



# A second-order approach to the Kato square root problem on open sets

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*Abstract.* We obtain the Kato square root property for coupled second-order elliptic systems in divergence form subject to mixed boundary conditions on an open and possibly unbounded set in  $\mathbb{R}^n$  under two simple geometric conditions: The Dirichlet boundary parts for the respective components are Ahlfors–David regular and a quantitative connectivity property in the spirit of locally uniform domains holds near the remaining Neumann boundary parts. In contrast with earlier work, our proof is not based on the first-order approach due to Axelsson–Keith–McIntosh but uses a second-order approach in the spirit of the original solution to the Kato square root problem on Euclidean space. This way, the proof becomes substantially shorter and technically less demanding.

## 1. Introduction

Let  $L$  be a coupled second-order elliptic system in divergence form on an open set  $O \subseteq \mathbb{R}^n$ ,  $n \geq 2$ , with bounded, measurable, elliptic coefficients in  $\mathcal{L}(C^m)$ , formally given by


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

The number  $m$  is the system size. Precise assumptions on the coefficients are presented in Assumption (B). For each component  $i = 1, \dots, m$ , let  $D_i \subseteq \partial O$  be a closed, possibly empty, subset of the boundary. Group them in the array  $\vec{D} = (D_i)_{i=1}^m$ . As an abuse of notation, we also identify  $\vec{D}$  with a subset of  $(\partial O)^m$ . Then, we complement the system  $L$  with Dirichlet boundary conditions on  $\vec{D}$ . On the remaining (Neumann) boundary  $(\partial O)^m \setminus \vec{D}$ , natural boundary conditions are imposed.

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To make the definition precise, define  $W_{D_i}^{1,2}(O)$  as the closure in  $W^{1,2}(O)$  of test functions vanishing in a neighborhood of  $D_i$  (see Definition 2.9), and put  $\mathbb{W}_{\mathbb{D}}^{1,2}(O) = \bigoplus_{i=1}^m W_{D_i}^{1,2}(O)$ . The system  $L$  can be properly defined using a sesquilinear form

$$a: \mathbb{W}_{\mathbb{D}}^{1,2}(O) \times \mathbb{W}_{\mathbb{D}}^{1,2}(O) \rightarrow \mathbb{C}$$

using Kato’s form method. The form  $a$  is obtained from the (formal) definition of  $L$  above by virtue of integration by parts, see (3).

The system  $L$  is invertible and  $m$ -accretive in  $L^2(O)^m$ . In particular, it possesses a (unique)  $m$ -accretive square root  $\sqrt{L}$  with the property  $(\sqrt{L})^2 = L$ . The question whether or not the identity  $D(\sqrt{L}) = \mathbb{W}_{\mathbb{D}}^{1,2}(O)$  holds has become famous as the *Kato square root problem*. Let us mention that, if the coefficients of the system are self-adjoint, then this property is essentially trivial. However, in the non-symmetric case, even the case  $O = \mathbb{R}^n$  and  $m = 1$  has resisted all attempts of a resolution for more than 40 years. Eventually, it was the breakthrough result due to Auscher, Hofmann, Lacey, McIntosh, and Tchamitchian [8] that answered Kato’s question in the affirmative in the Euclidean case.

Given that  $L$  is an elliptic operator of second order, it might not seem too surprising that the proof in [8] relies on harmonic analysis techniques for second-order elliptic operators. Now, however, comes the plot twist: Few years after the original solution of the Kato square root problem, Axelsson, Keith, and McIntosh proposed in their seminal paper [10] a new framework, called the *first-order approach*, in which the Kato square root problem (and many other problems from the so-called Calderón program) could be casted by reformulating them in terms of certain first-order differential operators (the so-called *perturbed Dirac operators*). Moreover, using this approach, they were also capable of resolving first cases of the Kato square root problem when the operator  $L$  is subject to mixed boundary conditions [9]. Eventually, using the first-order approach became the gold standard when treating the Kato square root problem on manifolds [31] or rough open sets subject to mixed boundary conditions [15,21,22].

Applications on sets with rough geometry come from various fields including, with exemplary references, elliptic and parabolic regularity [16,27], Lions’ non-autonomous maximal regularity problem [1,23], and boundary value problems [4,5].

The reader might wonder why the second-order proof on  $\mathbb{R}^n$  does *not* generalize to the setting on an open set  $O$ . To give an explanation, we have to dive a bit into the structure of the proof. What is common in both the second- and first-order approaches is that the original problem is reduced to the validity of some quadratic estimate. In our case, the quadratic estimate reads

$$\int_0^\infty \left\| \Theta_t \begin{bmatrix} u \\ \nabla u \end{bmatrix} \right\|_2^2 \frac{dt}{t} \lesssim \|u\|_{\mathbb{W}^{1,2}(O)}^2, \quad u \in \mathbb{W}_{\mathbb{D}}^{1,2}(O). \tag{♡}$$

The operator  $\Theta_t$  transforms a “vector field” in  $\mathbb{C}^{(n+1)m}$  into a vector in  $\mathbb{C}^m$ ; see Sect. 6 for a precise definition of  $\Theta_t$  and more details. To obtain the quadratic estimate (♡),

the task is further reduced to a Carleson measure estimate. The latter is the heart of the matter and relies on involved local  $T(b)$ -techniques, see Sect. 8. The bottleneck for the treatment of open sets is, however, the reduction to a Carleson measure estimate, presented in Sect. 7. Indeed, to obtain the desired estimates, suitable smoothing operators in the spirit of Littlewood–Paley theory have to be introduced. In the original proof, these smoothing operators are convolution operators with a nice kernel which are applied component-wise to the vector field  $\nabla u$ , see [8, Lem. 4.4]. In the same lemma, a crucial argument is performed: Using the Fourier transform, these component-wise smoothing operators commute nevertheless with any partial derivatives. Also in modern treatments of the Kato square root problem on Euclidean space, the same argument is crucially invoked [20, Rem. 13.8]. Such a reasoning is, of course, impossible in our setting, nourishing the need for the first-order approach.

The objective of the current manuscript is hence the following: We aim to reprove the state-of-the-art result [15] on the Kato square root problem subject to mixed boundary conditions by virtue of a second-order approach, that is, with a proof in the spirit of [8,20]. Moreover, in [15] only the case  $D_i \equiv D$  was treated. We are going to generalize [15] to allow a varying Dirichlet part among the different components, which was already possible in [21] in a more restrictive geometric setting.

Our main result reads as follows.

**Theorem 1.1** (Solution of the Kato square root problem). *Let  $O \subseteq \mathbb{R}^n$  be an open set and, for  $i = 1, \dots, m$ , let  $D_i \subseteq \partial O$  be a closed subset of the boundary. Set  $\vec{D} = (D_i)_{i=1}^m$ . Suppose for every  $i$  that  $D_i$  is Ahlfors–David regular (Definition 2.1) and that  $O$  is locally uniform near  $\partial O \setminus D_i$  (Definition 2.5). Then,  $D(\sqrt{L}) = \mathbb{W}_{\vec{D}}^{1,2}(O)$  holds with equivalence of norms*

$$\|u\|_2 + \|\nabla u\|_2 \approx \|\sqrt{L}u\|_2 \quad \left(u \in \mathbb{W}_{\vec{D}}^{1,2}(O)\right),$$

and the implicit constants depend on the coefficients of  $L$  only through the coefficient bounds.

The geometric setting announced in the theorem is very general and includes settings way below the Lipschitz class, including fractals like the von Koch snowflake. We will give more information on the geometrical setting in Sect. 2.

Before we explain the central idea of our proof, let us comment on the motivation for a second-order proof for Theorem 1.1. The first-order approach introduces an extra layer of information and complexity, which is crucial for applications to related areas such as elliptic boundary value problems (see the recent monograph [6] for background), but can also impede extensions to other settings and questions. One example is the Kato square root problem for parabolic operators. First, it was solved by Auscher et al. [7] using the first-order approach. Their proof is incredibly technical. Later, Ataei et al. [3] gave another proof using the second-order approach, which is not only substantially shorter and easier, but also generalizes the previous result in several aspects. So far, the Kato square root problem for parabolic operators on cylindrical

domains was only treated by Ouhabaz [33] using regularity in time of the coefficients. We expect that the methods developed in this article will prove useful in the treatment of the Kato square root problem for parabolic operators on cylindrical domains without any regularity of the coefficients, taking [3] as a blueprint. Some of the authors of this article will pursue this question in future work.

We would also like to mention the recent result of Haardt and Tolksdorf [25] on the Kato square root problem for generalized Stokes operators, which employs likewise the second-order approach instead of the first-order approach due to reduced complexity.

Now, we shed some light on the central insight underlying this article. As we have already mentioned, the standard proofs of the Kato square root problem using the second-order approach use smoothing operators that belong to the functional calculus of  $-\Delta$  (or, if  $L$  contains lower-order terms as in our case,  $-\Delta + 1$ ) and apply them component-wise to the vector field  $\nabla u$  (or, with lower-order terms, to  $[u, \nabla u]^t$ ). For simplicity, we stick to the inhomogeneous case with lower-order terms from now on. Write  $Tu = [u, \nabla u]^t$ . Then, at least formally,  $-\Delta + 1 = T^*T$ . Now, reversing the order of terms on the right-hand side of the last identity, we define the operator  $M := TT^*$ . Similar to  $-\Delta + 1$ , the operator  $M$  can be defined using a sesquilinear form and shares many desirable properties such as self-adjointness,  $m$ -accretivity, the square root property (for self-adjoint operators), and so forth with it. We will introduce the operators  $-\Delta + 1$  and  $M$ , both subject to mixed boundary conditions, in detail in Sect. 3.2. The crucial change in our approach is that we define the smoothing operators within the functional calculus of  $M$  instead of  $-\Delta + 1$ . Since  $M$  acts on vector fields by definition, the same is true for the smoothing operators that we define. Hence, we do not need to employ component-wise constructions. More concretely, our smoothing operators are simply resolvents of  $M$ , see Definition 7.3. For them, the following beautiful identity, which is a consequence of Proposition 3.10, holds

$$(1 + t^2 M)^{-1} T u = T (1 + t^2 (-\Delta + 1))^{-1} u, \quad u \in \mathbb{W}_D^{1,2}(O), t > 0. \quad (1)$$

With (1), we can still commute the “inhomogeneous gradient”  $T$  with the smoothing operator, similar to the commutation property using the Fourier transform on Euclidean space, but this operation will transform the “vector-valued” operator  $M$  into the “scalar-valued” operator  $-\Delta + 1$  and vice versa.

Also, we mention here that the operator  $M$  has its place in the  $T(b)$ -type argument that is key to the solution of the Kato square root problem. We are going to perturb the operator  $M$  by the elliptic coefficient matrix

$$B = \begin{bmatrix} d & c \\ b & A \end{bmatrix} : O \rightarrow \mathbb{C}^{(n+1)m \times (n+1)m}$$

to obtain the (still sectorial) operator  $MB$ . Its resolvents will be used to define the  $T(b)$ -type test functions, see (22).

We tried to keep the present article as self-contained as possible. However, to avoid too much repetition, results and arguments that can literally be taken from [15] or [20]

will not be carried out again. Hence, the reader is advised to keep copies of these manuscripts handy.

