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# $L^p$ -estimates for the square root of elliptic systems with mixed boundary conditions II

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## Abstract

We show  $L^p$ -estimates for square roots of second order complex elliptic systems  $L$  in divergence form on open sets in  $\mathbb{R}^d$  subject to mixed boundary conditions. The underlying set is supposed to be locally uniform near the Neumann boundary part, and the Dirichlet boundary part is Ahlfors–David regular. The lower endpoint for the interval where such estimates are available is characterized by  $p$ -boundedness properties of the semigroup generated by  $-L$ , and the upper endpoint by extrapolation properties of the Lax–Milgram isomorphism. Also, we show that the extrapolation range is relatively open in  $(1, \infty)$ .

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## 1. Introduction and main results

Let  $L$  be a second order complex elliptic system in divergence form on an open set  $O \subseteq \mathbb{R}^d$ ,  $d \geq 2$ , formally given by

$$Lu = - \sum_{i,j=1}^d \partial_i (a_{ij} \partial_j u) - \sum_{i=1}^d \partial_i (b_i u) + \sum_{j=1}^d c_j \partial_j u + du.$$

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The function  $u$  takes its values in  $\mathbb{C}^m$ , where  $m \geq 1$  is the size of the system, and the coefficients  $a_{ij}, b_i, c_j, d$  are valued in  $\mathcal{L}(\mathbb{C}^m)$  and are only supposed to be bounded, measurable, and elliptic in the sense of (2). We refer to  $d$  and  $m$  as *dimensions*, and to the implied constants in boundedness and ellipticity as *coefficient bounds*. The system  $L$  is subject to mixed boundary conditions in the following sense: We fix some closed subset  $D \subseteq \partial O$ , on which we impose homogeneous Dirichlet boundary conditions, and in the complementary boundary part  $N := \partial O \setminus D$  we impose natural boundary conditions.

To make this more precise, denote by  $W_D^{1,2}(O)$  the first-order Sobolev space on  $O$  with a homogeneous Dirichlet boundary condition on  $D$ . A proper definition will be given in Section 2.2. Put  $\mathbb{W}_D^{1,2}(O) := W_D^{1,2}(O)^m$  and define the sesquilinear form  $a : \mathbb{W}_D^{1,2}(O) \times \mathbb{W}_D^{1,2}(O) \rightarrow \mathbb{C}$  by

$$a(u, v) = \int_O \sum_{i,j=1}^d a_{ij} \partial_j u \cdot \overline{\partial_i v} + \sum_{i=1}^d b_i u \cdot \overline{\partial_i v} + \sum_{j=1}^d c_j \partial_j u \cdot \overline{v} + du \cdot \overline{v} \, dx.$$

Define  $L$  as the operator in  $L^2(O)^m$  associated with  $a$ . Then  $L$  is invertible, maximal accretive, and sectorial. We take a closer look on the properties of  $L$  in Section 2.3. In particular,  $L$  possesses a square root  $L^{\frac{1}{2}}$ . The question if  $D(L^{\frac{1}{2}}) = \mathbb{W}_D^{1,2}(O)$  with equivalent norms became famous as *Kato’s square root problem*, and could be answered in the affirmative, first on the whole space [4], and later under suitable geometric requirements on open sets [5,7,12].

Phrased differently, Kato’s square root property asserts that  $L^{\frac{1}{2}}$  is an isomorphism  $\mathbb{W}_D^{1,2}(O) \rightarrow L^2(O)^m$ . It is then a natural question if  $L^{\frac{1}{2}}$  also extrapolates in a suitable range of  $p$  to an isomorphism  $\mathbb{W}_D^{1,p}(O) \rightarrow L^p(O)^m$ , where  $\mathbb{W}_D^{1,p}(O) := W_D^{1,p}(O)^m$ . In the case  $O = \mathbb{R}^d$  and  $m = 1$ , an optimal range of such  $p$  was given by Auscher [1]. When  $O$  is a bounded and interior thick domain,  $D$  is Ahlfors–David regular (see Assumption D),  $O$  satisfies the so-called *weak Lipschitz condition around  $N$* , and the coefficients are real and scalar, then a first result for mixed boundary conditions was given by Auscher, Badr, Haller-Dintelmann, and Rehberg [2]. Under the same geometric assumptions, but with complex and matrix-valued coefficients, Egert showed in [11] that  $L^{\frac{1}{2}}$  extrapolates to an isomorphism  $\mathbb{W}_D^{1,p}(O) \rightarrow L^p(O)^m$  if  $p \in (p_-(L), 2 + \varepsilon)$ . Here,  $p_-(L)$  is the infimum of  $\mathcal{I}(L)$ , where

$$\mathcal{I}(L) := \{p \in (1, \infty) : \{e^{-tL}\}_{t>0} \text{ is } L^p\text{-bounded}\},$$

and  $\varepsilon > 0$  depends on geometry, dimensions, and coefficient bounds. We will write  $\llbracket p \rrbracket := \sup_{t>0} \|e^{-tL}\|_{L^p \rightarrow L^p}$  whenever  $p \in \mathcal{I}(L)$ . In the situation of [2] one has, for instance,  $p_-(L) = 1$ , see [2, Prop. 4.6 (i)]. The notion of  $L^p$ -bounded families of operators is made precise in Definition 3.1. Under *extrapolation* we understand that  $L^{\frac{1}{2}}$  and  $L^{-\frac{1}{2}}$ , initially defined on  $\mathbb{W}_D^{1,p}(O) \cap \mathbb{W}_D^{1,2}(O)$  and  $L^p(O)^m \cap L^2(O)^m$ , respectively, extend by continuity to bounded operators  $\mathbb{W}_D^{1,p}(O) \rightarrow L^p(O)^m$  and  $L^p(O)^m \rightarrow \mathbb{W}_D^{1,p}(O)$ . In this case, we say that  $L^{\frac{1}{2}}$  is a  $p$ -isomorphism. Similarly, we say that  $L^{\frac{1}{2}}$  and  $L^{-\frac{1}{2}}$  are  $p$ -bounded and so on.

The geometric constellation in [2,11] was primarily dictated by the available  $L^2$ -theory for the Kato square root problem from [12,13]. Meanwhile, by a recent result of the author together with Egert and Haller-Dintelmann [7], Kato’s square root problem could be solved in the affirmative if  $O$  is a possibly unbounded, non-connected, not interior thick open set which is *locally*

uniform near  $N$  (see Assumption **N**), and whose Dirichlet part  $D$  is Ahlfors–David regular (see Assumption **D**). It is one aim of this article to extend the results of [11] to this setting.

Also, it was shown in [11] that if  $p < p_-(L)$ , then  $L^{\frac{1}{2}}$  is not a  $p$ -isomorphism, but sharpness for the endpoint  $p = p_-(L)$  was not treated. Moreover, it was left as an open question in [11, p. 5] to characterize the optimal range of  $p > 2$  in the case of mixed boundary conditions.

In summary, it is the goal of this paper to establish the following improvements of the state of the art presented in [11]. In fact our article should be seen as a part II to [11], which is also the motivation for our title.

- (i) The square root isomorphism  $L^{\frac{1}{2}} : \mathbb{W}_D^{1,2}(O) \rightarrow L^2(O)^m$  can be extrapolated away from 2 even if  $O$  is only supposed to be open, locally uniform near  $N$ , and with Ahlfors–David regular Dirichlet part  $D$ ,
- (ii) the interior of the optimal range in which  $L^{\frac{1}{2}}$  is a  $p$ -isomorphism is  $(p_-(L), \tilde{q}_+(L))$ ,
- (iii) if  $p_-(L) > 1$ , then  $L^{\frac{1}{2}}$  is not a  $p_-(L)$ -isomorphism, similarly for  $\tilde{q}_+(L) < \infty$ .

Here,  $\tilde{q}_+(L)$  is defined as follows: We know from the Lax–Milgram lemma that  $\mathcal{L} : \mathbb{W}_D^{1,2}(O) \rightarrow \mathbb{W}_D^{-1,2}(O)$  is an isomorphism, where we put  $\mathbb{W}_D^{-1,p}(O) := (\mathbb{W}_D^{1,p'}(O))^*$  for  $p \in (1, \infty)$ . Here,  $p'$  is the Hölder-conjugate exponent to  $p$ . Similarly to the case of  $L^{\frac{1}{2}}$ , we say that  $\mathcal{L}$  is a  $p$ -isomorphism if  $\mathcal{L}^{-1}$  extends from  $\mathbb{W}_D^{-1,p}(O) \cap \mathbb{W}_D^{-1,2}(O)$  to a bounded operator  $\mathbb{W}_D^{-1,p}(O) \rightarrow \mathbb{W}_D^{1,p}(O)$ . Then define the set

$$\mathcal{J}(L) := \{p \in (1, \infty) : \mathcal{L} \text{ is a } p\text{-isomorphism}\},$$

and put  $\tilde{q}_+(L) := \sup \mathcal{J}(L)$ . Moreover, for  $q \in \mathcal{J}(L)$ , put  $\langle q \rangle := \|\mathcal{L}^{-1}\|_{\mathbb{W}_D^{-1,p}(O) \rightarrow \mathbb{W}_D^{1,p}(O)}$ . The quantities  $\llbracket p \rrbracket$  and  $\langle q \rangle$  will be useful to quantify dependence of implicit constants in Theorem 1.2.

**Remark 1.1.** Clearly,  $\mathcal{L}$  always extends from  $\mathbb{W}_D^{1,p}(O) \cap \mathbb{W}_D^{1,2}(O)$  to a bounded operator  $\mathbb{W}_D^{1,p}(O) \rightarrow \mathbb{W}_D^{-1,p}(O)$ , and the operator norm of this extension is controlled by the coefficient bounds. If  $p \in \mathcal{J}(L)$ , then this extension is one-to-one and onto, and its inverse coincides on  $\mathbb{W}_D^{-1,p}(O) \cap \mathbb{W}_D^{-1,2}(O)$  with the inverse provided by the Lax–Milgram lemma. The compatibility with the inverse operator in the case  $p = 2$  is the main advantage of our definition, as it enables us to invoke interpolation arguments.

On  $\mathbb{R}^d$ , a characterization of the upper endpoint using  $\tilde{q}_+(L)$  already appeared in [1, Cor. 4.24]. However, the version back then contained a flaw that originates from compatibility issues (confer with Remark 1.1) due to the unbounded geometry. This was pointed out by the author of [1] and Egert in their recent monograph [3, p. 135]. They also resolve the issue using compatible Hodge decompositions. Our characterization does not use this detour and works on domains with mixed boundary conditions.

The precise formulation of our main theorem then reads as follows.

