, u = \partial_y J(S(u^*),\, u^*)\, S'(u^*)\, u + \partial_u J(S(u^*),\, u^*)\, u\,. \tag{51}$$

Next we discuss the existence of Lagrange multipliers associated with the pointwise state constraints. Due to the well-known duality between the space of Borel-regular Radon-measures and the continuous functions, these constraints lead to measure-valued Lagrange-multipliers.

Definition 4.2. *The Lagrange functional* $\mathscr{L} \,:\, U_{\mathit{ad}} \times [\mathcal{M}(\overline{G} \times \overline{\Omega})]^2 \times \mathcal{M}(\overline{\Omega}) \to \mathbb{R}$ *associated with* (P_{opt}) *has the expression*

$$\begin{aligned} &\mathscr{L}(u,\, \mu_a,\, \mu_b,\, \mu_\gamma) := f(u) \\ &\quad + \int_{\overline{G}\times\overline{\Omega}} (y_a - \mathcal{S}(u))\, d\mu_a + \int_{\overline{G}\times\overline{\Omega}} (\mathcal{S}(u) - y_b)\, d\mu_b + \int_{\overline{\Omega}} (\partial_z \mathcal{S}_2(u) - \gamma)\, d\mu_\gamma\,. \end{aligned}$$

with $y_a = (-L',\, \theta_{\mathit{min}})$ *and* $y_b = (L',\, \theta_{\mathit{max}})$.

Here we identify for the sake of brevity $\mu_a,\, \mu_b \,\in\, \mathcal{M}(\overline{G} \times \overline{\Omega})$ with pairs $(\mu_{a,1},\, \mu_{a,2})$ and $(\mu_{b,1},\, \mu_{b,2})$ in $\mathcal{M}(\overline{G}) \times \mathcal{M}(\overline{\Omega})$. We have for instance

$$\int_{\overline{G}\times\overline{\Omega}} (y_a - \mathcal{S}(u))\, d\mu_a = \int_{\overline{G}} (-L' - \mathcal{S}_1(u))\, d\mu_{a,1} + \int_{\overline{\Omega}} (\theta_{\mathsf{min}} - \mathcal{S}_2(u))\, d\mu_{a,2}\,.$$

Definition 4.3. *Let* $u^* \in U_{\mathit{ad}}$ *be a local solution to* (P_{opt}). *Then,* $(\mu_a,\, \mu_b,\, \mu_\gamma) \in [\mathcal{M}(\overline{G} \times \overline{\Omega})]^2 \times \mathcal{M}(\overline{\Omega})$ *is called a Lagrange multiplier associated with the state constraints* (47)*,* (48) *and* (49) *if and only if*

$$\begin{gathered} \partial_u \mathscr{L}(u^*,\, \mu_a,\, \mu_b,\, \mu_\gamma)\, (u - u^*) \geq 0, \quad \forall\, u \in U_{\mathit{ad}} \\ \mu_a,\, \mu_b,\, \mu_\gamma \geq 0 \\ \int_{\overline{G}\times\overline{\Omega}} (y_a - \mathcal{S}(u^*))\, d\mu_a = 0 = \int_{\overline{G}\times\overline{\Omega}} (\mathcal{S}(u^*) - y_b)\, d\mu_b = \int_{\overline{\Omega}} (\partial_z \mathcal{S}_2(u) - \gamma)\, d\mu_\gamma\,. \end{gathered}$$

In the presence of box constraints, the adjoint state associated with the optimal control problem (P_{opt}) has usually low regularity. Due to the pointwise constraint (49) on the gradient of the state, the regularity is even getting worse. In order to introduce the adjoint state in the present situation, we assume that there are $\alpha > 0$, $s > 3$ such that

$$\partial_\psi J \,:\, Y \to [C^{2,\alpha}(\overline{G})]*, \quad \partial_\theta J \,:\, Y \to [W^{2,s}(\Omega)]^*\,. \tag{52}$$

Here and for the remainder of the paper, we identify a measure $\mu \in \mathcal{M}(\overline{\Omega})$ with the functional $\mu(\phi) := \int_{\overline{\Omega}} \phi\, d\mu$, $\phi \in C(\overline{\Omega})$. For ease of writing, we moreover set

$$\partial_z \mu(\phi) := \mu(\partial_z \phi), \quad \mu \in \mathcal{M}(\overline{\Omega}), \quad \phi \in C^1(\overline{\Omega})\,.$$

Proposition 4.4. *Let $u^* \in U_{ad}$ be feasible. Define $(\psi^*, \theta^*) = y^* := \mathcal{S}(u^*) \in Y$. Let $(\mu_1, \mu_2, \mu_3) \in \mathcal{M}(\overline{G}) \times \mathcal{M}(\overline{\Omega}) \times \mathcal{M}(\overline{\Omega})$. Assume that $J : Y \to \mathbb{R}$ satisfies* (52)*. Then, there exists a unique pair $p = (p_1, p_2) \in [C^\alpha(\overline{G})]^* \times L^{q'}(\Omega)$ such that*

$$\Big\langle p_1, \Big(-\frac{d}{dx_i}(F_{p_i,p_j}(x, \nabla\psi^*)\,\partial_{x_j}\xi) - \lambda'(\theta^*(x, \psi^*))\,\theta^*_z(x, \psi^*)\,\xi\Big)\Big\rangle$$
$$= \partial_\psi J(y^*)(\xi) + \mu_1(\xi) \quad \forall \xi \in C^{2,\alpha}(\overline{G}) \, : \, \partial_\psi B_1(y^*)\,\xi = 0\,, \tag{53}$$
$$\int_\Omega p_2\,(-\operatorname{div}(k\nabla\phi)) + \langle p_1, \lambda'(\theta^*(x,\psi^*))\,\phi(x, \psi^*)\rangle = \partial_\theta J(y^*)(\phi) + (\mu_2 + \partial_z\mu_3)(\phi)$$
$$\forall \phi \in W^{2,q}(\Omega) \, : \, \partial_\theta B_2(y^*)\,\phi = 0\,. \tag{54}$$

Proof. For $\psi^* \in C^{2,\alpha}(\overline{G})$, the matrix $\{F_{p_i,p_j}(x, \nabla\psi^*)\}$ is uniformly elliptic, and belongs to $C^{1,\alpha}(\overline{G})$. The coefficient $\theta^*_z(x, \psi^*)$ is of class $C^\alpha(\overline{G})$, and uniformly negative. Let $g \in C^\alpha(\overline{G})$ arbitrary. Due to classical results of regularity theory for linear second order uniformly elliptic equations ([Tro87], Theorem 3.28), there is a unique $\xi \in C^{2,\alpha}(\overline{G})$ satisfying the linear problem

$$-\frac{d}{dx_i}(F_{p_i,p_j}(x, \nabla\psi^*)\,\partial_{x_j}\xi) - \lambda'(\theta^*(x, \psi^*))\,\theta^*_z(x, \psi^*)\,\xi = g \text{ in } G \tag{55}$$
$$n_i\,F_{p_i,p_j}(x, \nabla\psi^*)\,\partial_{x_j}\xi = 0 \text{ on } \partial G\,. \tag{56}$$

Moreover, there is a constant depending on ψ^*, θ^* and on the domain G, but not on g such that $\|\xi\|_{C^{2,\alpha}(\overline{G})} \leq c\,\|g\|_{C^\alpha(\overline{G})}$. We denote $\mathcal{A}_1^{-1}$ the solution operator $g \mapsto \xi$. Obviously

$$|\mu_1 \circ \mathcal{A}_1^{-1}(g)| \leq \|\mu_1\|_{\mathcal{M}(\overline{G})}\,\|\mathcal{A}_1^{-1}(g)\|_{C(\overline{G})} \leq c\,\|g\|_{C^\alpha(\overline{G})}\,. \tag{57}$$