Notation

Given vectors  $\xi, \eta \in \mathbb{C}^k$ , put  $\xi \cdot \eta := \sum_{i=1}^k \xi_i \eta_i$ . Their inner product can hence be written as  $\langle \xi, \eta \rangle = \xi \cdot \bar{\eta}$ . For  $x \in \mathbb{R}^n$  and  $r > 0$ , write  $B(x, r)$  for the Euclidean ball centered in  $x$  of radius  $r$ . If  $B = B(x, r)$ , put  $r(B) := r$ . Moreover, if  $c > 0$  and  $B$  is an Euclidean ball, write  $cB$  for the concentric ball of radius  $cr(B)$ . Similarly, for  $x \in \mathbb{R}^n$  and  $\ell > 0$ , write  $Q(x, \ell)$  for the Euclidean (axis-parallel) cube centered in  $x$  of sidelength  $\ell$ . If  $Q = Q(x, \ell)$ , put  $\ell(Q) := \ell$ . Moreover, if  $c > 0$  and  $Q$  is an Euclidean cube, write  $cQ$  for the concentric cube of sidelength  $c\ell(Q)$ . For a fixed (open) ambient set  $O \subseteq \mathbb{R}^n$ , write  $B_O(x, r) := B(x, r) \cap O$  and  $Q_O(x, r) := Q(x, r) \cap O$ . For  $\varphi \in (0, \pi)$ , define the open sector of opening angle  $2\varphi$  around the positive real axis by  $S_\varphi := \{z \in \mathbb{C} \setminus \{0\} : |\arg(z)| < \varphi\}$ . In the case  $\varphi = 0$ , put  $S_0 := (0, \infty)$ . The corresponding closed sectors are denoted by  $\bar{S}_\varphi$ . Given  $A \subseteq \mathbb{R}^n$  and  $\delta > 0$ , write  $A_\delta := \{x \in \mathbb{R}^n : d(x, A) < \delta\}$  for the tube of size  $\delta$  around  $A$ . Write  $d(A, B)$  for the Euclidean distance of sets  $A, B \subseteq \mathbb{R}^n$ . For  $A \subseteq \mathbb{R}^n$  measurable with  $|A| > 0$  and  $f$  an integrable function on  $A$ , write  $(f)_A := \int_A f(y) dy$  for the average of  $f$  over  $A$ . Write  $C_0^\infty(\mathbb{R}^n)$  for the space of smooth and compactly supported functions on  $\mathbb{R}^n$ . Let  $\mathcal{L}(H, K)$  denote the bounded linear operators between two Hilbert spaces  $H$  and  $K$ , and put  $\mathcal{L}(H) := \mathcal{L}(H, H)$ . The space  $H^\infty(\Xi)$  denotes the bounded, holomorphic functions on an open set  $\Xi \subseteq \mathbb{C}$ .

2. Geometric setup

We adopt the geometric setting used in [15]. For convenience of the reader, we summarize below the concepts that are necessary to understand our article.

By  $\mathcal{H}^s(E)$ ,  $s \in (0, n]$ , we denote the  $s$ -dimensional Hausdorff measure of  $E \subseteq \mathbb{R}^n$  defined as follows. For  $\varepsilon > 0$ , we put

$$\mathcal{H}_\varepsilon^s(E) := \inf \left\{ \sum_i r(B_i)^s : \bigcup_i B_i \supseteq E, r(B_i) \leq \varepsilon \right\},$$

and since this value is increasing as  $\varepsilon \rightarrow 0$ , we define  $\mathcal{H}^s(E) := \lim_{\varepsilon \rightarrow 0} \mathcal{H}_\varepsilon^s(E)$ , see [2, Sec. 5.1].

**Definition 2.1.** A closed set  $D \subseteq \mathbb{R}^n$  is called Ahlfors–David regular if there is comparability

$$\mathcal{H}^{n-1}(B \cap D) \approx r(B)^{n-1}$$

uniformly for all open balls  $B$  of radius  $r(B) < \text{diam}(D)$  centered in  $D$ .

*Remark 2.2.* A practical interpretation is that Ahlfors–David regular sets behave  $(n - 1)$ -dimensional at all scales. When  $D$  is bounded, then, for any  $C \in (0, \infty)$ , the restriction on the radius may equivalently be changed to  $r(B) \leq C$ , at the cost of changing the implicit constants, see [14, Lem. A.4]. Sets with the latter property for  $C = 1$  are called  $(n - 1)$ -sets in [30].

**Definition 2.3.** An open set  $O \subseteq \mathbb{R}^n$  is called *interior thick* if

$$|B \cap O| \gtrsim |B|$$

uniformly for all open balls  $B$  of radius  $r(B) \leq 1$  centered in  $O$ .

In analogy with Remark 2.2, the restriction  $r(B) \leq 1$  is arbitrary and can be changed to  $r(B) \leq C$  for any fixed constant  $C \in (0, \infty)$ , up to a change in the implicit constant.

Throughout the manuscript, we are going to employ the following notational convention.

**Convention 2.4** (*Boldface symbols.*) If the underlying set  $O$  of an elliptic system is supposed to be interior thick, we write  $\mathbf{O}$  instead of  $O$ . All other objects related to the interior thick set  $\mathbf{O}$ , such as an elliptic system  $L$ , the Dirichlet boundary parts  $\vec{D}$ , and so on, will likewise be denoted by the corresponding bold letters  $\mathbf{L}$ ,  $\vec{\mathbf{D}}$ , and so on.

### 2.1. Locally uniform domains

**Definition 2.5.** Let  $\varepsilon \in (0, 1]$  and  $\delta \in (0, \infty]$ . Let  $O \subseteq \mathbb{R}^n$  be open and  $N \subseteq \partial O$ . Recall the notation  $N_\delta = \{z \in \mathbb{R}^n : d(z, N) < \delta\}$ . Then  $O$  is called *locally an  $(\varepsilon, \delta)$ -domain near  $N$*  if the following properties hold.

1. 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

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

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

If the values of  $\varepsilon$  and  $\delta$  need not be specified, then  $O$  is simply called *locally uniform near  $N$* .

*Remark 2.6.* Definition 2.5 describes a quantitative local connectivity property of  $O$  near  $N$ . For an illustration of  $\varepsilon$ -cigars with respect to  $\partial O$ , the reader can refer, for instance, to [35, Fig. 3.1]. Having positive radius is of course only a restriction if  $O$  has infinitely many connected components.

Locally uniform domains near  $N$  are compared to other popular geometric frameworks for mixed boundary conditions in [15, Prop. 2.5] and the subsequent remarks. We refer the reader to this discussion for more information.

Locally uniform domains satisfy the following corkscrew condition around the Neumann part  $N$ .

**Proposition 2.7** (Corkscrew condition). *Suppose that  $O \subseteq \mathbb{R}^n$  is open and locally an  $(\varepsilon, \delta)$ -domain near  $N \subseteq \partial O$ . Then, there exists a constant  $\kappa \in (0, 1]$  such that:*

$$\forall x \in \overline{N_{\delta/2} \cap O}, r \leq 1 \quad \exists z \in B(x, r): \quad B(z, \kappa r) \subseteq O \cap B(x, r).$$

In Sects. 6–8, we are going to establish Theorem 1.1 first under the additional assumption that  $O$  is interior thick. Afterward, we are going to use the corkscrew condition to verify interior thickness of some auxiliary set in Sect. 9, which will enable us to get rid of the interior thickness condition in Theorem 1.1. Moreover, in combination with Ahlfors–David regularity of  $D := \partial O \setminus N$ , the corkscrew condition yields porosity (see the following proposition for a definition) of the full boundary  $\partial O$ , see [15, Cor. 2.11] for a proof.

**Proposition 2.8** (Porosity of  $\partial O$ ). *Let  $O \subseteq \mathbb{R}^n$  be open and  $D \subseteq \partial O$  be closed. Suppose that  $D$  is Ahlfors–David regular and that  $O$  is locally uniform near  $\partial O \setminus D$ . Then  $\partial O$  is porous, that is to say, there exists  $\kappa \in (0, 1]$  with the property:*

$$\forall x \in \partial O, r \leq 1 \quad \exists z \in B(x, r): \quad B(z, \kappa r) \subseteq B(x, r) \setminus \partial O.$$

In Sect. 4, we are going to introduce so-called “dyadic structures”, which mimic the concept of dyadic cubes within an interior thick set  $O$ . Porosity of  $\partial O$  will provide additional properties of the dyadic structures.

## 2.2. Sobolev spaces

The Hilbert space  $W^{1,2}(O)$  on an open set  $O \subseteq \mathbb{R}^n$  is the collection of all  $u \in L^2(O)$  such that  $\nabla u \in L^2(O)^n$  with norm

$$\|u\|_{W^{1,2}(O)} := \left( \|u\|_{L^2(O)}^2 + \|\nabla u\|_{L^2(O)^n}^2 \right)^{1/2}. \tag{2}$$

We introduce the subspace of functions that vanish on a subset of  $\partial O$  as follows.

**Definition 2.9** (Sobolev space subject to mixed BC). *Let  $O \subseteq \mathbb{R}^n$  be open and  $D \subseteq \partial O$  be closed. The Hilbert space  $W_D^{1,2}(O)$  is the  $W^{1,2}(O)$ -closure of the set of test functions*

$$C_D^\infty(O) := \left\{ u|_O : u \in C_0^\infty(\mathbb{R}^n) \text{ and } d(\text{supp}(u), D) > 0 \right\}.$$

If  $\vec{D} = (D_i)_{i=1}^m$  is an array consisting of sets  $D_i \subseteq \partial O$ , then define the vector-valued space

$$W_{\vec{D}}^{1,2}(O) := \bigoplus_{i=1}^m W_{D_i}^{1,2}(O).$$

Due to the product structure, it is often possible to restrict one’s attention to the case  $m = 1$ , at least when pure function space questions are concerned. We will do so whenever possible. The given definition is standard in the modeling of mixed boundary conditions, see, for instance, [32, Sec. 4.1]. In the geometric context of Theorem 1.1, the space  $W_D^{1,2}(O)$  can equivalently be defined by virtue of a more natural class of test functions, see [13, Sec. 7].

For pure Dirichlet boundary conditions, we recover  $W_{\partial O}^{1,2}(O) = W_0^{1,2}(O)$ . To the contrary, in the case of pure Neumann boundary conditions it is possible that  $W_{\emptyset}^{1,2}(O)$  does *not* coincide with  $W^{1,2}(O)$ . Indeed, a disk with a slit serves as a counterexample [18, Ex. 1.1.10]. A sufficient condition for the validity of the identity  $W^{1,2}(O) = W_{\emptyset}^{1,2}(O)$  is the existence of a bounded Sobolev extension operator. This is, for instance, the case if  $O$  is locally uniform, by virtue of Jones’ result [29].

The following result provides a bounded extension operator for the space  $W_D^{1,2}(O)$ . It can be obtained by combining [15, Prop. 2.5] with the main result of [13]. In the case  $D = \emptyset$ , it is compatible with Jones’ result.

