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Second order sufficient optimality conditions for parabolic optimal control problems with pointwise state constraints

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ABSTRACT. In this paper we study optimal control problems governed by semilinear parabolic equations where the spatial dimension is two or three. Moreover, we consider pointwise constraints on the control and on the state. We formulate first order necessary and second order sufficient optimality conditions. We make use of recent results regarding elliptic regularity and apply the concept of maximal parabolic regularity to the occurring partial differential equations.

1. INTRODUCTION

In this paper we extend the theory of second order sufficient optimality conditions for state constrained optimal control problems, governed by semilinear parabolic partial differential equations, to spatial domains up to dimension three. It is well known that second order sufficient optimality conditions for nonlinear optimal control problems are essential both, in the numerical analysis, and for reliable optimization algorithms. For instance, the strong convergence of optimal controls and states for numerical discretizations of the problem heavily rests on second order sufficient optimality conditions. Moreover, one can show that numerical algorithms such as SQP methods are locally convergent if second order sufficient optimality conditions hold true.

Meanwhile, there are several contributions regarding second order sufficient optimality condition for state constrained optimal control problems governed by partial differential equations. For the case of elliptic equations we mention Casas, Tröltzsch and Unger [9], where especially boundary control problems where considered. Furthermore, we refer to Casas and Mateos in [8], where new second order conditions for problems with finitely many state constraints were introduced. This theory was extended to the case of pointwise state constraints in the contribution of Casas, de los Reyes and Tröltzsch, see [7]. Furthermore, we refer to Bonnans and Zidani [5] where beside finitely many state constraints also polyhedric constraints on the control were discussed. In the case of parabolic equations second order sufficient conditions were investigated by Raymond and Tröltzsch [35] and again in [7].

Let us emphasize the differences of our work to former contributions: in [35] and [7] it was necessary that the parabolic solution operator for the state equation of the optimal control problem is continuous from L^2 on the space-time cylinder to the space of (uniformly) continuous functions – due to the presence of pointwise state constraints. Furthermore, this is also caused by the well known two-norm discrepancy, see for instance Ioffe [27] and Maurer [31]. Thus, those authors were restricted to distributed control problems and spatial dimension one. Since the above mentioned mapping property of the parabolic solution operator does not hold in dimensions $d > 1$ we introduce here a quite different approach, heavily resting on maximal parabolic regularity and optimal embedding results. Moreover, the parabolic state equation is discussed under mild assumptions concerning the spatial domain and the coefficient function in the elliptic differential operator. Furthermore, we are able to deal with mixed boundary conditions. In order to do so, we will use very recent results from elliptic/parabolic regularity theory.

The paper is organized as follows: in the next section we introduce the optimal control problem, and we specify assumptions on given the quantities of the problem. Furthermore, we will make use of the concept of maximal parabolic regularity in order to analyze the state equation and a linearized version of it. The third section is devoted to the formulation of first order necessary optimality condition using an adjoint state equation. Since our state space will be chosen as a reflexive Banach space, the formulation of the respective adjoint state equation can be carried out intuitively. Here we mainly follow the ideas from [26, Ch.6.2-6.3]. The fourth section concerns the elaboration of second order sufficient optimality conditions adapting ideas in [9] to the parabolic case. The appendix is devoted to the proof

of the elliptic regularity result which is one of the cornerstones in the foregoing chapters.

2. Semilinear parabolic problems

We will consider the following parabolic optimal control problem with distributed control.

$$\left.\begin{aligned} \min J(y,u) := \iint_Q L(x,t,y,u)dxdt + \int_0^T \int_{\partial\Omega} l(x,t,y)d\sigma\, dt \\ y_t - \nabla\cdot\kappa\nabla y + d(x,t,y) = u \quad \text{in } Q := \Omega\times(0,T) \\ \nu\cdot\kappa\nabla y = 0 \quad \text{on } \Sigma_N = \Gamma\times(0,T) \\ y = 0 \quad \text{on } \Sigma_D = (\partial\Omega\setminus\Gamma)\times(0,T) \\ y(x,0) = 0 \quad \text{in } \Omega \\ u_a \le u(x,t) \le u_b \quad \text{a.e. in } Q. \\ y(x,t) \ge y_c(x,t) \quad \text{for all } (x,t)\in K\subset\overline{Q}. \end{aligned}\right\} \tag{P}$$

Moreover, we incorporate pointwise constraints on the control and on the state. In this setting, Ω is a subset of $\mathbb{R}^d$, $d\in\{2,3\}$ with boundary $\partial\Omega$, where Γ denotes an open subset of the boundary. Moreover, ν defines the outward unit normal at the boundary part Γ. In the sequel we abbreviate $\partial\Omega\times(0,T) =: \Sigma$. K is a non-empty compact subset of $\overline{Q}$.

2.1. Notations and assumptions.

Throughout the paper, all occurring spatial domains are generally supposed to be Lipschitzian (see [32, Ch. 1.1.9]), in particular, $\Omega\subset\mathbb{R}^d$, $d\in\{2,3\}$ always denotes a bounded Lipschitz domain.

Remark 2.1. *The Lipschitz property of the domain assures (besides other usefull things) a continuous extension operator $W^{1,q}(\Omega)\to W^{1,q}(\mathbb{R}^d)$ – universal for all $q\in[1,\infty]$. This yields immediately the usual Sobolev embeddings $W^{1,q}(\Omega)\hookrightarrow L^r(\Omega)$.*

Γ is an open subset of the boundary $\partial\Omega$ and is supposed to satisfy throughout the whole paper the following general assumption:

Assumption 2.2. *i) If $d=2$, then $\partial\Omega\setminus\Gamma$ is the finite union of closed arc pieces – non of which is degenerated to a single point.*

ii) If $d=3$, then $\partial\Omega\setminus\Gamma$ is the closure of its interior (within $\partial\Omega$). Moreover, the boundary of Γ within $\partial\Omega$ is locally bi-Lipschitz diffeomorphic to the unit interval $(0,1)$.

Remark 2.3. *In fact, the conditions in Assumption 2.2 are an equivalent (but much more intuitive) for $\Omega\cup\Gamma$ to be a regular set in the sense of* [21] *(see* [23, Ch. 5] *for a proof). In this spirit, this latter property is always implicitly understood when quoting results concerning this geometrical setting.*

In all what follows, the space $C^\delta(Q)$ denotes the space of Hölder continuous functions with index $\delta>0$. $W^{1,q}(\Omega)$ denotes the usual (real) Sobolev space on Ω. We use the symbol $W^{1,q}_\Gamma(\Omega)$ for the closure of

$$C^\infty_\Gamma(\Omega) := \left\{v|_\Omega : v\in C^\infty_0(\mathbb{R}^d), supp\, v\cap(\partial\Omega\setminus\Gamma)=\emptyset\right\}$$

in $W^{1,q}(\Omega)$. We write (as usual) $W_0^{1,q}(\Omega)$ instead of $W_\emptyset^{1,q}(\Omega)$. $W^{-1,q'}(\Omega)$ denotes the space of continuous linear forms on $W_0^{1,q}(\Omega)$ and $W_\Gamma^{-1,q'}(\Omega)$ denotes the dual to $W_\Gamma^{1,q}(\Omega)$ when $\frac{1}{q}+\frac{1}{q'}=1$ holds. In particular, the dual of $W^{1,q'}(\Omega)$ is denoted by $W_{\partial\Omega}^{-1,q}(\Omega)$. If the domain Ω is understood, we will abbreviate $W_\Gamma^{1,q}$ and $W_\Gamma^{-1,q}$, respectively. For two Banach spaces X and Y we denote the space of linear, bounded operators from X into Y by $\mathcal{L}(X;Y)$. If $X=Y$, then we abbreviate $\mathcal{L}(X)$. As usual, we define for a (matrix valued) coefficient function κ the operator

$$-\nabla\cdot\kappa\nabla : W_\Gamma^{1,2}(\Omega) \longmapsto W_\Gamma^{-1,2}(\Omega)$$

by

$$\langle -\nabla\cdot\kappa\nabla v, w\rangle := \int_\Omega \kappa\nabla v\cdot\nabla w\,dx \quad v,w\in W_\Gamma^{1,2}(\Omega), \tag{2.1}$$

where here and in the sequel $\langle\cdot,\cdot\rangle$ denotes the dual pairing between $W_\Gamma^{-1,2}(\Omega)$ and $W_\Gamma^{1,2}(\Omega)$. The restriction of the operator to spaces $W_\Gamma^{1,q}(\Omega)$, $q\geq 2$ will also be denoted by $-\nabla\cdot\kappa\nabla$.

Remark 2.4. *When restricting the range space of the operator $-\nabla\cdot\kappa\nabla$ to $L^2(\Omega)$, one obtains an operator for which the elements ψ of its domain satisfy the conditions $\psi|_{\partial\Omega\setminus\Gamma}=0$ in the sense of traces and $\nu\cdot\mu\nabla\psi=0$ on Γ in a generalized sense – ν being the outward unit normal of the domain, compare* [10, Ch. 1.2] *or* [16, Ch II.2]*.*
In this spirit, the operator $-\nabla\cdot\kappa\nabla$ is to be understood as one with mixed boundary conditions.

In all what follows, we will make the following general assumption:

Assumption 2.5. *Let κ be a measurable, bounded function on Ω, taking its values in the set of real symmetric $d\times d$ matrices. Moreover, κ has to fulfil the usual strong ellipticity condition*

$$\xi^T\kappa(x)\xi\geq c_\kappa|\xi|^2, \qquad \forall\xi\in\mathbb{R}^d$$

for almost all $x\in\Omega$ and some constant $c_\kappa>0$.

Assumption 2.6. *There is a $q_0>d$, such that*

$$-\nabla\kappa\cdot\nabla+1 : W_\Gamma^{1,q}(\Omega)\longmapsto W_\Gamma^{-1,q}(\Omega) \tag{2.2}$$

is a topological isomorphism for all $q\in[q_0',q_0]$, where $q_0'=\frac{q_0}{q_0-1}$ is the conjugate exponent to q_0.

Remark 2.7. *The appendix of the paper is devoted to specify assumptions on the domain Ω, the boundary part Γ and the coefficient function κ such that Assumption 2.6 holds true. Since this is a black box in view of the rest of the paper, and its discussion is of quite different character, we postponed this to the appendix.*

Remark 2.8. *In view of Shamir's famous counterexample* [37] *one cannot expect that* (2.2) *is a topological isomorphism for a $q\geq 4$ in general, if mixed boundary conditions are imposed. In this spirit we assume that q_0 is taken from the interval $(d,4)$ in the sequel, see also Proposition 2.10 below.*

Next, we will formulate assumptions on the given quantities of the optimal control problem:

(A1) For each pair $(x,t)\in Q$ or $(x,t)\in\Sigma$, respectively, the functions $L(x,t,y,u)$, $l(x,t,y)$ and $d(x,t,y)$ are of Carathèodory type, i.e. for all fixed $(y,u)\in\mathbb{R}^2$ or $y\in\mathbb{R}$ they are measurable with respect to $(x,t)\in Q$ or $(x,t)\in\Sigma$, respectively. The function $L(x,t,y,u)$ is twice partially differentiable w.r.t. to (y,u) for almost all $(x,t)\in Q$. Analogously, the functions d and l are twice partially differentiable w.r.t. y.

(A2) There is a constant C_d and, for all $M > 0$, a constant $C_{d,M}$ such that

$$|d(x,t,0)| + \left|\frac{\partial d}{\partial y}(x,t,0)\right| + \left|\frac{\partial^2 d}{\partial y^2}(x,t,0)\right| \le C_d$$
$$\left|\frac{\partial^2 d}{\partial y^2}(x,t,y_1) - \frac{\partial^2 d}{\partial y^2}(x,t,y_2)\right| \le C_{d,M}|y_1 - y_2|$$

hold for almost all $(x,t) \in Q$ and all $|y_i| \le M$, $i = 1,2$.

(A3) We assume that there is C_l and, for all $M > 0$, a constant $C_{l,M}$ such that

$$|l(x,t,0)| + \left|\frac{\partial l}{\partial y}(x,t,0)\right| + \left|\frac{\partial^2 l}{\partial y^2}(x,t,0)\right| \le C_l$$
$$\left|\frac{\partial^2 l}{\partial y^2}(x,t,y_1) - \frac{\partial^2 l}{\partial y^2}(x,t,y_2)\right| \le C_{l,M}|y_1 - y_2|$$

hold for almost all $(x,t) \in \Sigma$ and all $|y_i| \le M$, $i = 1,2$.

(A4) There is a constant C_L and, for all $M > 0$, a constant $C_{L,M}$ such that

$$|L(x,t,0)| + |L'(x,t,0)| + |L''(x,t,0)| \le C_L$$
$$|L''(x,t,y_1,u_1) - L''(x,t,y_2,u_2)| \le C_{L,M}(|y_1 - y_2| + |u_1 - u_2|)$$

for almost all $(x,t) \in Q$ and all $|y_i| \le M$, $|u_i| \le M$, $i = 1,2$, where L' and L'' denote the gradient and the Hessian matrix of L with respect to (y,u).

(A5) u_a, u_b are assumed to be real numbers satisfying $u_a < u_b$

(A6) $y_c(x,t)$ denotes a continuous function on the compact subset $K \subset \overline{Q}$ with $y_c(x,0) < 0$ for almost all $x \in \partial\Omega \setminus \Gamma$

2.2. **Discussion of the state equation.** This subsection is devoted to the analysis of the state equation from problem (P). Let us first recall the concept of maximal parabolic regularity and point out some basis facts on this: Let X be a Banach space and let A be a closed operator with dense domain $\mathcal{D} \subset X$, the latter equipped with the associated graph norm. Moreover, let $J = (T_0, T) \subset \mathbb{R}$ be a bounded interval. Suppose $r \in (1,\infty)$, then A is said to satisfy maximal parabolic $L^r(J;X)$-regularity if for any $f \in L^r(J;X)$ there is a unique function $w \in W^{1,r}(J;X) \cap L^r(J;\mathcal{D})$ such that

$$w_t + Aw = f, \qquad w(T_0) = 0.$$

This means, the mapping $W^{1,r}(J;X) \cap L^r(J;\mathcal{D}) \cap \{w : w(T_0) = 0\} \ni w \mapsto w_t + Aw \in L^r(J;X)$ is a continuous bijection. Hence the inverse is continuous by the open mapping theorem, and the solution w admits an estimate

$$\|w\|_{W^{1,r}(J;X)} + \|w\|_{L^r(J;\mathcal{D})} \le c\|f\|_{L^r(J;X)} \tag{2.3}$$

for some constant $c > 0$ independent of f. Note that by $W^{1,r}(J;X)$ we denote the set of those functions from $L^r(J;X)$ whose distributional derivate also belongs to $L^r(J;X)$.