**Theorem 1.2.** *Let  $O \subseteq \mathbb{R}^d$  be open, and  $D \subseteq \partial O$  be closed. Assume that  $(O, D)$  satisfies Assumption **N** and Assumption **D**. Then the system  $L$  satisfies the following:*

- (i) If  $p_-(L) < r < p < 2$ , then  $L^{\frac{1}{2}}$  is a  $p$ -isomorphism and implicit constants depend on  $p$ ,  $r$ ,  $\llbracket r \rrbracket$ , dimensions, geometry, and coefficient bounds. If  $2 < q < r < \tilde{q}_+(L)$ , then  $L^{\frac{1}{2}}$  is a  $q$ -isomorphism, and implicit constants depend on  $q$ ,  $r$ ,  $\llbracket r \rrbracket$ , dimensions, geometry, and coefficient bounds,
- (ii) if  $p \in (1, \infty)$  and  $L^{\frac{1}{2}}$  is a  $p$ -isomorphism, then  $p_-(L) \leq p \leq \tilde{q}_+(L)$ ,
- (iii) if  $p_-(L) > 1$ , then  $L^{\frac{1}{2}}$  is not a  $p_-(L)$ -isomorphism, and if  $\tilde{q}_+(L) < \infty$ , then  $L^{\frac{1}{2}}$  is not a  $\tilde{q}_+(L)$ -isomorphism.

**Remark 1.3.** The number  $p_-(L)$  is at most  $2_*$ , see [11, Thm. 1.6], and the number  $\tilde{q}_+(L)$  is at least 2 by the Lax–Milgram lemma. If  $d \geq 3$ ,  $p_-(L)$  can be improved to  $2_* - \varepsilon$ , see again [11, Thm. 1.6], and  $\tilde{q}_+(L)$  can be improved to  $2 + \varepsilon$  in any dimension, see Proposition 7.1.

In the next section, we will introduce all necessary definitions and make precise our geometric assumptions. Section 3 provides preliminary results, including some  $p$ -bounds for  $L^{-\frac{1}{2}}$  and the  $H^\infty$  calculus, most of them taken from [11] without proof. Therefore, we advise the reader to keep a copy of that article handy. In Section 4, we review results on the  $p$ -bound for  $L^{\frac{1}{2}}$  when  $p < 2$ . They rely on a weak-type argument which is based on a Calderón–Zygmund decomposition for Sobolev functions. Its proof relies on a new Hardy’s inequality related to mixed boundary conditions presented in Section 4.1. Finally, we prove Theorem 1.2 in the Sections 5–7. The respective sections correspond to items (i)–(iii) in the theorem.

**Notation.** Write  $\text{diam}(\cdot)$  for the diameter of a set and  $d(\cdot, \cdot)$  for the distance between two sets. We employ the shorthand notation  $d_E(x) := d(E, \{x\})$ . The  $(d - 1)$ -dimensional Hausdorff measure is denoted by  $\mathcal{H}^{d-1}$ . If  $\varphi \in (0, \pi)$ , then write  $S_\varphi$  for the (open) sector  $\{z \in \mathbb{C} \setminus \{0\} : |\arg(z)| < \varphi\}$ , and put  $S_0 := (0, \infty)$ . Also, write  $\overline{S}_\varphi := \overline{S}_\varphi$  for the closed sector. For  $\Xi \subseteq \mathbb{C}$  open, denote the space of bounded and holomorphic functions on  $\Xi$  by  $H^\infty(\Xi)$  and equip it with the supremum norm. Inductively, we introduce the shorthand notation  $2^{[0]} := 2$  and  $2^{[j+1]} := (2^{[j]})^*$  for iterated Sobolev exponents.

## 2. Elliptic systems & function spaces

We properly introduce the  $(m \times m)$ -elliptic system  $L$  on  $O \subseteq \mathbb{R}^d$ ,  $d \geq 2$ , from the introduction. To this end, we also need to define Sobolev spaces subject to mixed boundary conditions, and we discuss geometric properties of the pair  $(O, D)$ .

### 2.1. Geometry

Let  $O \subseteq \mathbb{R}^d$  be open and  $D \subseteq \partial O$  be closed. Fix the pair  $(O, D)$  for the rest of this article. In particular, implicit constants might depend on this choice of geometry, as well as on dimensions. Introduce the following set of geometric assumptions.

**Assumption N.** There are  $\varepsilon \in (0, 1]$  and  $\delta \in (0, \infty]$  such that with  $N_\delta := \{z \in \mathbb{R}^d : d(z, N) < \delta\}$  one has the following properties.

- (i) All points  $x, y \in O \cap N_\delta$  with  $|x - y| < \delta$  can be joined in  $O$  by an  $\varepsilon$ -cigar with respect to  $\partial O \cap N_\delta$ , that is to say, a rectifiable curve  $\gamma \subseteq O$  of length  $\ell(\gamma) \leq \varepsilon^{-1}|x - y|$  such that

$$d(z, \partial O \cap N_\delta) \geq \frac{\varepsilon |z - x| |z - y|}{|x - y|} \quad (z \in \gamma).$$

(ii)  $O$  has *positive radius near  $N$* , that is, there exists  $\lambda > 0$  such that all connected components  $O'$  of  $O$  with  $\partial O' \cap N \neq \emptyset$  satisfy  $\text{diam}(O') \geq \lambda \delta$ .

**Assumption D.** There are constants  $C, c > 0$  such that

$$\forall x \in D, r \in (0, \text{diam}(D)]: \quad cr^{d-1} \leq \mathcal{H}^{d-1}(\mathbf{B}(x, r) \cap D) \leq Cr^{d-1}.$$

**Assumption D'.** There are constants  $C, c > 0$  such that

$$\forall x \in D, r \in (0, 1]: \quad cr^{d-1} \leq \mathcal{H}^{d-1}(\mathbf{B}(x, r) \cap D) \leq Cr^{d-1}.$$

Assumption **N** means that  $O$  is *locally uniform near  $N$* , see [7, Sec. 2.1] for further information and a comparison with other geometric frameworks, including that used in [2,11]. Assumption **D** means that  $D$  is *Ahlfors–David regular* and Assumption **D'** that  $D$  is  $(d - 1)$ -regular. If  $D$  is bounded, then Assumption **D** and Assumption **D'** are equivalent, and in the unbounded case, Assumption **D** implies Assumption **D'**, but the converse might be false.

Throughout, assume that Assumption **N** is in place.

### 2.2. Sobolev spaces

Let  $p \in [1, \infty)$ . Write  $W^{1,p}(O)$  for the usual first-order Sobolev space of  $L^p$ -functions on  $O$  whose distributional gradient is in  $L^p(O)^d$ . Also, introduce the set of test functions

$$C_D^\infty(O) := \{u|_O : u \in C_0^\infty(\mathbb{R}^d) \quad \& \quad d(\text{supp}(u), D) > 0\}, \tag{1}$$

where  $C_0^\infty(\mathbb{R}^d)$  denotes the set of smooth and compactly supported functions on  $\mathbb{R}^d$ . Then the closed subspace  $W_D^{1,p}(O)$  of  $W^{1,p}(O)$  corresponding to *mixed boundary conditions on  $D$*  is given as the closure of  $C_D^\infty(O)$  in  $W^{1,p}(O)$ . See [6, Sec. 2.2] for an alternative set of test functions that leads to the same closure. Moreover, define the space  $W_D^{-1,p}(O)$  by  $W_D^{1,p'}(O)^*$ . Here,  $X^*$  denotes the space of antilinear functionals on  $X$ , and the  $W_D^{-1,p}(O)$ – $W_D^{1,p'}(O)$  duality extends the  $L^2(O)$ -duality. Replacing  $W$  by  $\mathbb{W}$ , we extend all definitions to  $m$ -fold product spaces as before. All definitions can be extended to the more general case that  $\Xi \subseteq \mathbb{R}^d$  is open and  $E \subseteq \overline{\Xi}$ ; Then we obtain for instance  $W_E^{1,p}(\Xi)$ .

Often, we will need that the space  $W_D^{1,p}(O)$  has the following (inhomogeneous) *extension property*. This is the main result in [6].

**Proposition 2.1.** *Suppose Assumption N. Then there exists a linear extension operator  $E$  on  $L_{\text{loc}}^1(O)$  that restricts for any  $p \in (1, \infty)$  to a bounded operator  $E : W_D^{1,p}(O) \rightarrow W_D^{1,p}(\mathbb{R}^d)$ .*

Here, extension operator refers to the property that  $(Eu)|_O = u$  for any  $u \in L_{\text{loc}}^1(O)$ . A consequence of Proposition 2.1 is that classical inequalities like the Sobolev embedding  $W^{1,p}(\mathbb{R}^d) \subseteq$

$L^{p^*}(\mathbb{R}^d)$  valid for  $p < d$  translate to  $W_D^{1,p}(O)$ . Here,  $p^* := \frac{pd}{d-p}$  is the (upper) Sobolev exponent to  $p$  if  $p < d$ , otherwise put  $p^* = \infty$ . Similarly, define the lower Sobolev exponent by  $p_* := \frac{pd}{d+p}$ .

### 2.3. The elliptic system

We give a precise definition for the elliptic system  $L$  from the introduction. Consider the coefficients  $a_{ij}, b_i, c_j, d: O \rightarrow \mathcal{L}(\mathbb{C}^m)$ . Here,  $i$  and  $j$  refer to row and column notation and  $m \geq 1$  is the size of the system. Put  $A = (a_{ij})_{ij}, b = (b_i)_i, c = (c_j)_j$ . We assume the upper bound

$$\left\| \begin{bmatrix} d & c \\ b & A \end{bmatrix} \right\|_{L^\infty(O; \mathcal{L}(\mathbb{C}^{dm+m}))} \leq \Lambda$$

for the coefficients. Using the spaces from Section 2.2, define the sesquilinear form

$$a: W_D^{1,2}(O) \times W_D^{1,2}(O) \rightarrow \mathbb{C}, \quad a(u, v) = \int_O \begin{bmatrix} d & c \\ b & A \end{bmatrix} \begin{bmatrix} u \\ \nabla u \end{bmatrix} \cdot \overline{\begin{bmatrix} v \\ \nabla v \end{bmatrix}} dx.$$

To ensure ellipticity of  $a$ , assume for some  $\lambda > 0$  the (inhomogeneous) *Gårding inequality*

$$\operatorname{Re} a(u, u) \geq \lambda (\|u\|_2^2 + \|\nabla u\|_2^2) \quad (u \in W_D^{1,2}(O)). \tag{2}$$

Associate with  $a$  the operator

$$\mathcal{L}: W_D^{1,2}(O) \rightarrow W_D^{-1,2}(O), \quad \langle \mathcal{L}u, v \rangle = a(u, v).$$

In virtue of (2) and the Lax–Milgram lemma,  $\mathcal{L}$  is invertible. Define  $L$  to be the maximal restriction of  $\mathcal{L}$  in  $L^2(O)^m$  in virtue of the inclusion  $L^2(O)^m \subseteq W_D^{-1,2}(O)$ . Clearly,  $L$  is again invertible. By ellipticity it follows that  $L$  is densely defined. Moreover, for some  $\omega' \in [0, \pi/2)$  that depends on coefficient bounds, the numerical range  $\Theta(L)$  is contained in the closed sector  $\overline{S}_{\omega'}$ . This is a consequence of  $\Theta(L) \subseteq \Theta(a)$  together with ellipticity of  $a$ . Define  $\omega$  as the infimum over all such  $\omega'$ . In particular,  $L$  is sectorial and maximal accretive, hence generates a contraction semigroup on  $L^2(O)^m$ .