**Theorem 2.10** (Extension operator). *Let  $O \subseteq \mathbb{R}^n$  be open and  $D \subseteq \partial O$  be closed. If  $O$  is locally uniform near  $\partial O \setminus D$ , then there exists a bounded linear extension operator  $\mathcal{E} : W_D^{1,2}(O) \rightarrow W_D^{1,2}(\mathbb{R}^n)$ . Moreover, the operator  $\mathcal{E}$  is local and homogeneous in the following sense: There are  $c \geq 1$  and  $r_0 > 0$ , depending on geometry, such that, for  $x \in \overline{O}$  and  $r \in (0, r_0]$ , there holds the estimate*

$$\|\nabla \mathcal{E}u\|_{L^2(B(x,r))} \lesssim \|\nabla u\|_{L^2(B_O(x,cr))}, \quad u \in W_D^{1,2}(O).$$

Using the local and homogeneous estimates for the extension operator, a local Poincaré inequality can be deduced for  $W_D^{1,2}(O)$ . This is carried out in [15, Prop. 3.9 & Rem. 3.10].

**Corollary 2.11** (Local Poincaré inequality). *In the setting of Theorem 2.10, there are  $c \geq 1$  and  $r_0 > 0$  depending on geometry such that, for  $x \in \overline{O}$  and  $r \in (0, r_0]$ , there holds the estimate*

$$\|u - (u)_{B_O(x,r)}\|_{L^2(B_O(x,r))} \lesssim r \|\nabla u\|_{L^2(B_O(x,cr))}.$$

*Remark 2.12.* Using a telescoping sum, the following extension of Corollary 2.11 is possible. Let  $x \in \overline{O}$  and  $\ell$  a positive integer such that  $2^\ell r \leq r_0$ . Then, there holds the estimate

$$\|u - (u)_{B_O(x,r)}\|_{L^2(B_O(x,2^\ell r))} \lesssim (\ell 2^{n\ell/2}) 2^\ell r \|\nabla u\|_{L^2(B_O(x,c2^\ell r))}.$$

### 3. Elliptic operator

In this section, we properly define the elliptic system appearing in the formulation of Theorem 1.1. Then, we collect some basic, but important, properties for it. Moreover, we define and discuss a counterpart to the Laplacian acting on vector fields, which will play a crucial role in the later analysis.

### 3.1. Elliptic systems in divergence form

The main player in the Kato square root problem is the *elliptic system* of second order in divergence form

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

on  $O$  subject to Dirichlet boundary conditions on  $\vec{D} \subseteq (\partial O)^m$  and Neumann boundary conditions on  $(\partial O)^m \setminus \vec{D}$ , where  $m \geq 1$  denotes the size of the system.

Throughout this article, we work under the following implicit assumption on the coefficients  $A, b, c$ , and  $d$ .

**Assumption (B).** The coefficients of  $L$  are bounded functions on  $O$ , that is,  $A \in L^\infty(O; \mathbb{C}^{nm \times nm}), b \in L^\infty(O; \mathbb{C}^{nm \times m}), c \in L^\infty(O; \mathbb{C}^{n \times nm})$  and  $d \in L^\infty(O; \mathbb{C}^{m \times m})$ , and they satisfy the (inhomogeneous) Gårding inequality: There is some  $\lambda > 0$  such that

$$\alpha(u, u) \geq \lambda (\|u\|_2^2 + \|\nabla u\|_2^2), \quad u \in \mathbb{W}_{\vec{D}}^{1,2}(O),$$

where the form  $\alpha$  is given by

$$\alpha(u, v) = \int_O A \nabla u \cdot \nabla \bar{v} + bu \cdot \nabla \bar{v} + (c \nabla u) \bar{v} + (du) \bar{v}, \quad u, v \in \mathbb{W}_{\vec{D}}^{1,2}(O). \quad (3)$$

Formally,  $L$  can be written as the composition

$$Lu = \begin{bmatrix} 1 & -\operatorname{div} \end{bmatrix} \begin{bmatrix} d & c \\ b & A \end{bmatrix} \begin{bmatrix} 1 \\ \nabla \end{bmatrix} u = T^* B T u,$$

where the inhomogeneous gradient is given by  $T = [1 \ \nabla]^t$ , has (formal) adjoint  $T^* = [1 \ -\operatorname{div}]$ , and  $B$  denotes the matrix

$$B = \begin{bmatrix} d & c \\ b & A \end{bmatrix} : O \rightarrow \mathbb{C}^{(n+1)m \times (n+1)m}$$

considered as a bounded multiplication operator on  $L^2(O)^{(n+1)m}$ .

To make this precise, we define the gradient with appropriate boundary conditions as a closed operator on  $L^2(O)^m$  and set the divergence as its Hilbert space adjoint.

**Definition 3.1** (*Gradient and divergence*). Denote by  $\nabla_{\vec{D}} : \mathbb{W}_{\vec{D}}^{1,2}(O) \subseteq L^2(O)^m \rightarrow L^2(O)^{nm}$  the gradient with Dirichlet boundary conditions on  $\vec{D}$ . This is a closed and densely defined operator, and we denote its (unbounded) adjoint by  $-\operatorname{div}_{\vec{D}} = (\nabla_{\vec{D}})^* : D(\operatorname{div}_{\vec{D}}) \subseteq L^2(O)^{nm} \rightarrow L^2(O)^m$ .

Before we define the inhomogeneous gradient, we fix the convenient notation

$$N = (n + 1)m.$$

Elements  $F \in L^2(O)^N$  will sometimes be referred to as vector fields.

**Definition 3.2** (The operators  $T_{\vec{D}}$  and  $T_{\vec{D}}^*$ ). Define the inhomogeneous gradient  $T_{\vec{D}} = [1, \nabla_{\vec{D}}]^t : \mathbb{W}_{\vec{D}}^{1,2}(O) \subseteq L^2(O)^m \rightarrow L^2(O)^N$  with Dirichlet boundary conditions on  $\vec{D}$ , and denote by  $T_{\vec{D}}^* : D(T_{\vec{D}}^*) \subseteq L^2(O)^N \rightarrow L^2(O)^m$  its adjoint. By a slight abuse of notation, we occasionally let  $T_{\vec{D}}^*$  also denote the bounded extension  $T_{\vec{D}}^* : L^2(O)^N \rightarrow (\mathbb{W}_{\vec{D}}^{1,2}(O))^*$ .

Note that  $\|T_{\vec{D}}u\|_2 = \|u\|_{\mathbb{W}_{\vec{D}}^{1,2}(O)}$  for  $u \in \mathbb{W}_{\vec{D}}^{1,2}(O)$ . If no confusion can arise, we sometimes write  $T$  instead of  $T_{\vec{D}}$ , and  $T^*$  instead of  $T_{\vec{D}}^*$  to ease notation.

**Definition 3.3.** We define the elliptic operator  $L$  as the composition

$$L = T_{\vec{D}}^* B T_{\vec{D}} : D(L) \subseteq L^2(O)^m \rightarrow L^2(O)^m$$

with maximal domain in  $L^2(O)^m$ .

While the direct definition is useful for algebraic manipulation,  $L$  can equivalently be defined as the operator on  $L^2(O)^m$  associated with the sesquilinear form  $\mathfrak{a}$  from (3). To this end, observe the identity

$$\mathfrak{a}(u, v) = \int_O B T_{\vec{D}} u \cdot \overline{T_{\vec{D}} v}, \quad u, v \in \mathbb{W}_{\vec{D}}^{1,2}(O).$$

Assumption (B) ensures that the form  $\mathfrak{a}$  is sectorial, so that the associated operator on  $L^2(O)^m$  is well defined. For a proof of the equivalence of these two definitions, see [12, Lemma 12.1]. Also associated with  $\mathfrak{a}$  is a bounded operator

$$\mathcal{L} : \mathbb{W}_{\vec{D}}^{1,2}(O) \rightarrow \left(\mathbb{W}_{\vec{D}}^{1,2}(O)\right)^*$$

extending  $L$  to  $\mathbb{W}_{\vec{D}}^{1,2}(O)$ . As for  $L$ , the bounded extension  $\mathcal{L}$  is given as the composition

$$\mathcal{L} = T_{\vec{D}}^* B T_{\vec{D}},$$

where this time  $T_{\vec{D}}^*$  is understood in the “very weak sense”, that is, as the bounded operator  $T_{\vec{D}}^* : L^2(O)^N \rightarrow (\mathbb{W}_{\vec{D}}^{1,2}(O))^*$ .

One easily verifies that the adjoint  $L^*$  is the operator associated with the adjoint form  $\mathfrak{a}^*$ , which shares the same properties as  $L$  for Assumption (B) is invariant under taking adjoints. We collect some more important properties of the operator  $L$  and refer to [12, Chapter 6] and [20] for background and proofs.

**Proposition 3.4.** *The operator  $L$  is  $m$ -accretive and sectorial. In particular, the resolvent family  $\{(1 + t^2 L)^{-1}\}_{t>0}$  is uniformly bounded in  $\mathcal{L}(L^2(O))^m$ .*

By the von Neumann inequality and McIntosh’s theorem, we obtain quadratic estimates for  $L$ .

**Corollary 3.5.** *The operator  $L$  has a bounded  $H^\infty$ -calculus and satisfies quadratic estimates.*

Besides uniform boundedness of resolvents, we sometimes need to control terms of the form  $T_{\vec{D}}(1 + t^2L)^{-1}$ , which can be achieved via the following simple result.

**Lemma 3.6.** *The family  $\{tT_{\vec{D}}(1 + t^2L)^{-1}\}_{t>0}$  is uniformly bounded in  $\mathcal{L}(L^2(O)^m, L^2(O)^N)$ , and its adjoint family is given by  $\{t(1 + t^2\mathcal{L})^{-1}T_{\vec{D}}^*\}_{t>0}$ , where  $T_{\vec{D}}^*$  is the bounded operator  $L^2(O)^N \rightarrow (\mathbb{W}_{\vec{D}}^{1,2}(O))^*$ .*

3.2. Operators  $-\Delta_{\vec{D}} + 1$  and  $M_{\vec{D}}$

Setting  $B \equiv \text{id}_{\mathbb{C}^N}$ , we obtain the inhomogeneous Laplacian  $-\Delta_{\vec{D}} + 1$  given by the composition  $-\Delta_{\vec{D}} + 1 = T_{\vec{D}}^*T_{\vec{D}}$  with corresponding form

$$a(u, v) = \left\langle T_{\vec{D}}u, T_{\vec{D}}v \right\rangle, \quad u, v \in \mathbb{W}_{\vec{D}}^{1,2}(O) = D(T_{\vec{D}}).$$

Considering the sesquilinear form derived from  $T_{\vec{D}}^*$ ,

$$b(F, G) = \left\langle T_{\vec{D}}^*F, T_{\vec{D}}^*G \right\rangle, \quad F, G \in D(T_{\vec{D}}^*),$$

we obtain a natural operator  $M_{\vec{D}}$  acting on vector fields  $F \in L^2(O)^N$ .