Consider now the linear functional

$$\langle p_1, g\rangle := (\partial_y J(y^*) + \mu_1) \circ \mathcal{A}_1^{-1}(g), \quad g \in C^\alpha(\overline{G})\,.$$

Due to (57) and the assumption (52), p_1 is continuous on $C^\alpha(\overline{G})$, and

$$\|p_1\|_{[C^\alpha(\overline{G})]^*} \leq c\,(\|\mu_1\|_{\mathcal{M}(\overline{G})} + \|\partial_y J(y^*)\|_{[C^{2,\alpha}(\overline{G})]^*})\,. \tag{58}$$

Choosing $g = \mathcal{A}_1(\xi)$, $\xi \in C^{2,\alpha}(\overline{G})$ arbitrary such that (56) is valid (that is $\partial_\psi B_1(y^*)\,\xi = 0$), we easily show that p_1 satisfies (53).

We now turn our attention to the relation (54). We introduce a linear functional

$$F_1(\phi) := \langle p_1, \lambda'(\theta^*(x,\psi^*))\,\phi(x, \psi^*)\rangle \tag{59}$$

Due to the continuity of the embedding $W^{1,q}(\Omega) \hookrightarrow C^\alpha(\overline{\Omega})$ for $q > 3$ and $\alpha \leq 1 - 3/q$, and to the estimate (58), it follows that

$$|F_1(\phi)| \leq \|p_1\|_{[C^\alpha(\overline{G})]^*}\,\|\lambda'(\theta^*(x,\psi^*))\,\phi(x, \psi^*)\|_{C^\alpha(\overline{G})} \leq c\,\|\phi\|_{W^{1,q}(\Omega)}\,. \tag{60}$$

Here we use the assumption (19) and the regularity $\theta^* \in C^1(\overline{\Omega})$. For $g \in L^q(\Omega)$, there is according to Lemma A.1 a unique $\phi \in W^{2,q}(\Omega)$ satisfying

$$-\operatorname{div}(k\nabla\phi) = g \text{ in } \Omega, \quad -k\nabla\phi \cdot n = 4\,\beta\,|\theta^*|^3\,\phi \text{ on } \partial\Omega\,.$$

and the estimate $\|\phi\|_{W^{2,q}(\Omega)} \leq c\,\|g\|_{L^q(\Omega)}$. We denote $\mathcal{A}_2^{-1}$ the solution operator $g \mapsto \phi$. Since the embedding $W^{1,q}(\Omega) \to C(\overline{\Omega})$ is continuous, there is c independent of g such that

$$|(\mu_2 + \partial_z \mu_3) \circ \mathcal{A}_2^{-1}(g))| \leq (\|\mu_2\|_{\mathcal{M}(\overline{\Omega})} + \|\mu_3\|_{\mathcal{M}(\overline{\Omega})})\,\|\mathcal{A}_2^{-1}(g)\|_{W^{1,\infty}(\Omega)} \\ \leq c\,\|g\|_{L^q(\Omega)}\,. \tag{61}$$

Consider the linear functional

$$F(g) := (\partial_\theta J(y^*) + \mu_2 + \partial_z \mu_3 - F_1) \circ \mathcal{A}_2^{-1})(g), \quad g \in L^q(\Omega)\,.$$

Due to the Riesz representation theorem for $L^q(\Omega)$, there is $p_2 \in L^{q'}(\Omega)$ such that $\int_\Omega p_2\, g = F(g)$ for all $g \in L^q(\Omega)$. For $g = \mathcal{A}_2(\phi)$, $\phi \in W^{2,q}(\Omega)$ such that $-k\nabla\phi \cdot n = 4\,\beta\,(\theta^*)^3\,\phi$ on $\partial\Omega$, the relation (54) follows. ☐

In order to interpret the adjoint state as the solution to a boundary value problem, we assume that the functional J satisfies a stronger assumption: There are $r > 1$, $s > 3$ such that

$$\partial_\psi J : Y \to [W^{2,r}(G)]^*, \quad \partial_\theta J : Y \to [W^{2,s}(\Omega)]^*\,. \tag{62}$$

We then have a regularity result.

Proposition 4.5. *Assumptions of Proposition 4.4 with* (62)*. Then, the pair* $(p_1,\, p_2)$ *belongs to* $L^{r'}(G) \times L^{q'}(\Omega)$ *and solves the following boundary value problem in the distributional sense:*

$$-\frac{d}{dx_i}(F_{p_i,p_j}(x,\,\nabla\psi^*)\,\partial_{x_j} p_1) - \lambda'(\theta^*(x,\,\psi^*))\,\theta_z^*(x,\,\psi^*)\,p_1 \\ = \partial_\psi J(y^*) + \mu_1 \quad \text{in } G \tag{63}$$

$$n_i\,F_{p_i,p_j}(x,\,\nabla\psi^*)\,\partial_{x_j} p_1 = 0 \quad \text{on } \partial G \tag{64}$$

$$-\operatorname{div}(k\,\nabla p_2) = \partial_\theta J(y^*) + \mu_2 + \partial_z \mu_3 \quad \text{in } \Omega \tag{65}$$

$$[-k\nabla p_2 \cdot \nu^*] = \nu_3^*\,\lambda'(\theta^*)\,p_1 \quad \text{on } S^* \tag{66}$$

$$-k\nabla p_2 \cdot n = 4\,\beta\,(\theta^*)^3\,p_2 \quad \text{on } \partial\Omega\,. \tag{67}$$

Here we have used the convention to write functionals in the right-hand side of the equation *and not to recall their contribution in the boundary or transmission conditions.*

Proof. Due to standard results of regularity theory for linear second order uniformly elliptic equations in smooth domains (cf. [Dau92], Theorem 3.2), the operator $\mathcal{A}_1^{-1}$ of the proof of Proposition 4.4 $g \mapsto \xi$ is continuous from $L^r(G)$ into $W^{2,r}(G)$. Since $r > 1$ and $G \subset \mathbb{R}^2$, the embedding $W^{2,r}(G) \to C(\overline{G})$ is continuous, and therefore

$$|\mu_1 \circ \mathcal{A}_1^{-1}(g)| \leq \|\mu_1\|_{\mathcal{M}(\overline{G})}\,\|\mathcal{A}_1^{-1}(g)\|_{C(\overline{G})} \leq c\,\|g\|_{L^r(G)}\,. \tag{68}$$

Thus, due to (62), the functional p_1 is continuous on $L^r(G)$. In view of the Riesz representation theorem for L^r, there is $p_1 \in L^{r'}(G)$ such that $\int_G p_1\, g = F(g)$ for all $g \in L^r(G)$, and

$$\|p_1\|_{L^{r'}(G)} = \|F\|_{[L^r(G)]^*} \leq c\,(\|\mu_1\|_{\mathcal{M}(\overline{G})} + \|\partial_y J(y^*)\|_{[W^{2,r}(G)]^*})\,. \tag{69}$$

Thus, the function p_1 is a distributional solution to the problem (63), (64). The surface measure on the surface $S^* := \mathrm{graph}(\psi^*; G)$ is given by $dS = \sqrt{1+|\nabla\psi^*|^2}\,dx$, where dx is the Lebesque measure in G. Since the upper unit normal ν^* is given by $\nu^* = (1 + |\nabla\psi^*|^2)^{-1/2}\,(-\nabla\psi^*,\,1)$, we have $dS = 1/\nu_3^*\,dx$ on S^*. Using the regularity of p_1, the functional F_1 of the proof of Proposition 4.4, (59) has the representation

$$F_1(\phi) = \int_G p_1(x)\,\lambda'(\theta^*(x,\psi^*))\,\phi(x,\,\psi^*)\,dx = \int_{S^*} \nu_3^*\,p_1\,\lambda'(\theta^*)\,\phi\,dS\,. \tag{70}$$

Thus, p_2 solves the problem (65), (66), (67) in the distributional sense. □

Since we obtain p_2 only in $L^{q'}$, the boundary condition (67) has to be interpreted in a very weak sense as in the following statement. Similar ideas were used in [CF93], Th. 5 in the context of optimal control. Trace theorems in spaces of negative order (dual spaces) were introduced in [LM63], Th. 7.1.