We will freely use the sectorial functional calculus of  $L$  and assume that the reader is familiar with this concept. The reader can consult the monograph [14] for further information on this topic.

The following theorem is the main result from [7] and establishes Kato’s square root property for  $L$ .

**Theorem 2.2** (*Kato’s square root property*). *Assume that the pair  $(O, D)$  satisfies Assumption N and Assumption D. Then  $D(L^{\frac{1}{2}}) = W_D^{1,2}(O)$  holds with equivalence of norms*

$$\|u\|_2 + \|\nabla u\|_2 \approx \|L^{\frac{1}{2}}u\|_2 \quad (u \in W_D^{1,2}(O)),$$

where the implicit constants depend only on geometry, dimensions,  $\lambda$ , and  $\Lambda$ .

### 2.4. Decomposition of $\mathcal{L}^{-1}$

We use a representation formula for  $\mathcal{L}^{-1}$ . A similar formula, but for  $\mathcal{L}$  itself, was also used in [11]. In fact, the lemma below follows from the result in [11] and Theorem 2.2. For convenience of the reader, we include the short and direct proof. The reason why we need a formula for  $\mathcal{L}^{-1}$  is that in unbounded sets the question of compatibility becomes a non-trivial task.

**Lemma 2.3.** *One has the identity*

$$(L^{\frac{1}{2}}\mathcal{L}^{-1}u | f)_2 = \langle u, (L^*)^{-\frac{1}{2}}f \rangle \quad (u \in \mathbb{W}_D^{-1,2}(O), f \in L^2(O)^m).$$

**Proof.** First, let  $u \in L^2(O)^m$  and  $v \in \mathbb{W}_D^{1,2}(O)$ . Then  $\mathcal{L}^{-1}u \in D(L)$ , hence, taking Theorem 2.2 into account, deduce

$$(u | v)_2 = a(\mathcal{L}^{-1}u, v) = (L\mathcal{L}^{-1}u | v) = (L^{\frac{1}{2}}\mathcal{L}^{-1}u | (L^*)^{\frac{1}{2}}v).$$

We specialize to  $v := (L^*)^{-\frac{1}{2}}f$  to conclude

$$\langle u, (L^*)^{-\frac{1}{2}}f \rangle = (u | (L^*)^{-\frac{1}{2}}f)_2 = (L^{\frac{1}{2}}\mathcal{L}^{-1}u | f).$$

Owing to Theorem 2.2 (applied with  $L$  and  $L^*$ ) and the Lax–Milgram lemma, both sides are continuous in  $u$  with respect to the  $\mathbb{W}_D^{-1,2}(O)$  topology. Hence, the claim follows by density.  $\square$

## 3. Review on off-diagonal estimates and $L^p$ extrapolation

### 3.1. Off-diagonal estimates

We review decay properties in  $L^p$  of operator families related to  $L$ . Definition 3.1 also clarifies the notion that the family  $\{e^{-tL}\}_{t>0}$  is  $L^p$ -bounded, which was used in the definition of  $p_-(L)$  in the introduction. The results obtained in this section will be used frequently in the course of this article.

**Definition 3.1.** Let  $\Xi \subseteq \mathbb{R}^d$  be measurable,  $m_1, m_2$  natural numbers and let  $U \subseteq \mathbb{C} \setminus \{0\}$  and  $\mathcal{T} = \{T(z)\}_{z \in U}$  be a family of bounded operators  $L^2(\Xi)^{m_1} \rightarrow L^2(\Xi)^{m_2}$ . Given  $1 \leq p \leq q \leq \infty$ , say that  $\mathcal{T}$  is  $L^p \rightarrow L^q$  bounded if there exists a constant  $C > 0$  such that for all  $u \in L^p(\Xi)^{m_1} \cap L^2(\Xi)^{m_1}$  and  $z \in U$  one has

$$\|T(z)u\|_{L^q(\Xi)^{m_2}} \leq C|z|^{-\frac{d}{2}(\frac{1}{p}-\frac{1}{q})}\|u\|_{L^p(\Xi)^{m_1}}.$$

If in addition there is  $c \in (0, \infty)$  such that, whenever  $E, F \subseteq \Xi$  and  $\text{supp}(u) \subseteq E$ , the more restrictive estimate

$$\|T(z)u\|_{L^q(F)^{m_2}} \leq C|z|^{-\frac{d}{2}(\frac{1}{p}-\frac{1}{q})}e^{-c\frac{d(E,F)^2}{|z|}}\|u\|_{L^p(E)^{m_1}}$$

holds, then say that  $\mathcal{T}$  satisfies  $L^p \rightarrow L^q$  off-diagonal estimates. Finally, if  $p = q$  in the above situations, we simply talk about  $L^p$ -boundedness and  $L^p$  off-diagonal estimates.



If  $\mathcal{T} = \{e^{-tL}\}_{t>0}$  and  $\mathcal{T}$  is  $L^p \rightarrow L^q$  bounded for some values  $1 \leq p < q \leq \infty$ , then we say that the semigroup is *hypercontractive*.

Using Davies’ trick one can show  $L^2$  off-diagonal estimates without any geometrical requirements.<sup>1</sup> The general argument is well-known, see [1] for a version on  $\mathbb{R}^d$  and [11] for a version on open sets. The following formulation follows with the proof presented in [11] when using Young’s inequality also for the term of order zero (this also eliminates the dependence of the implicit constants on  $\text{diam}(O)$  that appeared in [11]) and when replacing the function  $\varphi$  appearing in the proof by functions  $\varphi_n := d_E(x) \wedge n$  and taking the limit  $n \rightarrow \infty$  in the end.

**Proposition 3.2.** *For  $\psi \in [0, \pi/2 - \omega)$ , the operator families  $\{e^{-zL}\}_{z \in S_\psi}$ ,  $\{z \nabla e^{-z^2 L}\}_{z \in S_\psi}$ , and  $\{z L e^{-zL}\}_{z \in S_\psi}$  satisfy  $L^2$  off-diagonal estimates, and the implied constants depend on  $L$  only via its coefficient bounds.*

We continue with estimates in  $L^p$ . The following result allows to translate  $L^p$ -boundedness into  $L^q \rightarrow L^2$  off-diagonal estimates up to a slight loss in the integrability parameter. Its proof can be obtained by concatenating the relevant parts in [11, Prop. 4.4]. Note that geometry in that result is only needed to have an extension operator at ones disposal. This is ensured by Proposition 2.1 in our case.

**Proposition 3.3** (*Off-diagonal estimates from boundedness*). *Let  $q \in (p_-(L), 2)$ ,  $p \in (q, 2)$ , and let  $\psi \in [0, \pi/2 - \omega)$ . Then  $\{e^{-zL}\}_{z \in S_\psi}$  satisfies  $L^p \rightarrow L^2$  off-diagonal estimates, and the implicit constants depend on  $p, q, \llbracket q \rrbracket, \psi$ , and coefficient bounds.*

To the contrary, the following result yields  $L^p$ -boundedness from hypercontractivity. The argument is similar to that in [11, Prop. 4.4] and we only present the necessary changes.

**Proposition 3.4** (*Boundedness from hypercontractivity*). *Let  $1 \leq q < p < r \leq \infty$  be such that  $\{e^{-tL}\}_{t>0}$  is  $L^q \rightarrow L^r$  bounded. Then  $\{e^{-tL}\}_{t>0}$  is  $L^p$ -bounded, and  $\llbracket p \rrbracket$  depends only on  $p, q, r$ , coefficient bounds, and the implicit constant in the assumption.*

**Proof.** Let  $\theta \in (0, 1)$  be such that  $\frac{1}{p} = \frac{1-\theta}{2} + \frac{\theta}{r}$  and define  $[q, 2]_\theta \in (q, 2)$  by  $\frac{1}{[q, 2]_\theta} := \frac{1-\theta}{q} + \frac{\theta}{2}$ . Interpolate the  $L^q \rightarrow L^r$  bounds from the assumption with the  $L^2$  off-diagonal bounds from Proposition 3.2 to see that  $\{e^{-tL}\}_{t>0}$  satisfies  $L^{[q, 2]_\theta} \rightarrow L^p$  off-diagonal estimates, where the implicit constants depend on  $p, r$ , and implied constants in the hypothesis. Then the claim follows from [11, Lem. 4.5] with the same choices of  $s$  and  $g$  as in the proof [11, Prop. 4.4 (v)].  $\square$

As an application [11, Thm. 1.6] one can derive upper bounds for  $p_-(L)$  and lower bounds for  $p_+(L)$ . Geometry is only used to have an extension operator in hand.

**Corollary 3.5.** *One has  $p_-(L) = 1$  and  $p_+(L) = \infty$  if  $d = 2$  and  $p_-(L) \leq 2_*$  and  $p_+(L) \geq 2^*$  if  $d \geq 3$ .*

<sup>1</sup> In fact, using test functions as in (1) that are restrictions from  $\mathbb{R}^d$  constitutes a form of “geometry”. To see that one can use test function classes that only use information on  $O$  one has to impose restrictions on the geometry, see the discussion in Section 2.2.

### 3.2. Boundedness of the $H^\infty$ -calculus and Riesz transforms

In this section, we recall results from [1,11] on  $L^p$ -boundedness of the  $H^\infty$ -calculus and the Riesz transform associated with  $L$ . They are consequences of Proposition 3.3 and an extrapolation result due to Blunck and Kunstmann [9]. The use of geometry is completely hidden in the results providing off-diagonal estimates.

The following result is taken from [11, Thm. 1.3]. Observe that the operator  $f(L)$  is well-defined on  $L^2(O)^m$  owing to the Crouzeix–Delyon theorem for  $m$ - $\omega$ -accretive operators [14, Cor. 7.1.17]. Note that in the last line of [11, Thm. 1.3], the argument using the inclusion  $L^2(\Omega) \subseteq L^p(\Omega)$  has to be substituted by a standard argument using Fatou’s lemma.