**Definition 3.7** (The operator  $M_{\vec{D}}$ ). Define the operator  $M_{\vec{D}} : D(M_{\vec{D}}) \subseteq L^2(O)^N \rightarrow L^2(O)^N$  as the composition  $M_{\vec{D}} = T_{\vec{D}}T_{\vec{D}}^*$  with maximal domain

$$D(M_{\vec{D}}) = \left\{ F \in D(T_{\vec{D}}^*) : T_{\vec{D}}^*F \in D(T_{\vec{D}}) \right\}.$$

*Remark 3.8.* We claim that  $\text{ran}(M_{\vec{D}}) = \text{ran}(T_{\vec{D}})$ , and this is a closed subspace of  $L^2(O)^N$ . First, closedness of  $\text{ran}(T_{\vec{D}})$  is equivalent to the fact that the Sobolev space  $\mathbb{W}_{\vec{D}}^{1,2}(O)$  is complete. Second,  $\text{ran}(T_{\vec{D}}) \subseteq \text{ran}(M_{\vec{D}})$  follows from invertibility of  $-\Delta_{\vec{D}} + 1$ . Indeed, let  $u \in \mathbb{W}_{\vec{D}}^{1,2}(O)$  and write  $u = (-\Delta_{\vec{D}} + 1)v = T_{\vec{D}}^*T_{\vec{D}}v$  for some  $v \in D(-\Delta_{\vec{D}} + 1)$ . Hence,  $T_{\vec{D}}u = T_{\vec{D}}T_{\vec{D}}^*T_{\vec{D}}v = M_{\vec{D}}F$ , where  $F := T_{\vec{D}}v \in D(M_{\vec{D}})$ .

Formally,  $M_{\vec{D}}$  is given by the operator matrix  $\begin{bmatrix} 1 & -\text{div}_{\vec{D}} \\ \nabla_{\vec{D}} & -\nabla_{\vec{D}} \text{div}_{\vec{D}} \end{bmatrix}$ . Note, however, that for  $F = [F_0, F']^t \in L^2(O)^m \times L^2(O)^{nm}$ ,  $F \in D(M_{\vec{D}})$  does not imply  $F' \in D(\nabla_{\vec{D}} \text{div}_{\vec{D}})$ , but only  $F_0 - \text{div}_{\vec{D}} F' \in D(\nabla_{\vec{D}})$ .

From the sesquilinear form  $b$ , the operator  $M_{\vec{D}}$  inherits the same desirable properties as the inhomogeneous Laplacian.

**Proposition 3.9.** *The operator  $M_{\vec{D}}$  is self-adjoint and non-negative. In particular,  $M_{\vec{D}}$  has a bounded  $H^\infty$ -calculus on its (closed) range and satisfies quadratic estimates as well as the square root property*

$$\|\sqrt{M_{\vec{D}}}F\|_2 = \|T_{\vec{D}}^*F\|_2, \quad F \in D(T_{\vec{D}}^*) = D(\sqrt{M_{\vec{D}}}).$$

The following intertwining property between  $M_{\vec{D}}$  and  $-\Delta_{\vec{D}} + 1$  is essential for our arguments in Sect. 7.

**Proposition 3.10** (Intertwining between  $M_{\vec{D}}$  and  $-\Delta_{\vec{D}} + 1$ ). *Let  $f \in H^\infty(S_\varphi)$  for some  $\varphi \in (0, \pi)$ . Then, one has the intertwining relation*

$$T_{\vec{D}} f(-\Delta_{\vec{D}} + 1)u = f(M_{\vec{D}})T_{\vec{D}}u \quad (u \in \mathbb{W}_{\vec{D}}^{1,2}(O)).$$

*Proof.* We suppose familiarity with the construction and basic properties of the sectorial functional calculus. A reader who is not yet familiar with this concept can consult the monograph [26] or [20, Sec. 5].

Fix  $u \in \mathbb{W}_{\vec{D}}^{1,2}(O)$ . Also, let  $\varphi \in (0, \pi)$  and  $f \in H^\infty(S_\varphi)$ . We comment first why the identity from the statement is well defined. First of all,  $f(-\Delta_{\vec{D}} + 1)$  is well defined since the operator  $-\Delta_{\vec{D}} + 1$  is sectorial of angle zero and injective (even invertible). Next, write  $u = (-\Delta_{\vec{D}} + 1)^{-\frac{1}{2}}v$  for a suitable  $v \in L^2(O)^m$ , which uses the Kato square root property for  $-\Delta_{\vec{D}} + 1$ . Then, the representation  $f(-\Delta_{\vec{D}} + 1)u = (-\Delta_{\vec{D}} + 1)^{-\frac{1}{2}}f(-\Delta_{\vec{D}} + 1)v$  shows that  $f(-\Delta_{\vec{D}} + 1)u$  is indeed an element of  $\mathbb{W}_{\vec{D}}^{1,2}(O) = D(T_{\vec{D}})$ , where we used a basic commutation property of the functional calculus and boundedness of the  $H^\infty$ -calculus for  $-\Delta_{\vec{D}} + 1$ . Therefore, the left-hand side of the claimed identity is well defined. For the right-hand side, note that  $M_{\vec{D}}$  is in general not injective. However, if we restrict  $M_{\vec{D}}$  to  $\text{ran}(M_{\vec{D}}) = \text{ran}(M_{\vec{D}})$  (see Remark 3.8 for this identity), then  $M_{\vec{D}}$  becomes injective and  $f(M_{\vec{D}})$  can be defined as an operator on  $\text{ran}(M_{\vec{D}})$ . We are not going to distinguish  $M_{\vec{D}}$  from its injective part notation-wise. Since  $T_{\vec{D}}u \in \text{ran}(M_{\vec{D}})$  by Remark 3.8,  $f(M_{\vec{D}})$  is indeed defined on the “gradient field”  $T_{\vec{D}}u$  appearing in the statement.

We split the proof into 3 steps.

**Step 1:** Show  $T_{\vec{D}}(z - (-\Delta_{\vec{D}} + 1))^{-1}u = (z - M_{\vec{D}})^{-1}T_{\vec{D}}u$  for all  $z \in \mathbb{C} \setminus [0, \infty)$ .

The operators  $-\Delta_{\vec{D}} + 1$  and  $M_{\vec{D}}$  are sectorial of angle zero; hence, their resolvents for  $z \in \mathbb{C} \setminus [0, \infty)$  are well defined. Put  $v := (z - (-\Delta_{\vec{D}} + 1))^{-1}u$  for convenience. We can apply  $(z - (-\Delta_{\vec{D}} + 1))$  to the definition of  $v$  to find  $(z - (-\Delta_{\vec{D}} + 1))v = u$ . Since  $u \in \mathbb{W}_{\vec{D}}^{1,2}(O)$ , we can apply  $T_{\vec{D}}$  to the last identity. In conjunction with  $T_{\vec{D}}(-\Delta_{\vec{D}} + 1) = M_{\vec{D}}T_{\vec{D}}$ , this gives

$$T_{\vec{D}}u = T_{\vec{D}}(z - (-\Delta_{\vec{D}} + 1))v = (z - M_{\vec{D}})T_{\vec{D}}v.$$

Finally, we apply  $(z - M_{\vec{D}})^{-1}$  to the last identity and plug in the definition of  $v$  to conclude

$$(z - M_{\vec{D}})^{-1}T_{\vec{D}}u = T_{\vec{D}}v = T_{\vec{D}}(z - (-\Delta_{\vec{D}} + 1))^{-1}u.$$

**Step 2:** Show the intertwining relation for  $f \in H_0^\infty(S_\varphi)$ .

Since  $f \in H_0^\infty(S_\varphi)$ , we can write  $f(M_{\vec{D}})$  and  $f(-\Delta_{\vec{D}} + 1)$  via Cauchy integrals. Then, the claim follows from Step 1 by standard arguments.

**Step 3:** The general case  $f \in H^\infty(S_\phi)$ .

Recall the standard regularizer  $e(z) = z(1+z)^{-2}$  for the  $H^\infty$ -calculus of an injective sectorial operator. By definition,  $f(-\Delta_{\vec{D}} + 1)u = e(-\Delta_{\vec{D}} + 1)^{-1}(ef)(-\Delta_{\vec{D}} + 1)u$ . As discussed at the start of the proof,  $f(-\Delta_{\vec{D}} + 1)u$  is again in  $\mathbb{W}_{\vec{D}}^{1,2}(O)$ . Therefore, we can apply  $T_{\vec{D}}$  to the last identity to get  $T_{\vec{D}}f(-\Delta_{\vec{D}} + 1)u = T_{\vec{D}}e(-\Delta_{\vec{D}} + 1)^{-1}(ef)(-\Delta_{\vec{D}} + 1)u$ . By construction of the functional calculus,  $v := (ef)(-\Delta_{\vec{D}} + 1)u$  is in the range of  $e(-\Delta_{\vec{D}} + 1)$ . Furthermore,  $v \in \mathbb{W}_{\vec{D}}^{1,2}(O)$ . Put  $w := e(-\Delta_{\vec{D}} + 1)^{-1}v$ . We claim that also  $w \in \mathbb{W}_{\vec{D}}^{1,2}(O)$ . Indeed,  $w = f(-\Delta_{\vec{D}} + 1)u \in \mathbb{W}_{\vec{D}}^{1,2}(O)$  as observed above.

Next, we show  $T_{\vec{D}}e(-\Delta_{\vec{D}} + 1)^{-1}v = e(M_{\vec{D}})^{-1}T_{\vec{D}}v$ . To this end, write  $T_{\vec{D}}v = T_{\vec{D}}e(-\Delta_{\vec{D}} + 1)w = e(M_{\vec{D}})T_{\vec{D}}w$ , where we used Step 2 for the last manipulation. Therefore,  $T_{\vec{D}}v \in \text{ran}(e(M_{\vec{D}}))$  and we conclude  $e(M_{\vec{D}})^{-1}T_{\vec{D}}v = T_{\vec{D}}w = T_{\vec{D}}e(-\Delta_{\vec{D}} + 1)^{-1}v$  as desired.

In summary, we deduce with another application of Step 2 to  $ef \in H_0^\infty(S_\phi)$  that

$$\begin{aligned} T_{\vec{D}}f(-\Delta_{\vec{D}} + 1)u &= T_{\vec{D}}e(-\Delta_{\vec{D}} + 1)^{-1}(ef)(-\Delta_{\vec{D}} + 1)u \\ &= e(M_{\vec{D}})^{-1}T_{\vec{D}}(ef)(-\Delta_{\vec{D}} + 1)u \\ &= e(M_{\vec{D}})^{-1}(ef)(M_{\vec{D}})T_{\vec{D}}u \\ &= f(M_{\vec{D}})T_{\vec{D}}u. \end{aligned} \quad \square$$

*Remark 3.11.* The last proposition is our substitute for the observation made in [10, Rem. 4.5].

One important property of elliptic operators in divergence form is their off-diagonal decay. A standard way to derive them is by using Davies’ trick. In our geometric setting, this was done in [11, 19] for the families  $\{e^{-t^2L}\}_{t>0}$  and  $\{t\nabla e^{-t^2L}\}_{t>0}$ . The same proof also applies to the family  $\{te^{-t^2L}\}_{t>0}$ . Indeed, it suffices to observe that the coercivity condition used in the treatment of the gradient family is in fact an inhomogeneous coercivity condition. Using the Laplace transform, these bounds can be transferred to the respective resolvent families.

