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Hölder continuity for second order elliptic problems with nonsmooth data

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Abstract

The well known De Giorgi result on Hölder continuity for solutions of the Dirichlet problem is re-established for mixed boundary value problems, provided that the underlying domain is a Lipschitz domain and the border between the Dirichlet and the Neumann boundary part satisfies a very general geometric condition. Implications of this result for optimal control theory are presented.

1 Introduction

In the last decades it has been anticipated in applied analysis that many elliptic problems originating from science, engineering, and technology possess nonsmooth data. This means that they often live on nonsmooth domains, the coefficients are nonsmooth and, thirdly, they often exhibit mixed boundary conditions, see [3], [43] and the references cited therein, see also [45] and [22]. In this paper we prove the Hölder continuity for the solution u of

$$-\nabla \cdot \rho \nabla u + u = f + \sum_{j=1}^{d} \frac{\partial f_j}{\partial x_j}, \quad f \in L^{q/2},\ f_j \in L^q, \tag{1.1}$$

where q is larger than the space dimension, and mixed boundary conditions are incorporated, see Theorem 3.3. The result is to be seen in the tradition of Stampacchia's paper [49] (see also [40, 41]), where Hölder continuity already was achieved for mixed boundary value problems, but under rather technical conditions – difficult to verify in applications. Here, we generalize the Stampacchia result in space dimensions $d = 2, 3$ and 4 to Lipschitz domains, provided that the Dirichlet boundary part satisfies a very general compatibility condition – purely topological in nature and easy to check at least for $d = 2, 3$, see Theorem 5.2 and Theorem 5.4 below.
Note that the admissible distributional right hand sides in (1.1) allow for jumps in the conormal derivative of solutions across internal interfaces. This means, e.g. in electrostatics, that the jump in the normal component of the displacement $\nu_+ \cdot \varepsilon \nabla \varphi - \nu_- \cdot \varepsilon \nabla \varphi$ across a prescribed interface equals the surface charge density on the interface, and this surface charge density is represented by a distribution on the underlying domain Ω.

Divergence type operators as in (1.1) are of fundamental significance in many application areas. This is the case not only in mechanics (see [38, Ch. IV/V]), thermodynamics (see [48]) and electrodynamics (see [47]) of heterogeneous media, but also in mining, multiphase flow, mathematical biology (see [20, 6]) and semiconductor device simulation (see [45, 22, 24]), in particular quantum electronics (see [55, 5, 36, 54, 39]).

The non-homogeneous coefficient function ρ represents varying material properties as the context requires. It may be thermal conductivity in a heat equation (see [48, §21]) or dielectric permittivity in a Poisson equation, or diffusivity in a transport equation (see for instance [45, §2.2] for carrier continuity equations) or effective electron mass in a Schrödinger equation (see [36]).

Continuity of solutions to (1.1) plays an important role for the discussion of state-constrained optimal control problems (see for instance [8]). Hence it is rather natural to use the above mentioned result for the discussion of semilinear elliptic control

problems with pointwise inequality constraints on the state, which is done here in a very general setting. Such problems have been discussed by numerous authors before (see for instance [8, 1, 12] and the references therein). Concerning second-order sufficient optimality conditions, some progress has recently been made in a contribution of Casas et. al [11]. Here we show that, based on the regularity results of Theorem 3.3, the analysis, developed in [11], is also applicable to problems with mixed boundary conditions, which are not considered in [11]. Thus the consideration of mixed boundary conditions for semilinear elliptic state-constrained optimal control problems represents the genuine contribution of this paper from the viewpoint of optimal control theory.

The outline of the paper is as follows: first we introduce some notation. In Section 3 we formulate our regularity result, which is proved in Section 4. In Section 5 we give an alternative characterization for Gröger's regular sets, which represent the geometric setting for the domains under consideration and the associated Dirichlet boundary parts, in the $2d$ and $3d$ case. Finally, the relevance of the Hölder property for the discussion of semilinear elliptic optimal control problems with pointwise state constraints is pointed out in Section 6.

2 Notation

Throughout this paper, $\Omega \subset \mathbb{R}^d$ always denotes a bounded Lipschitz domain (see [31, Ch. 1.2] for the definition) and $\Gamma \subset \partial\Omega$ is an open part of its boundary. In particular, we often use the cube $K := \{\mathrm{x} \in \mathbb{R}^d : -1 < x_j < 1 \text{ for } 1 \le j \le d\}$, the half cube $K_- := \{\mathrm{x} \in K : x_d < 0\}$, its upper plate $\Sigma := \{\mathrm{x} \in K : x_d = 0\}$ and, lastly, the half of this, $\Sigma_0 := \{\mathrm{x} \in \Sigma : x_{d-1} < 0\}$. The symbol $C^\alpha(\Omega)$ stands for the usual Hölder space on Ω, see [35] or [51]. $W^{1,p}(\Omega)$ denotes the Sobolev space on Ω consisting of those $L^p(\Omega)$ functions whose first order distributional derivatives also belong to $L^p(\Omega)$ (see [31] or [42]). We use the symbol $W^{1,p}_\Gamma(\Omega)$ for the closure of

$$\big\{v|_\Omega : v \in C^\infty(\mathbb{R}^d),\ \operatorname{supp} v \cap (\partial\Omega \setminus \Gamma) = \emptyset\big\}$$

in $W^{1,p}(\Omega)$. Note that Ω enjoys the extension property for $W^{1,p}(\Omega)$ in view of being a bounded Lipschitz domain, see [23, Thm. 3.10] or [42, Ch. 1.1.16]. Thus, in case of $\Gamma = \partial\Omega$ the space $W^{1,p}_\Gamma(\Omega)$ is identical with the usual Sobolev space $W^{1,p}(\Omega)$. If $\Gamma = \emptyset$ we write as usual $W^{1,p}_0(\Omega)$ instead of $W^{1,p}_\emptyset(\Omega)$. $W^{-1,p'}_\Gamma(\Omega)$ denotes the dual to $W^{1,p}_\Gamma(\Omega)$ and $W^{-1,p'}(\Omega)$ denotes the dual to $W^{1,p}_0(\Omega)$, when $\frac{1}{p} + \frac{1}{p'} = 1$ holds. If Ω is understood, then we sometimes abbreviate $W^{\pm1,p}_\Gamma$, $W^{1,p}_0$ and $W^{-1,p}$, respectively. Please notice that all functional spaces under consideration are regarded as complex ones. By $\langle\cdot,\cdot\rangle_X$ we indicate the duality between a Banach space X and its dual. Finally, γ denotes a generic constant not always of the same numerical value.

3 The regularity result

Definition 3.1. Let $\Lambda \subset \mathbb{R}^d$ be a bounded domain and Υ a (relatively) open part of its boundary $\partial\Lambda$. Then we call $\Lambda \cup \Upsilon$ *regular* (in the sense of Gröger [29]), if for every $\mathrm{x} \in \partial\Lambda$ there are two open sets $\mathcal{U}_\mathrm{x}, \mathcal{V}_\mathrm{x} \subset \mathbb{R}^d$ and a bi-Lipschitz transform Ψ_x from $\mathcal{U}_\mathrm{x}$ onto $\mathcal{V}_\mathrm{x}$, such that $\mathrm{x} \in \mathcal{U}_\mathrm{x}$, $\Psi_\mathrm{x}(\mathrm{x}) = 0$ and $\Psi_\mathrm{x}\big(\mathcal{U}_\mathrm{x} \cap (\Lambda \cup \Upsilon)\big)$ either coincides with K_- or with $K_- \cup \Sigma$ or with $K_- \cup \Sigma_0$.

Assumption 3.2. Let ρ be a Lebesgue measurable, essentially bounded function on Ω, taking its values in the set of real $d \times d$ matrices, that additionally satisfies the usual (strong) ellipticity condition

$$\mathrm{y} \cdot \rho(\mathrm{x})\, \mathrm{y} \geq \iota |\mathrm{y}|^2, \quad \mathrm{y} \in \mathbb{R}^d, \tag{3.1}$$

for almost all $\mathrm{x} \in \Omega$ and some $\iota > 0$.

Given a coefficient function ρ, satisfying this assumption, we define the operator $-\nabla \cdot \rho \nabla + 1 : W_\Gamma^{1,2}(\Omega) \to W_\Gamma^{-1,2}(\Omega)$ by

$$\langle -\nabla \cdot \rho \nabla v + v, w \rangle_{W_\Gamma^{-1,2}} := \int_\Omega (\rho \nabla v \cdot \nabla w + v w)\, d\mathrm{x}\,, \quad v, w \in W_\Gamma^{1,2}(\Omega). \tag{3.2}$$

Then our first main result reads as follows.

Theorem 3.3. *Suppose $2 \leq d \leq 4$ and $q > d$. Suppose further that $\Omega \cup \Gamma$ is regular and that Assumption 3.2 is satisfied. Then there is an $\alpha > 0$, such that $(-\nabla \cdot \rho \nabla + 1)^{-1}$ maps $W_\Gamma^{-1,q}(\Omega)$ continuously into $C^\alpha(\Omega)$.*

Remark 3.4. a) The cases $\Gamma = \emptyset$ (Dirichlet boundary condition) and $\Gamma = \partial\Omega$ (Neumann boundary condition) are explicitly allowed.
b) It is not hard to see that the right hand side of (1.1) defines an element of $W_\Gamma^{-1,q}(\Omega)$. Conversely, any element from $W_\Gamma^{-1,q}(\Omega)$ may be represented this way, see [56, Ch. 4.3].

Corollary 3.5. *The result of Theorem 3.3 carries over to problems with Robin boundary conditions on Γ, if the representing function $\varkappa$ is from $L^\infty(\Gamma, \sigma)$ (σ being the induced boundary measure on Γ, cf. [33, Section 3]).*

Corollary 3.6. *Let a non-negative function $V \in L^\infty(\Omega)$ be given. Moreover, assume that, if $\mathrm{meas}(\partial\Omega \setminus \Gamma) = 0$, then there is a subset Ω_+ of Ω of positive measure, where V is strictly positive. Then, similarly to Corollary 3.5, Theorem 3.3 also applies to problems of the form $-\nabla \cdot \rho \nabla v + V v = f$, $f \in W_\Gamma^{-1,q}(\Omega)$.*

Corollary 3.7. *Let D_q denote the domain of the maximal restriction of $-\nabla \cdot \rho \nabla + 1$ to the space $W_\Gamma^{-1,q}(\Omega)$. Then, under the suppositions of Theorem 3.3, even the complex interpolation space $[D_q, W_\Gamma^{-1,q}]_\tau$ continuously embeds into a Hölder space $C^\beta(\Omega)$, if τ and β are sufficiently close to 0.*

Remark 3.8. Corollary 3.7 may be of use for the treatment of parabolic equations, see [46, 2, 44].

4 Proof of the regularity result

Let us start by commenting on the philosophy of the proof: the problem will be localized by means of a suitably chosen partition of unity, afterwards transformed by bi-Lipschitz mappings and, if necessary, by reflection. In any case one ends up with a Dirichlet problem on either a ball, the half cube K_- or the cube K. Then a well known regularity result (see Proposition 4.3) may be applied.

In order to perform this procedure we first quote two results from the literature and afterwards establish some auxiliary results, which will justify the required technical steps.

4.1 Known results

Proposition 4.1 ([30], see also [29])**.** *Suppose that ρ satisfies Assumption 3.2. If $\Omega \cup \Gamma$ is regular, then there is a $q_0 > 2$ such that for all $q \in [2, q_0[$ the operator $-\nabla \cdot \rho \nabla + 1$ provides a topological isomorphism between $W^{1,q}_\Gamma(\Omega)$ and $W^{-1,q}_\Gamma(\Omega)$.*

Remark 4.2. It is clear by Sobolev embedding that in the two dimensional case the assertion of Theorem 3.3 already follows from Proposition 4.1.

Proposition 4.3 (see [37, Ch. III.14], [35, Thm. C.2], [13, Ch. 4], see also [15])**.** *Let Λ be a ball or a cuboid and let the coefficient function ω (mutatis mutandis) satisfy Assumption 3.2. If $q > d$, then there is an $\alpha > 0$, such that*

$$\big(-\nabla \cdot \omega \nabla\big)^{-1} : W^{-1,q}(\Lambda) \to C^\alpha(\Lambda) \tag{4.1}$$

is continuous.

Remark 4.4. Usually, Proposition 4.3 is proved only for real spaces, but it is straightforward to extend this to the complex case: one considers for any element T of the complex Sobolev space $W^{-1,q}_\Gamma$ the linear forms $\frac{T+T^*}{2}$ and $\frac{T-T^*}{2i}$, where T^* is defined by $T^*\psi := \overline{T\overline{\psi}}$. Obviously, both take real values when applied to real functions and satisfy $\frac{T+T^*}{2} + i\frac{T-T^*}{2i} = T$. Thus, one may use the result for the corresponding real spaces.