Remark 2.9. *The following things on maximal parabolic $L^r(J;X)$-regularity are known:*

(i) *If A satisfies maximal parabolic $L^r(J;X)$-regularity, then it does for any other bounded interval $\hat{J}$, see* [13]

(ii) *If A satisfies maximal parabolic $L^r(J;X)$-regularity, then it satisfies maximal parabolic $L^s(J;X)$-regularity for all $s \in (1,\infty)$, see e.g. also* [13]

(iii) *There is a continuous embedding* [2]

$$W^{1,r}(J;X)\cap L^r(J;\mathcal{D})\hookrightarrow C^\beta(\bar{J};(X,\mathcal{D})_{\varsigma,1})\quad \textit{if}\quad 0\le\beta<1-\frac{1}{r}-\varsigma, \tag{2.4}$$

where $(X,\mathcal{D})_{\varsigma,1}$ *denotes the real interpolation space between* X *and* $\mathcal{D}$*, see* [39, Ch. 1]*.*

We will apply this concept to our problem. To this end, we need the following result (see [25, Theorem 5.4.]).

Proposition 2.10. *Let, under Assumption 2.2,* $q\in[2,\infty($ *in case of* $d=2$ *or* $q\in[2,6]$ *in case of* $d=3$*. Then, for every* $r>1$ *and any bounded interval* J *the operator* $-\nabla\cdot\kappa\nabla$ *satisfies maximal parabolic* $L^r(J;W_\Gamma^{-1,q})$*-regularity.*

Remark 2.11. *If, additionally, Assumption 2.6 is satisfied, then the domain* $\mathcal{D}$ *of* $-\nabla\cdot\kappa\nabla$ *equals* $W_\Gamma^{1,q}$*.*

Theorem 2.12. *Let the Assumptions 2.2/2.6 be satisfied and* $q\in(d,q_0]$ *be given. Moreover, we assume* $r>\frac{2q}{q-d}$ *and* $p\ge\frac{dq}{d+q}$*. Then, there is a* $T_{>0}$*, such that for all* $u\in L^r(0,T;L^p(\Omega))$ *the state equation of problem (P) admits a unique solution* $y=y(u)\in W^{1,r}(0,T;W_\Gamma^{-1,q})\cap L^r(0,T;W_\Gamma^{1,q})$*, which belongs to* $C^\gamma(Q)$ *with some* $\gamma>0$*. The number* T *may be taken uniformly for all functions* u *with* $u_a\le u\le u_b$*.*

Proof. According to Proposition 2.10, the operator $-\nabla\cdot\kappa\nabla$ in the state equation enjoys maximal parabolic $L^r(J;W_\Gamma^{-1,q})$-regularity. Furthermore, the control $u\in L^r(0,T;L^p(\Omega))$ is an element in $L^r(0,T;W_\Gamma^{-1,q})$ due to $p\ge\frac{dq}{d+q}$ and the resulting Sobolev embedding. We refer to [24, Theorem 6.17] that gives the existence of a $T_{>0}$ such that the state equation of problem (P) admits a unique solution $y=y(u)$ on $(0,T)$ satisfying $y\in W^{1,r}(0,T;W_\Gamma^{-1,q})\cap L^r(0,T;W_\Gamma^{1,q})$. Let us prove now the Hölder continuity of the solution. Due to the supposition $r>\frac{2q}{q-d}$ and $q>d$ the interval $(\frac12+\frac{d}{2q},1-\frac1r)$ is not empty. Assume now $\varsigma\in(\frac12+\frac{d}{2q},1-\frac1r)$. Then (2.4) gives

$$W^{1,r}(0,T;W_\Gamma^{-1,q})\cap L^r(0,T;W_\Gamma^{1,q})\hookrightarrow C^\beta([0,T];(W_\Gamma^{-1,q},W_\Gamma^{1,q})_{\varsigma,1}) \tag{2.5}$$

as long as $\beta<1-\frac1r-\varsigma$. On the other hand we have, thanks to Corollary 5.28 and Remark 5.29, for $\varsigma>\frac12+\frac{d}{2q}$

$$(W_\Gamma^{-1,q}(\Omega),W_\Gamma^{1,q}(\Omega))_{\varsigma,1}\hookrightarrow(W_\Gamma^{-1,q}(\Omega),W_\Gamma^{1,q}(\Omega))_{\varsigma,q}\hookrightarrow W_\Gamma^{2\varsigma-1,q}(\Omega)\hookrightarrow C^\alpha(\Omega) \tag{2.6}$$

with $\alpha:=2\varsigma-1-\frac{d}{q}>0$. Finally, (2.5) in combination with (2.6) give the asserted Hölder continuity. The uniformity in u can also be obtained from [24, Theorem 6.17.], see also [33]. □

Remark 2.13. *In this article we do not care how large the interval is where the solution exists. In general, these are highly nontrivial problems even in the case of smooth data, compare e.g.* [1]*. In this spirit, the occurring time intervals below shall be always understood as the existence interval* $(0,T)$ *from Theorem 2.12.*

Remark 2.14. *We will note here, that it is also possible to treat boundary conditions of Robin-type instead of pure Neumann-type boundary conditions, see* [24, Ch. 5.3]*. Furthermore, we are also able to deal with inhomogeneous Dirichlet boundary data, provided that they are smooth enough.*

2.3. **Analysis of the linearized state equation.** In this section we discuss the following linear initial boundary value problem that covers a linearized version of the state equation of problem (P).

$$\begin{aligned} w_t - \nabla \cdot \kappa \nabla w + c_0 w &= f \quad \text{in } Q \\ \nu \cdot \kappa \nabla w &= 0 \quad \text{on } \Sigma_N \\ w &= 0 \quad \text{on } \Sigma_D \\ w(x,0) &= 0 \quad \text{in } \Omega, \end{aligned} \tag{2.7}$$

where $c_0 \in L^\infty(Q)$ is given. We note that c_0 represents the partial derivative $\frac{\partial d}{\partial y}$. Analogously to the previous section, we will use the concept of maximal parabolic regularity for the solvability of (2.7).

Theorem 2.15. *Let Assumption 2.6 be satisfied and $q \in (d, q_0)$ be given. Moreover, we assume $r > \frac{2q}{q-d}$ and $p \geq \frac{dq}{d+q}$. Then, for all $f \in L^r(0,T;L^p(\Omega))$ the solution $w \in W^{1,r}(0,T;W_\Gamma^{-1,q}) \cap L^r(0,T;W_\Gamma^{1,q})$ of (2.7) belongs to $C^\alpha(Q)$ with some $\alpha > 0$. Furthermore, the mapping $f \mapsto w$ is continuous from $f \in L^r(0,T;L^p(\Omega))$ to $C^\alpha(Q)$.*

Proof. Again, according to Proposition 2.10, the operator $-\nabla \cdot \kappa \nabla$ in the state equation enjoys maximal parabolic $L^r(0,T;W_\Gamma^{-1,q})$-regularity and the right hand side f belongs to $L^r(0,T;W_\Gamma^{-1,q})$ by Sobolev embedding. Then a perturbation result, see e.g. [4, Prop. 1.3], gives the maximal parabolic $L^r(0,T;W_\Gamma^{-1,q})$-regularity of the operator $-\nabla \cdot \kappa \nabla + \tilde{c}_0$, where $\tilde{c}_0$ denotes the multiplication operator induced by c_0. Thus, we have

$$\|w\|_{W^{1,r}(0,T;W_\Gamma^{-1,q})} + \|w\|_{L^r(0,T;W_\Gamma^{1,q})} \leq c \|f\|_{L^r(0,T;L^p(\Omega))}.$$

Moreover, we have the continuous embedding

$$W^{1,r}(0,T;W_\Gamma^{-1,q}) \cap L^r(0,T;W_\Gamma^{1,q}) \hookrightarrow C^\alpha(Q).$$

for some $\alpha > 0$, see the proof of Theorem 2.12. □

Within the discussion of second order sufficient optimality conditions for problem (P), it is necessary to consider the solution of a linearized state equation with respect to right hand sides being elements from $L^2(Q)$. In order to obtain optimal a priori estimates for the solution in this case we prove the following result, which is another keypoint for all what follows:

Theorem 2.16. *Let Ω and Γ be as above.*

i) The restriction of the operator $-\nabla \cdot \kappa \nabla$ to $L^2(\Omega)$ satisfies maximal parabolic regularity, i.e. for every $f \in L^2(Q)$ the equation (2.7) admits a unique solution $w \in W^{1,2}(0,T;L^2(\Omega)) \cap L^2(0,T;\mathcal{D}_{L^2})$, where $\mathcal{D}_{L^2}$ denotes the domain of the operator $-\nabla \cdot \kappa \nabla$, when considered on $L^2(\Omega)$.

ii) Let $w \in W^{1,2}(0,T;L^2(\Omega)) \cap L^2(0,T;\mathcal{D}_{L^2})$ be the solution of (2.7) with respect to the right hand side $f \in L^2(Q)$. If $d = 2$, then w even belongs to every space $C([0,T];L^p(\Omega))$, if $p \in [1,\infty)$.

If $d = 3$, then w belongs to the space $L^{\frac{2}{\zeta}}(0,T;L^{\frac{6}{1-\zeta}}(\Omega))$ for all $\zeta \in (0,1)$, and one has the estimate

$$\|w\|_{L^{\frac{2}{\zeta}}(0,T;L^{\frac{6}{1-\zeta}}(\Omega))} \leq c \|f\|_{L^2(Q)}.$$

Proof. i) Due to the symmetry of the coefficient function κ, the operator $-\nabla \cdot \kappa \nabla|_{L^2}$ is selfadjoint and positive. Hence, it generates an analytic semigroup on $L^2(\Omega)$, due to functional calculus.

But this implies maximal parabolic regularity since $L^2(\Omega)$ is a Hilbert space, see [12]. This yields an a priori estimate like (2.3) – there taken $r = 2$. It is well-known ([3, Thm. 4.10.2]) that the space $W^{1,2}(0,T;L^2(\Omega)) \cap L^2(0,T;\mathcal{D}_{L^2})$ continuously embeds into $C([0,T];(L^2(\Omega),\mathcal{D}_{L^2})_{\frac{1}{2},2})$. But $(L^2(\Omega),\, \mathrm{dom}_{L^2(\Omega)}(\nabla\cdot\kappa\nabla))_{\frac{1}{2},2}$ equals $\mathrm{dom}_{L^2(\Omega)}(-\nabla\cdot\kappa\nabla+1)^{1/2}$ including the equivalence of norms, cf. [39, Ch. 1.18.10]. Moreover, $\mathrm{dom}_{L^2(\Omega)}(-\nabla\cdot\kappa\nabla+1)^{1/2}$ is nothing else but the form domain of $-\nabla\cdot\kappa\nabla$ (see [29, Ch. VI.2.6]); and this form domain equals $W^{1,2}_\Gamma(\Omega)$. Thus, the space $C([0,T];(L^2(\Omega),\mathcal{D}_{L^2})_{\frac{1}{2},2})$ is identical with $C([0,T];W^{1,2}_\Gamma(\Omega))$. Hence, the assertion for the $2d$-case results from the embedding $W^{1,2}_\Gamma(\Omega)) \hookrightarrow L^p(\Omega)$, whenever $p \in [1,\infty)$.
In the case of $d = 3$ one has, on one hand, the Sobolev embedding $W^{1,2}_\Gamma(\Omega) \hookrightarrow L^6(\Omega)$. Thus,

$$w \in C([0,T];W^{1,2}_\Gamma(\Omega)) \hookrightarrow L^\infty(0,T;L^6(\Omega)). \tag{2.8}$$

On the other hand, one knows the continuous embedding $\mathcal{D}_{L^2} \hookrightarrow L^\infty(\Omega)$, if $d \le 3$, cf. [19] or [38]. This gives

$$w \in L^2(0,T;L^\infty(\Omega)), \tag{2.9}$$

together with a corresponding estimate with respect to f. Let us show that (2.8) together with (2.9) implies $w \in L^{\frac{2}{\zeta}}(0,T;L^{\frac{6}{1-\zeta}}(\Omega))$, for all $\zeta \in (0,1)$. For doing so, one first observes that (2.9) implies the (Bochner-) measurability of w, when the function is considered as $L^{\frac{6}{1-\zeta}}(\Omega)$-valued. Secondly, one has for any $\psi \in L^\infty(\Omega)$

$$\|\psi\|_{L^{\frac{6}{1-\zeta}}(\Omega)} = \Big(\int_\Omega \big(|\psi|^{1-\zeta}|\psi|^\zeta\big)^{\frac{6}{1-\zeta}} d\mathrm{x}\Big)^{\frac{1-\zeta}{6}} \le \|\psi\|^{1-\zeta}_{L^6(\Omega)}\|\psi\|^\zeta_{L^\infty(\Omega)}.$$

Thus, one obtains

$$\begin{aligned}\Big(\int_0^T \|w(t)\|^{\frac{2}{\zeta}}_{L^{\frac{6}{1-\zeta}}(\Omega)} dt\Big)^{\frac{\zeta}{2}} &\le \Big(\int_0^T \big(\|w(t)\|^{1-\zeta}_{L^6(\Omega)}\|w(t)\|^\zeta_{L^\infty(\Omega)}\big)^{\frac{2}{\zeta}} dt\Big)^{\frac{\zeta}{2}}\\ &\le \|w\|^{1-\zeta}_{L^\infty(0,T;L^6(\Omega))}\|w\|^\zeta_{L^2(0,T;L^\infty(\Omega))},\end{aligned}$$

and the right hand side is finite, according to (2.8)/(2.9). □

3. Necessary optimality conditions

Let us first recall that here and in the following chapter we always impose the Assumptions 2.2, 2.5 and 2.6 without any further comment. We start with the introduction of a control-to-space mapping based on Theorem 2.12. For the subsequent we define $J := (0,T)$ and $W^{1,r}_0(J;W^{-1,q}_\Gamma) := W^{1,r}(J;W^{-1,q}_\Gamma) \cap \{\psi : \psi(0) = 0\}$. Further, we introduce the state space

$$Y := W^{1,r}_0(J;W^{-1,q}_\Gamma) \cap L^r(J;W^{1,q}_\Gamma),$$

thereby assuming $r > \frac{2q}{q-d}$ and $q \in (d, q_0)$.