**Proposition 3.6** ( *$H^\infty$ -calculus*). *Let  $p_-(L) < q < p_+(L)$ ,  $p \in (q, 2) \cup (2, q)$ , and  $\varphi \in (\omega, \pi)$ . Then for every  $f \in H^\infty(S_\varphi)$  one has*

$$\|f(L)u\|_p \lesssim \|f\|_\infty \|u\|_p \quad (u \in L^p(O)^m \cap L^2(O)^m),$$

where the implicit constant depends on  $p, q, \llbracket q \rrbracket, \varphi$ , and coefficient bounds.

In the same spirit, we obtain  $L^p$ -boundedness of the Riesz transform, which upgrades to a  $p$ -bound for  $L^{-\frac{1}{2}}$ . The result is taken from [11, Lem. 6.1 & Cor. 6.2]. As above, geometry is only used to provide off-diagonal estimates for  $\{t\nabla e^{-t^2L}\}_{t>0}$ . For this it is crucial that  $p < 2$ . Indeed, in this case the decomposition  $\sqrt{2t}\nabla e^{-2tL} = \sqrt{2}(\sqrt{t}\nabla e^{-tL})e^{-tL}$  lets us conclude  $L^p \rightarrow L^2$  off-diagonal estimates for  $\{t\nabla e^{-t^2L}\}_{t>0}$  from  $L^q$ -boundedness of  $\{e^{-tL}\}_{t>0}$  and  $L^2$  off-diagonal bounds for  $\{t\nabla e^{-t^2L}\}_{t>0}$  using composition, Proposition 3.3 and Proposition 3.2.

**Proposition 3.7** (*Riesz transform*). *Let  $p_-(L) < q < p < 2$ . Then the Riesz transform  $\nabla L^{-\frac{1}{2}}$  is  $L^p$ -bounded. Moreover, this bound can be upgraded to the  $p$ -bound*

$$\|L^{-\frac{1}{2}}u\|_{\mathbb{W}^{1,p}(O)} \lesssim \|u\|_p \quad (u \in L^p(O)^m \cap L^2(O)^m),$$

where implicit constant depends on  $p, q, \llbracket q \rrbracket$ , and coefficient bounds.

## 4. Survey on the $p$ -bound for $L^{\frac{1}{2}}$ when $p < 2$

In Proposition 3.7 we have seen the  $p$ -bound for  $L^{-\frac{1}{2}}$  when  $p < 2$ . The goal of this section is to investigate the complementing  $p$ -bound for  $L^{\frac{1}{2}}$ . The argument is in large parts already known in the literature. Therefore, we will mainly review these known results here. Of course we will indicate all necessary modifications to adapt these results to our setting. There is, however, one ingredient needed in this section that is really novel: the global Hardy inequality adapted to an unbounded Dirichlet part in Theorem 4.1. We will start with this result.

### 4.1. Hardy’s inequality

The main result of this subsection is the following Hardy’s inequality.

**Theorem 4.1** (Hardy’s inequality). Assume that the pair  $(O, D)$  satisfies Assumption  $N$  and that  $D$  satisfies Assumption  $D'$ , and let  $p \in (1, \infty)$ . Then Hardy’s inequality holds true for  $W_D^{1,p}(O)$ , that is, for all  $f \in W_D^{1,p}(O)$  one has

$$\int_O \left| \frac{f}{d_D} \right|^p dx \lesssim \|f\|_{W_D^{1,p}(O)}^p.$$

Using the extension operator from Proposition 2.1, Theorem 4.1 is a direct consequence of the following whole-space version.

**Lemma 4.2.** Assume Assumption  $D'$ , and let  $p \in (1, \infty)$ . Then Hardy’s inequality holds for  $W_D^{1,p}(\mathbb{R}^d)$ , that is, for all  $f \in W_D^{1,p}(\mathbb{R}^d)$  holds

$$\int_{\mathbb{R}^d} \left| \frac{f}{d_D} \right|^p dx \lesssim \|f\|_{W_D^{1,p}(\mathbb{R}^d)}^p.$$

The proof of Lemma 4.2 relies on the following Hardy’s inequality with pure Dirichlet boundary conditions, which is essentially contained in [16], see also [15]. Dependence of the implicit constants becomes apparent from an inspection of the proof.

**Proposition 4.3.** Let  $\Xi \subseteq \mathbb{R}^d$  be open. Assume that  $\partial\Xi$  is Ahlfors–David regular, where either  $\Xi$  is bounded or  $\partial\Xi$  is unbounded. Then one gets the estimate

$$\int_{\Xi} \left| \frac{f}{d_{\partial\Xi}} \right|^p dx \lesssim \int_{\Xi} |\nabla f|^p dx \quad (f \in C_{\partial\Xi}^\infty(\Xi)).$$

The implicit constant depends on geometry only via the implied constants from Ahlfors–David regularity of  $\partial\Xi$ . The inequality extends to  $W_{\partial\Xi}^{1,p}(\Xi)$  owing to Fatou’s lemma.

Let us come back to the proof of Lemma 4.2.

**Proof of Lemma 4.2.** Let  $(Q_k)_k$  be a grid of open cubes of diameter  $1/4$ . We consider the sets  $O_k := 2Q_k \setminus D$ . Each  $O_k$  has an Ahlfors–David regular boundary where the implicit constants depend only on the implied constants in Assumption  $D'$  and dimension.

To see this, take a ball  $B$  centered in  $\partial O_k$  with radius  $r$  at most  $1/2$  (which equals the diameter of  $O_k$ ). One has  $\partial O_k = \partial(2Q_k) \cup (D \cap 2Q_k)$ , which follows from porosity of  $D$  (see [7, discussion before Cor. 2.11]) and closedness of  $D$  by elementary geometric arguments. Consequently, the lower bound follows from the  $(d - 1)$ -regularity of  $\partial(2Q_k)$  or the  $(d - 1)$ -regularity of  $D$ , depending on the location of the center of  $B$ . The upper bound follows similarly if  $B$  doesn’t intersect either  $\partial(2Q_k)$  or  $D$ . Otherwise, say  $B$  is centered in  $\partial(2Q_k)$  and intersects  $D$  in  $x$ . Then we estimate  $\mathcal{H}^{d-1}(B \cap \partial O_k) \leq \mathcal{H}^{d-1}(B \cap \partial(2Q_k)) + \mathcal{H}^{d-1}(B(x, 2r) \cap D)$  and the estimate follows again from the  $(d - 1)$ -regularity of the two portions of the boundary. Note that all constants are uniform in  $k$ .

Now pick cutoff function  $\chi_k$  which are supported in  $2Q_k$  and equal 1 on  $\overline{Q}_k$ . Up to translation, we can use the same cut-off function for each  $k$ . Let  $f \in \mathbb{W}_D^{1,p}(\mathbb{R}^d)$  and estimate using Proposition 4.3 and the bounded overlap of  $(O_k)_k$  that

$$\int_{\mathbb{R}^d \setminus D} \left| \frac{f}{d_D} \right|^p dx \leq \sum_k \int_{O_k} \left| \frac{\chi_k f}{d_{\partial O_k}} \right|^p dx \lesssim \sum_k \|\chi_k f\|_{\mathbb{W}^{1,p}(2Q_k)}^p \lesssim \|f\|_{\mathbb{W}^{1,p}(\mathbb{R}^d)}^p.$$

Note that at the first “ $\lesssim$ ” we crucially use the control of implicit constants in the Dirichlet Hardy inequality.  $\square$

### 4.2. Calderón–Zygmund decomposition

The goal of this subsection is to investigate a Calderón–Zygmund decomposition for functions in the Sobolev space  $\mathbb{W}_D^{1,p}(O)$ . The reason for this is that the  $p$ -bound for  $L^{\frac{1}{2}}$  in Corollary 4.10 will follow from a weak-type estimate. Such a decomposition was first shown by Auscher on the whole space [1, Appendix A]. This idea was refined in [2,11] to work on domains, including the idea to use Hardy’s inequality to include (partial) Dirichlet boundary conditions (and this is the reason why we have investigated Hardy’s inequality in the previous subsection). To formulate the precise result, we introduce  $\mathbb{C}^m$ -valued Sobolev spaces subject to different boundary conditions in the individual components.

**Definition 4.4.** Let  $p \in [1, \infty)$ ,  $\Xi \subseteq \mathbb{R}^d$  open and  $E_k \subseteq \overline{\Xi}$  for  $k = 1, \dots, m$ . With the array  $\mathbb{E} := (E_k)_{k=1}^m$  define the space

$$\mathbb{W}_{\mathbb{E}}^{1,p}(\Xi) := \bigotimes_{k=1}^m \mathbb{W}_{E_k}^{1,p}(\Xi),$$

equipped with the subspace topology inherited from  $\mathbb{W}^{1,p}(\Xi)$ . Moreover, introduce the abbreviation  $\|\cdot\|_{\mathbb{W}^{1,p}(\Xi)}$  for the norm on  $\mathbb{W}_{\mathbb{E}}^{1,p}(\Xi)$ .

**Remark 4.5.** Here, we stay slightly more general than is necessary for our application. Compared to the  $L^2$  result used in [11], we cannot deal with different Dirichlet boundary parts in different components in Theorem 2.2. This is an artifact of the fact that  $O$  might not be a doubling space.

The main result of this subsection reads as follows.

**Theorem 4.6 (Sobolev Calderón–Zygmund – open set).** Let  $O \subseteq \mathbb{R}^d$  be open,  $D_k \subseteq \partial O$  be closed and  $(d - 1)$ -regular for  $k = 1, \dots, m$ , such that  $O$  is a locally uniform domain near  $\partial O \setminus D_k$  for all  $k$ , and let  $1 < p < \infty$ . Then for every  $u \in \mathbb{W}_D^{1,p}(O)$  and every  $\alpha > 0$  there exist an (at most) countable index set  $J$ , a family of cubes  $(Q_j)_{j \in J}$ , and functions  $g, b_j : O \rightarrow \mathbb{C}^m$  for  $j \in J$  such that the following holds.