4.2 Auxiliary Results

Lemma 4.5. *Let $\Omega \cup \Gamma$ be regular and let $\mathcal{U} \subset \mathbb{R}^d$ be open, such that $\Omega_\bullet := \Omega \cap \mathcal{U}$ is also a Lipschitz domain. Furthermore, we put $\Gamma_\bullet := \Gamma \cap \mathcal{U}$ and fix an arbitrary*

function $\eta \in C_0^\infty(\mathbb{R}^d)$ with $\operatorname{supp}\eta \subset \mathcal{U}$. Then for any $q \in [1,\infty[$ we have the following assertions.

i) If $v \in W^{1,q}_\Gamma(\Omega)$, then $\eta v|_{\Omega_\bullet} \in W^{1,q}_{\Gamma_\bullet}(\Omega_\bullet)$.

ii) Let for any $v \in L^1(\Omega_\bullet)$ the symbol $\tilde{v}$ indicate the extension of v to Ω by zero. Then the mapping

$$W^{1,q}_{\Gamma_\bullet}(\Omega_\bullet) \ni v \mapsto \widetilde{\eta v}$$

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

Proof. For the proof of both points we will employ the following well known set inclusion (cf. [16, Ch. 3.8]):

$$(\partial\Omega \cap \mathcal{U}) \cup (\Omega \cap \partial\mathcal{U}) \subset \partial\Omega_\bullet \subset (\partial\Omega \cap \mathcal{U}) \cup (\overline{\Omega} \cap \partial\mathcal{U}). \tag{4.2}$$

i) First one observes that the multiplication with η and the restriction is a continuous mapping from $W^{1,q}_\Gamma(\Omega)$ into $W^{1,q}(\Omega_\bullet)$. Thus, it suffices to show the assertion only for elements of the dense subset

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

what we will do now. One has by (4.2)

$$\operatorname{supp}(\eta v) \cap (\partial\Omega_\bullet \setminus \Gamma_\bullet) \subset \operatorname{supp}\eta \cap \operatorname{supp} v \cap \Big[\big((\partial\Omega \cap \mathcal{U}) \cup (\overline{\Omega} \cap \partial\mathcal{U}) \big) \setminus \big(\Gamma \cap \mathcal{U} \big) \Big].$$

Since $(\overline{\Omega} \cap \partial\mathcal{U}) \cap (\Gamma \cap \mathcal{U}) = \emptyset$, we see

$$\begin{aligned} \big((\partial\Omega \cap \mathcal{U}) \cup (\overline{\Omega} \cap \partial\mathcal{U}) \big) \setminus \big(\Gamma \cap \mathcal{U} \big) &= \big((\partial\Omega \cap \mathcal{U}) \setminus (\Gamma \cap \mathcal{U}) \big) \cup \big((\overline{\Omega} \cap \partial\mathcal{U}) \setminus (\Gamma \cap \mathcal{U}) \big) \\ &= \big((\partial\Omega \setminus \Gamma) \cap \mathcal{U} \big) \cup (\overline{\Omega} \cap \partial\mathcal{U}). \end{aligned}$$

This, together with $\operatorname{supp}\eta \subset \mathcal{U}$ yields

$$\operatorname{supp}(\eta v) \cap (\partial\Omega_\bullet \setminus \Gamma_\bullet) \subset \operatorname{supp}\eta \cap \operatorname{supp} v \cap \big((\partial\Omega \setminus \Gamma) \cap \mathcal{U} \big) = \emptyset.$$

ii) Let $v \in C_0^\infty(\mathbb{R}^d)$ with $\operatorname{supp} v \cap (\partial\Omega_\bullet \setminus \Gamma_\bullet) = \emptyset$. Since by the right hand side of (4.2) we have

$$\partial\Omega_\bullet \setminus \Gamma_\bullet \supseteq (\partial\Omega \cap \mathcal{U}) \setminus \Gamma_\bullet = \mathcal{U} \cap (\partial\Omega \setminus \Gamma),$$

it follows $\operatorname{supp} v \cap \big(\mathcal{U} \cap (\partial\Omega \setminus \Gamma) \big) = \emptyset$. Combining this with $\operatorname{supp}\eta \subset \mathcal{U}$, we obtain

$$\operatorname{supp}(\eta v) \cap (\partial\Omega \setminus \Gamma) = \operatorname{supp}(\eta v) \cap \big(\mathcal{U} \cap (\partial\Omega \setminus \Gamma \big) = \emptyset,$$

so $\eta v|_\Omega \in W^{1,q}_\Gamma(\Omega)$. Furthermore, it is not hard to see that $\|\eta v\|_{W^{1,q}(\Omega)} \leq \gamma_\eta \|v\|_{W^{1,q}(\Omega_\bullet)}$, where the constant γ_η is independent from v. Thus, the assertion follows, since $\{ v|_{\Omega_\bullet} \,:\, v \in C_0^\infty(\mathbb{R}^d),\ \operatorname{supp}(v) \cap (\partial\Omega_\bullet \setminus \Gamma_\bullet) = \emptyset \}$ is dense in $W^{1,q}_{\Gamma_\bullet}(\Omega_\bullet)$ and $W^{1,q}_\Gamma(\Omega)$ is closed in $W^{1,q}(\Omega)$. □

Lemma 4.6. *Let Ω, Γ, $\mathcal{U}$, η, $\Omega_\bullet$ and $\Gamma_\bullet$ be as in the foregoing lemma. Denote by $\rho_\bullet$ the restriction of the coefficient function ρ to $\Omega_\bullet$ and let the operator $-\nabla\cdot\rho_\bullet\nabla : W^{1,2}_{\Gamma_\bullet}(\Omega_\bullet)\to W^{-1,2}_{\Gamma_\bullet}(\Omega_\bullet)$ be defined analogously to (3.2). Assume $v\in W^{1,2}_\Gamma(\Omega)$ to be the solution of*

$$-\nabla\cdot\rho\nabla v + v = f \in W^{-1,2}_\Gamma(\Omega). \tag{4.3}$$

Then the following holds true.

i) For all $q\in\,]1,\infty[$ the linear form

$$f_\bullet : w\mapsto \langle f, \widetilde{\eta w}\rangle_{W^{-1,2}_\Gamma(\Omega)},$$

where $\widetilde{\eta w}$ again means the extension by zero to the whole Ω, is well defined and continuous on $W^{1,q'}_{\Gamma_\bullet}(\Omega_\bullet)$, whenever $f\in W^{-1,q}_\Gamma(\Omega)$.

ii) If we denote the linear form

$$W^{1,2}_{\Gamma_\bullet}(\Omega_\bullet)\ni w\mapsto \int_{\Omega_\bullet} v\rho_\bullet\nabla\eta\cdot\nabla w\,\mathrm{dx},$$

by T_v, then $u:=\eta v|_{\Omega_\bullet}$ satisfies

$$-\nabla\cdot\rho_\bullet\nabla u = -\eta v|_{\Omega_\bullet} - \rho_\bullet\nabla v|_{\Omega_\bullet}\cdot\nabla\eta|_{\Omega_\bullet} + T_v + f_\bullet =: f^\bullet. \tag{4.4}$$

iii) Assume now $2\le d\le 4$. If $f\in W^{-1,q}_\Gamma(\Omega)$ for a $q>d$, then there is a $p>d$ such that $f^\bullet\in W^{-1,p}_{\Gamma_\bullet}(\Omega_\bullet)$. Moreover, the mapping $W^{-1,q}_\Gamma(\Omega)\ni f\mapsto f^\bullet\in W^{-1,p}_{\Gamma_\bullet}(\Omega_\bullet)$ is continuous.

Proof. i) The mapping $f\mapsto f_\bullet$ is the adjoint to $v\mapsto\widetilde{\eta v}$, which maps by the preceding lemma $W^{1,q'}_{\Gamma_\bullet}(\Omega_\bullet)$ continuously into $W^{1,q'}_\Gamma(\Omega)$.

ii) For every $w\in W^{1,2}_{\Gamma_\bullet}(\Omega_\bullet)$ we have

$$\begin{aligned}
&\langle -\nabla\cdot\rho_\bullet\nabla u, w\rangle_{W^{-1,2}_{\Gamma_\bullet}(\Omega_\bullet)} + \int_{\Omega_\bullet}\eta v w\,\mathrm{dx} = \int_{\Omega_\bullet}\rho_\bullet\nabla(\eta v)\cdot\nabla w\,\mathrm{dx} + \int_{\Omega_\bullet}\eta v w\,\mathrm{dx}\\
&= \int_{\Omega_\bullet} v\rho_\bullet\nabla\eta\cdot\nabla w\,\mathrm{dx} + \int_{\Omega_\bullet}\eta\rho_\bullet\nabla v\cdot\nabla w\,\mathrm{dx} + \int_\Omega v\,\widetilde{\eta w}\,\mathrm{dx}\\
&= \int_{\Omega_\bullet} v\rho_\bullet\nabla\eta\cdot\nabla w\,\mathrm{dx} + \int_{\Omega_\bullet}\rho_\bullet\nabla v\cdot\nabla(\eta w)\,\mathrm{dx} - \int_{\Omega_\bullet} w\rho_\bullet\nabla v\cdot\nabla\eta\,\mathrm{dx} + \int_\Omega v\,\widetilde{\eta w}\,\mathrm{dx}
\end{aligned}$$

and by (4.3) we see

$$\begin{aligned}
\int_{\Omega_\bullet}\rho_\bullet\nabla v\cdot\nabla(\eta w)\,\mathrm{dx} + \int_\Omega v\,\widetilde{\eta w}\,\mathrm{dx} &= \int_\Omega \rho\nabla v\cdot\nabla(\widetilde{\eta w})\,\mathrm{dx} + \int_\Omega v\,\widetilde{\eta w}\,\mathrm{dx}\\
&= \langle f, \widetilde{\eta w}\rangle_{W^{-1,2}_\Gamma(\Omega)}.
\end{aligned}$$

Applying the definition of T_v and $f_\bullet$ and afterwards subtracting $\int_{\Omega_\bullet} \eta v w \, d\mathrm{x}$ from both sides yields the assertion.

iii) We regard the terms in (4.4) from left to right. For the first summand the assertion is obvious.

According to Proposition 4.1 there is an $\epsilon > 0$ such that the solution v of $-\nabla\cdot\rho\nabla v + v = f$ is from $W^{1,2+\epsilon}_\Gamma(\Omega)$, what implies $\nabla v \in L^{2+\epsilon}(\Omega)$. Furthermore, $|\nabla\eta| \in L^\infty(\Omega_\bullet)$ and $|\rho_\bullet \nabla v| \in L^{2+\epsilon}(\Omega_\bullet)$. Consequently we have $\rho_\bullet \nabla v \cdot \nabla\eta \in L^{2+\epsilon}(\Omega_\bullet)$. Now, whenever $1/p \geq (d-2-\epsilon)/(d(2+\epsilon))$ we have the embedding $L^{2+\epsilon}(\Omega_\bullet) \hookrightarrow W^{-1,p}_{\Gamma_\bullet}(\Omega_\bullet)$. Since we restricted the dimension to $2 \leq d \leq 4$, there is always a $p > 4 \geq d$ satisfying that condition, so the second term is also fine.

On the other hand, we have $v \in W^{1,2+\epsilon}_\Gamma(\Omega) \hookrightarrow L^{4+\delta}(\Omega)$ for a $\delta = \delta(d) > 0$. Thus, concerning T_v, we can estimate

$$|\langle T_v, w\rangle_{W^{-1,4+\delta}_{\Gamma_\bullet}(\Omega_\bullet)}| \leq \|v\|_{L^{4+\delta}(\Omega_\bullet)} \, \|\rho\|_{L^\infty(\Omega;\mathbb{C}^{d\times d})} \, \|\nabla\eta\|_{L^\infty(\Omega_\bullet)} \, \|w\|_{W^{1,(4+\delta)'}_{\Gamma_\bullet}(\Omega_\bullet)}.$$

The claim on $f_\bullet$ follows from i), while the proof of the last assertion is implicitly contained in the above considerations. □

Remark 4.7. It is the lack of integrability of the gradient of v (see the counterexample in [18, Ch. 4]) together with the quality of the needed Sobolev embeddings, which prevents the applicability of this localization procedure to higher dimensions and thus limits our central result to the dimensions up to 4.
The reader may wonder why we start with the operator $-\nabla\cdot\rho\nabla+1$ and consider the operator $-\nabla\cdot\rho_\bullet\nabla$ after the localization. The reason for this is the following: in order to include the pure Neumann case one should consider the operator $-\nabla\cdot\rho\nabla+1$. On the other hand, the resulting localized operators $-\nabla\cdot\rho_\bullet\nabla$ exhibit in any case a nontrivial Dirichlet boundary part (making them invertible) and the subsequent transformation techniques are technically simpler for the pure operator $-\nabla\cdot\rho_\bullet\nabla$.

Proposition 4.8. *Let $\Lambda \subset \mathbb{R}^d$ be a bounded Lipschitz domain and Υ be an open subset of its boundary. Assume that ϕ is a mapping from a neighborhood of Λ into $\mathbb{R}^d$ that is bi-Lipschitz. Let us denote $\phi(\Lambda) =: \Lambda_\triangle$ and $\phi(\Upsilon) =: \Upsilon_\triangle$. Then the following is true.*

i) For any $p \in]1,\infty[$, the mapping ϕ induces a linear, topological isomorphism

$$\Phi_p : W^{1,p}_{\Upsilon_\triangle}(\Lambda_\triangle) \to W^{1,p}_\Upsilon(\Lambda),$$

which is given by $(\Phi_p f)(\mathrm{x}) = f(\phi(\mathrm{x})) = (f\circ\phi)(\mathrm{x})$.

ii) $\Phi^*_{p'}$ is a linear, topological isomorphism between $W^{-1,p}_\Upsilon(\Lambda)$ and $W^{-1,p}_{\Upsilon_\triangle}(\Lambda_\triangle)$.

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

$$\Phi_{p'}^* \nabla \cdot \omega \nabla \Phi_p = \nabla \cdot \omega_\triangle \nabla \tag{4.5}$$

with

$$\omega_\triangle(\mathrm{y}) := \frac{1}{\left|\det(D\phi)(\phi^{-1}(\mathrm{y}))\right|} (D\phi)(\phi^{-1}(\mathrm{y}))\, \omega(\phi^{-1}(\mathrm{y}))\, \big(D\phi\big)^T(\phi^{-1}(\mathrm{y})) \tag{4.6}$$

for almost all $\mathrm{y} \in \Lambda_\triangle$. Here, $D\phi$ denotes the Jacobian of ϕ and $\det(D\phi)$ the corresponding determinant.

iv) If ω satisfies Assumption 3.2, then $\omega_\triangle$ also does.

Proof. The proof of i) is contained in [26, Thm. 2.10)]. Assertion ii) follows from i) by duality, while iii) is well known, see [32] for an explicit verification or [4, Ch. 0.8]. Finally, iv) is implied by (4.6) and the fact that for a bi-Lipschitz ϕ the Jacobian $D\phi$ and its inverse $(D\phi)^{-1}$ are essentially bounded (see [19, Ch. 3.1]). □

The next lemma makes clear that within the class of bi-Lipschitz transformations one only needs the two local model sets K_- and $K_- \cup \Sigma$, if one dispenses with the condition $\Psi_{\mathrm{x}}(\mathrm{x}) = 0$ (cf. Definition 3.1):

Lemma 4.9. *There is a bi-Lipschitz mapping $\Psi : \mathbb{R}^d \to \mathbb{R}^d$ which maps $K_- \cup \Sigma_0$ onto $K_- \cup \Sigma$.*

Proof. Let us first consider the case $d = 2$. We define on the lower halfspace $\{(x, y) : y \le 0\}$

$$\chi_1(x,y) := \begin{cases} (x - y/2, y/2), & \text{if } x \le 0, y \ge x, \\ (x/2, -x/2 + y), & \text{if } x \le 0, y < x, \\ (x/2, x/2 + y), & \text{if } x > 0, y < -x, \\ (x + y/2, y/2), & \text{if } x > 0, y \ge -x. \end{cases} \tag{4.7}$$

Observing that χ_1 acts as the identity on the x-axis, we may define χ_1 on the upper half space $\{(x, y) : y > 0\}$ also as the identity and thus obtain a globally bi-Lipschitz transformation χ_1 from $\mathbb{R}^2$ onto itself that transforms $K_- \cup \Sigma_0$ onto the triangle shown in Figure 1.

Next, we define the bi-Lipschitz mapping $\chi_2 : \mathbb{R}^2 \to \mathbb{R}^2$ by

$$\chi_2(x,y) := \begin{cases} (x, x + 2y + 1), & \text{if } x \le 0, \\ (x, -x + 2y + 1), & \text{if } x > 0, \end{cases} \tag{4.8}$$

in order to get the geometric constellation in Figure 2.