Definition 3.1. *Based on Theorem 2.12, we introduce for $p > \frac{dq}{q+d}$ the control-to-state operator $G : L^r(J;L^p(\Omega)) \to Y$ by $y = G(u)$, which assigns to $u \in L^r(J;L^p(\Omega))$ the unique solution $y(u) \in Y$ of the state equation of problem (P).*

Following the lines of the proof of Theorem 2.12, we obtain that the unique state $y = G(u)$ is Hölder continuous. By means of the analysis for the linearized state equation and the implicit function theorem one can easily prove the Frèchet-differentiability of the solution operator G:

Theorem 3.2. *Let assumptions (A1)-(A2) be satisfied. Then, the control-to-state operator G is twice Frèchet differentiable from $L^r(J;L^p(\Omega))$ to Y. Its derivative $y_h := G'(u)h$ at point u in direction $h \in L^r(J;L^p(\Omega))$ is given by the solution of*

$$\begin{aligned} (y_h)_t - \nabla \cdot \kappa \nabla y_h + d_y(x,t,y(u))y_h &= h \quad \text{in } Q \\ \nu \cdot \kappa \nabla y_h &= 0 \quad \text{on } \Sigma_N \\ y_h &= 0 \quad \text{on } \Sigma_D \\ y_h(x,0) &= 0 \quad \text{in } \Omega, \end{aligned} \tag{3.1}$$

where $y(u) = G(u)$. Furthermore, $y_{h_1h_2} = G''(u)h_1h_2$, $h_i \in L^r(J;L^p(\Omega))$, $i = 1,2$ is the solution of

$$\begin{aligned} (y_{h_1h_2})_t - \nabla \cdot \kappa \nabla y_{h_1h_2} + d_y(x,t,y(u))y_{h_1h_2} &= -d_{yy}(x,t,y(u))y_{h_1}y_{h_2} \quad \text{in } Q \\ \nu \cdot \kappa \nabla y_{h_1h_2} &= 0 \quad \text{on } \Sigma_N \\ y_{h_1h_2} &= 0 \quad \text{on } \Sigma_D \\ y_{h_1h_2}(x,0) &= 0 \quad \text{in } \Omega \end{aligned} \tag{3.2}$$

with $y_{h_i} = G'(u)h_i$, $i = 1,2$.

The following Proposition shows that the remainder term of the first derivative of the solution operator G can also be estimated with respect to the $L^2(Q)$-norm of the directions, which will be essential for second order sufficient conditions.

Proposition 3.3. *Let $\bar{u}, \hat{u} \in U_{ad}$ be given with associated states $\bar{y} = G(\bar{u})$ and $\hat{y} = G(\hat{u})$, respectively. Moreover, we introduce $y = G'(\bar{u})(\hat{u}-\bar{u})$ as the solution of the linearized state equation in direction $\hat{u} - \bar{u}$. Then, there is a constant $c > 0$ depending on $\bar{u}, \hat{u} \in U_{ad}$ such that*

$$\|\hat{y} - \bar{y} - y\|_Y \le c\|\hat{u} - \bar{u}\|^2_{L^2(Q)}. \tag{3.3}$$

Proof. Introducing the difference $z := \hat{y} - \bar{y} - y$ and using the first order expansion of d at $(x,t,\bar{y})$, one can easily see that z solves the following system

$$\begin{aligned} z_t - \nabla \cdot \kappa \nabla z + d_y(x,t,\bar{y})z &= -r_d \quad \text{in } Q \\ \nu \cdot \kappa \nabla z &= 0 \quad \text{on } \Sigma_N \\ z &= 0 \quad \text{on } \Sigma_D \\ z(x,0) &= 0 \quad \text{in } \Omega, \end{aligned}$$

where r_d denotes the remainder term of the first order expansion of d. According to Assumption (A2), we obtain for r_d

$$|r_d(x,t)| \le c_M |\hat{y}(x,t) - \bar{y}(x,t)|^2,$$

where c_M depends on $\|\hat{y}\|_{C(\overline{Q})}$ and $\|\bar{y}\|_{C(\overline{Q})}$, respectively. By means of Theorem 2.15, we conclude $z \in Y$ and the a priori estimate

$$\|z\|_Y \le c\|r_d\|_{L^r(J;L^p(\Omega))}$$

for $r > \frac{2q}{q-d}$ and $p \ge \frac{dq}{q+d}$. Note that $q > d$ implies directly $p > d/2$. Thus we end up with

$$\|z\|_Y \le c\|\hat{y} - \bar{y}\|^2_{L^{\tilde{r}}(J;L^{\tilde{p}}(\Omega))}$$

for $\tilde{r} > \frac{4q}{q-d}$ and $\tilde{p} > d$ and a constant depending on $\bar{u}, \hat{u} \in U_{ad}$ due to Theorem 2.12. According to differentiability of the solution operator G, there is a real number $0 < \eta < 1$ such that $\hat{y} - \bar{y} = G(\hat{u}) - G(\bar{u}) = G'(u)(\hat{u} - \bar{u})$ with $u = \eta\hat{u} + (1-\eta)\bar{u}$. Note that, $G'(u)(\hat{u} - \bar{u})$ is the solution

of a linear initial boundary value problem (2.7) with $c_0 := d_y(x,t,y(u))$ and the right hand side $f := \hat{u} - \bar{u}$. Thus we can exploit Theorem 2.16 and we derive the estimate

$$\|\hat{y} - \bar{y}\|_{L^r(J;L^p(\Omega))} \leq c\|\hat{u} - \bar{u}\|_{L^2(Q)}$$

taking ζ in Theorem 2.16(ii) sufficiently small. By means of this estimate the assertion is proven. □

It is known that Lagrange multipliers associated to pointwise state constraints are in general only regular Borel measures, see e.g. [6] and [34]. Let us define the Lagrange function associated to our problem (P) as follows:

$$\mathcal{L} : L^\infty(Q) \times \mathcal{M}(\overline{Q}) \to \mathbb{R},\ \mathcal{L}(u,\mu) = J(G(u),u) + < y_c - G(u), \mu >_{C(\overline{Q}),\mathcal{M}(\overline{Q})},$$

where the space of regular Borel measures on $\overline{Q}$ is denoted by $\mathcal{M}(\overline{Q})$. Note, that by Riesz representation theorem $\mathcal{M}(\overline{Q})$ can be identified with the dual space of $C(\overline{Q})$.

One can easily see that the Lagrange function is continuously differentiable w.r.t. to the control variable u from $L^\infty(Q)$ to $\mathbb{R}$ by Theorem 3.2, the chain rule and assumption (A1). Its derivative at point $u \in L^\infty(Q)$ in direction $h \in L^\infty(Q)$ is given by

$$\begin{aligned}\mathcal{L}'(u,\mu)h = &\iint_Q \frac{\partial L}{\partial u}(x,t,G(u),u)h + \frac{\partial L}{\partial y}(x,t,G(u),u)y_h dxdt \\ &+ \iint_\Sigma \frac{\partial l}{\partial y}(x,t,G(u))y_h d\sigma dt - < y_h, \mu >_{C(\overline{Q}),\mathcal{M}(\overline{Q})},\end{aligned} \tag{3.4}$$

where $y_h = G'(u)h$ is the solution of (3.1) w.r.t. $h \in L^\infty(Q)$. We continue with the definition of Lagrange multipliers associated to the state constraints in (P). Note that the control constraints were handled by a convex set of admissible controls:

$$U_{ad} = \{u \in L^\infty(Q) :\ u_a \leq u \leq u_b\}.$$

Definition 3.4. *Let $\bar{u} \in U_{ad}$ be a locally optimal control of (P), then $\mu \in \mathcal{M}(\overline{Q})$ is said to be a Lagrange multiplier associated to the state constraints of (P), if*

$$\mathcal{L}'(\bar{u},\mu)(u - \bar{u}) \geq 0 \qquad \forall u \in U_{ad} \tag{3.5}$$

$$< y_c - G(\bar{u}), \mu >_{C(\overline{Q}),\mathcal{M}(\overline{Q})} = 0 \tag{3.6}$$

$$\iint_Q \varphi d\mu \geq 0, \qquad \forall \varphi \in C(\overline{Q}), \varphi \geq 0 \tag{3.7}$$

hold true.

By means of an adjoint equation, we will reformulate the previous conditions into a optimality system. Moreover, it is well known that a certain constraint qualification is needed to ensure the existence of such a Lagrange multiplier, see e.g. [41]. We require a linearized Slater condition, which guarantees the existence of Lagrange multipliers in the sense of the previous definition.

Assumption 3.5. *Let $\bar{u} \in U_{ad}$ satisfy the following condition: there exist a feasible control $\hat{u} \in U_{ad}$, $G(\hat{u}) \geq y_c$ and a real number $\delta > 0$ such that*

$$G(\bar{u})(x,t) + G'(\bar{u})(\hat{u} - \bar{u})(x,t) \geq y_c(x,t) + \delta \qquad \forall (x,t) \in \overline{Q}.$$

Definition 3.6. *Let $q_0 > d$ be the number of Assumption 2.6 and let $q \in (d, q_0)$ be given. Further, we assume $r > \frac{2q}{q-d}$. We denote, for $s \in (1,\infty)$, by s' the conjugated exponent $\frac{s}{s-1}$ and observe*

$$q' \in (q_0', d/(d-1)) \qquad \text{and} \qquad r' \in (1,(2q)/(q+d)).$$

Regarding the numbers q, q', r and r' of the previous definition, we set

$$W_{r,0} = W_0^{1,r}(J; W_\Gamma^{-1,q}) \cap L^r(J; W_\Gamma^{1,q})$$
$$W_{r'} = W^{1,r'}(J; W_\Gamma^{-1,q'}) \cap L^{r'}(J; W_\Gamma^{1,q'})$$

The associated dual space are denoted by the superscript $*$.

Theorem 3.7. *Let $\bar u \in U_{ad}$ be local optimal control with associated state $\bar y = G(\bar u) \in Y = W_{r,0}$ satisfying Assumption 3.5. Then there exist a Lagrange multiplier $\bar\mu \in \mathcal{M}(\overline{Q})$ and an adjoint state $\bar p \in L^{r'}(J; W_\Gamma^{1,q'})$ such that the following optimality system is satisfied:*

$$\begin{aligned} \bar y_t - \nabla\cdot\kappa\nabla\bar y + d(x,t,\bar y) &= \bar u \quad \text{in } Q \\ \nu\cdot\kappa\nabla\bar y &= 0 \quad \text{on } \Sigma_N \\ \bar y &= 0 \quad \text{on } \Sigma_D \\ \bar y(x,0) &= 0 \quad \text{in } \Omega \end{aligned} \tag{3.8}$$

$$\begin{aligned} \int_J < z_t, \bar p >_{W_\Gamma^{-1,q}, W_\Gamma^{1,q'}} dt + \iint_Q \kappa\nabla z\cdot\nabla\bar p dxdt = \iint_Q \frac{\partial L}{\partial y}(x,t,\bar y,\bar u) z dxdt \\ + \iint_\Sigma \frac{\partial l}{\partial y}(x,t,\bar y) z d\sigma dt + \iint_Q z d\bar\mu \quad \forall z \in W_{r,0} \end{aligned} \tag{3.9}$$

$$\iint_Q (\bar p + \frac{\partial L}{\partial u}(x,t,\bar y,\bar u))(u-\bar u) dxdt \geq 0 \qquad \forall u \in U_{ad} \tag{3.10}$$

$$\iint_Q (y_c - \bar y) d\bar\mu = 0, \qquad \iint_Q \varphi d\mu \geq 0, \qquad \forall \varphi \in C(\overline{Q})^+ \tag{3.11}$$

Proof. Follow the lines of [26, Ch.6.2-6.3]. □

Please note, that the optimal adjoint state can be splitted into a regular part p_1 and a irregular part p_2, where on the one hand $p_2 \in L^{r'}(J; W_\Gamma^{1,q'})$ is the solution of (3.9) with respect to the measure $\bar\mu$ and on the other hand $p_1 \in W_{r'}$ solves the following equation in $L^{r'}(J; W_\Gamma^{-1,q'})$

$$\begin{aligned} -(p_1)_t - \nabla\cdot\kappa\nabla p_1 + d_y(x,t,\bar y)p_1 &= \tilde f \\ p_1(T) &= 0, \end{aligned}$$

where the right hand side $\tilde f \in L^{r'}(J; W_\Gamma^{-1,q'})$ is induced by $\frac{\partial L}{\partial y}(x,t,\bar y,\bar u)$ and $\frac{\partial l}{\partial y}(x,t,\bar y)$.