Lemma 4.6. *Assumptions of Proposition 4.4. Then, there is* $\widetilde{p}_2 \in [W^{1/q',q}(\partial\Omega)]^*$ *such that* $\forall\phi \in W^{2,q}(\Omega)$

$$\begin{aligned}\int_\Omega & p_2\,(-\,\mathrm{div}(k\nabla\phi)) + \langle\widetilde{p}_2,\,\big(-k\nabla\phi\cdot n - 4\,\beta\,(\theta^*)^3\,\phi\big)\rangle \\ &= -\langle p_1,\,\lambda'(\theta^*(x,\,\psi^*))\,\phi(x,\,\psi^*)\rangle + \partial_\theta J(y^*)\,\phi + (\mu_2 + \partial_z\mu_3)(\phi)\,.\end{aligned} \tag{71}$$

Proof. Let $p_2 \in L^{q'}(\Omega)$, $F \in [W^{2,q}(\Omega)]^*$ be such that

$$\int_\Omega p_2\,(-\,\mathrm{div}(k\nabla\phi)) = F(\phi) \quad \forall\phi \in W^{2,q}(\Omega),\ \partial_\theta B_2(y^*)\,\phi = 0\,, \tag{72}$$

as in the proof of Proposition 4.4. We show how to interpret the trace of p_2 as a functional $\widetilde{p}_2 \in [W^{1/q',q}(\partial\Omega)]^*$. Define

$$\mathcal{F}(\xi) := \int_\Omega p_2\,\mathrm{div}(k\nabla\phi) + F(\phi), \quad \phi \in W^{2,q}(\Omega)\,.$$

We easily show that $\mathcal{F} \in [W^{2,q}(\Omega)]^*$. On the other hand, according to Lemma A.1 it is possible to introduce an operator $\mathcal{B}:\ L^q(\Omega) \times W^{1/q',q}(\partial\Omega) \to W^{2,q}(\Omega)$, $(f,\,g) \mapsto \phi$, where ϕ is the solution to the linear problem

$$-\,\mathrm{div}(k\nabla\phi) = f \text{ in } \Omega\,, \quad -k\nabla\phi\cdot n - 4\,\beta\,(\theta^*)^3\,\phi = g \text{ on } \partial\Omega\,. \tag{73}$$

The functional $\mathcal{F}\circ\mathcal{B}$ clearly belongs to the dual of $L^q(\Omega) \times W^{1/q',q}(\partial\Omega)$. Moreover, due to (72) $\mathcal{F}\circ\mathcal{B}(f,\,0) = 0$ for all $f \in L^q(\Omega)$. This proves that the value of $\mathcal{F}\circ\mathcal{B}(f,\,g)$ depends only on g, and means nothing else but that there is $\widetilde{p}_2 \in [W^{1/q',q}(\partial\Omega)]^*$ such that

$$[\mathcal{F}\circ\mathcal{B}](f,\,g) = \langle\widetilde{p}_2,\,g\rangle \text{ for all } (f,\,g) \in L^q(\Omega) \times W^{1/q',q}(\partial\Omega)\,.$$

Choosing $(f,\,g) := \mathcal{B}^{-1}(\phi)$ with $\phi \in W^{2,q}(\Omega)$ arbitrary (cf. (73)), the claim follows. □

Remark 4.7. *In the Proposition 4.4, 4.5, we have only considered the case of* $u^* \in U_{ad}$ *feasible, because this is clearly the relevant one. If* $u^* \in U_{ad}$ *is not feasible, we can compute the adjoint state by instead solving:*

$$-\frac{d}{dx_i}(F_{p_i,p_j}(x,\,\nabla\psi^*)\,\partial_{x_j}p_1) - \lambda'(E(\theta^*)(x,\,\psi^*))\,\partial_z E(\theta^*)(x,\,\psi^*)\,p_1$$
$$= \partial_\psi J(y^*) + \mu_1 \text{ in } G \tag{74}$$
$$n_i\,F_{p_i,p_j}(x,\,\nabla\psi^*)\,\partial_{x_j}p_1 = 0 \text{ on } \partial G\,. \tag{75}$$

Once the distributional solution $p_1 \in L^r(G)$ *(resp.* $p_1 \in [C^\alpha(\overline{G})]^*$*) to* (74) *at hand,* (75)*, define* $\tilde{F}_1(\phi) := \int_{S^*} \nu_3^*\,\lambda'(E(\theta^*))\,p_1\,E'(\theta^*)\phi\,dS$*, and solve*

$$-\operatorname{div}(k\nabla p_2) = \partial_\theta J(y^*) + \mu_2 + \partial_z\mu_3 \text{ in } \Omega \tag{76}$$
$$[-k\nabla p_2\cdot\nu^*] = \tilde{F}_1 \text{ on } S^* \tag{77}$$
$$-k\nabla p_2\cdot n = 4\,\beta\,(\theta^*)^3\,p_2 \text{ on } \partial\Omega\,. \tag{78}$$

We now derive the first order optimality system under a classical linearized Slater condition.

Proposition 4.8. *Let* $u^* \in U_{ad}$ *be a local solution to* (P_{opt}) *which is regular in the sense of [ZK79]. Define* $y^* = \mathcal{S}(u^*)$*, and let the assumption* (52) *be valid. Then, there are a Lagrange multiplier (cf. the Definition 4.3) for the problem* (P_{opt})*, and an adjoint state* $p \in [C^\alpha(G)]^* \times L^{q'}(\Omega)$*, such that*

$$\rho\int_\Omega\{|\nabla u^*|^{q-2}\,\nabla u^*\cdot\nabla(u-u^*) + |u^*|^{q-2}\,u^*\,(u-u^*)\} - \langle\widetilde{p_2},\,4\beta\,(u^*)^3\,(u-u^*)\rangle$$
$$\geq 0 \quad \forall u \in U_{ad}\,.$$

Here, $\widetilde{p_2} \in [W^{1/q',q}(\partial\Omega)]^*$ *denotes the trace of* p_2 *(cp. Lemma 4.6).*

Proof. The existence of the Lagrange multipliers follows from [ZK79].