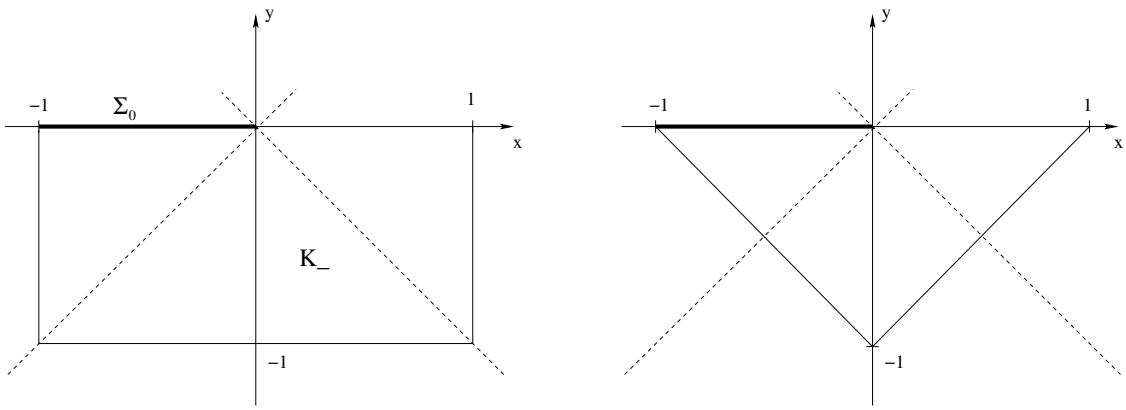

Figure 1: $K_- \cup \Sigma_0$ and $\chi_1(K_- \cup \Sigma_0)$

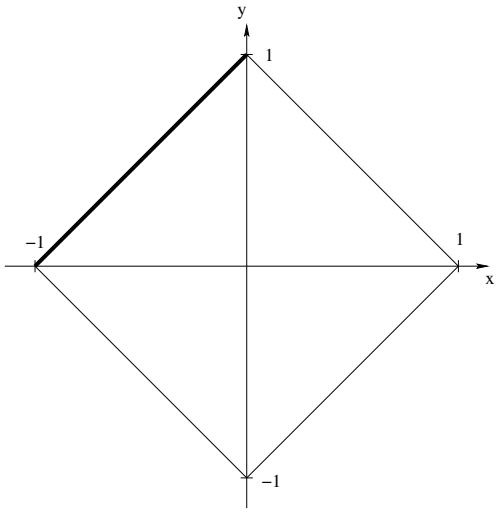

Figure 2: $\chi_2(\rho_1(K_- \cup \Sigma_0))$

If ϑ is the (clockwise) rotation by $\pi/4$, we thus achieved that $\chi := \vartheta\chi_2\chi_1 : \mathbb{R}^2 \to \mathbb{R}^2$ is bi-Lipschitz and satisfies

$$\chi(K_- \cup \Sigma_0) = \Big\{(x,y) \,:\, -\frac{1}{\sqrt{2}} < x < \frac{1}{\sqrt{2}},\ -\frac{1}{\sqrt{2}} < y \le \frac{1}{\sqrt{2}}\Big\}.$$

Let $\varsigma : \mathbb{R}^2 \to \mathbb{R}^2$ be the affine mapping $(x,y) \mapsto (\sqrt{2}x, \frac{1}{\sqrt{2}}y - \frac{1}{2})$. Then $\Psi_2 := \varsigma\chi$ maps $K_- \cup \Sigma_0$ bi-Lipschitzian onto $K_- \cup \Sigma$ in the $2d$ case.

If $d > 2$, one simply puts $\Psi(x_1, \dots, x_d) := (x_1, \dots, x_{d-2}, \Psi_2(x_{d-1}, x_d))$. □

Proposition 4.10. *Let for any* $\mathrm{x} = (x_1, \dots, x_d) \in \mathbb{R}^d$ *the symbol* x_- *denote the element* $(x_1, \dots, x_{d-1}, -x_d)$. *Further, for a* $d \times d$ *matrix* ϱ, *we define the matrix* ϱ^- *by*

$$\varrho^-_{j,k} := \begin{cases} \varrho_{j,k}, & \text{if } j,k < d, \\ -\varrho_{j,k}, & \text{if } j = d \text{ and } k \neq d \text{ or } k = d \text{ and } j \neq d, \\ \varrho_{j,k}, & \text{if } j = k = d. \end{cases} \tag{4.9}$$

Let ω *be a bounded, measurable function on* K_- *taking its values in the set of real, symmetric* $d \times d$ *matrices. We define the matrix valued function* $\hat{\omega}$ *on* K *by*

$$\hat{\omega}(\mathrm{x}) := \begin{cases} \omega(\mathrm{x}), & \text{if } \mathrm{x} \in K_-, \\ \big(\omega(\mathrm{x}_-)\big)^-, & \text{if } \mathrm{x}_- \in K_-, \\ 0, & \text{if } \mathrm{x} \in \Sigma. \end{cases} \tag{4.10}$$

Then we have the following assertions for every $p \in]1, \infty[$.

i) If $\psi \in W^{1,p}_\Sigma(K_-)$ *satisfies* $-\nabla \cdot \omega \nabla \psi = f \in W^{-1,p}_\Sigma(K_-)$, *then* $-\nabla \cdot \hat{\omega}\nabla\hat{\psi} = \hat{f} \in W^{-1,p}(K)$ *holds for* $\hat{\psi}$ *with*

$$\hat{\psi}(\mathrm{x}) = \begin{cases} \psi(\mathrm{x}), & \text{if } \mathrm{x} \in K_-, \\ \psi(\mathrm{x}_-), & \text{if } \mathrm{x}_- \in K_-, \end{cases}$$

and $\hat{f}$ *defined by* $\langle \hat{f}, \varphi\rangle_{W^{-1,p}(K)} := \langle f, \varphi|_{K_-} + \varphi_-|_{K_-}\rangle_{W^{-1,p}_\Sigma(K_-)}$. *Here, the function* φ_- *is defined by* $\varphi_-(\mathrm{x}) := \varphi(\mathrm{x}_-)$.

ii) The mapping $W^{-1,p}_\Sigma(K_-) \ni f \mapsto \hat{f} \in W^{-1,p}(K)$ *is continuous.*

Proof. i) It is known that $\hat{\psi}$ belongs to $W^{1,p}_0(K)$, see [23, Lemma 3.4]. Thus, it remains to show $-\nabla \cdot \hat{\omega}\nabla\hat{\psi} = \hat{f}$ as an equation in $W^{-1,p}(K)$. Since every test function from $W^{1,p}_0(K)$ may be split up into a symmetric and an anti-symmetric part, we may look at these two cases separately. For every anti-symmetric $\varphi \in W^{1,p}_0(K)$. i.e. $\varphi(\mathrm{x}_-) = -\varphi(\mathrm{x})$, the symmetry of $\hat{\omega}$, $\hat{\psi}$ and $\hat{f}$ yields immediately

$$\langle -\nabla \cdot \hat{\omega}\nabla\hat{\psi}, \varphi\rangle_{W^{-1,p}_0(K)} = 0 = \langle \hat{f}, \varphi\rangle_{W^{-1,p}_0(K)}.$$

In the case of symmetric functions φ the assertion is obtained by the definitions of $\hat{\psi}, \hat{f}, -\nabla \cdot \omega \nabla, -\nabla \cdot \hat{\omega} \nabla$ and straightforward calculations, based on Proposition 4.8 when applied to the transformation $\mathrm{x} \mapsto \mathrm{x}_-$.

ii) The operator $f \mapsto \hat{f}$ is the adjoint to $\varphi \mapsto (\varphi|_{K_-} + \varphi_-|_{K_-})$. □

4.3 Core of the proof

By Definition 3.1 and Lemma 4.9, for every $\mathrm{x} \in \partial\Omega$ there is an open neighborhood $\mathcal{U}_\mathrm{x}$ of x, an open set $\mathcal{W}_\mathrm{x}$ and a bi-Lipschitz mapping Ψ_x from $\mathcal{U}_\mathrm{x}$ onto $\mathcal{W}_\mathrm{x}$ such that $\Psi_\mathrm{x}\big((\Omega \cup \Gamma) \cap \mathcal{U}_\mathrm{x}\big)$ equals either K_- or $K_- \cup \Sigma$. Take for every point $\mathrm{x} \in \Omega$ a ball $\mathcal{B}_\mathrm{x} \subset \Omega$ centered at x. Obviously, the system $\{\mathcal{U}_\mathrm{x}\}_{\mathrm{x} \in \partial\Omega} \cup \{\mathcal{B}_\mathrm{x}\}_{\mathrm{x} \in \Omega}$ forms an open covering of $\overline{\Omega}$. Take a finite subcovering $\mathcal{U}_{\mathrm{x}_1}, \ldots, \mathcal{U}_{\mathrm{x}_k}, \mathcal{B}_{\mathrm{x}_1}, \ldots, \mathcal{B}_{\mathrm{x}_l}$ and choose a partition of unity $\eta_1, \ldots, \eta_k, \zeta_1, \ldots, \zeta_l$ over $\overline{\Omega}$, which is subordinated to this subcovering.

Assume now $f \in W_\Gamma^{-1,q}(\Omega)$ with $q > d$ and that v is the solution of $-\nabla \cdot \rho \nabla v + v = f$. Then, according to Proposition 4.6 with $\Gamma_\bullet = \emptyset$ and $\Omega_\bullet = B_{x_j}$, every function $\zeta_j v|_{\mathcal{B}_{\mathrm{x}_j}}$ satisfies an equation $-\nabla \cdot \rho \nabla (\zeta_j v|_{\mathcal{B}_{\mathrm{x}_j}}) = g_j$, where $g_j \in W^{-1,p}(\mathcal{B}_{\mathrm{x}_j})$ with $p > d$ and, additionally,

$$\|g_j\|_{W^{-1,p}(\mathcal{B}_{\mathrm{x}_j})} \le \gamma \|f\|_{W_\Gamma^{-1,q}(\Omega)} \tag{4.11}$$

with γ independent from f. Hence, by Proposition 4.3, we have $\zeta_j v|_{\mathcal{B}_{\mathrm{x}_j}} \in C^\alpha(\mathcal{B}_{\mathrm{x}_j})$ for an $\alpha = \alpha(j) > 0$ and, moreover,

$$\|\zeta_j v|_{\mathcal{B}_{\mathrm{x}_j}}\|_{C^\alpha(\mathcal{B}_{\mathrm{x}_j})} \le \gamma \|g_j\|_{W^{-1,p}(\mathcal{B}_{\mathrm{x}_j})}. \tag{4.12}$$

Clearly, (4.12) together with (4.11) implies

$$\|\zeta_j v\|_{C^\alpha(\Omega)} = \|\zeta_j v|_{\mathcal{B}_{\mathrm{x}_j}}\|_{C^\alpha(\mathcal{B}_{\mathrm{x}_j})} \le \gamma \|g_j\|_{W^{-1,p}(\mathcal{B}_{\mathrm{x}_j})} \le \gamma \|f\|_{W_\Gamma^{-1,q}(\Omega)}. \tag{4.13}$$

Let us now consider the functions $\eta_j v$ for fixed j: putting $\Omega_j := \Omega \cap \mathcal{U}_{\mathrm{x}_j}$ and $\Gamma_j := \Gamma \cap \mathcal{U}_{\mathrm{x}_j}$ we obtain by Lemma 4.5 i) that each $\eta_j v|_{\Omega_j}$ belongs to $W_{\Gamma_j}^{1,2}(\Omega_j)$. Furthermore, Proposition 4.6 shows that $\eta_j v|_{\Omega_j}$ satisfies an equation $-\nabla \cdot \rho \nabla (\eta_j v|_{\Omega_j}) = f_j$, where $f_j \in W_{\Gamma_j}^{-1,p}(\Omega_j)$ with $p > d$ and, additionally,

$$\|f_j\|_{W_{\Gamma_j}^{-1,p}(\Omega_j)} \le \gamma \|f\|_{W_\Gamma^{-1,q}(\Omega)} \tag{4.14}$$

with γ independent from f. Next we consider the 'transformed' function (cf. Proposition 4.8 with $\phi = \Psi_{\mathrm{x}_j}^{-1}$) $\psi_j := \Phi_p(\eta_j v|_{\Omega_j}) = (\eta_j v|_{\Omega_j}) \circ \Psi_{\mathrm{x}_j}^{-1}$ on K_-, from now on distinguishing the cases

$$\Psi_{\mathrm{x}_j}\big((\Omega \cup \Gamma) \cap \mathcal{U}_{\mathrm{x}_j}\big) = K_- \tag{4.15}$$

and

$$\Psi_{\mathrm{x}_j}\big((\Omega \cup \Gamma) \cap \mathcal{U}_{\mathrm{x}_j}\big) = K_- \cup \Sigma. \tag{4.16}$$

If (4.15) is true, then $\Gamma_j := \Gamma \cap \mathcal{U}_{\mathrm{x}_j} \subset \partial(\Omega \cap \mathcal{U}_{\mathrm{x}_j})$ must be empty, since K_- has only inner points and inner points pass to inner points and boundary points to boundary points under a bi-Lipschitz transformation. In particular, this means $\eta_j v|_{\Omega_j} \in W_0^{1,2}(\Omega_j)$. By Proposition 4.8 the function ψ_j belongs to $W_0^{1,2}(K_-)$ and satisfies an equation $-\nabla \cdot \omega \nabla \psi_j = h_j$ with $h_j = (\Phi_{p'}^*)^{-1} f_j \in W^{-1,p}(K_-)$ for the same $p > d$ as above. Thanks to Proposition 4.8 iv), the coefficient function ω again satisfies Assumption 3.2. Thus, by Proposition 4.3, $\psi_j \in C^\alpha(K_-)$, where α depends on j, and

$$\|\psi_j\|_{C^\alpha(K_-)} \le \gamma \|h_j\|_{W^{-1,p}(K_-)}$$

with α and γ independent from h_j. Transforming back, this gives $\eta_j v|_{\Omega_j} \in C^\alpha(\Omega_j)$ with

$$\|\eta_j v|_{\Omega_j}\|_{C^\alpha(\Omega_j)} \le \gamma \|f_j\|_{W^{-1,p}(\Omega_j)} \le \gamma \|f\|_{W_\Gamma^{-1,q}(\Omega)}, \tag{4.17}$$

where the last inequality is just (4.14). As the support of $\eta_j v$ has a positive distance to $\Omega \setminus \Omega_j$, the function $\eta_j v$ is from $C^\alpha(\Omega)$ with the norm equality $\|\eta_j v\|_{C^\alpha(\Omega)} = \|\eta_j v|_{\Omega_j}\|_{C^\alpha(\Omega_j)}$. This, together with (4.17) gives the desired estimate, where γ is independent from f.