- (i)  $u = g + \sum_j b_j$  holds pointwise almost everywhere,
- (ii) the family  $(Q_j)_{j \in J}$  is locally finite, and every  $x \in O$  is contained in at most  $12^d$  cubes,
- (iii)  $\sum_{j \in J} |Q_j| \lesssim \frac{1}{\alpha^p} \|u\|_{\mathbb{W}^{1,p}(O)}^p$ ,

- (iv)  $g \in \text{Lip}(O)^m$  with  $\|g\|_{\text{Lip}(O)^m} \lesssim \alpha$ ,
- (v)  $b_j \in \mathbb{W}_{\mathbb{D}}^{1,p}(O)$  with  $\|b_j\|_{\mathbb{W}^{1,p}(O)} \lesssim \alpha |Q_j|^{\frac{1}{p}}$  for every  $j \in J$ ,
- (vi) if  $p < d$ , then  $b_j \in L^q(O)^m$  for  $q \in [p, p^*]$  with  $\|b_j\|_q \lesssim \alpha |Q_j|^{1/p+(1-\theta)/d}$ , where  $\theta \in [0, 1]$  is such that  $1/q = (1-\theta)/p + \theta/p^*$ ,
- (vii)  $\|g\|_{\mathbb{W}^{1,p}(O)} + \|\sum_{j \in J'} b_j\|_{\mathbb{W}^{1,p}(O)} \lesssim \|u\|_{\mathbb{W}^{1,p}(O)}$  for all  $J' \subseteq J$ ,
- (viii)  $b_j$  is supported in  $Q_j \cap O$  for every  $j$ ,
- (ix) if  $1 < q < \infty$ ,  $u \in \mathbb{W}_{\mathbb{D}}^{1,q}(O)$ , and  $J' \subseteq J$ , then  $\sum_{j \in J'} b_j$  converges unconditionally in  $\mathbb{W}_{\mathbb{D}}^{1,q}(O)$ .

Let us point out the differences with [11, Lem. 7.2]. The most important difference is that we allow unbounded constellations in which  $O$  is only locally uniform and  $D$  does only fulfill a local  $d - 1$ -dimensionality condition. Property (vi) follows from an additional application of the Poincaré inequality and will be used for the case  $d = 2$  in Lemma 4.9 later on. The bound for  $J' \neq J$  in (vii) follows from an inspection of the proof, the same is true for the case  $q \neq p$  in (ix). The two last-mentioned properties are useful to circumvent convergence issues. These appear since we deal with operators that are a priori only bounded with respect to the  $L^2$  topology, and we cannot benefit from embedding relations as is the case of bounded domains.

In virtue of Proposition 2.1, Theorem 4.6 is an easy consequence of the following whole-space version. In particular, this shows that the only geometric ingredients are the availability of a Sobolev extension operator and Assumption  $D'$ .

**Lemma 4.7** (Sobolev Calderón–Zygmund – whole space). *Let  $D_k \subseteq \mathbb{R}^d$  be closed and  $(d - 1)$ -regular for  $k = 1, \dots, m$ , and let  $1 < p < \infty$ . For every  $u \in \mathbb{W}_{\mathbb{D}}^{1,p}(\mathbb{R}^d)$  and every  $\alpha > 0$  there exist an (at most) countable index set  $J$ , a family of cubes  $(Q_j)_{j \in J}$  and functions  $g, b_j : \mathbb{R}^d \rightarrow \mathbb{C}^m$  for  $j \in J$  such that the following holds.*

- (i)  $u = g + \sum_j b_j$  holds pointwise almost everywhere,
- (ii) the family  $(Q_j)_j$  is locally finite, and every  $x \in \mathbb{R}^d$  is contained in at most  $12^d$  cubes,
- (iii)  $\sum_j |Q_j| \lesssim \frac{1}{\alpha^p} \|u\|_{\mathbb{W}^{1,p}(\mathbb{R}^d)}^p$ ,
- (iv)  $g \in \mathbb{W}^{1,\infty}(\mathbb{R}^d)$  with  $\|g\|_{\mathbb{W}^{1,\infty}(\mathbb{R}^d)} \lesssim \alpha$ ,
- (v)  $b_j \in \mathbb{W}_{\mathbb{D}}^{1,p}(\mathbb{R}^d)$  with  $\|b_j\|_{\mathbb{W}^{1,p}(\mathbb{R}^d)} \lesssim \alpha |Q_j|^{\frac{1}{p}}$  for every  $j$ ,
- (vi)  $\|g\|_{\mathbb{W}^{1,p}(\mathbb{R}^d)} + \|\sum_{j \in J'} b_j\|_{\mathbb{W}^{1,p}(\mathbb{R}^d)} \lesssim \|u\|_{\mathbb{W}^{1,p}(\mathbb{R}^d)}$  for all  $J' \subseteq J$ ,
- (vii)  $b_j$  is compactly supported in  $Q_j$  for every  $j$ ,
- (viii) if  $1 < q < \infty$ ,  $u \in \mathbb{W}_{\mathbb{D}}^{1,q}(\mathbb{R}^d)$  and  $J' \subseteq J$ , then  $\sum_{j \in J'} b_j$  converges unconditionally in  $\mathbb{W}_{\mathbb{D}}^{1,q}(\mathbb{R}^d)$ .

The proof is similar to those in [11, Lem. 7.2] or [2, Lem. 7.1]. Indeed, in [11] they start with a function  $u$  on  $\Omega$  and decompose  $U := \eta(Eu)$ , where  $E$  is an extension operator for  $\Omega$  and  $\eta$  is a cutoff function that is constantly 1 on a ball  $B$  that compactly contains  $\Omega$ . This way, they construct a global decomposition of  $U$ , but can rely on a Hardy’s inequality on  $B$  with Dirichlet boundary condition on  $D \cup \partial B$ . It is crucial for them that the auxiliary domain and Dirichlet boundary part are still bounded. That being said, the central insight to show Lemma 4.7 is to follow their lines of argument, but directly work with a global function  $U$  and the global Hardy

inequality established in Lemma 4.2. We would like to point out that the order in which extension operator and Hardy’s inequality are applied is reversed in the approach presented in this article.

**Remark 4.8** (*boring cubes*). We would likewise use the opportunity to mention that the so-called *boring cubes* used in [11] are not needed. Indeed, they were introduced in [11] to treat Hardy-type estimates for bad functions directly in the construction. However, this bound can be deduced a posteriori using Hardy’s inequality. With this in mind, bad functions on boring cubes should be defined like bad functions on *usual cubes* and not like bad functions on *special cubes*. Gradient and non-gradient estimates for bad functions on usual cubes then apply directly to bad functions on “boring cubes”. This shortens and conceptually simplifies the proof given in [11].

4.3. Upper bound for the square root when  $p < 2$

In the case  $p < 2$ , we prove  $p$ -boundedness of the square root. The heart of the matter is the weak-type estimate in Lemma 4.9. A crucial observation is that we gain up to one Sobolev exponent in comparison to  $p_-(L)$ . We will benefit from this in Section 7 later on.

**Lemma 4.9.** *Let  $p_-(L)_* \vee 1 < q < p < 2$ , then one has for all  $\alpha > 0$  the weak-type bound*

$$|\{x \in O : |(L^{\frac{1}{2}}u)(x)| > \alpha\}| \lesssim \frac{1}{\alpha^p} \|u\|_{\mathbb{W}^{1,p}(O)}^p \quad (u \in \mathbb{W}_D^{1,p}(O) \cap \mathbb{W}_D^{1,2}(O)), \quad (3)$$

where implicit constants depend on  $p$ , coefficient bounds, and, if  $p^* < 2$ , on  $q$  and  $\llbracket q^* \rrbracket$ .

The proof of Lemma 4.9 is similar to that of [11, Prop. 8.1] and we will only explain the necessary changes, so the reader is strongly advised to keep a copy of that article handy. A key difference is that the argument in [11] assumes  $p^* < 2$ , which is not feasible in  $d = 2$ .<sup>2</sup> Property (vi) in our Calderón-Zygmund decomposition lets us circumvent this issue.

**Proof.** To start with, we claim that there exists  $r \in [p, p^*]$  satisfying

- (a)  $\{e^{-tL}\}_{t>0}$  satisfies  $L^r \rightarrow L^2$  off-diagonal estimates,
- (b) the  $H^\infty(S_\varphi)$ -calculus of  $L$  is  $L^r$ -bounded for all  $\varphi \in (\omega, \pi)$ ,
- (c)  $r \leq 2$ .

Note that, of course, (c) is necessary for (a) to hold, but we will also need to use (c) in conjunction with (b). Indeed, if  $p^* \geq 2$ , chose  $r = 2$ , which is admissible by Proposition 3.2 and the Crouzeix–Delyon theorem. Otherwise, when  $p^* < 2$ , let

$$p_-(L)_* \vee 1 < q < s_* < r_* < p < r.$$

Then, on the one hand,  $p_-(L) < s < r$ . On the other hand, by assumption of this case,  $r < p^* < 2$ . Hence,  $\{e^{-tL}\}_{t>0}$  satisfies  $L^r \rightarrow L^2$  off-diagonal estimates by Proposition 3.3, and the  $H^\infty(S_\varphi)$ -calculus of  $L$  is bounded on  $L^r$  for any  $\varphi \in (\omega, \pi)$  according to Proposition 3.6. Since

<sup>2</sup> After publication, the author of [11] resolved this problem in the arXiv version by a case distinction. We present a unified treatment here.

$\llbracket s \rrbracket \leq \llbracket q^* \rrbracket$  by interpolation with the contraction semigroup on  $L^2$ , implied constants depend on  $p, q, \llbracket q^* \rrbracket, \varphi$ , and coefficient bounds. Eventually, the dependence on  $\varphi$  will be replaced by a dependence on  $\omega$ , which in turn is under control using the coefficients bounds. Note also that we have  $r \in [p, p^*]$ .

Now let  $\alpha > 0, u \in \mathbb{W}_D^{1,p}(O)$ , and let  $u = g + \sum_j b_j$  be the Calderón–Zygmund decomposition from Theorem 4.6. Refer with (i)-(viii) to the respective properties of the decomposition. As in [11], the proof divides into 4 steps: Estimate of the good part, decomposition of the bad part into a local and a global integral, estimate of the local integral, and bound for the global integral.