Denote now $(\psi,\,\theta) \in Y$ the solution of the linearized system (cf. Lemma 3.1) with u replaced by $u - u^*$. Define $\mu_1 := \mu_{b,1} - \mu_{a,1} \in \mathcal{M}(\overline{G})$. Using the distributional formulation (53) of the equation (63) with the boundary condition (64) and the testfunction $\xi = \psi$, we obtain that

$$\left\langle p_1,\,\left(-\frac{d}{dx_i}(F_{p_i,p_j}(x,\,\nabla\psi^*)\,\partial_{x_j}\psi) - \lambda'(\theta^*(x,\,\psi^*))\,\theta_z^*(x,\,\psi^*)\,\psi\right)\right\rangle$$
$$= \partial_y J(y^*)\psi + \mu_1(\psi)\,. \tag{79}$$

On the other hand, we have $\theta \in W^{2,q}(\Omega)$, and

$$-k\nabla\theta\cdot n - 4\beta\,(\theta^*)^3\,\theta = -4\beta\,(u^*)^3\,(u-u^*)\,.$$

Choosing $\xi = \theta$ in the dirstributional formulation (71) with $\mu_2 := \mu_{b,2} - \mu_{a,2}$ and $\mu_3 := \mu_\gamma$, we obtain that

$$-\langle\widetilde{p_2},\,\left(4\,\beta\,(u^*)^3\,(u-u^*)\right)\rangle$$
$$+\langle p_1,\,\lambda'(\theta^*(x,\,\psi^*))\,\theta(x,\,\psi^*)\rangle = \partial_\theta J(y^*)(\theta) + (\mu_2 + \partial_z\mu_3)(\theta)\,. \tag{80}$$

Adding the relations (79) and (80), we identify

$$\begin{aligned}&\partial_y J(y^*)(\psi,\theta) + (\mu_b - \mu_a)(\psi,\theta) + \mu_\gamma(\partial_z\theta)\\ &\quad = \partial_y J(y^*)\psi + \mu_1(\psi) + \partial_\theta J(y^*)(\theta) + (\mu_2 + \partial_z\mu_3)(\theta)\\ &\quad = -\langle \widetilde{p}_2,\, 4\,\beta\,(u^*)^3\,(u-u^*)\rangle\,. \end{aligned} \tag{81}$$

Using now the variational inequality in the Definition 4.3 of the Lagrange multipliers, we obtain for $u^*,\ u \in U_{\text{ad}}$ arbitrary that

$$\begin{aligned}0 &\leq \partial_u \mathscr{L}(u^*,\, \mu_a,\, \mu_b,\, \mu_\gamma)\,(u-u^*)\\ &= -\langle \widetilde{p}_2,\, 4\,\beta\,(u^*)^3\,(u-u^*)\rangle + \partial_u J(y^*,u^*)\,(u-u^*)\,. \end{aligned} \tag{82}$$

proving the projection formula. ☐

5 One example

Finally we want to illustrate the theory at the example of the functional

$$J(\psi,\,\theta) := \frac{1}{2}\,\|\psi-\psi_d\|^2_{W^{2,2}(G)} + \frac{1}{2}\,\|\theta-\theta_d\|^2_{W^{1,2}(S)}\,. \tag{83}$$

We recall that here, $S := \mathrm{graph}(\psi;\, G)$.

The functional (83) is of interest because it does not entirely fits into the abstract setting of the precedent section. This gives us the occasion to point at two additional features of the practical problem. First, the natural domain of definition of J is not the entire Y, but the open subset $\{(\psi,\theta) \in Y\ :\ \|\psi\|_{L^\infty(G)} < L\}$. This is due to the fact (Remark 2.3) that J cannot be evaluated if parts of the surface $\mathrm{graph}(\psi;\, G)$ are not contained in the domain Ω. And, second, we need more regularity of the solution to establish the differentiability of J.

Throughout the section, we assume in this section that there is $p > 1$ (without loss of generality $p \leq q$) such that the data have the additional regularity

$$\|\partial_z f\|_{L^p(\Omega)} + \|\nabla\partial_z A\|_{L^p(\Omega)} < +\infty\,. \tag{84}$$

For $0 < M < L$, we introduce the Banach space

$$\begin{aligned} Y(p,\, M) &:= \{y = (\psi,\,\theta) \in Y\ :\ \|\partial_z\theta\|_{W^{2,p}(\Omega_M)} < +\infty\}\\ \|y\|_{Y(p,\,M)} &:= \|y\|_Y + \|\partial_z\theta\|_{W^{2,p}(\Omega_M)}\,, \end{aligned}$$

and an open subset $Y_0(p,\, M)$

$$Y_0(p,\, M) := \{y \in Y(p,\, M)\ :\ \|\psi\|_{L^\infty(G)} < M\}\,.$$

Lemma 5.1. *Assume that $\psi_d \in W^{2,2}(G)$ and $\theta_d \in W^{2,q}(\Omega)$ with $\partial_z\theta_d \in W^{2,p}(\Omega)$. Then, the functional J given by* (83) *is continuously differentiable in $Y_0(p,\, M)$. Moreover, the derivative $\partial_y J$ satisfies*

$$\partial_\psi J\,:\, Y_0(p,\, M) \to [W^{2,2}(G)]^*, \quad \partial_\theta J\,:\, Y_0(p,\, M) \to [W^{2,2}(\Omega)]^*\,.$$

Proof. Let $y^* = (\psi^*,\, \theta^*) \in Y_0(p;\, M)$. Denote $S^* := \mathrm{graph}(\psi^*,\, G)$. Throughout the proof, we use the abbreviation $w := \theta^* - \theta_d \in W^{2,q}(\Omega)$. We denote δ the tangential differential operator on S^*, that is

$$\delta f := \nabla f - (\nu^* \cdot \nabla f)\, \nu^* \quad f \in C^1(S^*)\,,$$

where ν^* denotes a unit normal to S^*. Let $J_1(\psi) := 1/2\, \|\psi - \psi_d\|^2_{W^{2,2}(G)}$. Obviously

$$\partial_\psi J_1(\psi^*)\, \psi = (\psi^* - \psi_d,\, \psi)_{W^{2,2}(G)}\,, \tag{85}$$

and it follows that $\partial_\psi J_1(y^*) \in [W^{2,2}(G)]^*$.

Consider $J_2(\psi,\, \theta) := 1/2\, \|\theta - \theta_d\|^2_{W^{1,2}(S)}$. Again, it is straightforward to compute that the derivative $\partial_\theta J_2(\psi^*,\, \theta^*)$ in some direction $\theta \in W^{2,2}(\Omega)$ has the expression

$$\partial_\theta J_2(\psi^*,\, \theta^*)\theta = \int_{S^*} \{w\, \theta + \delta\, w \cdot \delta\, \theta\}\, dS = (w,\, \theta)_{W^{1,2}(S^*)}\,.$$

Since S^* is of class $\mathcal{C}^{2,\alpha}$ and $S^* \subset \Omega_M$, the trace theorem implies that

$$|\partial_\theta J_2(\psi^*,\, \theta^*)\theta| \le \|w\|_{W^{1,2}(S^*)}\, \|\theta\|_{W^{1,2}(S^*)} \le c\, \|w\|_{W^{2,2}(\Omega_M)}\, \|\theta\|_{W^{2,2}(\Omega_M)}\,,$$

proving that $\partial_\theta J_2(y^*) \in [W^{2,2}(\Omega)]^*$.