**Proposition 3.12** (Off-diagonal estimates). *The families  $\{t(1 + t^2L)^{-1}\}_{t>0}$  and  $\{t\nabla(1 + t^2L)^{-1}\}_{t>0}$  satisfy  $L^2$  off-diagonal estimates, that is, there exist constants  $c, C > 0$  such that, for all  $t > 0$ , all measurable subsets  $E, F \subseteq O$  and all  $u \in L^2(O)$ , there holds*

$$\|\mathbf{1}_E t(1 + t^2L)^{-1}\mathbf{1}_F u\|_2 + \|\mathbf{1}_E t\nabla(1 + t^2L)^{-1}\mathbf{1}_F u\|_2 \leq C e^{-c\frac{d(E,F)}{t}} \|\mathbf{1}_F u\|_2 .$$

*By duality, also the adjoint family  $\{t(1 + t^2L)^{-1} \text{div}\}_{t>0}$  satisfies  $L^2$  off-diagonal estimates.*

### 3.3. Perturbations of $M_{\vec{D}}$

We perturb the operator  $M_{\vec{D}}$  by the elliptic coefficient function  $B$ . The resulting operator  $M_{\vec{D}}B$  is again sectorial, a fact that we are going to exploit in the construction of  $T(b)$ -type test functions in Sect. 8.

For instance in [18, Prop. 6.1.17], it is shown that the perturbation  $DB$  of a self-adjoint operator  $D$  is bisectorial. We make a minor adjustment to their argument to prove that, if  $D$  is non-negative, then  $DB$  is even sectorial. We formulate the subsequent result only for the choice  $D = M_{\vec{D}}$ . Let us mention that, if  $B$  were even strongly elliptic and not merely Gårding elliptic, then the subsequent result could be proved in an easier manner [12, Prop. 6.9].

**Lemma 3.13.** *If the coefficients  $B$  satisfy the Gårding ellipticity condition on  $\text{ran } T_{\vec{D}}$  as stated in Assumption (B), then the operator  $M_{\vec{D}}B$  is sectorial. Moreover, the family  $\{tT_{\vec{D}}^*B(1 + t^2M_{\vec{D}}B)^{-1}\}_{t>0}$  is uniformly bounded in  $\mathcal{L}(L^2(O)^N, L^2(O)^m)$ .*

*Proof.* To ease notation, write  $M, T$ , and  $T^*$  for the operators  $M_{\vec{D}}, T_{\vec{D}}$ , and  $T_{\vec{D}}^*$ , and write  $\|\cdot\|$  instead of  $\|\cdot\|_2$ . Recall that  $B$  satisfies Gårding’s inequality on  $\text{ran}(T) = \text{ran}(M)$ . The same is true for  $B^*$  because Assumption (B) is invariant under taking the adjoint. From [18, Prop. 6.1.17], we have the (non-orthogonal) topological decompositions of  $L^2(O)^N$  given by

$$L^2(O)^N = \ker(MB) \oplus \overline{\text{ran}(MB)}, \tag{4}$$

$$L^2(O)^N = \ker(B^*M) \oplus \overline{\text{ran}(B^*M)}. \tag{5}$$

Now, set

$$\omega := \sup_{0 \neq F \in \text{ran } M} |\arg \langle BF, F \rangle| \in [0, \frac{\pi}{2}),$$

and take  $\phi \in (\omega, \pi)$ . Using the decompositions above, we prove that, for all  $z \in \mathbb{C} \setminus \overline{S_\phi}$ , we have the estimates

$$\|(z - MB)U\| \gtrsim |z| \|U\|, \quad U \in \text{D}(MB), \tag{6}$$

$$\|(\bar{z} - B^*M)U\| \gtrsim |z| \|U\|, \quad U \in \text{D}(B^*M). \tag{7}$$

From this, we deduce that  $MB$  is sectorial as follows. Owing to (7), we find that  $\bar{z} - B^*M$  is injective and that its range is closed. Since  $B$  is bounded, we have  $(B^*M)^* = MB$ . Hence, (6) yields that  $\bar{z} - B^*M$  has dense range. Summarizing the two facts, we find  $\bar{z} \in \rho(B^*M)$ . Taking the estimate (7) into account, this shows sectoriality of  $B^*M$ . Next, using that  $B^*M$  is closed, it follows

$$(MB)^* = (B^*M)^{**} = \text{cl}(B^*M) = B^*M.$$

Thus, arguing similarly as above entails sectoriality of  $MB$ .

We turn our attention to proving (6). Let  $z \in \mathbb{C} \setminus \overline{S_\phi}$ . Let  $U \in \text{D}(MB)$  and, according to (4), write  $U = V + W$  with  $V \in \ker(MB)$  and  $W \in \overline{\text{ran}(MB)} \cap \text{D}(MB)$ .

Note that  $BW \in D(M)$ . Hence, by positivity of  $M$ , it holds  $\langle BW, MBW \rangle \geq 0$ . Moreover, since  $W \in \overline{\text{ran}(MB)} \subseteq \text{ran}(M)$ , we have  $\langle BW, W \rangle \in \overline{S}_\omega$ . Therefore,  $\bar{z} \langle BW, W \rangle \in \mathbb{C} \setminus \overline{S}_{\phi-\omega}$ . Cover  $\mathbb{C} \setminus \overline{S}_{\phi-\omega}$  by the set  $\mathbb{C} \setminus (\overline{S}_{\phi-\omega} \cup -\overline{S}_{\phi-\omega})$ , which is the complement of a bisector, and the (closed) sector around the negative real axis  $-\overline{S}_{\phi-\omega}$ . In the first case, if  $w \in \mathbb{C} \setminus (\overline{S}_{\phi-\omega} \cup -\overline{S}_{\phi-\omega})$ , then there holds comparability

$$|w| \approx_{\phi-\omega} |\text{Im } w| \tag{8}$$

as in [18, Prop. 6.1.17]. Otherwise, if  $w \in -\overline{S}_{\phi-\omega}$ , there holds comparability

$$|w| \approx |\text{Im } w| - \text{Re } w. \tag{9}$$

Suppose for the moment  $\langle BW, zW \rangle \in -\overline{S}_{\phi-\omega}$ . Then, from  $W \in \text{ran}(M) = \text{ran}(T)$  in conjunction with Gårding’s inequality, (9), positivity of  $M$ , and boundedness of  $B$ , we get

$$\begin{aligned} |z| \|W\|^2 &\lesssim |\bar{z}| \text{Re} \langle BW, W \rangle \\ &\lesssim |\langle BW, zW \rangle| \\ &\approx |\text{Im} \langle BW, zW \rangle| + \text{Re} \langle BW, -zW \rangle \\ &\leq |\text{Im} \langle BW, (z - MB)W \rangle| + \text{Re} \langle BW, (MB - z)W \rangle \\ &\leq 2 \|BW\| \|(z - MB)W\| \\ &\lesssim \|W\| \|(z - MB)W\|. \end{aligned}$$

Otherwise, if  $\langle BW, zW \rangle$  belongs to the complement of the bisector, a similar calculation using (8) instead of (9) yields

$$|z| \|W\|^2 \lesssim_{\phi-\omega} |\text{Im} \langle BW, (z - MB)W \rangle| \lesssim \|W\| \|(z - MB)W\|.$$

Combining both cases yields  $\|(z - MB)W\| \gtrsim |z| \|W\|$ . Furthermore,  $\|(z - MB)V\| = |z| \|V\|$  for  $V \in \ker(MB)$ . Since  $(z - MB)W \in \overline{\text{ran}(MB)}$  and  $MBV = 0 \in \ker(MB)$ , the topological decomposition (4) gives

$$\|(z - MB)U\| \approx \|(z - MB)V\| + \|(z - MB)W\| \gtrsim |z| (\|V\| + \|W\|) \approx |z| \|U\|,$$

which completes the proof of (6).

To prove (7), we split  $U \in D(B^*M)$  as  $U = V + Z$  with  $V \in \ker(B^*M)$  and  $Z \in \overline{\text{ran}(B^*M)} \cap D(B^*M)$ . Since  $\|B^*F\| \approx \|F\|$  on  $\text{ran}(M)$ , we have  $\overline{\text{ran}(B^*M)} = B^*(\text{ran}(M))$ . Therefore,  $Z = B^*W$  for some  $W \in \text{ran}(M) \cap D(B^*MB^*)$ . Reusing the calculation leading to (6) from above with  $B$  replaced by  $B^*$ , we have

$$\begin{aligned} |\bar{z}| \|B^*W\|^2 &\lesssim |z| \|W\|^2 \lesssim \|B^*W\| \|(\bar{z} - MB^*)W\| \\ &\lesssim \|B^*W\| \|B^*(\bar{z} - MB^*)W\|, \end{aligned}$$

where we used  $(\bar{z} - MB^*)W \in \text{ran}(M)$  in the last step. Thus, plugging in the definition of  $Z$ , deduce  $|\bar{z}| \|Z\| \lesssim \|(\bar{z} - B^*M)Z\|$ . Then, as before, we deduce from the splitting (5) the estimate (7).

Finally, let us prove uniform boundedness of  $tT^*B(1 + t^2MB)^{-1}$ . Observe that  $B(1 + t^2MB)^{-1}$  maps into the domain of  $M$  and that  $M$  is associated with the sesquilinear form  $\mathfrak{b}$ . Thus, for  $F \in L^2(O)^N$ , we have

$$\begin{aligned} \|tT^*B(1 + t^2MB)^{-1}F\|^2 &= \mathfrak{b}(t^2B(1 + t^2MB)^{-1}F, B(1 + t^2MB)^{-1}F) \\ &= \left\langle t^2MB(1 + t^2MB)^{-1}F, B(1 + t^2MB)^{-1}F \right\rangle \\ &\lesssim \left\| (1 - (1 + t^2MB)^{-1})F \right\| \left\| (1 + t^2MB)^{-1}F \right\| \lesssim \|F\|^2. \end{aligned}$$

The last two steps make use of the Cauchy–Schwarz inequality, the boundedness of  $B$ , and uniform boundedness of the resolvents  $(1 + t^2MB)^{-1}$  in  $\mathcal{L}(L^2(O)^N)$ , where the latter follows by sectoriality of  $MB$  established in the first part of the proof.  $\square$

### 4. Review on dyadic structures

Dyadic cubes are the foundation of dyadic harmonic analysis in  $\mathbb{R}^n$ . In this section, we recall a substitute on interior thick open sets for them, which will be fundamental for the analysis presented in Sects. 7 and 8.

To put things into a broader context, we note that an open and interior thick set  $O$  equipped with the restricted Euclidean metric and restricted Lebesgue measure is a locally doubling space, that is, there exists  $C \geq 2$  such that for all  $x \in O$  and  $r \in (0, 1]$  it holds

$$|B_O(x, 2r)| \leq C |B_O(x, r)|. \tag{10}$$

In [17, Thm. 11], Christ has constructed a full dyadic structure in spaces that fulfill the doubling property (10), even for all  $r \in (0, \infty)$ . With the local doubling property from above, the same construction gives a dyadic structure on small scales, that is, we can decompose the space  $O$  into small dyadic “cubes”, but not into large dyadic “cubes.” For our formulation here, we combine [22, Thm. 7.4] with the boundary estimate [15, Lem. 5.2] and the rescaling argument from [28, Prop. 2.12]. The boundary estimate, that is, property (5) in the subsequent proposition, is a consequence of porosity of  $\partial O$  established in Proposition 2.8. The remaining results hold for  $O$  merely interior thick.