Before we start discussing second order sufficient optimality conditions for problem (P), we will derive the second derivative of the Lagrangian w.r.t. the control u that will be widely used. From (3.4), we

obtain with the help of the introduced adjoint state:

$$\begin{aligned}\mathcal{L}''(u,\mu)h_1h_2 = \iint_Q \Big[&\frac{\partial^2 L}{\partial y^2}(x,t,y(u),u)y_{h_1}y_{h_2} + \frac{\partial^2 L}{\partial y \partial u}(x,t,y(u),u)(y_{h_1}h_2 + y_{h_2}h_1)\\ &+\frac{\partial^2 L}{\partial u^2}(x,t,y(u),u)h_1h_2 - p(u)\frac{\partial^2 d}{\partial y^2}(x,t,y(u))y_{h_1}y_{h_2}\Big]\,dxdt\\ &+\iint_\Sigma \frac{\partial^2 l}{\partial y^2}(x,t,y(u))y_{h_1}y_{h_2}d\sigma dt,\end{aligned} \tag{3.12}$$

where $p(u)$ is the solution of (3.9) with u, $y(u)$ and μ taken for $\bar{u}$, $\bar{y}$ and $\bar{\mu}$, respectively. The following proposition shows, that the second derivative of the Lagrangian w.r.t. u is bounded, when considered as quadratic form on $L^2(Q)$.

Proposition 3.8. *Let the assumptions (A1)-(A6) be satisfied. Moreover, let* $u,\ h \in L^\infty(Q)$ *and* $\mu \in \mathcal{M}(\overline{Q})$ *be given. Then there is a constant* $c > 0$ *such that*

$$\left|\mathcal{L}''(u,\mu)h^2\right| \le c\|h\|^2_{L^2(Q)}.$$

Proof. The result mainly depends on the estimate of the term of the form

$$\left|\iint_Q p(u)\frac{\partial^2 d}{\partial y^2}(x,t,y(u))y_h^2 dxdt\right|, \tag{3.13}$$

where $p(u)$ is the solution of (3.9) and $y_h = G'(u)h$. The other parts of $\mathcal{L}''(u,\mu)$ are discussed by means of assumptions (A1)-(A6), the continuity of the state $y(u)$ and standard a priori estimates for the solution of the linearized state equation. Let us come back to the estimation of (3.13). According to Theorem 3.7 and usual embedding results, we expect for the adjoint state

$$p(u) \in L^{r'}(J;W^{1,q'}_\Gamma) \hookrightarrow L^{r'}(J;L^{s'}(\Omega)), \qquad \text{for } r' < \frac{2q}{q+d},\ s' < \frac{dq'}{d-q'} < \frac{d}{d-2}$$

due to Definition 3.6 for the choice of q'. By means of Hölder inequality, assumptions on d_{yy} and the continuity of the state, we find

$$\begin{aligned}\left|\iint_Q p(u)\frac{\partial^2 d}{\partial y^2}(x,t,y(u))y_h^2\right| &\le c\|p(u)\|_{L^{r'}(J;L^{s'}(\Omega))}\|y_h\|^2_{L^r(J;L^s(\Omega))}\\ &\le c\|p(u)\|_{L^{r'}(J;W^{1,q'}_\Gamma(\Omega))}\|y_h\|^2_{L^r(J;L^s(\Omega))},\end{aligned}$$

with $s > d$ and $r > \frac{4q}{q-d}$. Relying on the regularity result given in Proposition 2.16, the linearized state y_h belongs to a space $L^{\frac{2}{\theta}}(J;L^{\frac{6}{1-\theta}}(\Omega))$ for all $\theta \in (0,1)$ considering the direction h as an element in $L^2(Q)$. Due to the estimate above, we have to require

$$\frac{2}{\theta} > \frac{4q}{q-d} \qquad \Rightarrow \qquad \theta < \frac{q-d}{2q}$$

that can be satisfied by a $\theta > 0$ since $q > d$. Fixing such θ, we of course fulfil the second assumption $\frac{6}{1-\theta} > d$ of the estimation for the case of $d = 2, 3$. Thus, we continue the estimate with some $\theta < \frac{q-d}{2q}$

$$\begin{aligned}\left| \iint_Q p(u) \frac{\partial^2 d}{\partial y^2}(x,t,y(u)) y_h^2 \right| &\leq c \|p(u)\|_{L^{r'}(J;W^{1,q'}_\Gamma(\Omega))} \|y_h\|^2_{L^r(J;L^s(\Omega))} \\ &\leq c \|p(u)\|_{L^{r'}(J;W^{1,q'}_\Gamma(\Omega))} \|y_h\|^2_{L^{\frac{2}{\theta}}(J;L^{\frac{6}{1-\theta}}(\Omega))} \\ &\leq c \|p(u)\|_{L^{r'}(J;W^{1,q'}_\Gamma(\Omega))} \|h\|^2_{L^2(Q)},\end{aligned}$$

see Proposition 2.16. □

Remark 3.9. *Please note that the estimate of Proposition 3.8 can only be proven, if the state variable y appears linearly in the pointwise state constraints. In order to deal with more general constraints like $g(y(x,t)) \leq 0$, where g is induced by a Nemytski operator, the continuity of solution operator G from $L^2(Q)$ to $C(\overline{Q})$ becomes necessary, since the term $< g_{yy}(\bar{y})(y_h)^2, \bar{\mu} >_{C(\overline{Q}),\mathcal{M}(\overline{Q})}$ occurs in the second derivative of the Lagrangian. However, in many real world applications pointwise state constraints are directly claimed to the state variable y, see e.g. the temperature variable in the thermistor problem discussed in* [26].

Based on the estimate in Proposition 3.8, we are able to discuss the remainders of the first and second Taylor expansion of the Lagrangian. A Taylor expansion of $\mathcal{L}$ is given by

$$\begin{aligned}\mathcal{L}(u,\bar{\mu}) - \mathcal{L}(\bar{u},\bar{\mu}) =& \mathcal{L}'(\bar{u},\bar{\mu})(u-\bar{u}) + r_{1,\mathcal{L}} \\ =& \mathcal{L}'(\bar{u},\bar{\mu})(u-\bar{u}) + \frac{1}{2}\mathcal{L}''(\bar{u},\bar{\mu})(u-\bar{u})^2 + r_{2,\mathcal{L}}\end{aligned}$$

Taking into account Assumptions (A1)-(A4), we are able to verify

$$\begin{aligned}|r_{1,\mathcal{L}}| &\leq c_{\mathcal{L}} \|u-\bar{u}\|^2_{L^2(Q)} \\ |r_{2,\mathcal{L}}| &\leq c_{\mathcal{L}} \|u-\bar{u}\|_{L^\infty(Q)} \|u-\bar{u}\|^2_{L^2(Q)}.\end{aligned} \tag{3.14}$$

The constant $c_{\mathcal{L}} > 0$ depends in particular on $\bar{u}$, $\bar{y} = G(\bar{u})$ and $\bar{p}$ as the solution of the adjoint equation, see (3.9). Note, that the $L^\infty(Q)$-norm in the second estimate can be weakened to a norm in $L^r(J;L^p(\Omega))$ with $r > \frac{2q}{q-d}$ and $p \geq \frac{dq}{d+q}$.

4. Second order sufficient optimality conditions

Our aim is to establish sufficient optimality conditions for problem (P), where we will follow the approach of Casas, Tröltzsch and Unger [9]. In the sequel $(\bar{u}, \bar{y} = G(\bar{u}))$ satisfies together with the dual variables $(\bar{p}, \bar{\mu})$ the first order necessary conditions given in Theorem 3.7. We associate to $\bar{u}$ the following cone of critical directions

$$C(\bar{u}) = \{h \in L^\infty(Q) : \ h \text{ satisfies (4.2) and (4.3)}\} \tag{4.1}$$

$$h(x,t) \begin{cases} \geq 0, & \text{if } \bar{u}(x,t) = u_a \\ \leq 0, & \text{if } \bar{u}(x,t) = u_b \end{cases} \tag{4.2}$$

$$y_h = G'(\bar{u})h \geq 0 \quad \text{if} \quad \bar{y}(x,t) = y_c(x,t) \tag{4.3}$$

Note, that $C(\bar{u})$ can be interpreted as the linearized cone at the point $\bar{u}$, see e.g. Maurer and Zowe [30]. The following theorem tells us that the difference of every feasible point u to $\bar{u}$ can be approximated by an element from the cone $C(\bar{u})$.

Theorem 4.1. *Suppose that Assumption 3.5 is satisfied. Then for all feasible controls $\hat{u} \in U_{ad}$ of problem (P) there is a $h \in C(\bar{u})$ such that the difference $r_h = \hat{u} - \bar{u} - h$ can be estimated by*

$$\|r_h\|_{L^\infty(Q)} \le c\|\hat{u} - \bar{u}\|^2_{L^2(Q)} \tag{4.4}$$

Moreover, the respective distance in the states $r_{y,h} = \hat{y} - \bar{y} - y_h$ with $y_h = G'(\bar{u})h$ can be estimated by

$$\|r_{y,h}\|_Y \le c\|\hat{u} - \bar{u}\|^2_{L^2(Q)}. \tag{4.5}$$

Proof. We will follow the lines of [9, Theorem 4.2]. Let $\hat{u} \in U_{ad}$ be a feasible control with associated state $\hat{y} = G(\hat{u})$. Moreover, we introduce $\tilde{y} = G'(\hat{u})(\hat{u} - \bar{u})$ as the solution of the linearized state equation in direction $\hat{u} - \bar{u}$. By Proposition 3.3, the estimate

$$\|\hat{y} - \bar{y} - \tilde{y}\|_Y \le c\|\hat{u} - \bar{u}\|^2_{L^2(Q)} \tag{4.6}$$

is valid. Let us introduce the mapping $\Phi(u) = G(u) - y_c$. Then the pointwise state constraints of problem (P) can be written in an abstract way by $\Phi(u) \in K$ or $\Phi(u) \ge_K 0$, where K is the positive convex cone $K := \{z \in C(\overline{Q}) : z(x,t) \ge 0 \quad \forall (x,t) \in \overline{Q}\}$. It is known that the linearized Slater condition in Assumption 3.5 is sufficient for the famous regularity condition by Zowe and Kurcyusz [41], see e.g. [40, Ch.6.1.2.]. This regularity condition can be written by

$$\Phi'(\bar{u})\mathcal{C}(\bar{u}) - \mathcal{K}(\Phi(\bar{u})) = C(\overline{Q}),$$

with $\mathcal{C}(\bar{u}) := \{\alpha(u - \bar{u}) : \alpha \ge 0, u \in U_{ad}\}$ and $\mathcal{K}(\bar{z}) := \{\beta(z - \bar{z}) : \beta \ge 0, z \in K\}$, respectively. Due to feasibility of $\hat{u}$, we have $\Phi(\hat{u}) \in K$ and a Taylor expansion gives

$$\Phi(\hat{u}) = \Phi(\bar{u}) + \Phi'(\bar{u})(\hat{u} - \bar{u}) + r_1^\Phi$$

where the remainder term can be estimated by

$$\|r_1^\Phi\|_{C(\overline{Q})} \le c\|\hat{u} - \bar{u}\|^2_{L^2(Q)}$$

due to (4.6) and the definition of Φ. Since $\Phi(\bar{u})$ and $\Phi(\hat{u})$ belong to K, the Taylor expansion implies

$$\Phi'(\bar{u})(\hat{u} - \bar{u}) \in \mathcal{K}(\Phi(\bar{u})) - r_1^\Phi.$$

Hence, we have $\hat{u} - \bar{u} \in \mathcal{C}(\bar{u})$ and $\Phi'(\bar{u})(\hat{u} - \bar{u}) \ge_{\mathcal{K}(\Phi(\bar{u}))} -r_1^\Phi$. According to [36], the last inequality is regular in the sense of Robinson, and we can thus apply the linear version of the Robinson-Ursescu theorem. Hence, we obtain the existence of a constant $c > 0$ and an element $h \in \mathcal{C}(\bar{u})$ satisfying

$$\|\hat{u} - \bar{u} - h\|_{L^\infty(Q)} \le c\|r_1^\Phi\|_{C(\bar{Q})} \le c\|\hat{u} - \bar{u}\|^2_{L^2(Q)}.$$

Moreover, we have $\Phi'(\bar{u})h \in \mathcal{K}(\Phi(\bar{u}))$ and thus $h \in C(\bar{u})$, see (4.1). The difference $r_{y,h} := \hat{y} - \bar{y} - y_h$ with $y_h = G'(\bar{u})h$ can be estimated as follows

$$\|r_{y,h}\|_Y \le \|\hat{y} - \bar{y} - \tilde{y}\|_Y + \|G'(\bar{u})(\hat{u} - \bar{u} - h)\|_Y.$$

Hence, the estimate (4.5) immediately follows from (4.6) and (4.4). □

Let us define, for a fixed $\tau > 0$, the set

$$Q_\tau = \{(x,t) \in Q : |\bar{p}(x,t) + \frac{\partial L}{\partial u}(x,t,\bar{y},\bar{u})| \ge \tau\}.$$

Hence, Q_τ is a subset of so called strongly active control constraints. Moreover, we introduce the projection operator $P_\tau : L^\infty(Q) \to L^\infty(Q)$, $u \mapsto P_\tau u = \chi_{Q \setminus Q_\tau} u$, i.e. $(P_\tau u)(x) = 0$ a.e. on

Q_τ. Following [9], it is also possible to incorporate "strongly active" state constraints. Therefore, we introduce the following subset of $C(\bar{u})$

$$C_{\beta,\tau}(\bar{u}) = \left\{ h \in C(\bar{u}) : < y_h, \bar{\mu} >_{C(\overline{Q}),\mathcal{M}(\overline{Q})} \leq \beta \iint_{Q\setminus Q_\tau} |h(x,t)| dxdt \right\}$$

for fixed constants $\tau > 0$ and $\beta > 0$. Now, we are in the position to require second order sufficient optimality conditions:

(SSC) There exist positive numbers β, τ and δ such that

$$\mathcal{L}''(\bar{u},\bar{\mu})h_2^2 \geq \|h_2\|^2_{L^2(Q)} \tag{4.7}$$

holds for all h_2 constructed in the following way: For every $h \in C_{\beta,\tau}(\bar{u})$ we split the direction h in $h_1 = h - P_\tau h$ and $h_2 = P_\tau h$.