The $\psi-$derivative of J_2 has a more complex expression. Due to the assumptions, $\partial_z w \in W^{2,p}(\Omega_M)$. We derive from elementary calculus that

$$\begin{aligned}
&\partial_\psi J_2(\psi^*,\, \theta^*)\, \psi \\
&= \underbrace{\frac{1}{2} \int_G \frac{\nabla\psi^* \cdot \nabla\psi}{\sqrt{1 + |\nabla\psi^*|^2}}\, [w^2 + |\, \delta\, w|^2](x,\, \psi^*) + \int_G \sqrt{1 + |\nabla\psi^*|^2}\, [w\, w_z](x,\, \psi^*)\, \psi}_{=:\langle a(w),\, \psi\rangle} \\
&+ \underbrace{\int_G \sqrt{1 + |\nabla\psi^*|^2}\, [\delta\, w\, \cdot \delta\, w_z](x,\, \psi^*)\, \psi - \int_G [(\nu^* \cdot \nabla w)\ \delta\, w](x,\, \psi^*)\ \cdot \delta\, \psi}_{=:\langle b(w),\, \psi\rangle}\,.
\end{aligned}$$

Using that $\psi^* \in C^{2,\alpha}(\overline{G})$ and $w \in W^{2,q}(\Omega) \hookrightarrow C^1(\overline{\Omega})$, we easily show that

$$|\langle a(w),\, \psi\rangle| \le c(w)\, \|\psi\|_{W^{1,1}(G)}\,. \tag{86}$$

The additional regularity is needed to handle the integral $\langle b(w),\, \psi\rangle$ that makes sense only if the tangential derivatives of the function $\partial_z w$ are available on the surface S^*. Under the additional assumptions, we have $\delta\, w_z \in W^{1/p',p}(S^*)$. Thus

$$\begin{aligned}
|\langle b(w),\, \psi\rangle| &\le c_1\, \|\, \delta\, w\|_{L^\infty(S^*)}\, \|\, \delta\, w_z\|_{L^p(S^*)}\, \|\psi\|_{L^{p'}(G)} + c_2\, \|\nabla w\|^2_{L^\infty(S^*)}\, \|\, \delta\, \psi\|_{L^1(G)} \\
&\le c(w)\, \|\psi\|_{W^{1,2}(G)}\,.
\end{aligned}$$

Thus, $\partial_\psi J_2(y^*) \in [W^{1,2}(G)]^*$, and using the standard Sobolev embedding, $\partial_\psi J_2(y^*) \in [W^{2,1}(G)]^*$. The claim follows. □

Lemma 5.2. *Let $u^* \in U$ be a feasible control. Then, there are $\rho_0 > 0$ and $0 < M < L$ such that the control to state mapping $\mathcal{S}$ maps $B_\rho(u^*;\, U)$ continously into $Y_0(p,\, M)$ for all $\rho \leq \rho_0$.*

Proof. Since u^* is feasible, the state $(\psi^*,\, \theta^*) = \mathcal{S}(u^*)$ satisfies $\|\psi^*\|_{L^\infty(G)} \leq L' < L$. Since $\mathcal{S}$ is continous, we easily obtain for $(\psi,\, \theta) = \mathcal{S}(u)$, $u \in B_\rho(u^*;\, U)$ that $\|\psi\|_{L^\infty(G)} \leq M < L$. It remains to prove that $\partial_z\theta \in W^{2,p}(\Omega_M)$. This is the object of Lemma 5.3 below. ☐

Lemma 5.3. *Under the additional assumption* (84)*, the solution $\theta = S_{heat}(u)$, $u \in U$ satisfies $\partial_z\theta \in W^{2,p}(\Omega_M)$ for $M < L$ arbitrary.*

Proof. According to Lemma 2.1, $\theta \in W^{2,q}(\Omega)$. Thus, $u := \partial_z\theta \in W^{1,q}(\Omega)$. It follows that $\theta^3\, u \in W^{1,q}(\Omega)$, and from the trace theorem, we get $\theta^3\, u \in W^{1/q',q}(\partial\Omega)$.

The function u satisfies

$$
\begin{aligned}
-\operatorname{div}(A\nabla u) &= \partial_z f + \operatorname{div}(\partial_z A\nabla\theta) \in L^p(\Omega) \\
-A\nabla u\cdot n &= 4\,\beta\,\theta^3\,\partial_z\theta + \partial_z A\nabla\theta\cdot n \in W^{1/p',p}(\Gamma_1)\,.
\end{aligned}
$$

The claim $u \in W^{2,p}(\Omega_M)$ near Γ_1 follows from local regularity results for the Neumann-problem near a surface of class $\mathcal{C}^2$ (special case of [Dau92], Th. 3.2 among others). ☐

To sum up, we can prove the following result.

Corollary 5.4. *Let* (84) *be valid. Assume that $\psi_d \in W^{2,2}(G)$ and $\theta_d \in W^{2,q}(\Omega)$, $\partial_z\theta_d \in W^{2,p}(\Omega)$ ($1 < p \leq q$). For every feasible $u^* \in U$, there is a neighbourhood $B_\rho(u^*)$ such that the operator $\partial_y J \circ \mathcal{S}$ exists and is continuous on $B_\rho(u^*)$. Moreover, $\partial_\psi J_2 \circ \mathcal{S} :\ B_\rho \to [W^{2,1}(G)]^*$, and $\partial_\theta J_2 \circ \mathcal{S} :\ B_\rho \to [W^{2,2}(\Omega)]^*$.*

Proof. Since $\mathcal{S}$ maps $B_\rho(u^*)$ into $Y_0(p,\, M)$ continuously (cf. Lemma 5.2), and since J is a C^1 mapping on this set according to Lemma 5.1, the claim follows from the chain rule for the Fréchet derivative. ☐

A The regularity result

Throughout this section, the domain Ω is the curvilinear polygon $G\times]-L, L[$ with $G \subset \mathbb{R}^2$ a bounded domain of class $\mathcal{C}^{2,\alpha}$ for some $\alpha \in [0, 1]$. Let n denote the outward unit normal on ∂G. We denote $\Gamma_1 := \partial G\times]-L, L[$ with outward unit normal n, and $\Gamma_2 = G \times \{-L, L\}$ with unit normal $n_{\Gamma_2} = \pm e_3$. We denote $W^{1,p}_{\Gamma_k}(\Omega)$, $k = 1, 2$ the subspace of $W^{1,p}(\Omega)$ the elements of which have a vanishing trace on Γ_k. We assume that there are $\tilde{A} \in C^1(\overline{\Omega};\, \mathbb{R}^{2\times 2})$, and $a_0 > 0$ such that

$$
\tilde{A}_{i,j}\,\eta_i\,\eta_j \geq a_0\,|\eta|^2 \quad \forall\eta \in \mathbb{R}^2\,, \tag{87}
$$

and we define a uniformly elliptic matrix $A \in C^1(\overline{\Omega};\, \mathbb{R}^{3\times 3})$ via

$$A = \begin{pmatrix} \tilde{A} & 0 \\ 0 & 1 \end{pmatrix} . \tag{88}$$

The following claim is proved for $Q = 0$ in [Dau92], Theorem 3.2.

Lemma A.1. *Assume that $A \in C^1(\overline{\Omega};\, \mathbb{R}^{3\times 3})$ satifies* (88)*, with $\tilde{A}$ satisfying* (87)*. Let $f \in L^q(\Omega)$ and $Q \in W^{1/q',q}(\partial\Omega)$ with $3 < q < \infty$. Assume that $u \in W^{1,2}(\Omega)$ satisfies $-\operatorname{div}(A\nabla u) = f$ in Ω, $-A\nabla u \cdot n = Q$ on $\partial\Omega$ in the weak sense. Then $u \in W^{2,q}(\Omega)$, and the estimate*

$$\|\nabla u\|_{W^{1,q}(\Omega)} \leq c\,(\|f\|_{L^q(\Omega)} + \|Q\|_{W^{1/q',q}(\partial\Omega)})\,, \tag{89}$$

is valid, with a constant c that depends only on Ω, q and A.