**Proposition 4.1** (Existence of a dyadic structure). *Suppose that  $O$  is interior thick and that  $\partial O$  is porous. Then, there exists a collection  $\{Q_\alpha^k \mid k \in \mathbb{N}_0, \alpha \in I_k\}$  of open sets, where  $I_k$  are countable index sets, and constants  $a_0, a_1, \eta, C > 0$  such that the following hold:*

1. For each  $k \in \mathbb{N}_0$ , it holds  $|O \setminus \cup_{\alpha \in I_k} Q_\alpha^k| = 0$ .
2. If  $\ell \geq k$ , then, for each  $\alpha \in I_k$  and each  $\beta \in I_\ell$ , either  $Q_\beta^\ell \subseteq Q_\alpha^k$  or  $Q_\beta^\ell \cap Q_\alpha^k = \emptyset$ .
3. If  $\ell \leq k$ , then, for each  $\alpha \in I_k$ , there is a unique  $\beta \in I_\ell$  such that  $Q_\alpha^k \subseteq Q_\beta^\ell$ .

4. For each  $Q_\alpha^k, k \in \mathbb{N}_0, \alpha \in I_k$ , there exists  $z_\alpha^k \in \mathbf{O}$  such that

$$Q(z_\alpha^k, a_0 2^{-k}) \cap \mathbf{O} \subseteq Q_\alpha^k \subseteq Q(z_\alpha^k, a_1 2^{-k}) \cap \mathbf{O}.$$

5. If  $k \in \mathbb{N}_0, \alpha \in I_k$ , and  $s > 0$ , then

$$\left| \{x \in Q_\alpha^k : d(x, \mathbb{R}^n \setminus Q_\alpha^k) \leq s 2^{-k}\} \right| \leq C s^\eta \left| Q_\alpha^k \right|.$$

**Definition 4.2** (Dyadic “cubes”). In the setting of Proposition 4.1, put  $\square_{2^{-k}} := \{Q_\alpha^k \mid \alpha \in I_k\}$ . Members of this collection are called *dyadic “cubes”* of generation  $2^{-k}$ . For  $t \in (2^{-(k+1)}, 2^{-k}]$ , define also  $\square_t := \square_{2^{-k}}$ . In this case, the *sidelength* of  $Q \in \square_t$  is  $\ell(Q) := 2^{-k}$ . Finally, the collection  $\square$  of all (local) *dyadic “cubes”* is given by  $\bigcup_k \square_{2^{-k}}$ .

**Definition 4.3** (Children and parents). Let  $\ell \geq k, R \in \square_{2^{-\ell}}$  and  $Q \in \square_{2^{-k}}$ . If  $R \subseteq Q$ , then  $R$  is called a *child* of  $R$ , and  $Q$  is called the (*unique*) *parent “cube”* of  $R$ .

With  $R$  and  $Q$  as in the preceding definition, Proposition 4.1 (2) asserts that  $R$  is either a child of  $Q$  or disjoint to  $Q$ . Moreover, Proposition 4.1 (3) asserts the existence of a parent “cube” to  $R$ . In conjunction with (2), this parent “cube” has to be unique, which justifies our terminology of unique parent “cubes” in Definition 4.3.

**Definition 4.4** (Double “cube”). If  $Q \in \square$ , then define the *doubled “cube”*  $2Q$  via  $2Q := \{x \in \mathbf{O} : d(x, Q) < \ell(Q)\}$ .

Using property (4) of dyadic “cubes”, interior thickness of  $\mathbf{O}$ , and elementary geometric considerations, we find  $|2Q| \lesssim |Q|$ .

*Remark 4.5.* (1) and (2) in Proposition 4.1 imply that, outside of a null set  $\mathfrak{N}$ , each  $x \in \mathbf{O} \setminus \mathfrak{N}$  is uniquely contained in a “cube”  $Q \in \square_t$  for each  $t \in (0, 1]$ .

In the following definition,  $L^1_{\text{loc}}(\mathbf{O})$  denotes the collection of measurable functions which are integrable over bounded subsets of  $\mathbf{O}$ .

**Definition 4.6.** For  $t \in (0, 1], x \in \mathbf{O} \setminus \mathfrak{N}$ , and  $u \in L^1_{\text{loc}}(\mathbf{O})$  define the *dyadic averaging operator* by

$$(\mathcal{A}_t u)(x) := \int_{Q_{x,t}} u(y) \, dy,$$

where  $Q_{x,t} \in \square_t$  is the unique “cube” containing  $x$ . For  $F \in L^1_{\text{loc}}(\mathbf{O})^k$ , via a minor abuse of notation, we define  $\mathcal{A}_t F$  by component-wise action, that is,

$$(\mathcal{A}_t F)(x) := \left( (\mathcal{A}_t F_i)(x) \right)_{i=1}^k,$$

where  $F = (F_i)_{i=1}^k$ .

We investigate some first properties.

**Proposition 4.7.**  $\mathcal{A}_t^2 = \mathcal{A}_t$ , and  $\mathcal{A}_t$  is a contraction on  $L^2(\mathbf{O})$  for all  $t \in (0, 1]$ .

*Proof.* Fix  $t \in (0, 1]$ . For the projection property, note that

$$(\mathcal{A}_t^2 u)(x) = \int_{Q_{x,t}} \left( \int_{Q_{z,t}} u(y) \, dy \right) \, dz = \int_{Q_{x,t}} (u)_{Q_{z,t}} \, dz = (u)_{Q_{x,t}} = \mathcal{A}_t u(x),$$

where we used  $Q_{z,t} = Q_{x,t}$  for  $z \in Q_{x,t}$  in the second step.

For the second claim, decomposing  $\mathbf{O} \setminus \mathfrak{N}$  into the dyadic “cubes”  $\square_t$  and applying Jensen’s inequality, we see for  $u \in L^2(\mathbf{O})$  that

$$\|\mathcal{A}_t u\|_2^2 = \sum_{Q \in \square_t} \int_Q |\mathcal{A}_t u|^2 = \sum_{Q \in \square_t} |Q| \left| \int_Q u \right|^2 \leq \sum_{Q \in \square_t} |Q| \int_Q |u|^2 = \|u\|_2^2.$$

□

The following is an important tool for later that is found in [31, Thm 4.3]. We will repeat the notion of a Carleson measure at the beginning of Sect. 8.

**Proposition 4.8** (Carleson’s inequality). *If  $\sigma$  is a Carleson measure on  $\mathbf{O} \times (0, 1]$  with Carleson norm  $\|\sigma\|_C$ , then*

$$\iint_{\mathbf{O} \times (0,1]} |\mathcal{A}_t u(x)|^2 \, d\sigma(x, t) \lesssim \|\sigma\|_C \|u\|_2^2.$$

### 5. A coercivity property

Throughout this section, we suppose that  $\mathbf{O} \subseteq \mathbb{R}^n$  is interior thick and that  $\mathbf{D} \subseteq \partial \mathbf{O}$  is closed and Ahlfors–David regular. In addition, we suppose that  $\mathbf{O}$  is locally uniform near  $\partial \mathbf{O} \setminus \mathbf{D}$ . The goal of this section is to prove the following result.

**Proposition 5.1** (Coercivity of  $-\Delta_{\mathbf{D}} + 1$ ). *There exists  $\alpha \in (0, 1]$  and a constant  $c > 0$  such that for every function  $v \in D(-\Delta_{\mathbf{D}} + 1)$  there holds the estimate*

$$\|(-\Delta_{\mathbf{D}} + 1)^{\frac{1+\alpha}{2}} v\|_2 \geq c \|T_{\mathbf{D}} v\|_{[L^2(\mathbf{O})^m, \mathbb{W}_{\mathbf{D}}^{1,2}(\mathbf{O})]_{\alpha}}.$$

In the Euclidean setting, that is to say, when  $\mathbf{O} = \mathbb{R}^n$ , one can take  $\alpha = 1$ . Indeed, this follows by using the Fourier transform. In [9], the authors introduce an abstract condition similar to Proposition 5.1 which they call (H8). For the Kato square root problem on  $\mathbb{R}^n$ , it amounts to showing that the domain of  $-\Delta$  coincides with  $W^{2,2}(\mathbb{R}^n)$  as well as that the Hessian of a function  $u \in D(-\Delta)$  is controlled by  $-\Delta u$  in norm. On domains, the analogue to Proposition 5.1 is [22, (H7)].

The proof of Proposition 5.1 will occupy the rest of this section.

### 5.1. Fractional Sobolev spaces

We will use fractional Sobolev spaces of functions that vanish on a subset  $D \subseteq \partial O$ . The starting point for their construction are the fractional Sobolev spaces  $W^{s,2}(\mathbb{R}^n)$ , which can be defined either as Bessel potential spaces or as Sobolev–Slobodeckij spaces if  $s$  is not an integer, see [34].

Since  $D$  is a  $(n - 1)$ -set, see Remark 2.2 for this terminology, a version of the Lebesgue differentiation theorem allows us to define traces on  $D$ . The following is a weakened version of [30, Thm. VI.1] that suffices for our purpose.

**Proposition 5.2.** *Let  $s \in (\frac{1}{2}, \frac{3}{2})$  and  $u \in W^{s,2}(\mathbb{R}^n)$ . For  $\mathcal{H}^{n-1}$ -almost every  $x \in D$  the limit*

$$(\mathcal{R}_D u)(x) := \lim_{r \rightarrow 0} \frac{1}{|B(x, r)|} \int_{B(x, r)} u(y) dy$$

*exists. The restriction operator  $\mathcal{R}_D$  maps  $W^{s,2}(\mathbb{R}^n)$  boundedly into  $L^2(D, \mathcal{H}^{n-1})$ .*

With the trace operator at hand, we introduce the closed subspace  $W_D^{s,2}(\mathbb{R}^n)$  of  $W^{s,2}(\mathbb{R}^n)$  by

$$W_D^{s,2}(\mathbb{R}^n) := \{u \in W^{s,2}(\mathbb{R}^n) : \mathcal{R}_D u = 0\}.$$

In the case  $s = 1$ , this notion is consistent with Definition 2.9, see, for instance, [14, Lem. 3.3]. Finally, we denote the distributional restriction to  $O$  by  $|_O$  and define fractional Sobolev spaces on  $O$  by restriction.

**Definition 5.3.** Let  $s \in [0, \frac{3}{2})$  and  $t \in (\frac{1}{2}, \frac{3}{2})$ . Put  $W^{s,2}(O) := \{u|_O : u \in W^{s,2}(\mathbb{R}^n)\}$  and  $W_D^{t,2}(O) := \{u|_O : u \in W_D^{t,2}(\mathbb{R}^n)\}$  and equip them with quotient norms.

*Remark 5.4.* These spaces are again Hilbert spaces by construction as quotients of Hilbert spaces. Since  $O$  is interior thick, we have that  $W_D^{t,2}(O)$  is a closed subspace of  $W^{t,2}(O)$  with an equivalent norm [14, Lem. 3.4]. As a cautionary tale, let us stress that in the context of this section  $W^{1,2}(O)$  is embedded into but possibly *not* equal to the collection of all  $u \in L^2(O)$  with  $\nabla u \in L^2(O)^d$  and norm (2). However, as a consequence of Theorem 2.10, the definition of  $W_D^{1,2}(O)$  above coincides with the original one from Definition 2.9 up to equivalent norms when working in the geometric setting of Theorem 1.1.

The (fractional) Sobolev spaces respect the following interpolation rule. The result was originally shown in [14] under the additional assumption that  $\partial O$  is a  $(n - 1)$ -set. Subsequently, the boundary regularity could be relaxed to porosity in [15, Prop. 4.16]. A reader who is not yet familiar with abstract interpolation theory can find further information in [34].