Let us now consider the case (4.16). Analogously as before Proposition 4.8 yields that ψ_j belongs to $W_\Sigma^{1,2}(K_-)$ and satisfies an equation $-\nabla \cdot \omega \nabla \psi_j = h_j$ with $h_j \in W_\Sigma^{-1,p}(K_-)$ and $p > d$, where ω again satisfies Assumption 3.2. Now, we apply the reflection principle from Proposition 4.10. This leads to a homogeneous Dirichlet problem $-\nabla \cdot \hat{\omega} \nabla \hat{\psi}_j = \hat{h}_j$, where $\hat{h}_j \in W^{-1,p}(K)$. But then Proposition 4.3 gives $\hat{\psi}_j \in C^\alpha(K)$ and $\|\hat{\psi}_j\|_{C^\alpha(K)} \le \gamma \|\hat{h}_j\|_{W^{-1,p}(K)}$ (α depending on j). Clearly, this, together with Proposition 4.10 ii), implies $\|\psi_j\|_{C^\alpha(K_-)} \le \gamma \|h_j\|_{W_\Sigma^{-1,p}(K_-)}$ and, consequently,

$$\|\eta_j v|_{\Omega_j}\|_{C^\alpha(\Omega_j)} \le \gamma \|f_j\|_{W_{\Gamma_j}^{-1,p}(\Omega_j)} \le \gamma \|f\|_{W_\Gamma^{-1,q}(\Omega)}.$$

Thus, we get $\eta_j v \in C^\alpha(\Omega)$ and $\|\eta_j v\|_{C^\alpha(\Omega)} \le \gamma \|f\|_{W_\Gamma^{-1,q}(\Omega)}$ with γ independent from f as in the previous case. Passing to the minimal $\alpha(j)$, this finishes the proof of Theorem 3.3.

Proof of Corollary 3.5. As is well known ([14, Ch. 1.2], [21, Ch II.2]), in case of a Robin boundary condition the operator is defined via the bilinear form

$$W_\Gamma^{1,2}(\Omega) \times W_\Gamma^{1,2}(\Omega) \ni (v, w) \mapsto \int_\Omega \rho \nabla v \cdot \nabla w \, d\mathrm{x} + \int_\Omega v w \, d\mathrm{x} + \int_\Gamma \varkappa \, v \, w \, d\sigma$$

for some $\varkappa \in L^\infty(\Gamma, \sigma)$. It is easy to see that the linear mapping $T : L^\infty(\Gamma, \sigma) \to W_\Gamma^{-1,p}(\Omega)$, given by

$$\langle T\psi, \varphi \rangle_{W_\Gamma^{-1,p}(\Omega)} = \int_\Gamma \varkappa \, \psi \, \varphi \, d\sigma,$$

is well defined and continuous. Denoting the domain of $-\nabla \cdot \rho\nabla + 1$ again by D_q, we have by Theorem 3.3 the compact embedding $D_q \hookrightarrow C^\alpha(\Omega) \hookrightarrow L^\infty(\Gamma, \sigma)$. Hence, the mapping T is relatively compact with respect to $-\nabla \cdot \rho\nabla + 1$ and a classical perturbation theorem [34, Ch. IV.1.3] applies. □

Proof of Corollary 3.6. We argue analogously to the proof of Corollary 3.5. Here, $T : L^\infty(\Omega) \to W_\Gamma^{-1,q}(\Omega)$ is defined by

$$\langle T\psi, \varphi\rangle_{W_\Gamma^{-1,q}(\Omega)} = \int_\Omega V\,\psi\,\varphi\,d\mathrm{x}.$$

Then, due to the compact embedding $D_q \hookrightarrow L^\infty(\Omega)$, the same perturbation argument as above yields that the domain of the maximal restriction of $-\nabla \cdot \rho\,\nabla + V$ to $W_\Gamma^{-1,q}(\Omega)$ coincides with D_q. Together with the coercivity of the associated bilinear form that follows from the assumptions on V stated in Corollary 3.6, this gives the assertion. □

Proof of Corollary 3.7. Applying a well known re-iteration result on complex interpolation (see [51, Ch 1.9.3]), we obtain for $\tau \in]0,1[$

$$[D_q, W_\Gamma^{-1,q}(\Omega)]_{\frac{\tau}{2}} \hookrightarrow [D_q, [D_q, W_\Gamma^{-1,q}(\Omega)]_{\frac{1}{2}}]_\tau. \tag{4.18}$$

But the embedding $W_\Gamma^{-1,q}(\Omega) \hookrightarrow W_\Gamma^{-1,2}(\Omega)$ gives $D_q \hookrightarrow W_\Gamma^{1,2}(\Omega)$. Together with $D_q \hookrightarrow C^\alpha(\Omega)$, we obtain by (4.18)

$$[D_q, W_\Gamma^{-1,q}(\Omega)]_{\frac{\tau}{2}} \hookrightarrow [C^\alpha(\Omega), [W_\Gamma^{1,2}(\Omega), W_\Gamma^{-1,2}(\Omega)]_{\frac{1}{2}}]_\tau.$$

One identifies the interpolation space $[W_\Gamma^{1,2}(\Omega), W_\Gamma^{-1,2}(\Omega)]_{\frac{1}{2}}$ as the space $L^2(\Omega)$ (see [51, Ch. 1.18.10]), what gives

$$[D_q, W_\Gamma^{-1,q}(\Omega)]_{\frac{\tau}{2}} \hookrightarrow [C^\alpha(\Omega), L^2(\Omega)]_\tau. \tag{4.19}$$

This latter interpolation space is known to embed into another Hölder space $C^\beta(\Omega)$, if $\tau > 0$ is chosen sufficiently small (see [27, Ch. 7], see also [52]). □

Remark 4.11. If the coefficient matrices are symmetric, the Hölder continuity of the solution for (1.1) may be deduced from the results of [28] and [25] by means of suitable (but nontrivial) embedding theorems. Unfortunately, this is not carried out there.

5 Alternative characterization for regular sets

Gröger's concept of regular sets [29] turned out to be a powerful tool for the treatment of mixed boundary value problems. Not only his regularity result [29], based

on this, is exploited in some tens of papers; but the regular sets proved also to be an adequate frame for establishing interpolation results for function spaces which include a trace zero condition on part of the boundary, see [26]. Moreover, it allowed to recover resolvent estimates and thus provided tools for the treatment of parabolic equations, which incorporate mixed boundary conditions, see [30], [27]. All of this shows that the concept of regular sets in itself deserves some investigation in order to simplify things.

In this spirit, the aim of this chapter is to prove that for two and three space dimensions the property of a set $\Lambda \cup \Upsilon$ to be regular in the sense of Gröger (see Definition 3.1) can be characterized by Λ being a Lipschitz domain and a certain topological property of Υ (to be specified in a moment). The point is that the resulting conditions usually can be checked 'by appearance' – in contrast to the original definition. Let us explicitly mention that the underlying class of Lipschitz domains is broad enough to contain e.g. the case of two balks, lying on each other with an angle $\neq \pi$, which together do not form a domain with Lipschitz boundary. We start with the following observation.

Theorem 5.1. *If $\Lambda \cup \Upsilon$ is regular, then Λ is a Lipschitz domain.*

Proof. Let $x \in \partial\Lambda$. Then there is, due to the definition, an open neighborhood $\mathcal{U}$ of x and a bi-Lipschitz mapping $\Psi : \mathcal{U} \to \mathbb{R}^d$, such that $\Psi(x) = 0$ holds and $\Psi(\mathcal{U} \cap (\Lambda \cup \Upsilon))$ equals $K_- \cup \tilde{\Sigma}$, where $\tilde{\Sigma} = \emptyset$ or $\tilde{\Sigma} = \Sigma$ or $\tilde{\Sigma} = \Sigma_0$. This means

$$\Psi(\mathcal{U} \cap (\Lambda \cup \Upsilon)) = \Psi((\mathcal{U} \cap \Lambda) \cup (\mathcal{U} \cap \Upsilon)) = K_- \cup \tilde{\Sigma} \tag{5.1}$$

and since inner points pass to inner points and boundary points to boundary points under a bi-Lipschitz transformation, (5.1) implies $\Psi(\mathcal{U} \cap \Lambda) = K_-$ in all three cases. Hence, $\mathcal{U}$ may serve as the local chart neighborhood required in the definition of a Lipschitz domain, see [31, Def. 1.2.1.2]. □

We first deal with the easier case of $d = 2$.

Theorem 5.2. *Let $\Lambda \subset \mathbb{R}^2$ be a bounded Lipschitz domain and $\Upsilon \subset \partial\Lambda$ be an open part of the boundary. Then $\Lambda \cup \Upsilon$ is regular in the sense of Gröger, iff the set $\overline{\Upsilon} \cap (\partial\Lambda \setminus \Upsilon)$ is finite and no connected component of $\partial\Lambda \setminus \Upsilon$ consists of a single point.*

Proof. In view of Theorem 5.1 and an application of the definition for regular sets it is clear that the condition is necessary. Sufficiency follows from the Lipschitz domain property and the fact that any point $x \in \partial\Lambda$ can only lie in Υ, $\overline{\Upsilon} \cap (\partial\Lambda \setminus \Upsilon)$ or in the (relative) interior of $\partial\Lambda \setminus \Upsilon$. □

Remark 5.3. It is not hard to see that the given condition is equivalent to the following: Υ is a finite union of open arc pieces from $\partial\Lambda$ and $\partial\Lambda \setminus \Upsilon$ is a finite union of (nondegenerate) closed arc pieces.

Now we come to an intrinsic characterization of regular sets in $\mathbb{R}^3$, which we regard as the second essential result of this work.

Theorem 5.4. *Let $\Lambda \subset \mathbb{R}^3$ be a bounded Lipschitz domain. Assume Υ to be an open subset of $\partial\Lambda$. Then $\Lambda \cup \Upsilon$ is regular in the sense of Gröger, iff the following two conditions are satisfied.*

i) $\partial\Lambda \setminus \Upsilon$ is the closure of its interior (within $\partial\Lambda$).

ii) For any $\mathrm{x} \in \overline{\Upsilon} \cap (\partial\Lambda \setminus \Upsilon)$ there is an open neighborhood $\mathcal{N}$ of x and a bi-Lipschitz mapping $\kappa : \mathcal{N} \cap \overline{\Upsilon} \cap (\partial\Lambda \setminus \Upsilon) \to]-1, 1[$.

Proof. According to the definition of regular sets the conditions are necessary.

In order to prove sufficiency, we have to show that for every $\mathrm{x} \in \partial\Lambda$ there is an open neighborhood $\mathcal{U}$ of x and a bi-Lipschitz mapping Ψ with $\Psi(\mathrm{x}) = 0$, such that $\Psi(\mathcal{U} \cap (\Lambda \cup \Upsilon))$ is either K_- or $K_- \cup \Sigma$ or $K_- \cup \Sigma_0$.

We first observe that

$$\partial\Lambda = \Upsilon \cup (\partial\Lambda \setminus \Upsilon)^\circ \cup \big[(\partial\Lambda \setminus \Upsilon) \cap \overline{\Upsilon}\big], \tag{5.2}$$

where the closure and the interior are again taken with respect to the topology of $\partial\Lambda$. In the following we will treat these three cases separately.

Let $\mathrm{x} \in \Upsilon$. Since Υ was supposed to be open, there is an open set $\mathcal{U}_1 \subset \mathbb{R}^d$ that contains x and satisfies $\mathcal{U}_1 \cap \partial\Lambda \subset \Upsilon$. Furthermore, as Λ is a Lipschitz domain, there is another open neighborhood $\mathcal{U}_2 \subset \mathbb{R}^d$ of x and a bi-Lipschitz transform Φ from $\mathcal{U}_2$ onto the (open) cube K, such that $\Phi(\mathrm{x}) = 0$, $\Phi(\Lambda \cap \mathcal{U}_2) = K_-$ and $\Phi(\partial\Lambda \cap \mathcal{U}_2) = \Sigma$. Since Φ is in particular a homeomorphism, the set $\Phi(\mathcal{U}_1 \cap \mathcal{U}_2)$ is an open neighborhood of 0 and it is contained in K. Thus, it contains a homothety tK of K for some $t > 0$. If we define $\mathcal{U} := \Phi^{-1}(tK)$, then $\Phi|_{\mathcal{U}}$ is a bi-Lipschitz mapping from the open neighborhood $\mathcal{U}$ of x onto tK, such that $\Phi(\mathcal{U} \cap (\Lambda \cup \Upsilon))$ is the set $t(K_- \cup \Sigma)$. Combining Φ with a homothety, we get a bi-Lipschitz mapping Ψ from $\mathcal{U}$ onto K that satisfies $\Psi(\mathrm{x}) = 0$ and $\Psi(\mathcal{U} \cap (\Lambda \cup \Upsilon)) = K_- \cup \Sigma$.

Analogously, one proves for the (relatively) inner points $\mathrm{x} \in (\partial\Lambda \setminus \Upsilon)^\circ$ the existence of a neighborhood $\mathcal{U}$ and a bi-Lipschitz mapping Ψ onto the open cube K such that $\Psi(x) = 0$ and $\Psi(\mathcal{U} \cap (\Lambda \cup \Upsilon))$ is the set K_-.

It remains to consider the points of $(\partial\Lambda \setminus \Upsilon) \cap \overline{\Upsilon}$. Let x be an element of this set. As Λ is a Lipschitz domain, there is an open neighborhood $\mathcal{O}$ of x in $\mathbb{R}^3$ and a bi-Lipschitz

mapping Φ from $\mathcal{O}$ onto the cube $K \subset \mathbb{R}^3$, such that $\Phi(\mathrm{x}) = 0$, $\Phi(\Lambda \cap \mathcal{O}) = K_-$ and $\Phi(\partial\Lambda \cap \mathcal{O}) = \Sigma$. Exploiting ii), we find another open neighborhood $\mathcal{N}$ of x and a bi-Lipschitz mapping κ, such that $\kappa(\overline{\Upsilon} \cap (\partial\Lambda \setminus \Upsilon) \cap \mathcal{N}) =]-1, 1[$. Without loss of generality we may assume $\kappa(\mathrm{x}) = 0 \in \mathbb{R}$.

Our job is now to combine the good properties of Φ and κ. In order to do so, we first define a smaller neighborhood of x that is contained in $\mathcal{O} \cap \mathcal{N}$. Since $\Phi(\mathcal{O} \cap \mathcal{N})$ is an open neighborhood of $0 \in \mathbb{R}^3$, we find a number $t \in]0, 1[$, such that $tK \subset \Phi(\mathcal{O} \cap \mathcal{N})$ and we set $\mathcal{X} := \Phi^{-1}(tK)$. Clearly, $\mathcal{X}$ then is an open neighborhood of x that is contained in $\mathcal{O} \cap \mathcal{N}$. Additionally, one has

$$\Phi(\Lambda \cap \mathcal{X}) = \Phi(\Lambda) \cap tK = \Phi(\Lambda \cap \mathcal{O}) \cap tK = K_- \cap tK = tK_-$$

and

$$\Phi(\partial\Lambda \cap \mathcal{X}) = \Phi(\partial\Lambda \cap \mathcal{O}) \cap tK = \Sigma \cap tK =]-t, t[\times]-t, t[\times \{0\}.$$

We define $P : \mathbb{R}^3 \to \mathbb{R}^2$ as the canonic projection onto the first two components and $\hat{\Phi} := P\Phi$ with $\mathcal{X} \cap \partial\Lambda$ as its domain of definition. Note that by the above considerations $\hat{\Phi} : \mathcal{X} \cap \partial\Lambda \to]-t, t[\times]-t, t[\times \{0\}$ is a bi-Lipschitz mapping with $\hat{\Phi}(\mathrm{x}) = 0 \in \mathbb{R}^2$. Let $]s_-, s_+[\subset]-1, 1[$ be the maximal interval containing 0, such that $\hat{\Phi}\kappa^{-1}(]s_-, s_+[) \subset]-t, t[\times]-t, t[$ and denote the set $\hat{\Phi}\kappa^{-1}(]s_-, s_+[)$ by $\mathcal{C}$. It is not hard to see, that $\mathcal{C}$ is the connected component of $\hat{\Phi}(\mathcal{X} \cap \overline{\Upsilon} \cap (\partial\Lambda \setminus \Upsilon))$, which contains $0 \in \mathbb{R}^2$ within $\hat{\Phi}(\mathcal{X} \cap \partial\Lambda) =]-t, t[\times]-t, t[$. We claim:

$$\hat{\Phi}(\mathcal{X} \cap \overline{\Upsilon} \cap (\partial\Lambda \setminus \Upsilon)) \setminus \mathcal{C} \quad \text{has a positive distance to } 0 \in \mathbb{R}^2. \tag{5.3}$$

In fact, the elements of $\hat{\Phi}(\mathcal{X} \cap \overline{\Upsilon} \cap (\partial\Lambda \setminus \Upsilon)) \setminus \mathcal{C}$ correspond to numbers from the set $]-1, s_-] \cup [s_+, 1[$ with respect to the mapping $\kappa\hat{\Phi}^{-1}$. Since κ is bi-Lipschitz, the image of this set under κ^{-1} has a positive distance to x. From this (5.3) follows from the bi-Lipschitz property of $\hat{\Phi}$.