Proof. Throughout the proof we need some preliminary regularity, whose proof can be found in the papers [Dau92, Dau88]:

$$\|\nabla u\|_{L^q(\Omega)} \leq c\,(\|f\|_{L^q(\Omega)} + \|Q\|_{W^{1/q',q}(\partial\Omega)})\,, \tag{90}$$

$$\|\nabla u\|_{H^{1/2+\delta}(\Omega)} \leq c\,(\|f\|_{L^q(\Omega)} + \|Q\|_{W^{1/q',q}(\partial\Omega)})\,, \tag{91}$$

for a $0 < \delta < 1/2$. In particular, it follows that

$$\|u\|_{W^{1+\delta,2}(\partial\Omega)} \leq c\,(\|f\|_{L^q(\Omega)} + \|Q\|_{W^{1/q',q}(\partial\Omega)})\,. \tag{92}$$

At the end of the proof, we show for $i = 1, 2, 3$ that u satisfies the relation

$$\begin{aligned} \int_\Omega \partial_{x_i} u \, \operatorname{div}(A\nabla\phi) + \int_{\partial\Omega} A\nabla\phi \cdot (\delta(u\, n_i) - \delta_i(u\, n)) \\ + \int_{\partial\Omega} Q\, \partial_{x_i} u = F_0(\phi)\,, \quad \forall \phi \in C^\infty(\overline{\Omega})\,, \end{aligned} \tag{93}$$

where $n =$ outward unit normal, $\delta = \nabla - n\,(n\cdot\nabla) =$ tangential differential operator on $\partial\Omega$, and the functional F_0 is defined via

$$F_0(\phi) := \int_\Omega \partial_{x_i} A\nabla\phi \cdot \nabla u + \int_\Omega f\, \partial_{x_i}\phi\,.$$

Due to the estimate (90), we easily prove for $F = F_0$ that

$$|F(\phi)| \leq c\,(\|f\|_{L^q(\Omega)} + \|Q\|_{W^{1/q',q}(\partial\Omega)})\, \|\nabla\phi\|_{L^{q'}(\Omega)}\,. \tag{94}$$

The regularity claim is well-known near the interior of the surfaces Γ_1 and Γ_2 (cf. [Tro87], Theorem 3.17). It is sufficient to prove the regularity in the neighbourhood of the edge $l := \overline{\Gamma_1} \cap \overline{\Gamma_2}$. For $s_0 \in l$, we simplify the discussion assuming that there is $R > 0$ such that the surface $\Gamma_{1,R} := B_R(s_0) \cap \Gamma_1$ is flat. Then, $l_R := l \cap B_R(s_0)$ is a line, and we can assume that $e_2 = (0, 1, 0)$ is the unit tangent to l_R. If these simplifying assumptions are not satisfied, we map the neighbourhood $\Omega_R(s_0) := B_R(s_0) \cap \Omega$ onto this model-configuration by means of a

C^2- diffeomorphism that flattens the boundary of the domain G and affects only the x direction. This transfomation clearly preserves the structural assumption (88) on the matrix A.

We define $\Sigma_R := \partial\Omega \cap B_R(s_0)$. Our assumptions imply that $H = 0$ on Σ_R, and $|\,\delta\, n| = 0$ on Σ_R. Let $\phi \in C^{\infty}(\overline{\Omega})$ arbitrary, and $\eta \in C^{\infty}_c(\Omega_R \cup \Sigma_R)$ fixed. We choose $\phi\,\eta$ as testfunction in (93), and we define $w_i := \eta\,\partial_{x_i} u$. It follows that

$$\begin{aligned} \int_{\Omega} w_i\, \operatorname{div}(A\nabla\phi) + \int_{\partial\Omega} A\nabla(\phi\,\eta) \cdot (\delta\, u\, n_i - \delta_i\, u\, n) + \int_{\partial\Omega} \eta\, Q\, \partial_{x_i}\phi = F_1(\phi) \\ := F_0(\eta\,\phi) - \int_{\Omega} \partial_{x_i} u\, (2\, A\nabla\eta \cdot \nabla\phi + \operatorname{div}(A\nabla\eta)\,\phi) - \int_{\partial\Omega} Q\, \partial_{x_i}\eta\,\phi\,. \end{aligned} \tag{95}$$

The linear functional $F = F_1$ satisfies the same estimate (94) with constants depending on η. We omit the proof of this straightforward estimate.

Note that $\delta\, u \in L^2(\partial\Omega)$ ((92)), and that $w_i \in L^q(\Omega)$ ((90)). Since $C^{\infty}(\overline{\Omega})$ is a dense subset of $W^{2,q'}(\Omega)$, the validity of (95) extends to all $\phi \in W^{2,q'}(\Omega)$. We now specialize the relation (95) to $i = 3$. The facts that $n_3 = 0$ on Γ_1, that $\delta_3 = 0$ on Γ_2, and that $|\,\delta\, n| = 0$ on supp$(\eta) \cap \partial\Omega$ yield the identity

$$\begin{aligned} \int_{\partial\Omega} A\nabla(\phi\,\eta) \cdot (\delta\, u\, n_i - \delta_i\, u\, n) \\ = - \int_{\Gamma_1} A\nabla(\eta\,\phi) \cdot n\ \delta_3\, u + \int_{\Gamma_2} A\nabla(\eta\,\phi) \cdot \delta\, u\, n_3\,. \end{aligned}$$

Observe also that if $\operatorname{trace}(\phi) = 0$ on Γ_2, then $\delta\, u \cdot A\nabla(\phi\,\eta) = 0$ on Γ_2. This is due to the property (88), that implies that $A\,\delta\, u$ is a tangential vector on Γ_2.

On the other hand, due again to the property (88) and the Gauss theorem,

$$\begin{aligned} \int_{\partial\Omega} \eta\, Q\, \partial_{x_3}\phi &= \int_{\Gamma_1} \eta\, Q\ \delta_3\,\phi + \int_{\Gamma_2} \eta\, Q\, n \cdot A\nabla\phi \\ &= \int_{\Gamma_1} \eta\, Q\, (\delta_3\,\phi - A\nabla\phi \cdot n) + \int_{\Omega} \operatorname{div}(Q\,\eta\, A\nabla\phi)\,. \end{aligned}$$

Thus, for $\tilde{w}_3 := w_3 + \eta\, Q$, it follows from (95) for all $\phi \in W^{2,q'}(\Omega) \cap W^{1,1}_{\Gamma_2}(\Omega)$ that

$$\begin{aligned} \int_{\Omega} \tilde{w}_3\, \operatorname{div}(A\nabla\phi) - \int_{\Gamma_1} (\delta_3\, u + Q)\,\eta\,(A\nabla\phi \cdot n) = F_2(\phi)\,, \\ := F_1(\phi) - \int_{\Omega} A\nabla\phi \cdot \nabla(\eta\, Q) - \int_{\Gamma_1} \eta\, Q\ \delta_3\,\phi + \int_{\Gamma_1} \delta_3\, u\,(A\nabla\eta \cdot n)\,\phi\,. \end{aligned} \tag{96}$$

For $\phi \in W^{2,q'}(\Omega) \cap W^{1,1}_{\Gamma_2}(\Omega)$, use the Gauss theorem again (recall that mean curvature vanishes on $\operatorname{supp}(\eta) \cap \partial\Omega$) to show that

$$\int_{\Gamma_1} \delta_3\, u\,(A\nabla\eta \cdot n)\,\phi = - \int_{\Gamma_1} u\ \delta_3((A\nabla\eta \cdot n)\,\phi)\,.$$