By means of this condition, we can formulate:

Theorem 4.2. *Let the feasible control $\bar{u} \in U_{ad}$ with associated state $\bar{y}$ satisfy Assumption 3.5 and the first order necessary optimality conditions* (3.8)-(3.11)*. Moreover, we require* ***(SSC).*** *Then there are constants $\rho > 0$ and $\delta' > 0$ such that*

$$J(\hat{y},\hat{u}) \geq J(\bar{y},\bar{u}) + \delta' \|\hat{u} - \bar{u}\|^2_{L^2(Q)}$$

holds for all feasible controls $\hat{u} \in U_{ad}$ with respective state $\hat{y} = G(\hat{u})$ satisfying $\|\hat{u} - \bar{u}\|_{L^\infty(Q)} \leq \rho$.

Proof. Let $\hat{u}$ be a feasible control with associated state $\hat{y} = G(\hat{u})$ and $\|\hat{u} - \bar{u}\|_{L^\infty(Q)} \leq \rho$. Due to definition of the Lagrangian we have

$$J(\hat{y},\hat{u}) - J(\bar{y},\bar{u}) = \mathcal{L}(\hat{u},\bar{\mu}) - \mathcal{L}(\bar{u},\bar{\mu}) - < G(\bar{u}) - G(\hat{u}), \bar{\mu} >_{C(\overline{Q}),\mathcal{M}(\overline{Q})} . \tag{4.8}$$

Next, we approximate $\hat{u} - \bar{u}$ by an element $h \in C(\bar{u})$ according to Theorem 4.1. In this way, we have the following remainder estimates for $r_h := \hat{u} - \bar{u} - h$ and $r_{y,h} = G(\hat{u}) - G(\bar{u}) - G'(\bar{u})h$:

$$\|r_h\|_{L^\infty(Q)} \leq c\|\hat{u} - \bar{u}\|^2_{L^2(Q)} \tag{4.9}$$

$$\|r_{y,h}\|_Y \leq c\|\hat{u} - \bar{u}\|^2_{L^2(Q)}, \tag{4.10}$$

where we recall that the state space Y is embedded in $C(\overline{Q})$. Now, we have to consider two different cases for the approximative direction h.

Case I: $h \in C_{\beta,\tau}(\bar{u})$

Here, we make use of first order and second order sufficient conditions. Due to complementary slackness conditions (3.11) and the feasibility of $\hat{u}$, we have

$$< G(\bar{u}) - G(\hat{u}), \bar{\mu} >_{C(\overline{Q}),\mathcal{M}(\overline{Q})} \leq 0.$$

Hence, we neglect this term in (4.8) and a Taylor expansion of $\mathcal{L}$ yields

$$\begin{aligned} J(\hat{y},\hat{u}) - J(\bar{y},\bar{u}) \geq & \mathcal{L}(\hat{u},\bar{\mu}) - \mathcal{L}(\bar{u},\bar{\mu}) \\ = & \mathcal{L}'(\bar{u},\bar{\mu})(u - \bar{u}) + \frac{1}{2}\mathcal{L}''(\bar{u},\bar{\mu})(u - \bar{u})^2 + r_{2,\mathcal{L}}. \end{aligned}$$

Using the variational inequality (3.10), one can easily find

$$J(\hat{y},\hat{u}) - J(\bar{y},\bar{u}) \geq \tau \iint_{Q_\tau} |\hat{u} - \bar{u}| dxdt + \frac{1}{2}\mathcal{L}''(\bar{u},\bar{\mu})(u - \bar{u})^2 + r_{2,\mathcal{L}}. \tag{4.11}$$

Let us introduce the abbreviation $B := \mathcal{L}''(\bar{u},\bar{\mu})$ for the bilinear form associated to the second derivative of the Lagrangian. We proceed with

$$B[\hat{u}-\bar{u}]^2 = B[h]^2 + 2B[h,r_h] + B[r_h]^2$$

since $\hat{u}-\bar{u} = h + r_h$. In this case we consider $h \in C_{\beta,\tau}(\bar{u})$ such that (SSC) applies to $B[h]^2$. By means of the splitting of $h = h_1 + h_2$ as described in (SSC), we obtain

$$\begin{aligned} B[h]^2 &= B[h_1]^2 + 2B[h_1,h_2] + B[h_2]^2 \\ &\geq \delta\|h_2\|^2_{L^2(Q)} - c\|h_1\|_{L^2(Q)}\|h_2\|_{L^2(Q)} - c\|h_1\|^2_{L^2(Q)} \end{aligned}$$

using the estimates of Proposition 3.8. Forthcoming, Young' inequality implies

$$\begin{aligned} B[h]^2 &\geq \frac{\delta}{2}\|h_2\|^2_{L^2(Q)} - c\|h_1\|^2_{L^2(Q)} \\ &= \frac{\delta}{2}\iint_{Q\setminus Q_\tau} |\hat{u}-\bar{u}-r_h|^2 dxdt - c\iint_{Q_\tau} |\hat{u}-\bar{u}-r_h|^2 dxdt \\ &\geq \frac{\delta}{2}\iint_{Q\setminus Q_\tau} |\hat{u}-\bar{u}|^2 dxdt - c\iint_{Q\setminus Q_\tau} |\hat{u}-\bar{u}||r_h| dxdt \\ &\quad - c\iint_{Q_\tau} |\hat{u}-\bar{u}|^2 dxdt - c\iint_{Q_\tau} |\hat{u}-\bar{u}||r_h| dxdt - c\iint_{Q_\tau} |r_h|^2 dxdt. \end{aligned}$$

Assume $\rho < 1$ is given and $\|\hat{u}-\bar{u}\|_{L^\infty(Q)} < \rho$. Using

$$\iint_{Q_\tau} |\hat{u}-\bar{u}|^2 dxdt \leq \|\hat{u}-\bar{u}\|_{L^\infty(Q)} \iint_{Q_\tau} |\hat{u}-\bar{u}| dxdt$$

and (4.9), we derive

$$B[h]^2 \geq \frac{\delta}{2}\iint_{Q\setminus Q_\tau} |\hat{u}-\bar{u}|^2 dxdt - c\rho\iint_{Q_\tau} |\hat{u}-\bar{u}| dxdt - c\rho\|\hat{u}-\bar{u}\|^2_{L^2(Q)}.$$

Similar estimates for the terms $B[h,r_h]$ and $B[r_h]^2$ yields altogether

$$\mathcal{L}''(\bar{u},\bar{\mu})(\hat{u}-\bar{u})^2 \geq \frac{\delta}{2}\iint_{Q\setminus Q_\tau} |\hat{u}-\bar{u}|^2 dxdt - c\rho\iint_{Q_\tau} |\hat{u}-\bar{u}| dxdt - c\rho\|\hat{u}-\bar{u}\|^2_{L^2(Q)}.$$

Substituting this estimate in (4.11) and choosing ρ sufficiently small, we derive

$$\begin{aligned} J(\hat{y},\hat{u}) - J(\bar{y},\bar{u}) \geq& (\tau - c\rho)\iint_{Q_\tau} |\hat{u}-\bar{u}| dxdt + \frac{\delta}{4}\iint_{Q\setminus Q_\tau} |\hat{u}-\bar{u}|^2 dxdt \\ &- c\rho\|\hat{u}-\bar{u}\|^2_{L^2(Q)} - |r_{2,\mathcal{L}}| \\ \geq& \frac{\tau}{2}\iint_{Q_\tau} |\hat{u}-\bar{u}| dxdt + \frac{\delta}{4}\iint_{Q\setminus Q_\tau} |\hat{u}-\bar{u}|^2 dxdt \\ &- c\rho\|\hat{u}-\bar{u}\|^2_{L^2(Q)} - |r_{2,\mathcal{L}}|. \end{aligned}$$

Since $\|\hat{u}-\bar{u}\|_{L^\infty(Q)} < \rho < 1$, we have $|\hat{u}-\bar{u}| \geq |\hat{u}-\bar{u}|^2$ almost everywhere in Q. Due to the remainder estimate (3.14), we can conclude

$$\begin{aligned} J(\hat{y},\hat{u}) - J(\bar{y},\bar{u}) \geq & \frac{\tau}{2}\iint_{Q_\tau} |\hat{u}-\bar{u}|^2 dxdt + \frac{\delta}{4}\iint_{Q\setminus Q_\tau} |\hat{u}-\bar{u}|^2 dxdt \\ & - c\rho\|\hat{u}-\bar{u}\|^2_{L^2(Q)} - c_{\mathcal{L}}\|\hat{u}-\bar{u}\|_{L^\infty(Q)}\|\hat{u}-\bar{u}\|^2_{L^2(Q)} \\ \geq & (\delta' - c\rho)\|\hat{u}-\bar{u}\|^2_{L^2(Q)} \\ \geq & \frac{\delta'}{2}\|\hat{u}-\bar{u}\|^2_{L^2(Q)} \end{aligned}$$

for sufficiently small $\rho > 0$.

Case II: $h \in C(\bar{u}) \setminus C_{\beta,\tau}(\bar{u})$

In this case we have to deduce the quadratic growth condition from the first order optimality conditions. Note that the linearized state $y_h = G'(\bar{u})h$ satisfies the following inequality

$$< y_h, \bar{\mu} >_{C(\overline{Q}),\mathcal{M}(\overline{Q})} > \beta \iint_{Q\setminus Q_\tau} |h(x,t)| dxdt \tag{4.12}$$

Now the first order Taylor expansion of the Lagrangian in (4.8) and the fact $G(\hat{u}) - G(\bar{u}) = G'(\bar{u})h + r_{y,h}$ yields

$$J(\hat{y},\hat{u}) - J(\bar{y},\bar{u}) = \mathcal{L}'(\bar{u},\bar{\mu})(u-\bar{u}) + r_{1,\mathcal{L}} + < G'(\bar{u})h + r_{y,h}, \bar{\mu} >_{C(\overline{Q}),\mathcal{M}(\overline{Q})} .$$

The variational inequality (3.10) and (4.12) gives

$$J(\hat{y},\hat{u}) - J(\bar{y},\bar{u}) \geq \tau \iint_{Q_\tau} |\hat{u}-\bar{u}| dxdt + \beta \iint_{Q\setminus Q_\tau} |h| dxdt + r_{1,\mathcal{L}} + < r_{y,h}, \bar{\mu} >_{C(\overline{Q}),\mathcal{M}(\overline{Q})}$$

By means of (4.9), (4.10) and (3.14), we obtain

$$\begin{aligned} J(\hat{y},\hat{u}) - J(\bar{y},\bar{u}) \geq & \min\{\tau,\beta\}\|\hat{u}-\bar{u}\|_{L^1(Q)} - c\|\hat{u}-\bar{u}\|^2_{L^2(Q)} \\ \geq & \delta\|\hat{u}-\bar{u}\|_{L^1(Q)} - \|\hat{u}-\bar{u}\|_{L^\infty(Q)}\|\hat{u}-\bar{u}\|_{L^1(Q)} \end{aligned}$$

As in case I, we assume $\rho < 1$ such that $|\hat{u}-\bar{u}| \geq |\hat{u}-\bar{u}|^2$ almost everywhere in Q. Thus, we conclude

$$\begin{aligned} J(\hat{y},\hat{u}) - J(\bar{y},\bar{u}) \geq & \delta\|\hat{u}-\bar{u}\|^2_{L^2(Q)} - \rho\|\hat{u}-\bar{u}\|^2_{L^2(Q)} \\ \geq & \delta'\|\hat{u}-\bar{u}\|^2_{L^2(Q)} \end{aligned}$$

for some $\delta' > 0$ provided $\rho > 0$ is chosen sufficiently small. □

Following the lines of [7, Section 7], a much smaller cone of critical directions was necessary in order to formulate second order sufficient conditions. Again, the continuity of the control-to-state mapping from $L^2(Q)$ to $C(\overline{Q})$ is decisive such that a restriction of the spatial dimension to one becomes necessary. Thus, the adaption of the ideas of the proof presented in [7], where the smallest possible cone of critical directions is used, to higher dimensional parabolic problems remains still an open question.

5. Appendix

In this appendix we describe geometric configurations and conditions on the coefficient function κ for which our Assumption 2.6 holds true. We will distinguish between the two-dimensional and the three-dimensional case since the requirements on the geometry and the coefficient function differ essentially.

5.1. **The elliptic regularity result: 2d.** The following proposition shows that Assumption 2.6 is satisfied under very weak conditions. This result was elaborated in Gröger's pioneering work [21].

Proposition 5.1. *Let $\Omega \subset \mathbb{R}^2$ be a Lipschitz domain and Γ be an open part of the boundary $\partial\Omega$. Assume that Γ satisfies Assumption 2.2 i). Finally, let κ be a measurable, bounded, elliptic coefficient function, taking its values in the set of real 2×2 matrices. Then there is a number $q_0 > 2$, such that*

$$-\nabla \cdot \kappa \nabla + 1 : W_\Gamma^{1,q}(\Omega) \to W_\Gamma^{-1,q}(\Omega) \tag{5.1}$$

is a topological isomorphism for all $q \in [2, q_0]$.