Let θ be the (bi-Lipschitz) mapping $\hat{\Phi}\kappa^{-1} :]s_-, s_+[\to \mathcal{C}$. We will identify $]s_-, s_+[$ by means of the (bi-Lipschitz) embedding $\mathbb{R} \ni x \mapsto (x, 0) \in \mathbb{R}^2$ with the set $]s_-, s_+[\times \{0\}$. Then by a deep lying theorem of Tukia, cf. [53, Thm. B], there exists a bi-Lipschitz extension of θ which maps $\mathbb{R}^2$ onto itself that we will denote by Θ.

Note that Θ maps $]s_-, s_+[\times \{0\}$ onto $\mathcal{C}$ and, in particular, $\Theta(0) = 0 \in \mathbb{R}^2$. As $\hat{\Phi}(\mathcal{X} \cap \partial\Lambda) =]-t, t[\times]-t, t[$ is open in $\mathbb{R}^2$ and due to (5.3) one finds an $\epsilon \in]0, \min\{-s_-, s_+, t\}]$, such that

$$\big[\hat{\Phi}\big(\mathcal{X} \cap \overline{\Upsilon} \cap (\partial\Lambda \setminus \Upsilon)\big) \setminus \mathcal{C}\big] \cap \Theta\big(]-\epsilon, \epsilon[\times]-\epsilon, \epsilon[\big) = \emptyset \tag{5.4}$$

and simultaneously

$$\Theta\big(]-\epsilon, \epsilon[\times]-\epsilon, \epsilon[\big) \subset]-t, t[\times]-t, t[$$

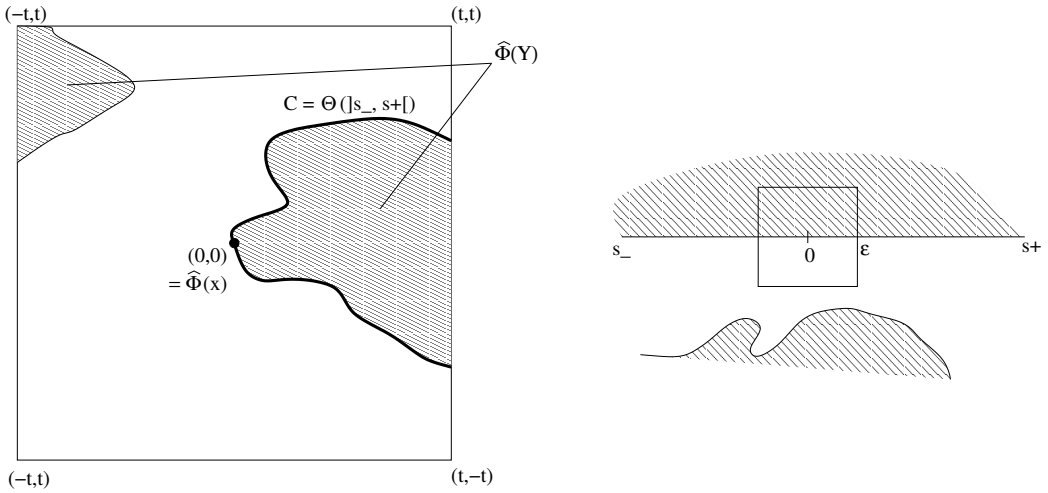

Figure 3: $\hat{\Phi}(\mathcal{X} \cap \partial\Lambda)$ and $\Theta^{-1}\big(\hat{\Phi}(\mathcal{X} \cap \partial\Lambda)\big)$

holds, see Figure 3.

This ϵ will provide us a suitable neighborhood $\mathcal{U}$ of x to complete our task. In fact, we set $\mathcal{Z} := \Theta\big(]-\epsilon,\epsilon[\times]-\epsilon,\epsilon[\big)$ and $\mathcal{U} := \Phi^{-1}(\mathcal{Z} \times]-\epsilon,\epsilon[)$. For the bi-Lipschitz mapping Ψ we define first the mapping ξ on $\mathcal{Z} \times]-\epsilon,\epsilon[$ by

$$\xi(y_1, y_2, y_3) := (\Theta^{-1}(y_1, y_2), y_3)$$

and then set $\Psi := \frac{1}{\epsilon}(\xi \circ \Phi)$ on $\mathcal{U}$. Note that $\Phi(\mathcal{U})$ is exactly $\mathcal{Z} \times]-\epsilon,\epsilon[$ by construction, which implies that everything is well defined. Furthermore, $\mathcal{U}$ is obviously a neighborhood of x and since ξ and Φ are bi-Lipschitz mappings, Ψ is of the same quality.

Regarding the desired mapping properties of Ψ, we already see

$$\Psi(\mathrm{x}) = \xi(\Phi(\mathrm{x}))/\epsilon = \xi(0)/\epsilon = \big(\Theta^{-1}(0,0), 0\big)/\epsilon = 0$$

and

$$\epsilon\Psi(\mathcal{U}) = \xi(\mathcal{Z} \times]-\epsilon,\epsilon[) = \Theta^{-1}(\mathcal{Z}) \times]-\epsilon,\epsilon[= \epsilon K.$$

Since $\mathcal{U} \subset \mathcal{O}$, we get

$$\begin{aligned}\epsilon\Psi(\mathcal{U} \cap \Lambda) &= \xi\big((\mathcal{Z} \times]-\epsilon,\epsilon[) \cap \Phi(\Lambda \cap \mathcal{O})\big) = \epsilon K \cap \xi(K_-) \\ &= \epsilon K \cap \big(\Theta^{-1}(]-1,1[^2) \times]-1,0[\big).\end{aligned}$$

Observing $\Theta(]-\epsilon,\epsilon[\times]-\epsilon,\epsilon[) \subset]-t,t[\times]-t,t[\subset]-1,1[^2$ and thus $]-\epsilon,\epsilon[\times]-\epsilon,\epsilon[\subset \Theta^{-1}(]-1,1[^2)$, this yields

$$\Psi(\mathcal{U} \cap \Lambda) = K_-. \tag{5.5}$$

For the boundary of Λ we get by analogous considerations

$$\Psi(\mathcal{U} \cap \partial\Lambda) = \Sigma, \tag{5.6}$$

so the only thing left to prove is $\Psi(\mathcal{U}\cap\Upsilon)=\Sigma_0$.

First, we focus on the interface $\mathcal{U}\cap\overline{\Upsilon}\cap(\partial\Lambda\setminus\Upsilon)$ and show that this is mapped to the line $]-1,1[\times\{0\}\times\{0\}$, i.e. the boundary of Σ_0 in Σ. Then, in a second step, we will show that $\Psi(\mathcal{U}\cap\Upsilon)$ must be exactly one of the half squares Σ_0 or $-\Sigma_0$. We first observe

$$\begin{aligned}&\Theta^{-1}\big(\mathcal{Z}\cap\hat{\Phi}(\mathcal{X}\cap\overline{\Upsilon}\cap(\partial\Lambda\setminus\Upsilon))\big)\\&=\Theta^{-1}\big(\mathcal{Z}\cap\big[\hat{\Phi}(\mathcal{X}\cap\overline{\Upsilon}\cap(\partial\Lambda\setminus\Upsilon))\setminus\mathcal{C}\big]\big)\cup\Theta^{-1}\big(\mathcal{Z}\cap\hat{\Phi}(\mathcal{X}\cap\overline{\Upsilon}\cap(\partial\Lambda\setminus\Upsilon))\cap\mathcal{C}\big).\end{aligned}$$

Now, the left part of this union is empty thanks to (5.4). Using $\mathcal{Z}=\Theta(]-\epsilon,\epsilon[\times]-\epsilon,\epsilon[)$ and $\mathcal{C}\subset\hat{\Phi}\big(\mathcal{X}\cap\overline{\Upsilon}\cap(\partial\Lambda\setminus\Upsilon)\big)$, we thus obtain

$$\begin{aligned}\Theta^{-1}\big(\mathcal{Z}\cap\hat{\Phi}(\mathcal{X}\cap\overline{\Upsilon}\cap(\partial\Lambda\setminus\Upsilon))\big)&=(]-\epsilon,\epsilon[\times]-\epsilon,\epsilon[)\cap\Theta^{-1}(\mathcal{C})\\&=(]-\epsilon,\epsilon[\times]-\epsilon,\epsilon[)\cap(]-\epsilon,\epsilon[\times\{0\})\\&=]-\epsilon,\epsilon[\times\{0\}.\end{aligned}\tag{5.7}$$

Having in mind that $\Phi(\mathcal{X}\cap\overline{\Upsilon}\cap(\partial\Lambda\setminus\Upsilon))=\hat{\Phi}(\mathcal{X}\cap\overline{\Upsilon}\cap(\partial\Lambda\setminus\Upsilon))\times\{0\}$ and $\mathcal{U}=\Phi^{-1}(\mathcal{Z}\times]-\epsilon,\epsilon[)$, this implies

$$\begin{aligned}\epsilon\Psi\big(\mathcal{U}\cap\overline{\Upsilon}\cap(\partial\Lambda\setminus\Upsilon)\big)&=\xi\big(\Phi\big(\mathcal{X}\cap\overline{\Upsilon}\cap(\partial\Lambda\setminus\Upsilon)\big)\cap\Phi(U)\big)\\&=\Theta^{-1}\big(\hat{\Phi}\big(\mathcal{X}\cap\overline{\Upsilon}\cap(\partial\Lambda\setminus\Upsilon)\big)\cap\mathcal{Z}\big)\times\{0\}\\&=]-\epsilon,\epsilon[\times\{0\}\times\{0\}\end{aligned}$$

and thus

$$\Psi\big(\mathcal{U}\cap\overline{\Upsilon}\cap(\partial\Lambda\setminus\Upsilon)\big)=]-1,1[\times\{0\}\times\{0\}.\tag{5.8}$$

Now, we claim:

(∗) (5.6) and (5.8) imply, that $\Psi(\mathcal{U}\cap\Upsilon)$ is either $]-1,1[\times]-1,0[\times\{0\}$ or $]-1,1[\times]0,1[\times\{0\}$.

Firstly, (5.6) and (5.8) imply that at least one of the two sets in this claim must contain a point from $\Psi(\mathcal{U}\cap\Upsilon)$. Let in this spirit $\mathcal{A}$ be any of the two sets $]-1,1[\times]-1,0[\times\{0\}$ or $]-1,1[\times]0,1[\times\{0\}$, which contains at least one point from $\Psi(\mathcal{U}\cap\Upsilon)$. Both the sets $\Psi(\mathcal{U}\cap\Upsilon)$ and $\Psi(\mathcal{U}\cap(\partial\Lambda\setminus\Upsilon)^\circ)$ are open in $\Psi(\mathcal{U}\cap\partial\Lambda)$ and, consequently, the – mutually disjoint – sets $\Psi(\mathcal{U}\cap\Upsilon)\cap\mathcal{A}$ and $\Psi(\mathcal{U}\cap(\partial\Lambda\setminus\Upsilon)^\circ)\cap\mathcal{A}$ are open in $\mathcal{A}$. Since by (5.8) no points from $\Psi(\mathcal{U}\cap\overline{\Upsilon}\cap(\partial\Lambda\setminus\Upsilon))$ can lie in $\mathcal{A}$, we have, according to (5.2) and (5.6), the identity

$$(\Psi(\mathcal{U}\cap\Upsilon)\cap\mathcal{A})\cup(\Psi(\mathcal{U}\cap(\partial\Lambda\setminus\Upsilon)^\circ)\cap\mathcal{A})=\Psi(\mathcal{U}\cap\partial\Lambda)\cap\mathcal{A}=\mathcal{A}.\tag{5.9}$$

$\mathcal{A}$ is connected, therefore (5.9) can only be true if $\Psi(\mathcal{U}\cap(\partial\Lambda\setminus\Upsilon)^\circ)\cap\mathcal{A}=\emptyset$. This means: if any of the two sets $]-1,1[\times]-1,0[\times\{0\}$ and $]-1,1[\times]0,1[\times\{0\}$ contains

a point from $\Psi(\mathcal{U} \cap \Upsilon)$, then it is a subset of $\Psi(\mathcal{U} \cap \Upsilon)$. But then the other cannot contain a point from $\Psi(\mathcal{U} \cap \Upsilon)$, because in this case it also would be a subset of $\Psi(\mathcal{U} \cap \Upsilon)$, which cannot be true in view of (5.8) and our supposition that $\partial\Lambda \setminus \Upsilon$ is the closure of its interior. This proves the claim $(*)$.

Together with (5.5) this gives $\Psi(\mathcal{U} \cap (\Lambda \cup \Upsilon)) = K_- \cup \Sigma_0$ or $\Psi(\mathcal{U} \cap (\Lambda \cup \Upsilon)) = K_-(\cup - \Sigma_0)$. In the first case we have finished the proof, in the second we compose Ψ with a reflection at the x-z-plane to conclude. □

Corollary 5.5. *If $\Lambda \subset \mathbb{R}^3$ is a Lipschitzian polyhedron and $\overline{\Upsilon} \cap (\partial\Lambda \setminus \Upsilon)$ is a finite union of line segments, then $\Lambda \cup \Upsilon$ is regular.*

Remark 5.6. Theorem 5.4 makes precise an old suggestion of Gröger, see [29, Remark 1]. Unfortunately, the given intrinsic characterization is restricted to the dimensions 2 and 3, because there is no analogue of the Tukia theorem in dimensions above 2. Nevertheless, the by far most important cases concerning applications are covered.