Using Lemma A.2, (1) we prove for $\phi \in W^{2,q'}(\Omega) \cap W^{1,1}_{\Gamma_2}(\Omega)$ the estimates

$$\left|\int_{\Gamma_1} \eta\, Q\ \delta_3\, \phi\right| \leq c\, \|\eta\, Q\|_{W^{1/q',q}(\partial\Omega)}\, \|\nabla\phi\|_{L^{q'}(\Omega)}$$
$$\left|\int_{\Gamma_1} \delta_3\, u\, (A\nabla\eta \cdot n)\, \phi\right| \leq c\, \|(A\nabla\eta \cdot n^{\Gamma_1})\, \phi\|_{W^{1,q'}(\Omega)}\, \|u\|_{W^{1,q}(\Omega)}\,,$$

showing that the functional $F = F_2$ again satisfies the continuity estimate (94) (since Γ_1 is of class $\mathcal{C}^2$, the normal n^{Γ_1} has an extension in $[C^1(\overline{\Omega})]^3$). For $k \in \{1, 2, 3\}$ arbitrary and $\psi \in C^\infty_c(\Omega_R)$, define v_0 to be the weak solution to the mixed problem

$$-\operatorname{div}(A\nabla v_0) = \partial_{x_k}\psi \text{ in } \Omega, \quad -A\nabla v_0 \cdot n = 0 \text{ on } \Gamma_1, \quad v = 0 \text{ on } \Gamma_2\,.$$

According to the result of [Dau92], Theorem 3.2, $v_0 \in W^{2,s}(\Omega)$ for all $1 < s < 2$, and for all $1 < p < \infty$, there is a constant depending on $\Omega,\ A,\ p$ such that

$$\|v_0\|_{W^{1,p}(\Omega)} \leq c\, \|\partial_{x_k}\psi\|_{[W^{1,p'}(\Omega)]^*} \leq c\, \|\psi\|_{L^p(\Omega)}\,.$$

Putting v_0 into (96), we obtain that

$$\left|\int_\Omega \tilde{w}_3\, \partial_{x_k}\psi\right| \leq |F_2(v_0)| \leq c\, (\|f\|_{L^q(\Omega)} + \|Q\|_{W^{1/q',q}(\partial\Omega)})\, \|v_0\|_{W^{1,q'}(\Omega)}$$
$$\leq c\, (\|f\|_{L^q(\Omega)} + \|Q\|_{W^{1/q',q}(\partial\Omega)})\, \|\psi\|_{L^{q'}(\Omega)}\,.$$

Thus, recalling the definition of $\tilde{w} := \eta\, (\partial_{x_3}u + Q)$, we obtain that $\nabla(\eta\, \partial_{x_3}u) \in [L^q(\Omega_R)]^3$. For $R' < R$ arbitrary and suitable choice of the localization η, we obtain that

$$\|\nabla\partial_{x_3}u\|_{L^q(\Omega_{R'})} \leq c\, (\|f\|_{L^q(\Omega)} + \|Q\|_{W^{1/q',q}(\partial\Omega)})\,. \tag{97}$$

We now consider (95) for $i = 2$. Since $n_2 = 0$ on supp$(\eta) \cap \partial\Omega$, it follows that

$$\int_\Omega w_2\, \operatorname{div}(A\nabla\phi) - \int_{\partial\Omega} A\nabla(\phi\, \eta) \cdot n\ \delta_2\, u + \int_{\partial\Omega} \eta\, Q\, \partial_{x_2}\phi = F_1(\phi)\,.$$

Note that $e_2 = (0, 1, 0)$ is everywhere tangent on Σ_R. Using Lemma A.2, (2) we can put the relation in the form

$$\int_\Omega w_2\, \operatorname{div}(A\nabla\phi) - \int_{\partial\Omega} \delta_2\, u\, \eta\, (A\nabla\phi \cdot n) = F_3(\phi)$$
$$:= F_1(\phi) - \int_{\partial\Omega} \{\eta\, Q\ \delta_2\, \phi - A\nabla\eta \cdot n\ \delta_2\, u\, \phi\}\,,$$

with a functional F_3 that again satisfies the estimate (94). Defining $v_0 \in W^{2,s}(\Omega)$, $s < \infty$ arbitrary (cp. [Dau92], Theorem 3.2) to be the weak solution to the homogeneuous Neumann problem

$$-\operatorname{div}(A\nabla v_0) = \partial_{x_k}\psi \text{ in } \Omega, \quad -A\nabla v_0 \cdot n = 0 \text{ on } \partial\Omega\,.$$

for $k \in \{1,2,3\}$ and $\psi \in C_c^\infty(\Omega_R)$ arbitrary, we argue as above to prove that

$$\|\nabla \partial_{x_2} u\|_{L^q(\Omega_{R'})} \leq c\,(\|f\|_{L^q(\Omega)} + \|Q\|_{W^{1/q',q}(\partial\Omega)})\,. \tag{98}$$

In the case $i = 1$, we know from the previous steps that the mixed weak derivatives $\partial^2_{x_1,x_j} u$ exist for $j \neq 1$ and belong to $L^q(\Omega)$. Due to standard interior regularity results, $u \in W^{2,q}_{\text{loc}}(\Omega)$. Using the equation $-\operatorname{div}(A\nabla u) = f$, we can show that $\partial_{x_1} u$ also has a x_1 weak derivative that almost everywhere satisfies

$$-\partial_{x_1}(a_{1,1}\,\partial_{x_1} u) = f + \partial_{x_1}(a_{1,2}\,\partial_{x_2} u) + \partial_{x_2}(a_{2,1}\,\partial_{x_1} u + a_{2,2}\,\partial_{x_2} u) + \partial^2_{x_3^3} u \in L^q(\Omega)\,.$$

In order to complete the proof, it remains to prove the relation (93). Since u is a weak solution,

$$-\int_\Omega u\,\operatorname{div}(A\nabla\phi) + \int_{\partial\Omega} u\,A\nabla\phi\cdot n + \int_{\partial\Omega} Q\,\phi = \int_\Omega f\,\phi\,,\quad \forall \phi \in C^\infty(\overline{\Omega})\,.$$

We choose in the latest relation ϕ of the form $\partial_{x_i}\phi$ ($i = 1,2,3$), and we use a few integration by parts to prove that

$$\begin{aligned}\int_\Omega \partial_{x_i} u\,\operatorname{div}(A\nabla\phi) - \int_{\partial\Omega} n_i\,u\,\operatorname{div}(A\nabla\phi) + \int_{\partial\Omega} u\,\partial_{x_i}(A\nabla\phi)\cdot n + \int_{\partial\Omega} Q\,\partial_{x_i}\phi\\ = \int_\Omega \partial_{x_i} A\nabla\phi\cdot\nabla u + \int_\Omega f\,\partial_{x_i}\phi = F_0(\phi)\,.\end{aligned} \tag{99}$$

Using the tangential differential operators δ and $\operatorname{div}_{\partial\Omega}$ on $\partial\Omega$, we have

$$-n_i\,\operatorname{div}(A\nabla\phi) + \partial_{x_i}(A\nabla\phi)\cdot n = -n_i\,\operatorname{div}_{\partial\Omega}(A\nabla\phi) + \delta_i(A\nabla\phi)\cdot n \text{ on } \partial\Omega\,.$$

Thus, (99) turns to be equivalent to

$$\begin{aligned}\int_\Omega \partial_{x_i} u\,\operatorname{div}(A\nabla\phi) + \int_{\partial\Omega} u\,(-n_i\,\operatorname{div}_{\partial\Omega}(A\nabla\phi) + \delta_i(A\nabla\phi)\cdot n)\\ + \int_{\partial\Omega} Q\,\partial_{x_i}\phi = F_0(\phi)\,.\end{aligned} \tag{100}$$