**Step 1:** Handling the good part. Decompose with the Calderón–Zygmund decomposition

$$|\{|L^{\frac{1}{2}}u > \alpha\}| \leq |\{|L^{\frac{1}{2}}g > \alpha/2\}| + |\{|L^{\frac{1}{2}}\sum_{j \in J} b_j > \alpha/2\}|.$$

We refer to the first term as the *good part* and to the second term as the *bad part*. With the exact same arguments as in [11, Step 1], we conclude

$$|\{|L^{\frac{1}{2}}g > \alpha/2\}| \lesssim \frac{1}{\alpha^p} \|u\|_{\mathbb{W}^{1,p}(O)}^p.$$

**Step 2:** Decomposition of the bad part. First of all, let us mention that it suffices to assume that  $J$  is finite, provided we can show a bound that does not depend on the size of  $J$ . This allows to rearrange terms without worrying about convergence issues. Indeed, put  $J_n := J \cap \{1, \dots, n\}$  for  $n \geq 1$ , then  $\sum_{j \in J_n} b_j \rightarrow b = \sum_{j \in J} b_j$  in  $\mathbb{W}_D^{1,2}(O)$  as  $n \rightarrow \infty$  by (ix), so we get from Tchebychev’s inequality

$$\begin{aligned} |\{|L^{\frac{1}{2}}b > \alpha/2\}| &\leq |\{|L^{\frac{1}{2}}(b - \sum_{j \in J_n} b_j) > \alpha/4\}| + |\{|L^{\frac{1}{2}}\sum_{j \in J_n} b_j > \alpha/4\}| \\ &\leq \frac{16}{\alpha^2} \|L^{\frac{1}{2}}(b - \sum_{j \in J_n} b_j)\|_2^2 + |\{|L^{\frac{1}{2}}\sum_{j \in J_n} b_j > \alpha/4\}|. \end{aligned}$$

Now, if the second term can be controlled by

$$|\{|L^{\frac{1}{2}}\sum_{j \in J_n} b_j > \alpha/4\}| \lesssim \frac{1}{\alpha^p} \|u\|_{\mathbb{W}^{1,2}(O)}^p$$

with an implicit constant independent of  $n$ , then, in the light of Theorem 2.2 and by convergence of  $\sum_{j \in J_n} b_j$  to  $b$  in  $\mathbb{W}_D^{1,2}(O)$ , the first term vanishes as  $n \rightarrow \infty$ , which lets us conclude.

Furthermore, to control  $|\{|L^{\frac{1}{2}}b > \alpha/2\}|$ , it suffices as in [11, Step 2] to control the *local* and *global integrals*

$$\left| \left\{ \left| \sum_j \int_{2^{-n}}^{r_j \sqrt{2}^{-n}} Le^{-t^2 L} b_j dt \right| > \frac{\sqrt{\pi} \alpha}{8} \right\} \right| + \left| \left\{ \left| \sum_j \int_{r_j \sqrt{2}^{-n}}^\infty Le^{-t^2 L} b_j dt \right| > \frac{\sqrt{\pi} \alpha}{8} \right\} \right|$$

for all  $n \geq 1$ , where  $r_j = 2^\ell$  with  $\ell$  the unique integer such that  $2^\ell \leq \ell_j \leq 2^{\ell+1}$ , and where  $\ell_j$  is the sidelength of  $Q_j$ .

**Step 3:** Handling the local integral. Put  $\gamma := d(1/r - 1/2) + 1$  and  $C_k(Q_j) := 2^{k+1}Q_j \setminus 2^kQ_j$  for  $k \geq 2$ . We only show the bound

$$\left\| \int_{2^{-n}}^{r_j \vee 2^{-n}} Le^{-tL^2} b_j \, dt \right\|_{L^2(C_k(Q_j) \cap O)^m} \lesssim \alpha \ell_j^{d/2} 2^{-k\gamma} e^{-c4^k} \tag{4}$$

for all  $k \geq 2$ ,  $j \in J$ , and  $n \geq 1$ . Then the bound for the local integral can be concluded as in [11, Step 3].

So, let us show (4). Clearly, we can assume  $r_j \geq 2^{-n}$ . Note that the off-diagonal bounds for  $\{e^{-tL}\}_{t>0}$  can be upgraded to off-diagonal bounds for  $\{tLe^{-tL}\}_{t>0}$  by composition (see for example [11, Prop. 4.4 (iv)]), and this imports no further dependence for the implied constants. With this in hand, and using the support property (vii), we calculate for the integrand of (4) that

$$\|Le^{-t^2L} b_j\|_{L^2(C_k(Q_j) \cap O)^m} \lesssim t^{-d(\frac{1}{r}-\frac{1}{2})-2} e^{-c4^{k-1}r_j^2/t^2} \|b_j\|_r.$$

Plugging this back into (4) and using (vi) leads to

$$\begin{aligned} \left\| \int_{2^{-n}}^{r_j} Le^{-t^2L} b_j \, dt \right\|_{L^2(C_k(Q_j) \cap O)^m} &\leq \int_{2^{-n}}^{r_j} \|Le^{-t^2L} b_j\|_{L^2(C_k(Q_j) \cap O)^m} \, dt \\ &\lesssim \alpha \ell_j^{\frac{d}{p}+1-\theta} \int_{2^{-n}}^{r_j} t^{-d(\frac{1}{r}-\frac{1}{2})-1} e^{-c4^{k-1}r_j^2/t^2} \frac{dt}{t}. \end{aligned}$$

Using the substitution  $s = 4^{k-1}r_j^2/t^2$ , we obtain

$$\lesssim \alpha \ell_j^{\frac{d}{p}+1-\theta} r_j^{-\gamma} 2^{-(k-1)\gamma} \int_{4^{k-1}}^{\infty} s^{\frac{\gamma}{2}} e^{-cs} \frac{ds}{s}.$$

Keeping in mind  $\ell_j \approx r_j$  and observing  $\theta = d(1/p - 1/r)$ , the prefactor reduces to  $\ell_j^{\frac{d}{2}}$ . Then we split the exponential term and use  $s \geq 4^{k-1}$  to find

$$\lesssim \alpha \ell_j^{\frac{d}{2}} 2^{-(k-1)\gamma} e^{-c4^{k-2}} \int_0^{\infty} s^{\frac{\gamma}{2}} e^{-cs/2} \frac{ds}{s}.$$

The integral in  $s$  is finite since  $\gamma \geq 1 > 0$ . This completes the proof of (4).

**Step 4:** Estimate for the global integral. To this end, put  $J_k := \{j \in J : r_j \vee 2^{-n} = 2^k\}$  for any integer  $k$ . Then, as in [11, Step 4], there exists a function  $f$  which belongs to  $H^\infty(S_\varphi)$  for any  $\varphi \in (\omega, \pi/2)$ , with which we can write



$$\sum_{j \in J} \int_{r_j}^{\infty} L e^{-t^2 L} b_j \, dt = \sum_k \sum_{j \in J_k} \frac{1}{2^k} f(4^k L) b_j.$$

Plug this back into the definition of the global integral and use Tchebychev’s inequality (compared to [11], we apply it with  $r$  instead of  $p^*$ ), followed by linearity (here, we use that  $J$  is supposed to be finite) to derive

$$\begin{aligned} \left| \left\{ \left| \sum_j \int_{r_j}^{\infty} L e^{-t^2 L} b_j \, dt \right| > \frac{\sqrt{\pi\alpha}}{8} \right\} \right| &\lesssim \frac{1}{\alpha^r} \left\| \sum_k \sum_{j \in J_k} 2^{-k} f(4^k L) b_j \right\|_r^r \\ &= \frac{1}{\alpha^r} \left\| \sum_k f(4^k L) \sum_{j \in J_k} 2^{-k} b_j \right\|_r^r. \end{aligned}$$

Now, use the square function estimate from [11, Lem. 8.2] with  $\varphi \in (\omega, \pi/2)$ , which is justified by (b), to give

$$\left\| \sum_k f(4^k L) \sum_{j \in J_k} 2^{-k} b_j \right\|_r^r \lesssim \left\| \left( \sum_k \left| \sum_{j \in J_k} 2^{-k} b_j \right|^2 \right)^{\frac{1}{2}} \right\|_r^r.$$

Write out the  $L^r$ -norm and employ (c) to give

$$= \int_O \left( \sum_k \left| \sum_{j \in J_k} 2^{-k} b_j \right|^2 \right)^{\frac{r}{2}} \, dx \leq \int_O \sum_k \left( \sum_{j \in J_k} |2^{-k} b_j| \right)^r \, dx.$$

Continuing as in [11], we arrive at

$$\lesssim \sum_{j \in J} \ell_j^{-r} \int_O |b_j|^r \, dx.$$

Plug this back in the calculation and use (vi) followed by (iii) to conclude (recall  $\theta = d(1/p - 1/r)$ )

$$\left| \left\{ \left| \sum_{j \in J} \int_{r_j}^{\infty} L e^{-t^2 L} b_j \, dt \right| > \frac{\sqrt{\pi\alpha}}{8} \right\} \right| \lesssim \sum_{j \in J} |Q_j|^{-\frac{r}{d} + \frac{r}{p} + (1-\theta)\frac{r}{d}} = \sum_{j \in J} |Q_j| \lesssim \alpha^{-p} \|u\|_{\mathbb{W}^{1,p}(O)}^p.$$

Combining the bounds for the good part, the local integral and the global integral, this gives (3).  $\square$

Using interpolation, we conclude a  $p$ -bound for  $L^{\frac{1}{2}}$ . The interpolation theory used in [2,11] does not apply as  $O$  might not be locally doubling.

**Corollary 4.10.** *Let  $p_-(L)_* \vee 1 < q < p < 2$ , then*

$$\|L^{\frac{1}{2}}u\|_p \lesssim \|u\|_{\mathbb{W}^{1,p}(O)} \quad (u \in \mathbb{W}_D^{1,p}(O) \cap \mathbb{W}_D^{1,2}(O)),$$

where the implicit constant depends on  $p, q, \omega$ , coefficient bounds, and, if  $p^* < 2$ , on  $\llbracket q^* \rrbracket$ .

**Proof.** Put  $r := (p+q)/2$ . Write  $L^{r,\infty}(O)$  for the usual weak  $L^r$ -space on  $O$ . Recall that  $L^{r,\infty}(O)$  is a complete quasi-normed space. Owing to Lemma 4.9,  $L^{\frac{1}{2}}$  extrapolates from  $\mathbb{W}_D^{1,r}(O) \cap \mathbb{W}_D^{1,2}(O)$  to a bounded operator

$$L^{\frac{1}{2}}: \mathbb{W}_D^{1,r}(O) \rightarrow L^{r,\infty}(O)^m.$$

Here, the implied constant depends on  $p, q, \omega$ , coefficient bounds, and, if  $p^* < 2$ , on  $\llbracket q^* \rrbracket$ . Moreover, by Theorem 2.2, we have

$$L^{\frac{1}{2}}: \mathbb{W}_D^{1,2}(O) \rightarrow L^2(O)^m.$$

Chose  $\theta \in (0, 1)$  such that  $1/p = (1-\theta)/r + \theta/2$ . Real interpolation yields an extension

$$L^{\frac{1}{2}}: (\mathbb{W}_D^{1,r}(O), \mathbb{W}_D^{1,2}(O))_{\theta,2} \rightarrow (L^{r,\infty}(O)^m, L^2(O)^m)_{\theta,2}.$$

It remains to determine the interpolation spaces. For this, it suffices to argue componentwise [18, Sec. 1.18.1]. This being said, the space on the right-hand side then coincides with  $L^p(O)^m$  according to [18, Sec. 1.18.6]. For the left-hand side, this follows from the whole space case in [8, Thm. 1.2] (here, we need Assumption  $D'$ ) together with the retraction-coretraction principle [18, Sec. 1.2.4] applied with  $R$  the pointwise restriction to  $O$  and  $S$  the extension operator from Proposition 2.1.  $\square$

### 5. Extrapolation of the square root property

In this part, we prove Theorem 1.2 (i). Most of the work in the case  $p < 2$  has already been done in Sections 3.2 and 4.3, so we mainly focus on the case  $p > 2$ .