6 Application to semilinear elliptic optimal control problems

In the subsequent we will employ the results of the previous sections, in particular Theorem 3.3, to derive necessary and sufficient optimality conditions for the following semilinear elliptic optimal control problem with pointwise state and control constraints and jumping boundary conditions:

$$
\text{(P)} \quad \left\{ \begin{array}{lll}
\text{minimize} & J(y,u) := \displaystyle\int_\Omega L(\mathrm{x}, y(\mathrm{x}))\, d\mathrm{x} + \int_\Gamma l(\mathrm{x}, y(\mathrm{x}), u(\mathrm{x}))\, d\sigma & \\
\text{subject to} & -\nabla \cdot a\, \nabla y + b(\mathrm{x}, y) = f & \text{in } \Omega \\
& \partial_n y = u & \text{on } \Gamma \\
& y = 0 & \text{on } \partial\Omega \setminus \Gamma \\
\text{and} & u_{\min}(\mathrm{x}) \le u(\mathrm{x}) \le u_{\max}(\mathrm{x}) & \text{a.e. on } \Gamma \\
& g(\mathrm{x}, y(\mathrm{x})) \le 0 & \text{for all } \mathrm{x} \in \overline{\Omega}.
\end{array} \right.
$$

As already mentioned in the introduction, necessary and sufficient optimality conditions for semilinear elliptic control problems have been addressed by numerous authors before (cf. for instance [8, 12, 11] and the references therein). In particular, we refer to the recent contribution of Casas et al. [11], where an optimal control problem is analyzed that is very similar to (P), but does not contain mixed boundary conditions. However, as we will see in the following, with the results of Section 3 at hand, the analysis of [11] can easily be adapted to (P).

Note that mixed boundary conditions play an important role in various applications. A typical example is the optimal control of an electric potential in a conducting material by adjusting the direct current inducing the potential. In the stationary case, this problem is modelled by the electrostatic equation, an elliptic PDE with homogeneous Neumann boundary conditions at isolated surfaces, homogeneous Dirichlet conditions at the anode and inhomogeneous Neumann boundary conditions at the cathode, where the control enters the system (see for instance [17]). Hence, the arising problem is covered by the general problem (P). We point out that state-constrained optimal control problems with mixed boundary conditions and distributed control can be discussed analogously to the following investgation of (P). However, to keep the discussion concise, we do not consider distributed controls here.

In addition to Assumption 3.2 for the coefficient function a, we require the following conditions to be satisfied by the quantities in (P):

Assumption 6.1. The domain $\Omega \subset \mathbb{R}^d$, $d \leq 4$, is a bounded Lipschitz domain, $\Gamma \subset \partial\Omega$ is an open part of its boundary and $\partial\Omega \setminus \Gamma$ has positive measure. Moreover, $\Omega \cup \Gamma$ is regular in the sense of Gröger (cf. Theorems 5.2 and 5.4 for the two and three dimensional case). The function $b : \Omega \times \mathbb{R} \to \mathbb{R}$ is twice continuously differentiable w.r.t. the second variable and monotone increasing, i.e., $\frac{\partial b}{\partial y}(\mathrm{x}, y) \geq 0$ a.e. in Ω. Furthermore, there is an $s > d/2$ such that

$$b(\cdot, 0) \in L^s(\Omega) \quad \text{and} \quad f \in L^s(\Omega).$$

Moreover, for all $M > 0$ there is a constant $C_{b,M} > 0$, such that

$$\begin{aligned} \Big|\frac{\partial b}{\partial y}(\mathrm{x}, y_1)\Big| + \Big|\frac{\partial^2 b}{\partial y^2}(\mathrm{x}, y_1)\Big| &\leq C_{b,M} \quad \text{and} \\ \Big|\frac{\partial^2 b}{\partial y^2}(\mathrm{x}, y_2) - \frac{\partial^2 b}{\partial y^2}(\mathrm{x}, y_1)\Big| &\leq C_{b,M}\,|y_2 - y_1| \end{aligned}$$

for almost all $\mathrm{x} \in \Omega$ and all $y_1, y_2 \in \mathbb{R}$ with $|y_1|, |y_2| \leq M$.

Assumption 6.2. The function $l : \Gamma \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is a Carathéodory function of class C^2 w.r.t. the second and third variables. In addition, l is convex w.r.t. the third variable. Moreover, $l(\cdot, 0, 0) \in L^1(\Gamma)$ and for all $M > 0$ there exist a constant $C_{l,M} > 0$ and a function $\psi_{l,M} \in L^2(\Gamma)$ with

$$\begin{aligned} \Big|\frac{\partial l}{\partial y}(\mathrm{x}, y_1, u_1)\Big| + \Big|\frac{\partial l}{\partial u}(\mathrm{x}, y_1, u_1)\Big| \leq \psi_{l,M}(\mathrm{x})\,, \quad |D^2_{(y,u)} l(\mathrm{x}, y_1, u_1)| \leq C_{l,M} \\ |D^2_{(y,u)} l(\mathrm{x}, y_2, u_2) - D^2_{(y,u)} l(\mathrm{x}, y_1, u_1)| \leq C_{l,M}\,(|y_2 - y_1| + |u_2 - u_1|) \end{aligned} \tag{6.1}$$

for almost all $\mathrm{x} \in \Gamma$ and all $|y_1|, |y_2|, |u_1|, |u_2| \leq M$. Here, $D^2_{(y,u)} l$ denotes the Hessian of l w.r.t. (y, u). Furthermore, $L : \Omega \times \mathbb{R} \to \mathbb{R}$ fulfills analogous conditions, i.e. it

is of class C^2 w.r.t. the second variable, $L(\cdot,0,0) \in L^1(\Omega)$ and for all $M > 0$ there exist $C_{L,M} > 0$ and $\psi_{L,M} \in L^2(\Omega)$ with

$$\begin{aligned} |\frac{\partial L}{\partial y}(\mathrm{x}, y_1)| \le \psi_{L,M}(\mathrm{x})\,, \quad |\frac{\partial^2}{\partial y^2} L(\mathrm{x}, y_1)| \le C_{L,M} \\ |\frac{\partial^2}{\partial y^2} L(\mathrm{x}, y_2) - \frac{\partial^2}{\partial y^2} L(\mathrm{x}, y_1)| \le C_{L,M}\,|y_2 - y_1| \end{aligned} \tag{6.2}$$

for almost all $\mathrm{x} \in \Omega$ and all $|y_1|, |y_2| \le M$.

Assumption 6.3. The bounds in the control constraints satisfy $u_{\min}, u_{\max} \in L^\infty(\Gamma)$ with $u_{\min}(\mathrm{x}) < u_{\max}(\mathrm{x})$ a.e. in Ω. Moreover, $g : \overline{\Omega} \times \mathbb{R} \to \mathbb{R}$ is continuous and twice continuously differentiable w.r.t. the second variable. In addition, $\frac{\partial g}{\partial y}$ and $\frac{\partial^2 g}{\partial y^2}$ are continuous on $\bar{\Omega} \times \mathbb{R}$, and $g(\mathrm{x}, 0) < 0$ is satisfied on $\partial\Omega \setminus \Gamma$.

Note that the last conditions in Assumption 6.3 allow for the existence of a Slater point, which is essential for the derivation of first-order necessary conditions (see Assumption 6.16 below).

6.1 Discussion of the state equation

We start the discussion of (P) with the analysis of the state equation, i.e.

$$\begin{aligned} -\nabla \cdot a\,\nabla y + b(\mathrm{x}, y) &= f \quad \text{in } \Omega \\ \partial_n y &= u \quad \text{on } \Gamma \\ y &= 0 \quad \text{on } \partial\Omega \setminus \Gamma. \end{aligned} \tag{6.3}$$

Definition 6.4. Let $q \in [2, \infty[$ and $\mathfrak{s}, \mathfrak{r} \in \mathbb{R}$ satisfy $\mathfrak{s} > 1$ and let $\mathfrak{r} > 1$, if $d = q = 2$, and $\mathfrak{s} \ge dq/(d+q)$ and $\mathfrak{r} \ge (d-1)q/d$, otherwise. Moreover, let $\varphi \in L^{\mathfrak{s}}(\Omega)$ and $\psi \in L^{\mathfrak{r}}(\Gamma)$ be given. Then we denote the elements of $W_\Gamma^{-1,q}(\Omega)$, associated to φ and ψ, by $\tilde{\varphi}$ and $\tilde{\psi}$, i.e.

$$\langle \tilde{\varphi}\,,\, w \rangle_{W_\Gamma^{-1,q}(\Omega)} := \int_\Omega \varphi\, w \, d\mathrm{x}, \quad \langle \tilde{\psi}\,,\, w \rangle_{W_\Gamma^{-1,q}(\Omega)} := \int_\Gamma \psi\, w \, d\sigma, \quad w \in W_\Gamma^{1,q'}(\Omega). \tag{6.4}$$

Since embedding and trace theorems guarantee $w \in L^{\mathfrak{s}'}(\Omega)$ and $\tau_\Gamma w \in L^{\mathfrak{r}'}(\Gamma)$, if $w \in W_\Gamma^{1,q'}(\Omega)$, the integrals in (6.4) are finite and, hence, $\tilde{\varphi}$ and $\tilde{\psi}$ are well defined.

Definition 6.5. Suppose that $f \in L^{\mathfrak{s}}(\Omega)$, $\mathfrak{s} > 2d/(d+2)$, and $u \in L^{\mathfrak{r}}(\Gamma)$, $\mathfrak{r} > (2d-2)/d$. Then a function $y \in W_\Gamma^{1,2}(\Omega) \cap L^\infty(\Omega)$ is said to be a *solution of* (6.3), if it fulfills the operator equation

$$-\nabla \cdot a\,\nabla y + \tilde{b}(y) = \tilde{f} + \tilde{u} \quad \text{in } W_\Gamma^{-1,2}(\Omega), \tag{6.5}$$

where $\tilde{f}, \tilde{u} \in W_\Gamma^{-1,2}(\Omega)$ are defined according to Definition 6.4 and $\tilde{b} : L^\infty(\Omega) \to W_\Gamma^{-1,2}(\Omega)$ is analogously given by

$$\langle \tilde{b}(y)\,,\, w\rangle_{W_\Gamma^{-1,2}(\Omega)} := \int_\Omega b(\mathrm{x}, y(\mathrm{x}))\, w(\mathrm{x})\, d\mathrm{x}, \quad w \in W_\Gamma^{1,2}(\Omega).$$

Note that, due to Assumption 6.1, the Nemyzki operator $\Phi_b(y) := b(\cdot, y(\cdot))$ is continuous from $L^\infty(\Omega)$ to $L^{\mathfrak{s}}(\Omega)$, $\mathfrak{s} > 2d/(d+2)$, so $\tilde{b}$ is well defined.

Theorem 6.6. *Let $f \in L^s(\Omega)$ with $s > d/2$ and $u \in L^r(\Gamma)$ with $r > d-1$. Then, under Assumption 6.1, there exists a unique solution of (6.3) in the sense of Definition 6.5. Moreover, there is an $\alpha > 0$ such that this solution belongs to $C^\alpha(\Omega)$.*

Proof. The existence of a unique solution in $W_\Gamma^{1,2}(\Omega) \cap L^\infty(\Omega)$ is standard (cf. for instance [8] or [1] and the references therein). For convenience of the reader, we recall the main arguments. First, one considers a modified nonlinearity given by

$$b_k(y) := \begin{cases} b(k), & \text{if } y > k, \\ b(y), & \text{if } -k \le y \le k, \\ b(-k), & \text{if } y < -k, \end{cases}$$

with some $k > 0$. For a nonlinearity of this form, Browder and Minty's theorem for monotone operators immediately implies the existence of a unique solution in $W_\Gamma^{1,2}(\Omega)$. Then a classical argument in the spirit of Stampacchia [50] yields

$$\|y\|_{L^\infty(\Omega)} \le c_\infty \left(\|f\|_{L^s(\Omega)} + \|u\|_{L^r(\Gamma)} + 1\right)$$

with a constant c_∞ independent of f and k. It is easily verified that the mixed boundary conditions do not influence the analysis in [50].
Hence, if we choose $k \ge \|y\|_{L^\infty(\Omega)}$, then the solution of the truncated problem coincides with the one of (6.3). It remains to verify the Hölder continuity of y, which follows from Theorem 3.3 together with a classical bootstrapping argument. To see this, rewrite (6.5) as

$$(-\nabla \cdot a\, \nabla + 1)y = g \tag{6.6}$$

with $g := \tilde{f} + \tilde{u} - \tilde{b}(y) + \tilde{y}$ and $\tilde{y}$ according to Definition 6.4. Due to $f, b(y) \in L^s(\Omega)$, $s > d/2$, $u \in L^r(\Gamma)$, $r > d-1$, and $y \in L^\infty(\Omega)$, Sobolev embedding theorems give that $g \in W_\Gamma^{-1,q}(\Omega)$ for a $q > d$. Therefore, Theorem 3.3 implies $y \in C^\alpha(\Omega)$. □

Definition 6.7. For the rest of this section, let $s > d/2$ and $r > d-1$ be fixed, but arbitrary. Moreover, f is a fixed inhomogeneity in $L^s(\Omega)$ (cf. Assumption 6.1). Based on Theorem 6.6, we introduce the *control-to-state operator* $S : L^r(\Gamma) \to W_\Gamma^{1,2}(\Omega) \cap C^\alpha(\Omega)$, mapping u to the solution of (6.3).