Corollary 5.2. *Under the Assumptions in Proposition 5.1, there is a $q_1 > 2$, such that* (5.1) *is a topological isomorphism even for all $q \in [q_1', q_1]$.*

Proof. Let κ^* be the adjoint coefficient function and q_0^* the number which is associated to $-\nabla\cdot\kappa^*\nabla+1$ via Proposition 5.1. It it not hard to see that $-\nabla \cdot \kappa \nabla + 1 : W_\Gamma^{1,q'}(\Omega) \to W_\Gamma^{-1,q'}(\Omega)$ is the adjoint of $-\nabla \cdot \kappa^* \nabla + 1 : W_\Gamma^{1,q}(\Omega) \to W_\Gamma^{-1,q}(\Omega)$. Thus, it is sufficient to take q_1 as $\min(q_0, q_0^*)$. □

Remark 5.3. *It is known that $q_0 - 2$ can be arbitrarily small in general.*

5.2. **The elliptic regularity result: 3d.** In the following we introduce geometric suppositions on the domain Ω, continuity properties of the coefficient function κ and geometric suppositions on the boundary part Γ which altogether assure that Assumption 2.6 is really fulfilled. We start with a first global

Assumption 5.4. *$\Omega \subset \mathbb{R}^3$ is a strong Lipschitz domain (see* [32, Ch. 1.1.9]*) Let $\Omega_\circ \subset \Omega$ be a C^1-subdomain whose closure is also contained in Ω. Assume that κ is an elliptic coefficient function, taking its values in the set of real, symmetric 3×3-matrices. Suppose further that the restriction of κ to $\Omega_\circ$ and to $\Omega \setminus \overline{\Omega_\circ}$ is uniformly continuous.*

Synonymous to 'strong Lipschitz domain' is 'domain with Lipschitz boundary', see [20, Ch. 1.2.2]. Moreover, a domain is a strong Lipschitz domain if and only if it has the uniform cone property, see [20, Thm. 1.2.2.2]. For instance, every bounded and convex domain is a strong Lipschitz domain.

We continue with the introduction of geometric assumptions on the boundary part Γ.

Definition 5.5. *Let us fix once and for all an open triangle $\triangle \subset \mathbb{R}^2$. Let further P_1 be one vertex of $\triangle$ and $\mathcal{S}_1$ one of the adjacent sides. Let $\mathcal{S}_1^+$ be one half of $\mathcal{S}_1$ with endpoints P_1, P_2. Define $\Pi := \triangle \times (-1, 1)$ and denote by $\mathcal{P}^-$ its (open) groundplate and by $\mathcal{P}^+$ its (open) coverplate. Finally, we define the boundary parts Σ, Υ by*

$$\Sigma := \mathcal{S}_1^+ \times (-1, 1), \quad \Upsilon := \mathcal{S}_1 \times (-1, 1).$$

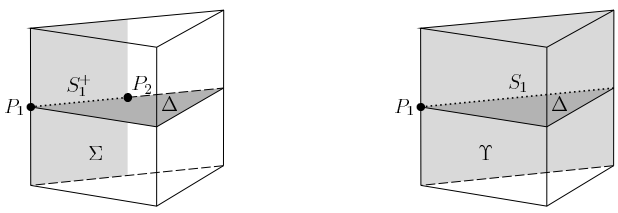

FIGURE 1. The two model constellations

Assumption 5.6. *Let $\Gamma \subset \partial\Omega$ be an open part of the boundary. If $\partial\Gamma$ denotes the boundary of Γ within $\partial\Omega$, then we demand: for every $\mathrm{x} \in \partial\Gamma$ there is a neighbourhood U_x of x and a C^1-diffeomorphism ϕ_x from a neighbourhood of $\overline{U_\mathrm{x}}$ into $\mathbb{R}^3$, such that $\phi_\mathrm{x}(\Omega \cap U_\mathrm{x}) = \Pi$, and either*

i) $\phi_\mathrm{x}(\mathrm{x}) = (P_2, 0) \in \mathbb{R}^3$ *and*
a) $\phi_\mathrm{x}(\Gamma \cap U_\mathrm{x}) = \Sigma$, *or*
b) $\phi_\mathrm{x}(\Gamma \cap U_\mathrm{x}) = \Sigma \cup \mathcal{P}^+ \cup (\mathcal{S}_1^+ \times \{1\})$ *or*
c) $\phi_\mathrm{x}(\Gamma \cap U_\mathrm{x}) = \Sigma \cup \mathcal{P}^- \cup (\mathcal{S}_1^+ \times \{-1\})$ *or*
d) $\phi_\mathrm{x}(\Gamma \cap U_\mathrm{x}) = \Sigma \cup (\mathcal{S}_1^+ \times \{-1, 1\}) \cup \mathcal{P}^+ \cup \mathcal{P}^-$
or
ii) $\phi_\mathrm{x}(\mathrm{x}) = (P_1, 0) \in \mathbb{R}^3$ *and*
e) $\phi_\mathrm{x}(\Gamma \cap U_\mathrm{x}) = \Upsilon$, *or*
f) $\phi_\mathrm{x}(\Gamma \cap U_\mathrm{x}) = \Upsilon \cup \mathcal{P}^+ \cup (\mathcal{S}_1 \times \{1\})$, *or*
g) $\phi_\mathrm{x}(\Gamma \cap U_\mathrm{x}) = \Upsilon \cup \mathcal{P}^- \cup (\mathcal{S}_1 \times \{-1\})$, *or*
h) $\phi_\mathrm{x}(\Gamma \cap U_\mathrm{x}) = \Upsilon \cup (\mathcal{S}_1 \times \{-1, 1\}) \cup \mathcal{P}^+ \cup \mathcal{P}^-$.

Remark 5.7. *Possibly diminishing the neighbourhoods U_x one can always arrange that U_x does not touch $\Omega_\circ$. In this spirit we will always assume that the coefficient function κ is uniformly continuous on any set $\Omega \cap U_\mathrm{x}$.*

We intend to prove the following theorem, which we consider as the main result of this section:

Theorem 5.8. *Under the Assumptions 5.4/5.6 there is $q_0 > 3$ such that for all $q \in [2, q_0]$*

$$-\nabla \cdot \kappa \nabla + 1 : W_\Gamma^{1,q}(\Omega) \to W_\Gamma^{-1,q}(\Omega) \tag{5.2}$$

is a topological isomorphism.

Corollary 5.9. *Under the Assumptions 5.4/5.6,* (5.2) *is a topological isomorphism even for all $q \in [q_0', q_0]$.*

Remark 5.10. *In fact, the model sets in Assumption 5.6 provide a great variety of admissible geometrical constellations. In particular, one can take Π itself as the domain Ω and Γ as one of the right hand sides in a) – h).*
Concerning the geometric settings we have in mind, Assumption 2.2 ii) is always fulfilled: For $\Omega = \Pi$ and Γ as any of the right hand sides of a) – h) it is obvious, and in case of $\Gamma \subset \partial\Omega$ this is implied by Assumption 5.6.

5.3. **The proof of Theorem 5.8.** Let us start this subsection by quoting some previous results which will later allow to deduce the proof of Theorem 5.8.

Lemma 5.11. *Let $\Lambda \subset \mathbb{R}^d$ be a bounded Lipschitz domain and Ξ be an open part of its boundary. Let ρ be a bounded, measurable coefficient function.*

i) For all $q \in (1, \infty)$ we have the estimate

$$\| -\nabla \cdot \rho \nabla \|_{\mathcal{L}(W_\Xi^{1,q}(\Lambda); W_\Xi^{-1,q}(\Lambda))} \leq \|\rho\|_{L^\infty(\Omega; \mathcal{L}(\mathbb{R}^d))}. \tag{5.3}$$

ii) If $(\nabla \cdot \rho \nabla)^{-1} \in \mathcal{L}(W_\Xi^{-1,q}(\Lambda); W_\Xi^{1,q}(\Lambda))$ and $\hat{\rho}$ is another coefficient function on Λ which satisfies

$$\|\rho - \hat{\rho}\|_{L^\infty(\Lambda)} \|(\nabla \cdot \rho \nabla)^{-1}\|_{\mathcal{L}(W_\Xi^{-1,q}(\Lambda); W_\Xi^{1,q}(\Lambda))} < 1,$$

then also $(\nabla \cdot \hat{\rho} \nabla)^{-1} \in \mathcal{L}(W_\Xi^{-1,q}(\Lambda); W_\Xi^{1,q}(\Lambda))$.

iii) Point ii) continues to hold, if there $\nabla\cdot\rho\nabla$ *and* $\nabla\cdot\hat{\rho}\nabla$ *are replaced by* $\nabla\cdot\rho\nabla-1$ *and* $\nabla\cdot\hat{\rho}\nabla-1$*, respectively.*

Proof. i) follows directly from the definition of $-\nabla\cdot\rho\nabla$ and Hölder's inequality.
ii) and iii) are implied by i) and a classical perturbation argument, cf. [29, Ch. IV.1.4, Thm. 1.16]. □

We proceed with quoting a result on real interpolation of Sobolev spaces from [17].

Proposition 5.12. *Let* $\Lambda\subset\mathbb{R}^3$ *be a bounded Lipschitz domain and let* Ξ *satisfy – mutatis mutandis – Assumption 2.2 ii). If* $q_0,q_1\in(1,\infty)$, $\varsigma\in(0,1)$ *and* $\frac{1}{q}=\frac{1-\varsigma}{q_0}+\frac{\varsigma}{q_1}$*, then one has the following identity concerning real interpolation:*

$$(W^{1,q_0}_{\Xi}(\Lambda);W^{1,q_1}_{\Xi}(\Lambda))_{\varsigma,q}=W^{1,q}_{\Xi}(\Lambda). \tag{5.4}$$

Corollary 5.13. *If* $q_0,q_1\in(1,\infty)$ *and* $\varsigma\in(0,1)$ *and* $\frac{1}{q}=\frac{1-\varsigma}{q_0}+\frac{\varsigma}{q_1}$*, then*

$$(W^{-1,q_0}_{\Xi}(\Lambda);W^{-1,q_1}_{\Xi}(\Lambda))_{\varsigma,q}=W^{-1,q}_{\Xi}(\Lambda). \tag{5.5}$$

Proof. Since also $\frac{1}{q'}=\frac{1-\varsigma}{q_0'}+\frac{\varsigma}{q_1'}$, one obtains from (5.4) and the duality formula for real interpolation (cf. [39, Ch. 1.11.2])

$$(W^{-1,q_0}_{\Xi}(\Lambda);W^{-1,q_1}_{\Xi}(\Lambda))_{\varsigma,q}=\big(\big(W^{1,q_0'}_{\Xi}(\Lambda)\big)';\big(W^{1,q_1'}_{\Xi}(\Lambda)\big)'\big)_{\varsigma,q}=$$

$$=\big((W^{1,q_0'}_{\Xi}(\Lambda);W^{1,q_1'}_{\Xi}(\Lambda))_{\varsigma,q'}\big)'=\big(W^{1,q'}_{\Xi}(\Lambda)\big)'=W^{-1,q}_{\Xi}(\Lambda).$$

□

The following corollary is a direct consequence of the two foregoing results.

Corollary 5.14. *Assume* $q_0,q_1\in(1,\infty)$ *and*

$$A\in\mathcal{L}(W^{-1,q_0}_{\Xi}(\Lambda);W^{1,q_0}_{\Xi}(\Lambda))\cap\mathcal{L}(W^{-1,q_1}_{\Xi}(\Lambda);W^{1,q_1}_{\Xi}(\Lambda)).$$

Then $A\in\mathcal{L}(W^{-1,q}_{\Xi}(\Omega);W^{1,q}_{\Xi}(\Lambda))$ *for every* $q\in(q_0,q_1)$*.*

Remark 5.15. *We will apply Corollary 5.14 in the situations* $A=\big(-\nabla\cdot\rho\nabla+1\big)^{-1}$ *or* $A=\big(-\nabla\cdot\rho\nabla\big)^{-1}$*.* $\big(-\nabla\cdot\rho\nabla+1\big)^{-1}$ *continuously acts between* $W^{-1,2}_{\Xi}(\Lambda)$ *and* $W^{1,2}_{\Xi}(\Lambda)$ *by Lax-Milgram, what is also the case for* $\big(-\nabla\cdot\rho\nabla\big)^{-1}$ *if* $\partial\Lambda\setminus\Xi$ *has positive boundary measure. If one knows that it also acts continuously between* $W^{-1,q}_{\Gamma}(\Omega)$ *and* $W^{1,q}_{\Gamma}(\Omega)$ *for one* $q>2$ *then this is also true for* all $\tilde{q}$ *from the interval* $[2,q]$*.*

In the sequel we also need instruments which allow us to localize the elliptic equation under consideration.

Lemma 5.16. *Let* $\Lambda\subset\mathbb{R}^3$ *be a bounded Lipschitz domain,* Ξ *an open part of its boundary and* U *an open subset of* $\mathbb{R}^3$*. We put* $\Lambda_\bullet:=\Lambda\cap U$*,* $\Xi_\bullet:=\Xi\cap U$ *and fix an arbitrary function* $\eta\in C^\infty_0(\mathbb{R}^3)$ *with supp* $\eta\subset U$*.*

i) If $v\in W^{1,q}_{\Xi}(\Lambda)$ *then* $\eta v|_{\Lambda_\bullet}\in W^{1,q}_{\Xi_\bullet}(\Lambda_\bullet)$*.*

ii) Let for any $w \in W^{1,1}(\Lambda_\bullet)$ the symbol $\tilde{w}$ indicate the extension of w to Λ by zero.
a) For every $q \in (1,\infty)$ the mapping

$$W^{1,q}_{\Xi_\bullet}(\Lambda_\bullet) \ni v \longmapsto \widetilde{\eta v}$$

has its image in $W^{1,q}_{\Xi}(\Lambda)$ and is continuous.
b) If $U \cap (\partial\Lambda \setminus \Xi) = \emptyset$ then for any $q \in (1,\infty)$ the mapping

$$W^{1,q}(\Lambda_\bullet) \ni v \longmapsto \widetilde{\eta v}$$

has its image in $W^{1,q}_{\Xi}(\Lambda)$ and is continuous.