Consider Fig. 1. Lemmas 5.1 and 5.2 make precise the following heuristic: If two out of three arrows in the diagram correspond to  $p$ -isomorphisms, then all arrows are  $p$ -isomorphisms.

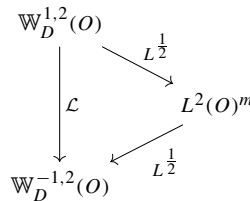


Fig. 1. Decomposition of  $\mathcal{L}$  into two square roots.

If  $\mathcal{L}$  is a  $p$ -isomorphism, then Lemma 5.3 and the case  $p < 2$  yield that the lower  $L^{\frac{1}{2}}$ -arrow comes for free. This leads to the proof of Theorem 1.2 (i) in the case  $p > 2$ . In the same spirit, but using Lemma 6.1, we are going to show necessity in the next section.

**Lemma 5.1.** *Let  $p \in (1, \infty)$  be such that  $L^{\frac{1}{2}}$  is a  $p$ -isomorphism and  $(L^*)^{\frac{1}{2}}$  is a  $p'$ -isomorphism. Then  $\mathcal{L}$  is a  $p$ -isomorphism, and implicit constants depend only on those in the assumptions.*

A similar correspondence appeared in [10, Thm. 6.5]. They work with realizations of  $L$  in  $L^p$  that rely on the fact that on bounded domains  $L^q \subseteq L^p$  if  $q \geq p$ . In particular, compatibility is never an issue. Our simple argument using compatible extensions extends also to the unbounded setting.

**Proof.** To show the  $p$ -isomorphism property we only have to show that  $\mathcal{L}^{-1}$  is  $\mathbb{W}_D^{-1,p}(O) \rightarrow \mathbb{W}_D^{1,p}(O)$  bounded on  $\mathbb{W}_D^{-1,p}(O) \cap \mathbb{W}_D^{-1,2}(O)$  in the case of  $\mathcal{L}$ , compare with Remark 1.1. Hence, let  $u \in \mathbb{W}_D^{-1,p}(O) \cap \mathbb{W}_D^{-1,2}(O)$ , and also let  $h \in L^{p'}(O)^m \cap L^2(O)^m$ . Calculate first using Lemma 2.3 and the  $p'$ -isomorphism property for  $L^*$  that

$$|(L^{\frac{1}{2}}\mathcal{L}^{-1}u | h)| = |\langle u, (L^*)^{-\frac{1}{2}}h \rangle| \leq \|u\|_{\mathbb{W}_D^{-1,p}(O)} \|(L^*)^{-\frac{1}{2}}h\|_{\mathbb{W}_D^{1,p'}(O)} \lesssim \|u\|_{\mathbb{W}_D^{-1,p}(O)} \|h\|_{p'}.$$

Taking the supremum over  $h$  yields

$$\|L^{\frac{1}{2}}\mathcal{L}^{-1}u\|_p \lesssim \|u\|_{\mathbb{W}_D^{-1,p}(O)}. \tag{5}$$

Implicit constants depend on the implied constants coming from the  $p'$ -isomorphism assumption. Write  $\mathcal{L}^{-1} = L^{-\frac{1}{2}}L^{\frac{1}{2}}\mathcal{L}^{-1}$  and use the  $p$ -isomorphism hypothesis along with (5) to give

$$\|\mathcal{L}^{-1}u\|_{\mathbb{W}_D^{1,p}(O)} = \|L^{-\frac{1}{2}}L^{\frac{1}{2}}\mathcal{L}^{-1}u\|_{\mathbb{W}_D^{1,p}(O)} \lesssim \|L^{\frac{1}{2}}\mathcal{L}^{-1}u\|_p \lesssim \|u\|_{\mathbb{W}_D^{-1,p}(O)}. \quad \square$$

The proof of the following lemma is similar, so we omit its proof.

**Lemma 5.2.** *Let  $p \in (1, \infty)$  be such that  $\mathcal{L}$  is a  $p$ -isomorphism and  $(L^*)^{\frac{1}{2}}$  is a  $p'$ -isomorphism. Then  $L^{\frac{1}{2}}$  is a  $p$ -isomorphism, and implicit constants depend only on those in the assumptions.*

To verify in the proof of Theorem 1.2 (i) that Lemma 5.2 is applicable, we will rely on the following lemma. Recall the notation  $2^{\lfloor j \rfloor}$  for iterated Sobolev exponents.

**Lemma 5.3.** *Let  $2 \leq p < r < \tilde{q}_+(L)^*$ . Then  $p \in \mathcal{I}(L)$ , and  $\llbracket p \rrbracket$  depends only on  $p, r, \langle r_* \rangle$ , coefficient bounds, and dimensions. In particular,  $p_+(L) \geq \tilde{q}_+(L)^*$ .*

**Proof.** First of all, we can assume that  $p \geq 2^*$  in the light of Corollary 3.5. Let  $\ell \geq 1$  denote the largest integer such that  $2^{\lfloor \ell \rfloor} \leq p < 2^{\lfloor \ell + 1 \rfloor}$ . Moreover, we can assume that  $r \in (p, 2^{\lfloor \ell + 1 \rfloor})$ , since otherwise we can replace  $r$  by some exponent  $s$  in this interval, and  $s$  and  $\langle s \rangle$  depend only on  $p, r$ , and  $\langle r \rangle$ , in virtue of interpolation.

Let  $p_j$  and  $r_j, j = 0, \dots, \ell$ , denote the sequences of numbers satisfying  $p_\ell = p, r_\ell = r$ , and  $p_{j+1} = p_j^*$  as well as  $r_{j+1} = r_j^*$  for  $j = 0, \dots, \ell - 1$ .

For  $j = 0, \dots, \ell - 1$ , we claim the following. Assume that  $p_j \in \mathcal{I}(L)$ . Then  $p_{j+1} \in \mathcal{I}(L)$  and  $\llbracket p_{j+1} \rrbracket$  depends only on  $p_j, r_j, r, \llbracket p_j \rrbracket, \langle r \rangle$ , coefficient bounds, and dimensions.

Indeed, observe first that  $(r_{j+1})_{**} = (r_j)_* < 2^{\lfloor j \rfloor} \leq p_j$ , and that  $(r_{j+1})_{**} \geq (r_1)_{**} > (p_1)_{**} \geq 2_*$ . Hence, by Proposition 3.6 (taking Corollary 3.5 into account), for some  $\varphi \in (0, \pi/2 - \omega)$

depending only on coefficient bounds and dimensions, the  $H^\infty(S_\varphi)$ -calculus of  $L$  is bounded on  $L^{(r_{j+1})^{**}}$ , with implied constant depending only on  $r_j, p_j, \llbracket p_j \rrbracket$ , coefficient bounds, and dimensions. Second, note that  $\mathcal{L}^{-1}$  is  $(r_{j+1})_*$ -bounded due to  $2 \leq (p_1)_* < (r_{j+1})_* \leq r_*$ , the assumption on  $r$ , and interpolation. The  $(r_{j+1})_*$ -bound for  $\mathcal{L}^{-1}$  only imports  $r$ , and  $\langle r_* \rangle$  as a further dependence. With these two ingredients, estimate for  $t > 0$  and  $u \in L^p(O)^m \cap L^2(O)^m$  that

$$\begin{aligned} \|e^{-tL}u\|_{r_{j+1}} &\lesssim \|\mathcal{L}^{-1}\mathcal{L}e^{-tL}u\|_{\mathbb{W}_D^{1,(r_{j+1})^*}(O)} \lesssim \|\mathcal{L}e^{-tL}u\|_{\mathbb{W}_D^{-1,(r_{j+1})^*}(O)} \\ &\lesssim t^{-1}\|t\mathcal{L}e^{-tL}u\|_{(r_{j+1})^{**}} \lesssim t^{-1}\|u\|_{(r_{j+1})^{**}}. \end{aligned} \tag{6}$$

Implicit constants depend only on the aforementioned quantities. Estimate (6) means that the family  $\{e^{-tL}\}_{t>0}$  is  $L^{(r_{j+1})^{**}} \rightarrow L^{r_{j+1}}$  bounded. Now, Proposition 3.4 yields  $p_{j+1} \in \mathcal{I}(L)$  with the claimed control over  $\llbracket p_{j+1} \rrbracket$ . This completes the proof of the claim.

Now,  $2 \leq p_0 < 2^*$ , so according to Corollary 3.5,  $p_0 \in \mathcal{I}(L)$  with  $\llbracket p_0 \rrbracket$  depending only on  $p_0$ , coefficient bounds, and dimensions. Hence, by induction over  $j = 0, \dots, \ell - 1$ , the claim yields  $p = p_\ell \in \mathcal{I}(L)$ . By finiteness of the sequence, and since  $p_j$  and  $r_j$  only depend on  $p, r$ , and  $j$ , the quantity  $\llbracket p \rrbracket$  depends only on  $p, r, \langle r_* \rangle$ , coefficient bounds and dimensions, as claimed.  $\square$

**Proof of Theorem 1.2 (i).** The case  $p_-(L) < r < p < 2$  is immediate by Corollary 4.10 and Proposition 3.7.

Now, let  $2 < q < r < \tilde{q}_+(L)$ . By definition,  $\mathcal{L}$  is a  $q$ -isomorphism. Then Lemma 5.2 lets us conclude provided we can ensure that  $(L^*)^{\frac{1}{2}}$  is a  $q'$ -isomorphism. To this end, we want to appeal to the first case above, but applied to  $L^*$  instead of  $L$ . By duality,  $p_-(L^*) < q' < 2$  if, and only if,  $2 < q < p_+(L)$ . But this is true by Lemma 5.3, since  $\mathcal{L}$  is moreover an  $r$ -isomorphism. Hence, we can indeed apply the case above. Note that  $\langle q \rangle$  is controlled by  $\langle r \rangle$  in virtue of interpolation, which gives the right constant dependencies.  $\square$

**6. Necessary conditions**

We show Theorem 1.2 (ii). For its proof we will need the following lemma, whose proof is similar to that of Lemma 5.3.