Lemma 6.8. *Suppose that there is a sequence $\{u_k\}$ converging weakly to u in $L^r(\Gamma)$. Then $S(u_k) \to S(u)$ in $W_\Gamma^{1,2}(\Omega) \cap C^\alpha(\Omega)$.*

Proof. With Theorem 3.3 at hand, the arguments are standard (cf. for instance [11]). Nevertheless, let us recall the basic ideas. In all what follows we use the notation $y_k := S(u_k)$ and $y := S(u)$. The weak convergence of $\{u_k\}$ implies the uniform boundedness of this sequence in $L^r(\Gamma)$ giving in turn that $\{y_k\}$ is uniformly bounded in $C(\overline{\Omega})$. Hence, $\{y_k\}$ and $\{\Phi_b(y_k)\}$, with Φ_b as defined above, converge weakly in $L^s(\Omega)$ with $s > d/2$, to some z_y and z_Φ, respectively. Now define the sequence $\{g_k\}$ in $W_\Gamma^{-1,q}(\Omega)$ by $g_k := \tilde{f} + \tilde{u}_k - \tilde{b}(y_k) + \tilde{y}_k$. Due to the compact embedding $L^s(\Omega) \hookrightarrow W_\Gamma^{-1,q}(\Omega)$ and the compactness of the trace operator $\tau_\Gamma : W_\Gamma^{1,q'}(\Omega) \to L^{r'}(\Gamma)$, weak convergences of $\{u_k\}$, $\{y_k\}$, and $\{\Phi_b(y_k)\}$ imply strong convergence of $\{g_k\}$ in $W_\Gamma^{-1,q}(\Omega)$ to $g := \tilde{f} + \tilde{u} - \tilde{z}_\Phi + \tilde{z}_y$, where $\tilde{z}_\Phi$ and $\tilde{z}_y$ again denote the elements in $W_\Gamma^{-1,q}(\Omega)$ associated to z_Φ and z_y, respectively. Now consider again the auxiliary equation (6.6) with g_k as inhomogeneity. Theorem 3.3 then implies

$$y_k \to \eta := (-\nabla \cdot a \nabla + 1)^{-1} g \quad \text{in } W_\Gamma^{1,2}(\Omega) \cap C^\alpha(\Omega).$$

This in particular guarantees $y_k \to \eta$ in $L^\infty(\Omega)$ and, hence, $\Phi_b(y_k) \to \Phi_b(\eta)$ in $L^s(\Omega)$, $s > d/2$, as well as $\tilde{y}_k \to \tilde{\eta}$ and $\tilde{b}(y_k) \to \tilde{b}(\eta)$ in $W_\Gamma^{-1,q}(\Omega)$. Consequently, η is the solution of (6.3) associated to u, which implies $y_k \to y$ in $W_\Gamma^{1,2}(\Omega) \cap C^\alpha(\Omega)$. □

Now, we turn to the linearized version of (6.3). Given a $\bar{y} \in L^\infty(\Omega)$, the linearized state equation reads as

$$-\nabla \cdot a \nabla y + \tilde{b}'(\bar{y}) y = \tilde{h} \quad \text{in } W_\Gamma^{-1,2}(\Omega), \tag{6.7}$$

where $\tilde{h} \in W_\Gamma^{-1,2}(\Omega)$ and $\tilde{b}'(\bar{y}) : W_\Gamma^{1,2}(\Omega) \to W_\Gamma^{-1,2}(\Omega)$ is defined by

$$\langle \tilde{b}'(\bar{y}) y \,,\, w \rangle_{W_\Gamma^{-1,2}(\Omega)} := \int_\Omega \frac{\partial b}{\partial y}(\mathrm{x}, \bar{y}(\mathrm{x})) y(\mathrm{x})\, w(\mathrm{x})\, d\mathrm{x}, \quad w \in W_\Gamma^{1,2}(\Omega).$$

Note that Assumption 6.1 implies $\frac{\partial b}{\partial y}(\mathrm{x}, \bar{y}(\mathrm{x})) \in L^\infty(\Omega)$ and that, due to the monotonicity of b, $\frac{\partial b}{\partial y}(\mathrm{x}, \bar{y}(\mathrm{x})) \geq 0$ holds true a.e. in Ω. Hence, an immediate consequence of Corollary 3.6 is the following

Lemma 6.9. *Let $\bar{y} \in L^\infty(\Omega)$ be given. For every $\tilde{h} \in W_\Gamma^{-1,2}(\Omega)$ there is a unique solution $y \in W_\Gamma^{1,2}(\Omega)$ of (6.7). Furthermore, if $\tilde{h} \in W_\Gamma^{-1,q}(\Omega)$ for some $q > d$, then $y \in W_\Gamma^{1,2}(\Omega) \cap C^\alpha(\Omega)$ for some $\alpha > 0$.*

In view of Assumption 6.1, the Nemyzki operator $\Phi_b(y) = b(\cdot, y(\cdot))$ clearly is twice continuously Fréchet differentiable in $L^\infty(\Omega)$. Thus, together with Lemma 6.9, the implicit function theorem implies the following result (for a detailed proof see for instance [10]).

Theorem 6.10. *Under Assumption 6.1 the control-to-state operator S is twice continuously Fréchet differentiable from $L^r(\Gamma)$ to $W^{1,2}_\Gamma(\Omega) \cap C^\alpha(\Omega)$. Its first derivative at $\bar u \in L^r(\Gamma)$ in direction $h \in L^r(\Gamma)$ solves*

$$-\nabla \cdot a\,\nabla y + \tilde b'(\bar y) y = \tilde h \quad \text{in } W^{-1,2}_\Gamma(\Omega), \tag{6.8}$$

where $\bar y = S(\bar u)$ and $\tilde h$ denotes the element of $W^{-1,2}_\Gamma(\Omega)$ associated to h. Furthermore, $\eta = S''(\bar u)[h_1, h_2]$, $h_i \in L^r(\Gamma)$, $i = 1, 2$, is the solution of

$$-\nabla \cdot a\,\nabla \eta + \tilde b'(\bar y)\eta = -\tilde b''(\bar y) y_1 y_2 \quad \text{in } W^{-1,2}_\Gamma(\Omega) \tag{6.9}$$

with $y_i = S'(\bar u)h_i$, $i = 1, 2$, i.e. the solution of (6.8), and

$$\langle \tilde b''(\bar y) y_1 y_2\,,\, w\rangle_{W^{-1,2}_\Gamma(\Omega)} := \int_\Omega \frac{\partial^2 b}{\partial y^2}(\mathrm{x}, \bar y(\mathrm{x})) y_1(\mathrm{x}) y_2(\mathrm{x})\, w(\mathrm{x})\, d\mathrm{x}, \quad w \in W^{1,2}_\Gamma(\Omega).$$

Note that, due to $h_i \in L^r(\Gamma)$, $i = 1, 2$, Lemma 6.9 yields $y_i \in L^\infty(\Omega)$. In addition, Assumption 6.1 implies $\frac{\partial^2 b}{\partial y^2}(\cdot, \bar y(\cdot)) \in L^s(\Omega)$, so $\tilde b''(\bar y) y_1 y_2$ is well defined.

6.2 An adjoint equation involving measures

It is well known that the Lagrange multipliers associated to pointwise state constraints are in general only regular Borel measures, which appear as inhomogeneity in the adjoint equation (cf. for instance [8]). Before we are in the position to discuss such an equation, the set D_q, introduced in Corollary 3.7, has to be investigated in more detail. Recall that D_q denotes the domain of the maximal restriction of $-\nabla \cdot a\,\nabla + 1$ to $W^{-1,q}_\Gamma(\Omega)$. Throughout this section we use the abbreviation $A_V := -\nabla \cdot a\,\nabla + V$, where $V \in L^\infty(\Omega)$ denotes a given, non-negative function. Since $|\partial\Omega \setminus \Gamma| > 0$ by Assumption 6.1, $A_V : D_q \to W^{-1,q}_\Gamma(\Omega)$ is continuously invertible.

Lemma 6.11. *The space $\big(D_q,\ \|\,.\,\|_{D_q} := \|-\nabla \cdot a\,\nabla\,. + .\,\|_{W^{-1,q}_\Gamma(\Omega)}\big)$ is a Banach space. Moreover, $W^{1,q}_\Gamma(\Omega)$ is dense in D_q.*

Proof. Clearly, since $A_1 = -\nabla \cdot a\,\nabla + 1$ is linear and injective, $\|\,.\,\|_{D_q}$ indeed represents a norm on D_q and is equivalent to the graph norm on D_q. Moreover, the completeness of D_q follows from the closedness of $A_1 : D_q \to W^{-1,q}_\Gamma(\Omega)$, which holds since A_1 is continuously invertible by Corollary 3.6. In order to show the density of $W^{1,q}_\Gamma(\Omega)$, consider the restriction of A_1 to functions in $W^{1,q}_\Gamma(\Omega)$, denoted by $\tilde A_1 : W^{1,q}_\Gamma(\Omega) \to W^{-1,q}_\Gamma(\Omega)$. Due to the continuous invertibility of A_1, the space $W^{1,q}_\Gamma(\Omega)$ is dense in D_q, if $R(\tilde A_1)$ is dense in $W^{-1,q}_\Gamma(\Omega)$, where $R(\tilde A_1)$ denotes the

range of $\tilde{A}_1$. Since $\overline{R(\tilde{A}_1)} = \ker(\tilde{A}_1^*)^\perp$, $R(\tilde{A}_1)$ is dense in $W_\Gamma^{-1,q}(\Omega)$, iff $\ker(\tilde{A}_1^*) = 0$, where $\tilde{A}_1^*$ is defined by

$$\langle \tilde{A}_1^* v, w \rangle_{W_\Gamma^{-1,q'}} := \int_\Omega (a^\top \nabla v \cdot \nabla w + vw)\, d\mathrm{x}\,, \quad v \in W_\Gamma^{1,q'}(\Omega), w \in W_\Gamma^{1,q}(\Omega).$$

Clearly, $\tilde{A}_1^*$ is injective due to the coercivity of the associated bilinear form, giving in turn the assertion. □

Next, let us consider the following PDE

$$\begin{aligned} -\nabla \cdot a^\top \nabla p + V\, p &= \mu_\Omega \quad \text{in } \Omega \\ \partial_n p &= \mu_\Gamma \quad \text{on } \Gamma \\ p &= 0 \quad \text{on } \partial\Omega \setminus \Gamma, \end{aligned} \tag{6.10}$$

where Ω and a are supposed to fulfill the assumptions of Theorem 3.3. Moreover, V is a fixed, but arbitrary non-negative function in $L^\infty(\Omega)$. Furthermore, the inhomogeneity μ is given in $\mathcal{M}(\overline{\Omega})$ which is the space of regular Borel measures that can be identified with the dual of $C(\overline{\Omega})$ by means of the Riesz representation theorem. Moreover, μ_Ω and μ_Γ denote the restrictions of μ to Ω and Γ, respectively. In view of formal integration by parts, we define solutions to (6.10) as follows.

Definition 6.12. A function $p \in W_\Gamma^{1,q'}(\Omega)$, $q' = q/(q-1) < d/(d-1)$, is said to be a *solution of* (6.10), if the equation

$$\int_\Omega (a^\top \nabla p \cdot \nabla w + V\, p\, w)\, d\mathrm{x} = \langle \mu\,,\, w \rangle_{\mathcal{M}(\overline{\Omega})} \quad \forall\, w \in W_\Gamma^{1,q}(\Omega) \tag{6.11}$$

is satisfied.

Lemma 6.13. *Let $V \in L^\infty(\Omega)$, $V(\mathrm{x}) \geq 0$ a.e. in Ω and $\mu \in \mathcal{M}(\overline{\Omega})$ be given. Then there is a unique solution to* (6.10) *in the sense of Definition 6.12. This solution satisfies*

$$\|p\|_{W_\Gamma^{1,q'}(\Omega)} \leq \gamma\, \|\mu\|_{\mathcal{M}(\overline{\Omega})}$$

with a constant $\gamma > 0$ independent of μ.

Proof. The variational formulation (6.11) is equivalent to

$$\langle \tilde{A}_V^*\, p\,,\, w \rangle_{W_\Gamma^{-1,q'}(\Omega)} = \langle p\,,\, \tilde{A}_V\, w \rangle_{W_\Gamma^{1,q'}(\Omega)} = \langle \mu\,,\, w \rangle_{\mathcal{M}(\overline{\Omega})} \quad \forall\, w \in W_\Gamma^{1,q}(\Omega), \tag{6.12}$$

where, as above, $\tilde{A}_V : W_\Gamma^{1,q}(\Omega) \to W_\Gamma^{-1,q}(\Omega)$ denotes the restriction of A_V to $W_\Gamma^{1,q}(\Omega)$. Since $W_\Gamma^{1,q}(\Omega)$ is dense in D_q by Lemma 6.11, we see that (6.12) is equivalent to

$$\langle p\,,\, A_V\, w \rangle_{W_\Gamma^{1,q'}(\Omega)} = \langle \mu\,,\, w \rangle_{\mathcal{M}(\overline{\Omega})} \quad \forall\, w \in D_q \quad \Leftrightarrow \quad A_V^*\, p = \hat{\mu} \quad \text{in } D_q^*.$$

Here, D_q^* denotes the dual to D_q. Moreover, $\hat{\mu}$ is the element in D_q^* associated to $\mu \in \mathcal{M}(\overline{\Omega})$ by

$$\langle \hat{\mu}\,,\, w\rangle_{D_q^*} = \langle \mu\,,\, w\rangle_{\mathcal{M}(\overline{\Omega})} = \int_{\overline{\Omega}} w(\mathrm{x})\, d\mu \quad \forall\, w \in D_q,$$

which is well defined due to $D_q \hookrightarrow C(\overline{\Omega})$ by Theorem 3.3. Now, Corollary 3.6 guarantees $(A_V^*)^{-1} \in \mathcal{B}(D_q^*, W_\Gamma^{1,q'}(\Omega))$. Hence, due to the equivalence of $A_V^* p = \hat{\mu}$ to (6.11), there is a unique solution in the sense of the above definition and it holds

$$\begin{aligned}\|p\|_{W_\Gamma^{1,q'}(\Omega)} &\le \|(A_V)^{-1}\|_{\mathcal{B}(W_\Gamma^{-1,q}(\Omega),D_q)}\, \|\hat{\mu}\|_{D_q^*} \\ &\le \gamma \sup_{\substack{w\in D_q\\ w\neq 0}} \frac{|\langle \hat{\mu}\,,\, w\rangle_{D_q}|}{\|w\|_{D_q}} \le \gamma \sup_{\substack{w\in C(\overline{\Omega})\\ w\neq 0}} \frac{|\langle \mu\,,\, w\rangle_{\mathcal{M}(\overline{\Omega})}|}{\|w\|_{C(\overline{\Omega})}} = \gamma\, \|\mu\|_{\mathcal{M}(\overline{\Omega})},\end{aligned}$$

which gives the assertion. □

6.3 Necessary and sufficient optimality conditions

With the above results, the analysis of this section is along the lines of [11]. Hence, we shorten the description, if the arguments are analogous to the ones in [11]. First, let us introduce the reduced objective functional $j : L^\infty(\Gamma) \to \mathbb{R}$ and the Lagrange function $\mathcal{L} : L^\infty(\Gamma) \times \mathcal{M}(\overline{\Omega}) \to \mathbb{R}$ by

$$j(u) := J(S(u), u) = \int_\Omega L(\mathrm{x}, S(u)(\mathrm{x}))\, d\mathrm{x} + \int_\Gamma l(\mathrm{x}, S(u)(\mathrm{x}), u(\mathrm{x}))\, d\sigma, \tag{6.13}$$

$$\mathcal{L}(u,\mu) := j(u) + \int_{\overline{\Omega}} g(\mathrm{x}, S(u)(\mathrm{x}))d\mu. \tag{6.14}$$

Lemma 6.14. *Let $\mu \in \mathcal{M}(\overline{\Omega})$ be arbitrary. Then the Lagrange function is twice continuously Fréchet differentiable w.r.t. u from $L^\infty(\Gamma)$ to $\mathbb{R}$. If $\mu_{\partial\Omega\setminus\Gamma} = 0$, then its first partial derivative at $\bar{u}$ in direction $h \in L^\infty(\Gamma)$ is given by*

$$\frac{\partial \mathcal{L}}{\partial u}(\bar{u},\mu)h = \int_\Gamma \Big[\frac{\partial l}{\partial u}(\mathrm{x}, \bar{y}(\mathrm{x}), \bar{u}(\mathrm{x})) + p(\mathrm{x})\Big] h(\mathrm{x})\, d\sigma, \tag{6.15}$$

where $\bar{y} = S(\bar{u})$ and $p \in W_\Gamma^{1,q'}(\Omega)$ solves

$$\begin{aligned} -\nabla\cdot a^\top \nabla p + \frac{\partial b}{\partial y}(\bar{y})p &= \frac{\partial L}{\partial y}(\bar{y}) + \frac{\partial g}{\partial y}(\bar{y})\mu_\Omega && \text{in } \Omega \\ \partial_n p &= \frac{\partial l}{\partial y}(\bar{y},\bar{u}) + \frac{\partial g}{\partial y}(\bar{y})\mu_\Gamma && \text{on } \Gamma \\ p &= 0 && \text{on } \partial\Omega\setminus\Gamma \end{aligned} \tag{6.16}$$

in the sense of Definition 6.12. Moreover, the second derivative of $\mathcal{L}$ *at* $\bar{u}$ *in directions* $h_1, h_2 \in L^\infty(\Gamma)$ *is given by*

$$\begin{aligned}\frac{\partial^2 \mathcal{L}}{\partial u^2}(\bar{u},\mu)h_1h_2 = \int_\Omega \Big[\frac{\partial^2 L}{\partial y^2}(\mathrm{x},\bar{y},\bar{u})y_1y_2 - p\,\frac{\partial^2 b}{\partial y^2}(\mathrm{x},\bar{y})y_1y_2\Big]\,d\mathrm{x} \\ + \int_\Gamma \Big[\frac{\partial^2 l}{\partial y^2}(\mathrm{x},\bar{y},\bar{u})y_1y_2 + \frac{\partial^2 l}{\partial y\partial u}(\mathrm{x},\bar{y},\bar{u})(y_1h_2+y_2h_1) \\ + \frac{\partial^2 l}{\partial u^2}(\mathrm{x},\bar{y},\bar{u})h_1h_2\Big]\,d\sigma + \int_{\overline{\Omega}} \frac{\partial^2 g}{\partial y^2}(\mathrm{x},\bar{y},\bar{u})y_1y_2\,d\mu\end{aligned} \tag{6.17}$$

with $y_i = S'(\bar{u})h_i$, $i = 1, 2$.