Using the Gauss Theorem, we obtain the identity

$$\begin{aligned}\int_{\partial\Omega} u\,(-n_i\,\operatorname{div}_{\partial\Omega}(A\nabla\phi) + \delta_i(A\nabla\phi)\cdot n) = \int_{\partial\Omega} A\nabla\phi\cdot(\delta(u\,n_i) - \delta_i(u\,n))\\ + \int_{\partial\Gamma_1} u\,(-A\nabla\phi\cdot n'\,n_i + A\nabla\phi\cdot n\,n_i')\\ + \int_{\partial\Gamma_2} u\,(-A\nabla\phi\cdot n'\,n_i + A\nabla\phi\cdot n\,n_i')\,,\end{aligned}$$

where $n' =$ conormal on the curve $l = \partial\Gamma_j$ from the respective surface. Using that $n'_{\Gamma_i} = n_{\Gamma_j}$ on l, $i,j = 1,2$ and $i \neq j$, the line integrals vanish, and (100) yields (93). ☐

Lemma A.2. *Let* $h \in W^{1/q',q}(\partial\Omega)$, $q > 3$.

(1) If $g \in W^{2,1}(\Omega) \cap W^{1,1}_{\Gamma_k}(\Omega)$, $k \in \{1,2\}$ then

$$\left| \int_{\Gamma_j} h\ \delta_i\, g \right| \le c\, \|h\|_{W^{1/q',q}(\partial\Omega)}\, \|\nabla g\|_{W^{1,q'}(\Omega)}, \quad j \in \{1,2\},\ j \neq k \text{ and } i = 1,2,3\,;$$

(2) Assume that $\tau \in [C^1(\overline{\Omega})]^3$ satisfies $\tau \cdot n = 0$ on $\partial\Omega$. For $g \in W^{2,1}(\Omega)$ it then follows that

$$\left| \int_{\partial\Omega} h\, \tau \cdot \delta\, g \right| \le c\, \|h\|_{W^{1/q',q}(\partial\Omega)}\, \|\nabla g\|_{W^{1,q'}(\Omega)}\,.$$

Proof. Due to the trace theorem, we can assume without loss of generality that $h \in W^{1,q}(\Omega)$. Moreover, since Γ_j is a $\mathcal{C}^2$ surface for $j = 1,2$, we can assume that there are extensions $n^{\Gamma_j} \in [C^1(\overline{\Omega})]^3$ for the normal vectors. Let $V \in [C^1(\overline{\Omega})]^3$. Using the Gauss theorem, we can compute for $j = 1,2$

$$\int_\Omega \operatorname{curl}(h\,(V \times n^{\Gamma_j})) \cdot \nabla g = \int_{\partial\Omega} h\,[(V \times n^{\Gamma_j}) \times n] \cdot \nabla g\,.$$

(1): Let $V = e_i - n_i^{\Gamma_j}\, n^{\Gamma_j}$. Then $[(V \times n) \times n] = -V$ on Γ_j. Since $[(V \times n^{\Gamma_j}) \times n]$ is tangent on Γ_k and $\operatorname{trace} g = 0$ on Γ_k, we obtain the representation

$$\int_{\Gamma_j} h\ \delta_i\, g = -\int_\Omega \operatorname{curl}(h\,(V \times n^{\Gamma_j})) \cdot \nabla g\,,$$

which clearly proves the claim.

(2): Let $V = \tau$. Then, $(V \times n^{\Gamma_j}) \times n^{\Gamma_j}] = -\tau$ on Γ_j, and $(V \times n^{\Gamma_j}) \times n^{\Gamma_k} = 0$ for $j \neq k$ and the claim follows from the representation

$$\sum_{j=1}^{2} \int_\Omega \operatorname{curl}(h\,(V \times n^{\Gamma_j})) \cdot \nabla g = \int_{\partial\Omega} h\,\tau \cdot \nabla g\,.$$

□

B The extension operator

We now turn to the problem of finding an operator E like in Assumption 2.4. First we have to 'monotonize' the function $\theta \in W^{2,q}(\Omega)$. A simple idea for $\gamma < 0$ is to use

$$P(\theta)(x,z) := \theta(x,z) - \|[\partial_z\theta - \gamma]^+\|_{L^\infty(\Omega)}\, z, \quad \theta \in W^{2,q}(\Omega),\ (x,z) \in \Omega\,.$$

But this only leads to a Lipschitz continuous operator. Therefore, we introduce $g_0(t) := [t-\gamma]^+$, $t \in \mathbb{R}$ and we choose a sequence of functions $\{g_k\}_{k\in\mathbb{N}} \subset C^1(\mathbb{R})$ such that

$$g_k(t) = 0 \text{ for } t \le \gamma, \quad g_k(t) \ge [t - \gamma + 1/k]^+, \quad g_k \to g_0 \text{ in } C_{\text{loc}}(\mathbb{R})\,.$$

Denote $c_0 =$ embedding constant for $W^{1,q}(\Omega) \to C(\overline{\Omega})$. We then define

$$P(\theta)(x,z) = \theta(x,z) - c_0^{-1}\,\|g_k(\theta_z)\|_{W^{1,q}(\Omega)}\,z, \quad \theta \in W^{2,q}(\Omega),\,(x,z) \in \Omega\,. \tag{101}$$

We verify that $P(\theta) = \theta$ in Ω if $\sup_\Omega \theta_z \le \gamma$. Moreover, in Ω

$$\begin{aligned}\partial_z P(\theta) &= \partial_z\theta - c_0^{-1}\,\|g_k(\theta_z)\|_{W^{1,q}(\Omega)} \le \partial_z\theta - \|g_k(\theta_z)\|_{C(\overline{\Omega})}\\ &\le \partial_z\theta - \|g_0(\theta_z)\|_{C(\overline{\Omega})} \le \partial_z\theta - [\partial_z\theta - \gamma + 1/k]^+\\ &\le \gamma + 1/k\,.\end{aligned}$$

Lemma B.1. *Let $\gamma < 0$, $0 < L' < L$. There is a continuously differentiable operator $E = E_{\gamma,L'} : W^{2,q}(\Omega) \to C^{1,\alpha}(\overline{G}\times\mathbb{R})$, such that $\sup_{G\times\mathbb{R}} \partial_z E(\theta) \le \gamma_0 < 0$ for all $\theta \in W^{2,q}(\Omega)$, and such that $E(\theta) = \theta$ in $\Omega_{L'}$ for all θ with $\partial_z\theta \le \gamma$ in Ω.*

Proof. For $\theta \in W^{2,q}(\Omega)$ we construct an extension operator. For $k \in \mathbb{N}$, let $f_k : \mathbb{R} \to]-L,\,L[$ be a smooth function such that

$$\begin{aligned} f_k(t) &\le f_0(t) := \operatorname{sign}(t)\,\min\{|t|,\,L\} \quad t \in \mathbb{R}\\ f_k(t) &= f_0(t) \quad \text{for } |t| \le L - 1/k\\ f_k' &> 0,\ t \in \mathbb{R} \quad f_k \to f_0 \text{ uniformly on compact sets as } k \to \infty\,.\end{aligned}$$

For $\theta \in W^{2,q}(\Omega)$, take P from (101), and define

$$E(\theta)(x,z) := P(\theta)(x,\,f_\delta(z)) \quad (x,z) \in G \times \mathbb{R}\,. \tag{102}$$

□

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