**Proposition 5.5** (Interpolation identity). *For  $s \in (0, 1)$ , one has the following interpolation identity*

$$[L^2(O), W_D^{1,2}(O)]_s = \begin{cases} W^{s,2}(O) & (\text{if } s < 1/2) \\ W_D^{s,2}(O) & (\text{if } s > 1/2) \end{cases}.$$

### 5.2. Identification of fractional power domains of the Laplacian

We recall an identification result from [15] that concerns certain fractional powers of  $-\Delta_{\vec{D}} + 1$ . This property relies on the geometric quality of  $\mathcal{O}$  and  $\vec{D}$  and invokes deep results from potential theory and related fields.

In analogy with the case  $\alpha = 1$ , we employ the notation  $\mathbb{W}_{\vec{D}}^{\alpha,2}(\mathcal{O}) := \oplus_{i=1}^m \mathbb{W}_{D_i}^{\alpha,2}(\mathcal{O})$ , where  $\vec{D} = (D_i)_{i=1}^m$  is a given array of Ahlfors–David regular boundary parts.

**Theorem 5.6.** *Under the geometric assumptions fixed at the beginning of this section, there exists  $\varepsilon \in (0, \frac{1}{2})$  such that the fractional power domains of  $-\Delta_{\vec{D}} + 1$  in  $L^2(\mathcal{O})^m$  are given by*

$$D((-\Delta_{\vec{D}} + 1)^{\frac{\alpha}{2}}) = \begin{cases} \mathbb{W}_{\vec{D}}^{\alpha,2}(\mathcal{O}) & \text{if } \alpha \in (\frac{1}{2}, 1 + \varepsilon), \\ \mathbb{W}^{\alpha,2}(\mathcal{O}) & \text{if } \alpha \in (0, \frac{1}{2}). \end{cases}$$

The identity holds with equivalence of norms, and, by invertibility of  $-\Delta_{\vec{D}} + 1$ , the graph norm can be replaced by the homogeneous graph norm.

The proof of the preceding result is found in [15, Thm. 1.2].

### 5.3. Proof of Proposition 5.1

Eventually, we can give the proof of the main result of this section.

*Proof of Proposition 5.1.* Set  $\alpha = \varepsilon/2$ , where  $\varepsilon$  is introduced in Theorem 5.6. Note that  $\alpha < 1/2$ . Now, let  $v \in D(-\Delta_{\vec{D}} + 1)$ . Using Proposition 5.5 and the definition of  $T = T_{\vec{D}}$ , calculate

$$\|Tv\|_{[L^2(\mathcal{O})^m, \mathbb{W}_{\vec{D}}^{1,2}(\mathcal{O})]_{\alpha}}^2 \approx \|Tv\|_{\mathbb{W}^{\alpha,2}(\mathcal{O})}^2 = \|v\|_{\mathbb{W}^{\alpha,2}(\mathcal{O})}^2 + \|\nabla v\|_{\mathbb{W}^{\alpha,2}(\mathcal{O})}^2.$$

By definition of the scale of spaces  $\mathbb{W}^{s,2}(\mathcal{O})$ , the gradient maps  $\mathbb{W}^{1+\alpha,2}(\mathcal{O}) \rightarrow \mathbb{W}^{\alpha,2}(\mathcal{O})$  (see [15, Lem. 4.10] for details). Hence, taking Remark 5.4 and  $1 + \alpha \in [1, 1 + 1/2]$  into account, we continue by

$$\|Tv\|_{[L^2(\mathcal{O})^m, \mathbb{W}_{\vec{D}}^{1,2}(\mathcal{O})]_{\alpha}} \lesssim \|v\|_{\mathbb{W}^{1+\alpha,2}(\mathcal{O})} \approx \|v\|_{\mathbb{W}_{\vec{D}}^{1+\alpha,2}(\mathcal{O})}.$$

Eventually, Theorem 5.6 lets us conclude

$$\|Tv\|_{[L^2(\mathcal{O})^m, \mathbb{W}_{\vec{D}}^{1,2}(\mathcal{O})]_{\alpha}} \lesssim \|(-\Delta_{\vec{D}} + 1)^{\frac{1+\alpha}{2}} v\|_2.$$

□

### 6. Reduction to a quadratic estimate

In Sects. 6–8, we are going to prove our main result, Theorem 1.1, under the additional assumption that  $\mathbf{O}$  is interior thick. This statement is equivalent to the validity of certain quadratic estimates. The argument is well known in the literature (see [20, Chap. 13] for instance), but we are going to briefly recap on it in this section for the reader’s convenience. Eventually, we will remove the interior thickness condition in Sect. 9 to complete the proof of Theorem 1.1.

The contents of this section are still valid without the interior thickness condition, so we will not yet employ the bold letter convention (Convention 2.4) here. However, interior thickness will be crucial in the verification of the quadratic estimate (QE) appearing in the following proposition.

**Proposition 6.1** (Reduction to a quadratic estimate). *In the situation of Theorem 1.1, the validity of Kato’s square root property is equivalent to the quadratic estimate*

$$\int_0^\infty \|tL(1 + t^2L)^{-1}u\|_2^2 \frac{dt}{t} \lesssim \|u\|_{\mathbb{W}^{1,2}(O)}^2, \quad u \in \mathbb{W}^{1,2}_D(O), \tag{QE}$$

for every elliptic system in divergence form  $L$  on  $O$  subject to Dirichlet boundary conditions in  $\vec{D} \subseteq (\partial O)^m$

Hence, instead of showing Theorem 1.1 right away, we are going to establish (QE) in the following two sections.

As in [20], the quadratic estimate (QE) can be reformulated in terms of the bounded operator  $\mathcal{L} : \mathbb{W}^{1,2}_D(O) \rightarrow (\mathbb{W}^{1,2}_D(O))^*$ . More precisely, writing

$$\Theta_t = t(1 + t^2\mathcal{L})^{-1}T_D^*B$$

with  $T_D^*$  in the “very weak formulation” and keeping  $\|u\|_{\mathbb{W}^{1,2}(O)}^2 = \|T_D u\|_2^2$  in mind, (QE) takes the form

$$\int_0^\infty \|\Theta_t T_D u\|_2^2 \frac{dt}{t} \lesssim \|T_D u\|_2^2, \quad u \in \mathbb{W}^{1,2}_D(O).$$

**Lemma 6.2.** *The family  $\{\Theta_t\}_{t>0}$  is uniformly bounded in  $\mathcal{L}(L^2(O)^N, L^2(O)^m)$  and satisfies  $L^2$  off-diagonal estimates.*

*Proof.* Since the coefficient matrix  $B$  acts as a bounded multiplication operator on  $L^2(O)^N$  and preserves the support, the claim is a direct consequence of Proposition 3.12. □

### 7. Principal part approximation

Throughout this section, we suppose that the pair  $(\mathbf{O}, \vec{D})$  satisfies the geometric assumptions from Theorem 1.1 as well as that  $\mathbf{O}$  is interior thick. Recall Convention 2.4 on the usage of bold symbols. The goal of this section is to reduce the validity of (QE) to a Carleson measure estimate. The latter is verified in Sect. 8.

### 7.1. Presentation of the relevant operators

It is well known that, owing to the off-diagonal estimates from Lemma 6.2,  $\Theta_t$  extends to a bounded operator  $L^\infty(\mathcal{O})^N \rightarrow L^2_{\text{loc}}(\mathcal{O})^m$  for all  $t$ , see, for instance, [20, Prop. 11.12 & Def. 11.14]. We exploit this fact in the subsequent definition of the principal part.

**Definition 7.1** (Principal part). Identifying the standard unit vectors  $e_1, e_2, \dots, e_N \in \mathbb{C}^N$  with their respective constant functions on  $\mathcal{O}$ , we define for  $t \in (0, 1]$  the *principal part* of  $\Theta_t$  by

$$\gamma_t := [\Theta_t(e_1), \dots, \Theta_t(e_N)] \in L^2_{\text{loc}}(\mathcal{O}, \mathbb{C}^{m \times N})$$

*Remark 7.2.* For almost every  $x \in \mathcal{O}$ , the principal part  $\gamma_t(x)$  is a linear map from  $\mathbb{C}^N$  to  $\mathbb{C}^m$  acting as

$$\gamma_t(x)w = \Theta_t(w\mathbf{1}_{\mathbb{R}^n})(x), \quad w \in \mathbb{C}^N.$$

In particular, for  $F \in L^2(\mathcal{O})^N$ ,  $t \in (0, 1]$  and a dyadic ‘‘cube’’  $Q \in \square_t$  we have

$$\mathbf{1}_Q(\Theta_t - \gamma_t \mathcal{A}_t)F = \mathbf{1}_Q \Theta_t(F - (F)_Q).$$

**Definition 7.3** (Smoothing operators). For  $t > 0$ , we define the smoothing operators

$$P_t = (1 + t^2 M_{\vec{D}})^{-1} \in \mathcal{L}(L^2(\mathcal{O})^N), \quad Q_t = t T_{\vec{D}}^* P_t \in \mathcal{L}(L^2(\mathcal{O})^N, L^2(\mathcal{O})^m).$$

A direct consequence of Proposition 3.10 with the function  $f : z \rightarrow (1 + t^2 z)^{-1}$  is the commuting relation

$$P_t T_{\vec{D}} = T_{\vec{D}} (1 + t^2 (-\Delta_{\vec{D}} + 1))^{-1}. \tag{11}$$

**Lemma 7.4.** *The families  $\{P_t\}$  and  $\{Q_t\}$  are uniformly bounded in  $\mathcal{L}(L^2(\mathcal{O})^N)$  and  $\mathcal{L}(L^2(\mathcal{O})^N, L^2(\mathcal{O})^m)$ , respectively. Thus, also the adjoint family  $\{Q_t^*\}$  is uniformly bounded in  $\mathcal{L}(L^2(\mathcal{O})^m, L^2(\mathcal{O})^N)$ , and  $Q_t^*$  is given by the bounded extension of  $t P_t T_{\vec{D}}$  to  $L^2(\mathcal{O})^m$ .*

*Proof.* Uniform boundedness of  $\{P_t\}$  is by  $m$ -accretivity of  $M_{\vec{D}}$ , and for  $\{Q_t\}$  one can use the sesquilinear form  $\mathfrak{b}$ , see the proof of Lemma 3.13 or [20, Lem. 11.7].  $\square$

**Lemma 7.5.** *For  $F \in L^2(\mathcal{O})^N$ , one has*

$$\int_0^\infty \|Q_t F\|_2^2 \frac{dt}{t} \lesssim \|F\|_2^2.$$

*If in addition  $F \in \text{ran}(T_{\vec{D}})$ , then we have the reproducing formula*

$$2 \int_0^\infty Q_t^* Q_t F \frac{dt}{t} = F.$$

*Proof.* Owing to Proposition 3.9, the square root property for the self-adjoint operator  $M_{\vec{D}}$  gives

$$\|Q_t F\|_2 = \|t T_{\vec{D}}^* (1 + t^2 M_{\vec{D}})^{-1} F\|_2 = \|\sqrt{t^2 M_{\vec{D}}} (1 + t^2 M_{\vec{D}})^{-1} F\|_2.$$

Hence, the first assertion follows by quadratic estimates for  $M_{\vec{D}}$ .