Proof. The arguments are standard (cf. [10]). Nevertheless, we shortly describe the derivation of (6.15) to see how the associated theory is influenced by the analysis of the adjoint equation as carried out in Section 6.2. The differentiability of $\mathcal{L}$ is an immediate consequence of Assumptions 6.1–6.3 and Theorem 6.10. Concerning the explicit form of $\frac{\partial \mathcal{L}}{\partial u}$, the chain rule yields

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial u}(\bar{u},\mu)h = \int_\Omega \frac{\partial L}{\partial y}(\bar{y},\bar{u})y\,d\mathrm{x} \\ + \int_\Gamma \Big(\frac{\partial l}{\partial y}(\bar{y},\bar{u})y + \frac{\partial l}{\partial u}(\bar{y},\bar{u})h\Big)\,d\sigma + \langle \mu\,,\,\frac{\partial g}{\partial y}(\bar{y})y\rangle_{\mathcal{M}(\overline{\Omega})}\end{aligned} \tag{6.18}$$

with $\bar{y} = S(\bar{u})$ and $y = \frac{\partial S}{\partial u}(\bar{u})h$, i.e. $y \in D_q$ solves $A_{b'(\bar{y})}\,y = -\nabla\cdot a\,\nabla y + \tilde{b}'(\bar{y})y = \tilde{h}$ in $W_\Gamma^{-1,q}(\Omega)$. According to the analysis of Section 6.2, the variational formulation of (6.16) is equivalent to

$$\langle A^*_{b'(\bar{y})}\,p\,,\,v\rangle_{D_q^*} = \int_\Omega \frac{\partial L}{\partial y}(\bar{y},\bar{u})v\,d\mathrm{x} + \int_\Gamma \frac{\partial l}{\partial y}(\bar{y},\bar{u})v\,d\sigma + \langle \mu\,,\,\frac{\partial g}{\partial y}(\bar{y})v\rangle_{\mathcal{M}(\overline{\Omega})} \quad \forall\, v \in D_q$$

(cf. the proof of Lemma 6.13). Choosing $v = y$ as test function yields

$$\begin{aligned}&\int_\Omega \frac{\partial L}{\partial y}(\bar{y},\bar{u})y\,d\mathrm{x} + \int_\Gamma \frac{\partial l}{\partial y}(\bar{y},\bar{u})y\,d\sigma + \langle \mu\,,\,\frac{\partial g}{\partial y}(\bar{y})y\rangle_{\mathcal{M}(\overline{\Omega})} \\ &\quad = \langle A^*_{b'(\bar{y})}\,p\,,\,y\rangle_{D_q^*} = \langle A_{b'(\bar{y})}\,y\,,\,p\rangle_{W_\Gamma^{-1,q}(\Omega)} = \langle \tilde{h}\,,\,p\rangle_{W_\Gamma^{-1,q}(\Omega)} = \int_\Gamma h\,p\,d\sigma.\end{aligned}$$

Inserting this into (6.18) gives (6.15). Finally, (6.17) follows from an analogous argument. □

Definition 6.15. A function $u \in L^\infty(\Gamma)$ is called *feasible* for (P), if it fulfills

$$u_{\min}(\mathrm{x}) \le u(\mathrm{x}) \le u_{\max}(\mathrm{x}) \quad \text{a.e. on } \Gamma$$
$$g(\mathrm{x}, S(u)(\mathrm{x})) \le 0 \quad \text{for all } \mathrm{x} \in \overline{\Omega}.$$

Under Assumptions 6.1–6.3 there is at least one (global) solution of (P), provided that a feasible function exists (see [9, Thm. 8] for the proof).

Let us now turn to necessary optimality conditions for (P). It is well known that certain constraint qualifications are required to discuss pointwise inequality constraints on the state as they occur in (P). Here, we rely on the following *linearized Slater condition*.

Definition 6.16. Let $\bar{u} \in L^\infty(\Gamma)$ be feasible for (P). We say that the *linearized Slater condition* is fulfilled at $\bar{u}$, if there exists a function $\hat{u} \in L^\infty(\Gamma)$, such that

$$u_{\min}(\mathrm{x}) \le \hat{u}(\mathrm{x}) \le u_{\max}(\mathrm{x}) \quad \text{a.e. on } \Gamma, \tag{6.19}$$
$$g(\mathrm{x}, \bar{y}(\mathrm{x})) + \frac{\partial g}{\partial y}(\mathrm{x}, \bar{y}(\mathrm{x}))y(\mathrm{x}) < 0 \quad \text{for all } \mathrm{x} \in \overline{\Omega}, \tag{6.20}$$

where $\bar{y} = S(\bar{u})$ and $\hat{y} = S'(\bar{u})(\hat{u} - \bar{u})$.

Note that, due to $\hat{y}|_{\partial\Omega\setminus\Gamma} = 0$, (6.20) yields $g(\mathrm{x}, \bar{y}(\mathrm{x})) = g(\mathrm{x}, 0) < 0$ for all $x \in \partial\Omega \setminus \Gamma$ which is guaranteed by Assumption 6.3. With the existence and regularity results for the state and the adjoint equation obtained before, the theory of first-order necessary conditions for (P) is standard. For the corresponding theorem, we define the *Hamiltonian associated to* (P), denoted by $H : \Gamma \times \mathbb{R} \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$:

$$H(\mathrm{x}, y, u, p) := l(\mathrm{x}, y, u) + p\,(u - b(\mathrm{x}, y)).$$

The definition of H allows to formulate the first-order necessary conditions in form of Pontryagin's principle. For the corresponding proof we refer to [7].

Theorem 6.17. *Suppose that $\bar{u} \in L^\infty(\Gamma)$ is a local solution of* (P) *in the topology of $L^\infty(\Gamma)$, i.e., $j(\bar{u}) \le j(u)$ for all feasible u with $\|u - \bar{u}\|_{L^\infty(\Gamma)} \le \varepsilon$. Furthermore, denote the state associated to $\bar{u}$ by $\bar{y} \in W^{1,2}_\Gamma(\Omega) \cap C^\alpha(\Omega)$. Moreover, let Assumptions 6.1–6.3 hold and let the linearized Slater condition be satisfied at $\bar{u}$. Then there exist a function $p \in W^{1,q'}_\Gamma(\Omega)$ and a Borel measure $\mu \in \mathcal{M}(\overline{\Omega})$, such that the adjoint equation* (6.16) *is fulfilled in the sense of Definition 6.12 and it holds*

$$\int_{\overline{\Omega}} (v(\mathrm{x}) - g(\mathrm{x}, \bar{y}(\mathrm{x})))d\mu(\mathrm{x}) \le 0 \quad \textit{for all } v \in C(\overline{\Omega}) \textit{ with } v(\mathrm{x}) \le 0\ \forall\, x \in \overline{\Omega} \tag{6.21}$$

$$H(\mathrm{x}, \bar{y}(\mathrm{x}), \bar{u}(\mathrm{x}), p(\mathrm{x})) = \min_{t \in U_{\mathrm{ad}}(\mathrm{x}, \bar{u}(\mathrm{x}))} H(\mathrm{x}, \bar{y}(\mathrm{x}), t, p(\mathrm{x})) \quad \textit{a.e. on } \Gamma, \tag{6.22}$$

where $U_{\mathrm{ad}}(\mathrm{x}, \bar{u}(\mathrm{x})) := [\max\{u_{\min}(\mathrm{x}), \bar{u}(\mathrm{x}) - \varepsilon\}, \min\{u_{\max}(\mathrm{x}), \bar{u}(\mathrm{x}) + \varepsilon\}]$.

In [8], it is shown that the Lagrange multiplier associated to the state constraints is concentrated in the Borel set $\{\mathrm{x} \in \overline{\Omega} : g(\mathrm{x}, \bar{y}(\mathrm{x})) = 0\}$, such that $\mu_{\partial\Omega\setminus\Gamma} = 0$ since $g(\mathrm{x}, 0) < 0$ on $\partial\Omega \setminus \Gamma$ according to Assumption 6.3. Hence, we obtain homogeneous Dirichlet boundary conditions on $\partial\Omega \setminus \Gamma$ also in the adjoint equation (6.16). The first-order necessary conditions in Theorem 6.17 can also be formulated in terms of the Lagrangian (see [11] for details).

In all what follows, let $\bar{u}$ again be a fixed local optimum with associated state $\bar{y}$, adjoint state p, and Lagrange multiplier μ such that (6.21) and (6.22) are fulfilled. For the statement of second-order sufficient conditions accounting for strongly active sets, we have to restrict to the two dimensional case, since the underlying analysis heavily relies on the assumption that $S : L^2(\Omega) \to C(\overline{\Omega})$ (see [11, Sections 4 and 6.3]). In view of Theorem 6.6, this is not fulfilled in the three and four dimensional case. We start with the definition of the *critical cone associated to* $\bar{u}$:

$$C(\bar{u}) := \{h \in L^2(\Gamma) : h \text{ satisfies conditions (a), (b), and (c)}\},$$

where

$$h(\mathrm{x}) \begin{cases} \geq 0, & \text{if } \bar{u}(\mathrm{x}) = u_{\min}(\mathrm{x}), \\ \leq 0, & \text{if } \bar{u}(\mathrm{x}) = u_{\max}(\mathrm{x}), \\ = 0, & \text{if } \frac{\partial H}{\partial u}(x, \bar{y}(\mathrm{x}), \bar{u}(\mathrm{x}), p(\mathrm{x})) = 0, \end{cases} \tag{a}$$

$$\frac{\partial g}{\partial y}(\mathrm{x}, \bar{y}(\mathrm{x}))y(\mathrm{x}) \leq 0, \quad \text{if } g(\mathrm{x}, \bar{y}(\mathrm{x})) = 0, \tag{b}$$

$$\int_{\overline{\Omega}} \frac{\partial g}{\partial y}(\mathrm{x}, \bar{y}(\mathrm{x}))y(\mathrm{x})d\mu(\mathrm{x}) = 0 \tag{c}$$

and $y = S'(\bar{u})h$. Note that $y \in C(\overline{\Omega})$ in the two dimensional case. Moreover, the derivative of the Hamiltonian is given by $\frac{\partial H}{\partial u}(x, \bar{y}, \bar{u}, p) = \frac{\partial l}{\partial u}(\mathrm{x}, \bar{y}, \bar{u}) + p$.

Now, we are in the position to state the second-order sufficient conditions for (P). With the above results, in particular Lemma 6.8, the corresponding proof is completely analogous to the one presented in [11].

Theorem 6.18. *Let $d = 2$, let Assumptions 6.1–6.3 be satisfied and suppose that $\bar{u} \in L^\infty(\Gamma)$ with associated state $\bar{y} \in W^{1,2}_\Gamma(\Omega) \cap C^\alpha(\Omega)$ is feasible for* (P). *Moreover, let $p \in W^{1,q'}_\Gamma(\Omega)$ and $\mu \in \mathcal{M}(\Omega)$ exist such that* (6.16), (6.21), *and* (6.22) *are satisfied. In addition, it is assumed that there are two constants $\omega, \tau > 0$ with*

$$\frac{\partial^2 l}{\partial u^2}(\mathrm{x}, \bar{y}(\mathrm{x}), \bar{u}(\mathrm{x})) \geq \omega \quad \text{if} \quad \left|\frac{\partial H}{\partial u}(x, \bar{y}(\mathrm{x}), \bar{u}(\mathrm{x}), p(\mathrm{x}))\right| \leq \tau, \ \text{a.e. on } \Gamma \tag{6.23}$$

$$\frac{\partial^2 \mathcal{L}}{\partial u^2}(\bar{u}, \mu)h^2 > 0 \quad \text{for all } h \in C(\bar{u}) \setminus \{0\}. \tag{6.24}$$

Then there exist $\varepsilon, \delta > 0$*, such that*

$$j(u) \geq j(\bar{u}) + \frac{\delta}{2} \|u - \bar{u}\|^2_{L^2(\Gamma)}$$

for all feasible $u \in L^\infty(\Gamma)$ *with* $\|u - \bar{u}\|_{L^\infty(\Gamma)} < \varepsilon$*.*

Note that, according to Lemma 6.14, $\mathcal{L}$ is only continuously differentiable from $L^\infty(\Gamma)$ to $\mathbb{R}$. However, it is straightforward to see that Assumptions 6.1–6.3 ensure that $\frac{\partial \mathcal{L}}{\partial u}$ and $\frac{\partial^2 \mathcal{L}}{\partial u^2}$ can be extended from $L^\infty(\Gamma)$ to $L^2(\Gamma)$ using (6.15) and (6.17). This extension is also used in (6.24). Note further that the sufficient conditions (6.23) and (6.24) are natural in the sense that they are comparatively close to the necessary optimality conditions (see [11, Remark 4.2] for details).

Remark 6.19. We point out that the second-order analysis can be extended to the three dimensional case if distributed controls are applied instead of boundary control, since $L^2(\Omega) \hookrightarrow W_\Gamma^{-1,q}(\Omega)$ and thus continuous states are obtained with controls in $L^2(\Omega)$ (see [11, Thm. 4.1]). Nevertheless, up to the authors' best knowledge, there is no proof of second-order conditions accounting for strongly active sets in case of pointwise state constraints and boundary controls in three dimensions.

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