Proof. i) and iia) are proved in [23, Lemma 4.6], or see [24, Lemma 5.8]. It follows the proof of iib): obviously, supp η has a positive distance to $\overline{\Lambda} \setminus U$. Therefore, the continuation by zero to whole Λ preserves the $W^{1,q}$-property and, additionally, the corresponding operation is continuous. Thus, in order to show the property $\widetilde{\eta v} \in W^{1,q}_{\Xi}(\Lambda)$ it suffices to show that this indeed holds true for every element $v \in W^{1,q}(\Lambda_\bullet)$ which equals the restriction of a C^∞-function $\hat{v}$ on whole $\mathbb{R}^3$. But it is clear that in this case supp $\eta\hat{v}$ does not intersect $\partial\Lambda \setminus \Xi$ and, additionally, $\widetilde{\eta v} = \eta\hat{v}|_\Lambda$. □

Theorem 5.17. *Let $\Lambda, \Xi, U, \eta, \Lambda_\bullet, \Xi_\bullet$ be as in the foregoing lemma. Assume, additionally, that $\Lambda_\bullet := \Lambda \cap U$ is also a Lipschitz domain. Let $\kappa_\bullet$ denote the restriction of the coefficient function κ to $\Lambda_\bullet$ and let the operator*

$$-\nabla \cdot \kappa_\bullet \nabla : W^{1,2}_{\Xi_\bullet}(\Lambda_\bullet) \mapsto W^{-1,2}_{\Xi_\bullet}(\Lambda_\bullet)$$

be defined analogously to (2.1). *Assume $u \in W^{1,2}_{\Xi}(\Lambda)$ to be the solution of*

$$-\nabla \cdot \kappa \nabla u + u = f \in W^{-1,2}_{\Xi}(\Lambda). \tag{5.6}$$

Then the following holds true:

i) The function $v := \eta u|_{\Lambda_\bullet}$ is from $W^{1,2}_{\Xi_\bullet}(\Lambda_\bullet)$.
ii) The linear form

$$f_\bullet : w \mapsto \langle f, \widetilde{\eta w}\rangle$$

(where $\widetilde{\eta w}$ again means the extension by zero to whole Λ) is well defined and continuous on $W^{1,q'}_{\Xi_\bullet}(\Lambda_\bullet)$ whenever $f \in W^{-1,q}_{\Xi}(\Lambda)$.
iii) If we denote the linear form

$$w \longmapsto \int_{\Lambda_\bullet} u\kappa_\bullet \nabla\eta \cdot \nabla w \, dx$$

by T_u then v satisfies

$$-\nabla \cdot \kappa_\bullet \nabla v + v = -\kappa_\bullet \nabla u|_{\Lambda_\bullet} \cdot \nabla\eta|_{\Lambda_\bullet} + T_u + f_\bullet =: f^\bullet. \tag{5.7}$$

iv) Assume $q \in [2,6]$. Then the right hand side $f^\bullet$ of (5.7) *is from $W^{-1,q}_{\Xi_\bullet}(\Lambda_\bullet)$ provided that $f \in W^{-1,q}_{\Xi}(\Lambda)$. Moreover, the mapping $W^{-1,q}_{\Xi}(\Lambda) \ni f \mapsto f_\bullet \in W^{-1,q}_{\Xi_\bullet}(\Lambda_\bullet)$ is continuous.*
v) If $U \cap (\partial\Lambda \setminus \Xi) = \emptyset$, then one can also set $\Xi_\bullet := \partial\Lambda_\bullet$, and, hence, the right hand side $f^\bullet$ of (5.7) *may be interpreted as an element $f^\blacklozenge$ from $W^{-1,q}_{\partial\Omega}(\Lambda_\bullet)$.*

Proof. i) – iv) are proved in [23, Ch. 4.2.].
v) The condition $U \cap (\partial\Lambda \setminus \Xi) = \emptyset$ implies $U \cap \partial\Lambda = U \cap \Xi = \Xi_\bullet$. Since $\Lambda_\bullet = \Lambda \cap U$, one has

$$\partial\Lambda_\bullet \subset (\partial\Lambda \cap U) \cup (\Lambda \cap \partial U) \cup (\partial\Lambda \cap \partial U) = \Xi_\bullet \cup (\Lambda \cap \partial U) \cup (\partial\Lambda \cap \partial U).$$

Consequently, for any $\vartheta \in C^\infty(\mathbb{R}^d)$ with supp $\vartheta \subset U$ and any function $\psi \in W^{1,q'}(\Lambda_\bullet)$, the function $\vartheta|_{\Lambda_\bullet}\psi$ belongs to $W^{1,q'}_{\Xi_\bullet}(\Lambda_\bullet)$. We fix such a function ϑ, which, in addition, satisfies $\vartheta \equiv 1$ on $\operatorname{supp}\eta$ and define $\langle f^\blacklozenge, \psi\rangle := \langle f^\bullet, \vartheta|_{\Lambda_\bullet}\psi\rangle$ for $\psi \in W^{1,q'}(\Lambda_\bullet)$. Obviously, $f^\blacklozenge$ is an extension of $f^\bullet$ and does even not depend on our chosen ϑ. □

Lemma 5.18. *Let $\Lambda \subset \mathbb{R}^3$ be a Lipschitz domain and Ξ be an open part of its boundary. Assume that ρ is a uniform continuous function on $\overline{\Lambda}$, taking its values in the set of 3×3 matrices. If for every fixed $\mathrm{y} \in \overline{\Lambda}$, the operator*

$$-\nabla \cdot \rho(\mathrm{y})\nabla + 1 : W^{1,q}_\Xi(\Lambda) \to W^{-1,q}_\Xi(\Lambda) \tag{5.8}$$

is a topological isomorphism, then the operator

$$-\nabla \cdot \rho\nabla + 1 : W^{1,q}_\Xi(\Lambda) \to W^{-1,q}_\Xi(\Lambda) \tag{5.9}$$

also is.

Proof. Let, for every $\mathrm{y} \in \overline{\Lambda}$, $B(\mathrm{y})$ be an open ball around y, such that all $\mathrm{z} \in B(\mathrm{y}) \cap \Lambda$ satisfy

$$\|\rho(\mathrm{y}) - \rho(\mathrm{z})\| \|\big(-\nabla \cdot \rho(\mathrm{y})\nabla + 1\big)^{-1}\|_{\mathcal{L}(W^{-1,q}_\Xi(\Lambda);W^{1,q}_\Xi(\Lambda))} < 1. \tag{5.10}$$

We chose a finite covering of $\overline{\Lambda}$ by the finite family $B(\mathrm{y}_1), \dots, B(\mathrm{y}_m)$ and define $U = \cup_j B(\mathrm{y}_j)$. Let $\eta_1, \dots, \eta_m$ be smooth partition of unity on $\overline{\Lambda}$ which is subordinated to $B(\mathrm{y}_1), \dots, B(\mathrm{y}_m)$. According to Theorem 5.17 (U there taken as an open neighbourhood of $\overline{\Lambda}$), the equation

$$-\nabla \cdot \rho\nabla u + u = f \in W^{-1,q}_\Xi(\Lambda) \tag{5.11}$$

leads to the system of equations

$$-\nabla \cdot \rho\nabla(\eta_j u) = f_j \in W^{-1,q}_\Xi(\Lambda), \quad j = 1, \dots, m \tag{5.12}$$

with $\|f_j\|_{W^{-1,q}_\Xi(\Lambda)} \le c\|f\|_{W^{-1,q}_\Xi(\Lambda)}$, cf. Theorem 5.17. Let us now fix j and abbreviate y_j by y. We define a new coefficient function by setting

$$\rho_j(\mathrm{z}) := \begin{cases} \rho(\mathrm{z}), & \text{if} \quad \mathrm{z} \in B(\mathrm{y}) \cap \Lambda \\ \rho(\mathrm{y}), & \text{if} \quad \mathrm{z} \in \Lambda \setminus B(\mathrm{y}). \end{cases} \tag{5.13}$$

Thanks to its support property, the function $\eta_j u$ satisfies besides (5.12) also the equation

$$-\nabla \cdot \rho_j \nabla(\eta_j u) + \eta_j u = f_j \in W^{-1,q}_\Xi(\Lambda). \tag{5.14}$$

(5.10) and the definition of ρ_j together imply the inequality

$$\|\rho(\mathrm{y}) - \rho_j\|_{L^\infty(\Lambda)} \|\big(-\nabla \cdot \rho(\mathrm{y})\nabla + 1\big)^{-1}\|_{\mathcal{L}(W^{-1,q}_\Xi(\Lambda);W^{1,q}_\Xi(\Lambda))} < 1. \tag{5.15}$$

Since (5.8) is a topological isomorphism, (5.15), in conjunction with Proposition 5.11, tells us that $-\nabla \cdot \rho_j \nabla : W^{1,q}_\Xi(\Lambda) \to W^{-1,q}_\Xi(\Lambda)$ also is a topological isomorphism. Thus, $\eta_j u \in W^{1,q}_\Xi(\Lambda)$. Since $j \in \{1, \dots, m\}$ was arbitrary, this implies $u \in W^{1,q}_\Xi(\Lambda)$. Thus, (5.9) is a continuous bijection, and then the open mapping theorem implies the assertion. □

For the proof of the next proposition, we refer to [22, Prop. 16].

Proposition 5.19. *Let $\Lambda \subset \mathbb{R}^d$ be a bounded Lipschitz domain and Ξ be an open subset of its boundary. Assume that ϕ is a mapping from a neighbourhood of $\overline{\Lambda}$ into $\mathbb{R}^d$ which is bi-Lipschitz. Let us denote $\phi(\Lambda) = \Lambda_\bigstar$ and $\phi(\Xi) = \Xi_\bigstar$. Then*

i) For any $q \in (1,\infty)$ ϕ induces a linear, topological isomorphism

$$\Psi_q : W^{1,q}_{\Xi_\bigstar}(\Lambda_\bigstar) \to W^{1,q}_{\Xi}(\Lambda)$$

which is given by $(\Psi_q f)(x) = f(\phi(x)) = (f \circ \phi)(x)$.

ii) $\Psi^*_{q'}$ is a linear, topological isomorphism between $W^{-1,q}_{\Xi}(\Lambda)$ and $W^{-1,q}_{\Xi_\bigstar}(\Lambda_\bigstar)$.

iii) If ρ is a bounded measurable function on Λ, taking its values in the set of $d \times d$ matrices, then

$$\Psi^*_{q'} \nabla \cdot \rho \nabla \Psi_q = \nabla \cdot \rho_\bigstar \nabla \tag{5.16}$$

with

$$\rho_\bigstar(\mathrm{y}) = (D\phi)(\phi^{-1}(\mathrm{y}))\rho(\phi^{-1}(\mathrm{y}))\big(D\phi\big)^T(\phi^{-1}(\mathrm{y}))\frac{1}{\big|\det(D\phi)(\phi^{-1}\mathrm{y})\big|}. \tag{5.17}$$

($D\phi$ denotes the Jacobian of ϕ and $\det(D\phi)$ the corresponding determinant).

If $-\nabla \cdot \rho \nabla : W^{1,q}_{\Xi}(\Lambda) \to W^{-1,q}_{\Xi}(\Lambda)$ is a topological isomorphism, then $-\nabla \cdot \rho_\bigstar \nabla : W^{1,q}_{\Xi_\bigstar}(\Lambda_\bigstar) \to W^{-1,q}_{\Xi_\bigstar}(\Lambda_\bigstar)$ also is (and vice versa).

Remark 5.20. *If, in particular, the coefficient function ρ is (uniformly) continuous and ϕ is continuously differentiable, then the transformed coefficient function also is.*
On the other hand, if ρ is continuous, and the transforming function ϕ is only Lipschitzian, then one is confronted with a transformed coefficient function, the discontinuities of which are hardly to control. Since one has on the side of model constellations only few (with very peculiar discontinuities for the coefficient function) at hand, one is forced (more or less) to demand in Assumption 5.6 a transforming function from C^1.

The next two propositions contain the regularity results of our ultimate model constellations.

Proposition 5.21. *Under Assumption 5.4, the operators*

$$-\nabla \cdot \kappa \nabla + 1 : W^{1,q}_0(\Omega) \to W^{-1,q}(\Omega)$$

and

$$-\nabla \cdot \kappa \nabla + 1 : W^{1,q}(\Omega) \to W^{-1,q}_{\partial\Omega}(\Omega)$$

provide topological isomorphisms for a $q > 3$, cf. [15, Thm. 1.1/Rem. 3.17].

Remark 5.22. *It is known* [28] *that – even in the class of strong Lipschitz domains and even if in the case of the Dirichlet Laplacian – that q – 3 may arbitrarily small in general. This is, besides Shamir's counterexample (cf. Remark 2.8) the second reason why the concept of this kind of maximal elliptic regularity does not work in dimensions $d \geq 4$.*

Theorem 5.23. *Assume, in the notations of Definition 5.5 and Assumption 5.6, that $\Theta := \phi_{\mathrm{x}}(\Gamma \cap U_{\mathrm{x}})$ satisfies any of the conditions a)-d). If ρ is a real, symmetric, positive definite 3×3-matrix, then there is a number $q > 3$ such that*

$$-\nabla \cdot \rho \nabla : W^{1,q}_{\Theta}(\Pi) \to W^{-1,q}_{\Theta}(\Pi) \tag{5.18}$$

is a topological isomorphism.