**Lemma 6.1.** *Let  $p \in (2, \infty)$  be such that  $L^{\frac{1}{2}}$  is a  $p_*$ -isomorphism. Then  $p_+(L) \geq p$ .*

**Proof.** In the light of Corollary 3.5, it suffices to treat the case  $d \geq 3$ . We employ an iterative argument. To this end, we make for  $k \geq 0$  the following

**Claim:** If  $p_+(L) \geq 2^{[k]}, 2^{[k]} < q < 2^{[k+1]}$ , and  $L^{\frac{1}{2}}$  is a  $q_*$ -isomorphism, then  $p_+(L) \geq q$ .

**Proof of the claim.** We use the expansion  $e^{-t^2L} = L^{-\frac{1}{2}}L^{\frac{1}{2}}e^{-t^2L}$ . Observe that  $2_* < q_* < 2^{[k]} \leq p_+(L)$ . Hence, owing to Proposition 3.6 and taking Corollary 3.5 into account, the  $H^\infty(S_\varphi)$ -calculus of  $L$  is bounded on  $L^{q^*}(O)^m$  for any  $\varphi \in (\omega, \pi/2)$ . Using this in the last step, together with the Sobolev embedding and the  $q_*$ -isomorphism property of  $L^{\frac{1}{2}}$ , yields

$$\|e^{-t^2L}u\|_q \lesssim \|L^{-\frac{1}{2}}L^{\frac{1}{2}}e^{-t^2L}u\|_{\mathbb{W}_D^{1,q^*}(O)} \lesssim \|L^{\frac{1}{2}}e^{-t^2L}u\|_{q_*} \lesssim t^{-1}\|u\|_{q_*}.$$

This means that  $\{e^{-tL}\}_{t>0}$  is  $L^{q^*} \rightarrow L^q$  bounded. We conclude  $q \leq p_+(L)$  with Proposition 3.4.  $\square$

Now, fix  $\ell \geq 0$  such that  $2 < \dots < 2^{[\ell]} < p \leq 2^{[\ell+1]}$ . Observe that  $L^{\frac{1}{2}}$  is by interpolation a  $(2^{[j]})_*$ -isomorphism for  $j = 1, \dots, \ell$ . Hence, the claim yields by induction over  $j$  that  $p_+(L) \geq 2^{[\ell]}$ . In a second step, the claim applied with  $k = \ell$  and  $q = p$  gives the assertion.  $\square$

**Proof of Theorem 1.2 (ii).** We divide the proof into two cases.

**Case 1:**  $p < 2$ . This part was already shown in [11, Thm. 1.2 (ii)]. Note that geometry in-there was only used to ensure the continuous embedding  $\mathbb{W}_D^{1,q}(O) \subseteq L^{q^*}(O)^m$ , which is a consequence of Proposition 2.1 in our situation.

**Case 2:**  $p > 2$ . Assume that  $L^{\frac{1}{2}}$  is a  $p$ -isomorphism. From  $p = (p^*)_*$  and Lemma 6.1 it follows that  $p_+(L) \geq p^*$  if  $p < d$  and  $p_+(L) = \infty$  otherwise. In particular,  $2 < p < p_+(L)$ , which translates to  $p_-(L^*) < p' < 2$  by the duality formula  $(e^{-tL})^* = e^{-tL^*}$ . Hence, we obtain from the case  $p < 2$  for  $L^*$  in Theorem 1.2 (i) that  $(L^*)^{\frac{1}{2}}$  is a  $p'$ -isomorphism. Then we conclude with Lemma 5.1 that  $\mathcal{L}$  is a  $p$ -isomorphism. Consequently,  $\tilde{q}_+(L) \geq p$  as desired.  $\square$

### 7. Endpoint cases

To conclude this article, we show sharpness at the endpoints, provided they do not fall outside the interval  $(1, \infty)$ . This is Theorem 1.2 (iii).

The following result is an application of Šneřberg’s theorem [17]. Here, we exploit that  $\{\mathbb{W}_D^{1,p}(O)\}_{p \in (1, \infty)}$ ,  $\{L^p(O)^m\}_{p \in (1, \infty)}$ , and  $\{\mathbb{W}_D^{-1,p}(O)\}_{p \in (1, \infty)}$  are complex interpolation scales. For the second scale, this is clear. That the first scale is an interpolation scale was discussed in the proof of Theorem 1.2 (i) (note that the arguments in-there work both for the real and complex interpolation method). Finally, use duality to transfer the interpolation properties of the first scale to the last scale, see also [8, Prop. 5.2].

**Proposition 7.1.** *Assume that Assumption  $D'$  holds. Let  $p \in (1, \infty)$  be such that  $L^{\frac{1}{2}}$  is a  $p$ -isomorphism and suppose that there exists some  $\varepsilon' > 0$  such that  $L^{\frac{1}{2}}$  is  $q$ -bounded for  $q \in [p - \varepsilon', p + \varepsilon']$ . Then there is  $\varepsilon' > \varepsilon > 0$  such that  $L^{\frac{1}{2}}$  is a  $q$ -isomorphism for all  $q \in (p - \varepsilon, p + \varepsilon)$ . Similarly, if  $\mathcal{L}$  is a  $p$ -isomorphism, then there is again some  $\varepsilon > 0$  such that  $\mathcal{L}$  is a  $q$ -isomorphism for all  $q \in (p - \varepsilon, p + \varepsilon)$ .*

**Remark 7.2.** Observe that in Proposition 7.1 we did not assume that  $\mathcal{L}$  is  $q$ -bounded in an interval around  $p$ . This is because  $\mathcal{L}$  is automatically  $q$ -bounded for all  $q \in [1, \infty]$  by Hölder’s inequality applied to the definition of  $\mathcal{L}$ .

**Proof of Theorem 1.2 (iii).** To begin with, assume that  $p_-(L) > 1$  and  $L^{\frac{1}{2}}$  is a  $p_-(L)$ -isomorphism. By Corollary 4.10,  $L^{\frac{1}{2}}$  is  $q$ -bounded for  $q \in (p_-(L)_* \vee 1, 2)$ . Since  $p_-(L) > 1$  and  $p_-(L)_* < p_-(L)$ , we find  $\varepsilon' > 0$  as required by Proposition 7.1. Then, let  $\varepsilon > 0$  be provided by that proposition. It follows from Theorem 1.2 (ii) that  $p_-(L) \leq p_-(L) - \varepsilon$ , which is a contradiction.

Now assume that  $\tilde{q}_+(L) < \infty$  and that  $L^{\frac{1}{2}}$  is a  $\tilde{q}_+(L)$ -isomorphism. Then  $p_+(L) \geq \tilde{q}_+(L)^* > q_+(L)$  by Lemma 6.1. Duality reveals  $p_-(L^*) < (\tilde{q}_+(L))'$ . It follows from Theorem 1.2 (i)

that  $(L^*)^{\frac{1}{2}}$  is a  $(\tilde{q}_+(L))'$  isomorphism. Consequently, Lemma 5.1 gives that  $\mathcal{L}$  is a  $\tilde{q}_+(L)$ -isomorphism. Then, as above, Proposition 7.1 leads to the contradiction  $\tilde{q}_+(L) + \varepsilon \leq \tilde{q}_+(L)$ .  $\square$

## Data availability

No data was used for the research described in the article.

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## References

- [1] P. Auscher, On necessary and sufficient conditions for  $L^p$ -estimates of Riesz transforms associated to elliptic operators on  $\mathbb{R}^n$  and related estimates, *Mem. Am. Math. Soc.* 186 (871) (2007).
- [2] P. Auscher, N. Badr, R. Haller-Dintelmann, J. Rehberg, The square root problem for second order divergence form operators with mixed boundary conditions on  $L^p$ , *J. Evol. Equ.* 15 (1) (2015) 165–208.
- [3] P. Auscher, M. Egert, *Boundary Value Problems and Hardy Spaces for Elliptic Systems with Block Structure*, 2023, <https://doi.org/10.1007/978-3-031-29973-5>.
- [4] P. Auscher, S. Hofmann, M. Lacey, A. McIntosh, P. Tchamitchian, The solution of the Kato square root problem for second order elliptic operators on  $\mathbb{R}^n$ , *Ann. Math. (2)* 156 (2) (2002) 633–654.
- [5] A. Axelsson, S. Keith, A. McIntosh, The Kato square root problem for mixed boundary value problems, *J. Lond. Math. Soc. (2)* 74 (1) (2006) 113–130.
- [6] S. Bechtel, R. Brown, R. Haller-Dintelmann, P. Tolksdorf, Sobolev extension operators for functions with partially vanishing trace, arXiv preprint, available at <https://arxiv.org/abs/1910.06009>.
- [7] S. Bechtel, M. Egert, R. Haller-Dintelmann, The Kato square root problem on locally uniform domains, *Adv. Math.* 375 (2020), <https://doi.org/10.1016/j.aim.2020.107410>.
- [8] S. Bechtel, M. Egert, Interpolation theory for Sobolev functions with partially vanishing trace on irregular open sets, *J. Fourier Anal. Appl.* 25 (5) (2019) 2733–2781.
- [9] S. Blunck, P.C. Kunstmann, Calderón-Zygmund theory for non-integral operators and the  $H^\infty$  functional calculus, *Rev. Mat. Iberoam.* 19 (3) (2003) 919–942.
- [10] K. Disser, A.F.M. ter Elst, J. Rehberg, On maximal parabolic regularity for non-autonomous parabolic operators, *J. Differ. Equ.* 262 (3) (2017) 2039–2072.
- [11] M. Egert,  $L^p$ -estimates for the square root of elliptic systems with mixed boundary conditions, *J. Differ. Equ.* 265 (4) (2018) 1279–1323.
- [12] M. Egert, R. Haller-Dintelmann, P. Tolksdorf, The Kato square root problem for mixed boundary conditions, *J. Funct. Anal.* 267 (5) (2014) 1419–1461.
- [13] M. Egert, R. Haller-Dintelmann, P. Tolksdorf, The Kato square root problem follows from an extrapolation property of the Laplacian, *Publ. Math.* 61 (2) (2016) 451–483.
- [14] M. Haase, *The Functional Calculus for Sectorial Operators*, Operator Theory: Advances and Applications, vol. 169, Birkhäuser, Basel, 2006.
- [15] P. Hajlasz, Pointwise Hardy inequalities, *Proc. Am. Math. Soc.* 127 (2) (1999) 417–423.
- [16] J. Lehrbäck, Pointwise Hardy inequalities and uniformly fat sets, *Proc. Am. Math. Soc.* 136 (6) (2008) 2193–2200.
- [17] I. Šneĭberg, Spectral properties of linear operators in interpolation families of Banach spaces, *Mat. Issled.* 9 (2) (1974) 214–229, 254–255.
- [18] H. Triebel, *Interpolation Theory, Function Spaces, Differential Operators*, North-Holland Mathematical Library, vol. 18, North-Holland Publishing, Amsterdam, 1978.