Proof. Case a) is contained in [22, Thm. 1]. In case b) one reflects (see [22, Prop. 17]) the problem across the plane $\mathcal{H} := \{\mathrm{z} : \mathrm{z} = (x,y,z), z = 1\}$. The resulting problem on the cylinder $\widehat{\Pi} := \Pi \cup (\Delta \times [1,3[)$ has then a Dirichlet condition on the groundplate $\mathcal{P}^-$ and on the new coverplate $\Delta \times \{3\}$. Moreover, the resulting coefficient function is constant on both components of $\widehat{\Pi} \setminus \mathcal{H}$. Thus,

the resulting problem again fits into [22, Thm. 1]. Having the information for the problem on $\widehat{\Pi}$ at hand, one applies [22, Prop. 17] and obtains the claimed regularity for the original problem on Π. Case c) is treated like b), this time only reflecting across the plane $\{\mathrm{z} : \mathrm{z} = (x, y, z), z = -1\}$. Next we consider case d). Let for this $\square$ be a square which contains the closure of $\triangle$. Define $\Pi_+ := \square \times (-\frac{1}{2}, 2)$, and $\Pi_- := \square \times (-2, \frac{1}{2})$. Obviously, Π_+ and Π_- form an open covering of Π. Let η_+, η_- be two smooth functions with the properties supp $\eta_+ \subset \Pi_+$, supp $\eta_- \subset \Pi_-$ and $\eta_+ + \eta_- = 1$ on the closure of Π. Localizing the equation $-\nabla \cdot \mu \nabla u = f \in W_\Theta^{-1,q}(\Pi)$ according to Proposition 5.17, one ends up with two problems of type b) and c), respectively – which are already treated.
The cases e)-h) are treated analogously, this time employing [22, Thm. 2]. $\square$

Lemma 5.24. *Assume that M is a bounded set of real, symmetric 3×3 matrices which admit a common ellipticity bound. Then there is common $q_M > 3$ such that* (5.18) *are topological isomorphisms for all $\rho \in M$ and all $q \in [2, q_M]$.*

Proof. Assume that the assertion is false. Then, for every $n \in \mathbb{N}$ there is matrix $\rho_n \in M$ such that (5.18) is not a topological isomorphism, if ρ is there taken as ρ_n and $q = 3 + \frac{1}{n}$. Modulo extracting a subsequence, we may suppose that $\{\rho_n\}_n$ converges towards a matrix ρ – which is clearly real, positive definite and symmetric. Thus, according to Proposition 5.23 there is a $q > 3$ such that (5.18) is a topological isomorphism. But, since $||\rho - \rho_n||$ approaches 0, the operators $-\nabla \cdot \rho_n \nabla : W_\Theta^{1,q}(\Pi) \to W_\Theta^{-1,q}(\Pi)$ must also be continuously invertible for sufficiently large n and this same q, cf. Lemma 5.11. According to Remark 5.15, this carries over to all $\tilde{q} \in [2, q]$. This is a contradiction. $\square$

Lemma 5.25. *Assume $\mathrm{x} \in \partial\Gamma$, and let U_x be the corresponding neighbourhood from Assumption 5.6. Then there is a $q > 3$ such that*

$$-\nabla \cdot \kappa|_{\Omega \cap U_\mathrm{x}} \nabla + 1 : W^{1,q}_{\Gamma \cap U_\mathrm{x}}(\Omega \cap U_\mathrm{x}) \to W^{-1,q}_{\Gamma \cap U_\mathrm{x}}(\Omega \cap U_\mathrm{x}) \tag{5.19}$$

is a topological isomorphism.

Proof. First we will prove the assertion for $-\nabla \cdot \kappa|_{\Omega \cap U_\mathrm{x}} \nabla$ instead of $-\nabla \cdot \kappa|_{\Omega \cap U_\mathrm{x}} \nabla + 1$. For this, recall that, thanks to Remark 5.7, we may assume that the coefficient function κ is uniformly continuous on $\Omega \cap U_\mathrm{x}$. (In the sequel, $\kappa|_{\Omega \cap U_\mathrm{x}}$ is always identified with its canonic extension to the closure of $\Omega \cap U_\mathrm{x}$.) According to Proposition 5.19, one may transform the operator under the mapping ϕ_x, where the resulting operator is that in (5.18), ρ now being a uniformly continuous coefficient function on Π, cf. (5.17). But also in this case (5.18) is a topological isomorphism for a number $q > 3$, thanks to Theorem 5.23, Lemma 5.24 and Lemma 5.18. Transforming back, we obtain a $q > 3$ such that

$$-\nabla \cdot \kappa|_{\Omega \cap U_\mathrm{x}} \nabla : W^{1,q}_{\Gamma \cap U_\mathrm{x}}(\Omega \cap U_\mathrm{x}) \to W^{-1,q}_{\Gamma \cap U_\mathrm{x}}(\Omega \cap U_\mathrm{x}) \tag{5.20}$$

is a topological isomorphism. Hence, the resolvent of $-\nabla \cdot \kappa|_{\Omega \cap U_\mathrm{x}} \nabla$ is compact, and (5.19) can only fail to be an isomorphism if -1 is an eigenvalue of $-\nabla \cdot \kappa|_{\Omega \cap U_\mathrm{x}} \nabla$. The latter is, obviously, not the case. $\square$

Now we are in the position to prove the main result of this section, claimed in Theorem 5.8:

Proof. Let, for any $\mathrm{x} \in \partial\Gamma$, U_x be the corresponding neighbourhood from Assumption 5.6 and $U_{\mathrm{x}_1}, \ldots, U_{\mathrm{x}_n}$ be a finite subcovering of $\partial\Gamma$. Let $\mathcal{W}$ be an open neighbourhood of $\overline{\Omega}$ and put

$$U_+ := \mathcal{W} \setminus \overline{\Gamma}, \quad U_- := \mathcal{W} \setminus (\partial\Omega \setminus \Gamma). \tag{5.21}$$

It is clear that then the system $U_-, U_+, U_{\mathrm{x}_1}, \ldots, U_{\mathrm{x}_n}$ forms an open covering of $\overline{\Omega}$. Let $\eta_+, \eta_-, \eta_1, \ldots, \eta_n$ be a smooth partition of unity, subordinated to this covering. We abbreviate $\mathcal{U}_j := \Omega \cap U_{\mathrm{x}_j}$, $\Gamma_j := \Gamma \cap U_{\mathrm{x}_j}$. If $q \leq 6$ then the equation

$$-\nabla \cdot \kappa \nabla u + u = f \in W_\Gamma^{-1,q}(\Omega)$$

leads to the system of equations

$$-\nabla \cdot \kappa \nabla \eta_+ u + \eta_+ u = f_+ \in W^{-1,q}(\Omega);\ \eta_+ u \in W_0^{1,2}(\Omega), \tag{5.22}$$

$$-\nabla \cdot \kappa \nabla \eta_- u + \eta_- u = f_- \in W_{\partial\Omega}^{-1,q}(\Omega);\ \eta_- u \in W^{1,2}(\Omega), \tag{5.23}$$

$$-\nabla \cdot \kappa|_{\mathcal{U}_j} \nabla \eta_j u + \eta_j u = f_j \in W_{\Gamma_j}^{-1,q}(\mathcal{U}_j);\ \eta_j u \in W_{\Gamma_j}^{1,2}(\mathcal{U}_j), \tag{5.24}$$

according to Proposition 5.17. Then Proposition 5.21 tells us that

$$-\nabla \cdot \kappa \nabla + 1 : W_0^{1,q_+}(\Omega) \to W_0^{-1,q_+}(\Omega) \tag{5.25}$$

and

$$-\nabla \cdot \kappa \nabla + 1 : W^{1,q_-}(\Omega) \to W_{\partial\Omega}^{-1,q_-}(\Omega) \tag{5.26}$$

are topological isomorphisms for some $q_+, q_- > 3$. Moreover, Lemma 5.25 provides, for every $j \in \{1, \ldots, n\}$ a number $q_j > 3$ such that each of the operators

$$-\nabla \cdot \kappa|_{\mathcal{U}_j} \nabla + 1 : W_{\Gamma_j}^{1,q_j}(\mathcal{U}_j) \to W_{\Gamma_j}^{-1,q_j}(\mathcal{U}_j) \tag{5.27}$$

is a topological isomorphism. Define now $q := min(6, q_+, q_-, q_1, \ldots, q_n)$. Then (5.25), (5.26) and (5.27) remain topological isomorphisms, if $q_+, q_-, q_1, \ldots, q_n$ are all replaced by q, cf. Remark 5.15. This gives $\eta_+ u \in W_0^{1,q}(\Omega) \subset W_\Gamma^{1,q_+}(\Omega)$ and $\eta_- u \in W^{1,q}(\Omega)$. Let ϑ be a smooth function with supp $\vartheta \subset \mathcal{W}$ and $\vartheta \equiv 1$ on supp η and $\vartheta \equiv 0$ in a neighbourhood of $\partial\Omega \backslash \Gamma$. Since Ω is a Lipschitz domain, one may approximate the function $\eta_- u$ by a sequence of smooth functions $\{\psi_k\}_k$ in the $W^{1,q}(\Omega)$-norm. Obviously, the sequence $\{\psi_k \vartheta|_\Omega\}_k$ then also approximates $\eta_- u$ in the $W^{1,q}(\Omega)$-norm. Hence, $\eta_- u \in W_\Gamma^{1,q}(\Omega)$. Finally, each function $\eta_j u$ belongs to the space $W_{\Gamma_j}^{1,q}(\mathcal{U}_j)$. Choosing a function ϑ_j with supp $\vartheta_j \subset U_{\mathrm{x}_j}$ and $\vartheta_j \equiv 1$ on suppη, Lemma 5.16 gives $\widetilde{\eta_j u} = \widetilde{\vartheta_j \eta_j u} \in W_\Gamma^{1,q}(\Omega)$. Hence, the operator in (5.2) is a continuous bijection for a $q > 3$ and, consequently, by the open mapping theorem, continuously invertible. The assertion for all $q \in [2, q_0]$ follows by interpolation, cf. Corollary 5.14. □

It follows the proof of Corollary 5.9: Obviously, the adjoint operator of (5.2), acting between $W_\Gamma^{1,q'}(\Omega)$ and $W_\Gamma^{-1,q'}(\Omega)$ also is a topological isomorphism. Due to the proposed symmetry of the coefficient matrices, the restriction to $L^2(\Omega)$ is selfadjoint. Since the dual pairing between $W_\Gamma^{1,2}(\Omega)$ and $W_\Gamma^{-1,2}(\Omega)$ extends the scalar product in $L^2(\Omega)$, the adjoint operator is simply the closure of (5.2) in the space $W_\Gamma^{-1,q'}(\Omega)$. Having the cases $q = q_0'$ and $q = q_0$ at hand, one employs again Corollary 5.14.

Remark 5.26. *In fact, much more is known concerning the isomorphism property* (5.2)*. First, one may deviate from the Lipschitz-graph property of the domain, cf.* [14]*. Secondly, certain discontinuities of the coefficient function also at the boundary of the domain can be admitted, see* [14] *and* [15]*. Since the underlying theories are beyond the scope of this paper, we restricted here ourselves to this simplified concept.*

5.4. **Interpolation.** In this subsection we prove real interpolation results for Sobolev spaces needed in the proof of Theorem 2.12.

Theorem 5.27. *Let Ω and Γ be as above (in particular, Assumption 2.2 shall be satisfied). Let ρ be a bounded, elliptic, real coefficient function, taking its values in the set of symmetric $d \times d$-matrices.*

i) $-\nabla \cdot \rho\nabla$ is a positive operator (see [39, Ch. 1.14.1]*) on $W_\Gamma^{-1,q}(\Omega)$, and, hence, its fractional powers are well defined as long as $q \in [2, 6]$.*

ii) If $\varsigma \in (\frac{1}{2}, 1)$ and $r \in [1, \infty]$, then

$$(W_\Gamma^{-1,q}(\Omega), W_\Gamma^{1,q}(\Omega))_{\varsigma,r} \hookrightarrow (L^q(\Omega), \mathrm{dom}_{W_\Gamma^{-1,q}(\Omega)}(-\nabla \cdot \rho\nabla + 1))_{2\varsigma-1,r}. \tag{5.28}$$

Proof. i) See [25, Corollary 5.21].

ii) The continuity of $-\nabla\cdot\rho\nabla+1 : W_\Gamma^{1,q}(\Omega) \to W_\Gamma^{-1,q}(\Omega)$ yields a continuous embedding $W_\Gamma^{1,q}(\Omega) \hookrightarrow \mathrm{dom}_{W_\Gamma^{-1,q}(\Omega)}(-\nabla \cdot \rho\nabla + 1)$, if the latter space is equipped with the graph norm. Hence, one has, according to i),

$$(W_\Gamma^{-1,q}(\Omega), W_\Gamma^{1,q}(\Omega))_{\varsigma,r} \hookrightarrow (W_\Gamma^{-1,q}(\Omega), \mathrm{dom}_{W_\Gamma^{-1,q}(\Omega)}(-\nabla \cdot \rho\nabla + 1))_{\varsigma,r} =$$

$$= (\mathrm{dom}_{W_\Gamma^{-1,q}(\Omega)}(-\nabla \cdot \rho\nabla + 1)^{1/2}, \mathrm{dom}_{W_\Gamma^{-1,q}(\Omega)}(-\nabla \cdot \rho\nabla + 1))_{2\varsigma-1,r},$$

cf. [39, Ch. 1.15.4]. Further, one knows $(-\nabla \cdot \rho\nabla + 1)^{-1/2} \in \mathcal{L}(W_\Gamma^{-1,q}(\Omega); L^q(\Omega))$ (see [38, Thm. 3.2]). This gives $\mathrm{dom}_{W_\Gamma^{-1,q}(\Omega)}(-\nabla \cdot \rho\nabla + 1)^{1/2} \hookrightarrow L^q(\Omega)$, what implies (5.28). □

Corollary 5.28. *If, under the same suppositions as in Theorem 5.27, one additionally knows $\mathrm{dom}_{W_\Gamma^{-1,q}(\Omega)}(-\nabla \cdot \rho\nabla + 1) = W_\Gamma^{1,q}(\Omega)$, then one has the continuous embedding*

$$(W_\Gamma^{-1,q}(\Omega), W_\Gamma^{1,q}(\Omega))_{\varsigma,q} \hookrightarrow W_\Gamma^{2\varsigma-1,q}(\Omega).$$

Proof. We already know the embedding (5.28) – where the right hand side in case of $r = q$ now reads as $(L^q(\Omega, W_\Gamma^{1,q}(\Omega))_{2\varsigma-1,q}$. But, thanks to [17, Remark 3.6], this interpolation space is determined as the Sobolev-Slobodetskii space $W_\Gamma^{2\varsigma-1,q}(\Omega)$. □

Remark 5.29. *If $\alpha := 2\varsigma - 1 - \frac{d}{q} > 0$, then one has the embedding*

$$W_\Gamma^{2\varsigma-1,q}(\Omega) \hookrightarrow W^{2\varsigma-1,q}(\Omega) \hookrightarrow C^\alpha(\Omega),$$

cf. [39, Ch. 2.8.1].

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