For the reproducing formula, note that  $Q_t$  maps into  $D(T_{\vec{D}})$ , so we can compute

$$Q_t^* Q_t = t^2 (1 + t^2 M_{\vec{D}})^{-1} T_{\vec{D}} T_{\vec{D}}^* (1 + t^2 M_{\vec{D}})^{-1} = t^2 M_{\vec{D}} (1 + t^2 M_{\vec{D}})^{-2} = f(t^2 M_{\vec{D}}),$$

where  $f(z) = z(1 + z)^{-2}$ . By Remark 3.8, we have  $\text{ran}(T_{\vec{D}}) = \text{ran}(M_{\vec{D}})$ , so the Calderón reproducing formula [20, Thm. 6.16] yields the assertion.  $\square$

With these operators, we first split the left-hand side of (QE) as

$$\int_0^\infty \|\Theta_t T_{\vec{D}} u\|_2^2 \frac{dt}{t} \lesssim \int_0^\infty \|\Theta_t P_t T_{\vec{D}} u\|_2^2 \frac{dt}{t} + \int_0^\infty \|\Theta_t (1 - P_t) T_{\vec{D}} u\|_2^2 \frac{dt}{t}. \tag{12}$$

The second term on the right-hand side can be controlled via a simple algebraic manipulation.

**Proposition 7.6.** *For  $F \in L^2(\mathcal{O})^N$ , there holds the quadratic estimate*

$$\int_0^\infty \|\Theta_t (1 - P_t) F\|_2^2 \frac{dt}{t} \lesssim \|F\|_2^2.$$

*Proof.* Note that  $1 - P_t = t^2 M_{\vec{D}} P_t$  and  $T_{\vec{D}}^* B M_{\vec{D}} = T_{\vec{D}}^* B T_{\vec{D}} T_{\vec{D}}^* \subseteq \mathcal{L} T_{\vec{D}}^*$ . Thus, for  $F \in L^2(\mathcal{O})^N$ , we can compute

$$\begin{aligned} \Theta_t (1 - P_t) F &= t(1 + t^2 \mathcal{L})^{-1} T_{\vec{D}}^* B t^2 M_{\vec{D}} P_t F \\ &= t^2 (1 + t^2 \mathcal{L})^{-1} \mathcal{L} t T_{\vec{D}}^* P_t F \\ &= t^2 L(1 + t^2 L)^{-1} Q_t F = (1 - (1 + t^2 L)^{-1}) Q_t F. \end{aligned}$$

By  $m$ -accretivity, the resolvents  $(1 + t^2 L)^{-1}$  are uniformly bounded, so we arrive at

$$\int_0^\infty \|\Theta_t (1 - P_t) F\|_2^2 \frac{dt}{t} \lesssim \int_0^\infty \|Q_t F\|_2^2 \frac{dt}{t} \lesssim \|F\|_2^2,$$

where the last step follows from the quadratic estimate for  $Q_t$  from Lemma 7.5.  $\square$

### 7.2. Reduction to finite time

We want to approximate the first term in (12) by the principal part. However, since the dyadic structure on  $\mathcal{O}$  and hence the approximation  $\gamma_t, \mathcal{A}_t$  only exist on small scales, the integral for  $t \geq 1$  has to be treated separately.

**Proposition 7.7.** *It holds*

$$\int_1^\infty \left\| \Theta_t P_t T_{\vec{D}} u \right\|_2^2 \frac{dt}{t} \lesssim \left\| T_{\vec{D}} u \right\|_2^2, \quad u \in \mathbb{W}_{\vec{D}}^{1,2}(\mathcal{O}).$$

*Proof.* Denote by  $H_\alpha$  the complex interpolation space  $[L^2(\mathcal{O})^m, \mathbb{W}_{\vec{D}}^{1,2}(\mathcal{O})]_\alpha$ . Since  $\Theta_t$  is uniformly bounded in  $\mathcal{L}(L^2(\mathcal{O})^N, L^2(\mathcal{O})^m)$  and  $H^\alpha \hookrightarrow L^2(\mathcal{O})^m$ , we have

$$\left\| \Theta_t P_t T_{\vec{D}} u \right\|_2 \lesssim \left\| P_t T_{\vec{D}} u \right\|_2 \lesssim \left\| P_t T_{\vec{D}} u \right\|_{H_\alpha}.$$

Recall from (11) the commuting relation  $P_t T_{\vec{D}} u = T_{\vec{D}} (1 + t^2(-\Delta_{\vec{D}} + 1))^{-1} u$ . Since the resolvent  $(1 + t^2(-\Delta_{\vec{D}} + 1))^{-1}$  maps into  $D(-\Delta_{\vec{D}} + 1)$ , we can use Proposition 5.1 in conjunction with the square root property of  $-\Delta_{\vec{D}} + 1$  and the intertwining property from Proposition 3.10 with the  $H^\infty$ -function  $f(z) = \frac{z^\alpha}{1+t^2z}$  to obtain

$$\begin{aligned} \left\| P_t T_{\vec{D}} u \right\|_{H_\alpha} &= \left\| T_{\vec{D}} (1 + t^2(-\Delta_{\vec{D}} + 1))^{-1} u \right\|_{H_\alpha} \\ &\lesssim \left\| (-\Delta_{\vec{D}} + 1)^{\frac{1+\alpha}{2}} (1 + t^2(-\Delta_{\vec{D}} + 1))^{-1} u \right\|_2 \\ &= \left\| T_{\vec{D}} (-\Delta_{\vec{D}} + 1)^{\frac{\alpha}{2}} (1 + t^2(-\Delta_{\vec{D}} + 1))^{-1} u \right\|_2 \\ &= \left\| (M_{\vec{D}})^{\frac{\alpha}{2}} P_t T_{\vec{D}} u \right\|_2. \end{aligned}$$

We can then estimate  $1 \leq t^{2\alpha}$  to obtain a square function estimate for  $M_{\vec{D}}$  with  $f(z) = z^{\alpha/2}(1+z)^{-1}$ , which reads

$$\begin{aligned} \int_1^\infty \left\| \Theta_t P_t T_{\vec{D}} u \right\|_2^2 \frac{dt}{t} &\lesssim \int_1^\infty t^{2\alpha} \left\| (M_{\vec{D}})^{\frac{\alpha}{2}} (1 + t^2 M_{\vec{D}})^{-1} T_{\vec{D}} u \right\|_2^2 \frac{dt}{t} \\ &= \int_1^\infty \left\| f(t^2 M_{\vec{D}}) T_{\vec{D}} u \right\|_2^2 \frac{dt}{t} \lesssim \left\| T_{\vec{D}} u \right\|_2^2, \end{aligned}$$

where we used Proposition 3.9 in the final step. □

### 7.3. Smoothed principal part approximation

As the next step, we want to approximate  $\Theta_t P_t T_{\vec{D}}$  by the smoothed principle part  $\gamma_t \mathcal{A}_t P_t T_{\vec{D}}$ . This will be the content of Proposition 7.10. As a preparation, we establish the following lemma first. To this end, recall from Remark 7.2 the (pointwise) matrix action of  $\gamma_t$ .

**Lemma 7.8.** *The family  $\gamma_t \mathcal{A}_t$  is uniformly bounded in  $\mathcal{L}(L^2(\mathcal{O})^N)$  for  $t \in (0, 1]$ . Moreover, for  $F = [F_0, \dots, F_n] \in \mathbb{W}_{\vec{D}}^{1,2}(\mathcal{O})^{n+1}$ , there holds*

$$\left\| (\Theta_t - \gamma_t \mathcal{A}_t) F \right\|_2 \lesssim t \left\| T_{\vec{D}} F \right\|_2, \quad t \in (0, 1].$$

*Proof.* Fix  $t \in (0, 1]$  and the natural number  $k$  for which  $t \in (2^{-(k+1)}, 2^{-k}]$ . First, we work on a fixed  $Q \in \square_t$ . By utilizing Proposition 4.1 (4), there exist constants  $a_0, a_1 > 0$  and  $z \in \mathcal{O}$  such that

$$Q(z, a_0 2^{-k}) \cap \mathcal{O} \subseteq Q \subseteq Q(z, a_1 2^{-k}) \cap \mathcal{O}. \tag{13}$$

Let  $Q_* := Q(z, a_0 2^{-k})$  and  $Q^* := Q(z, a_1 2^{-k})$ . Then, the left-hand side of (13) becomes  $Q_* \cap \mathcal{O}$  and the right-hand side  $Q^* \cap \mathcal{O}$ . Owing to interior thickness of  $\mathcal{O}$ , there holds

$$|Q| \gtrsim |Q_*|. \tag{14}$$

For a bounded set  $K \subseteq \mathcal{O}$  and  $b \in L^\infty(\mathcal{O})^N$ , the limit  $\Theta_t b := \lim_{k \rightarrow \infty} \Theta_t(\mathbf{1}_{2^k Q_* \cap \mathcal{O}} b)$  exists in  $L^2(K)^N$  and is independent of  $Q^*$ . Indeed, this is a consequence of the off-diagonal estimates of  $\Theta_t$ , see, for instance, [20, Prop. 11.12]. We have already employed the same construction when defining the principal part in Definition 7.1. Now, we define *annuli* of a “cube”  $Q$  by

$$C_1(Q) := 4Q^* \cap \mathcal{O}, \quad C_\ell(Q) := (2^{\ell+1} Q^* \setminus 2^\ell Q^*) \cap \mathcal{O},$$

where  $\ell \geq 2$ . Using this notation in the definition of  $\Theta_t b$  yields

$$\gamma_t \mathcal{A}_t F = \lim_{k \rightarrow \infty} \Theta_t(\mathbf{1}_{2^k Q_* \cap \mathcal{O}}(F)_Q) = \lim_{k \rightarrow \infty} \sum_{\ell=1}^{k-1} \Theta_t(\mathbf{1}_{C_\ell(Q)}(F)_Q) = \sum_{\ell=1}^{\infty} \Theta_t(\mathbf{1}_{C_\ell(Q)}(F)_Q).$$

Now, note for  $\ell \geq 2$  that

$$\frac{d(C_\ell(Q), Q)}{t} \geq \frac{d(C_\ell(Q), Q^*)}{t} \gtrsim 2^\ell.$$

Both of the above, in conjunction with Lemma 6.2, allow us to see that

$$\begin{aligned} \|\mathbf{1}_Q(\gamma_t \mathcal{A}_t F)\|_2 &\leq \sum_{\ell=1}^{\infty} \|\mathbf{1}_Q \Theta_t(\mathbf{1}_{C_\ell(Q)}(F)_Q)\|_2 \\ &\lesssim \sum_{\ell=1}^{\infty} e^{-c2^\ell} \|\mathbf{1}_{C_\ell(Q)}(F)_Q\|_2. \end{aligned}$$

By Hölder’s inequality and (14), we have

$$\|\mathbf{1}_{C_\ell(Q)}(F)_Q\|_2 = \frac{|C_\ell(Q)|^{\frac{1}{2}}}{|Q|} \left| \int_Q F(y) \, dy \right| \leq \left( \frac{|C_\ell(Q)|}{|Q|} \right)^{\frac{1}{2}} \|\mathbf{1}_Q F\|_2 \lesssim 2^{\frac{\ell n}{2}} \|\mathbf{1}_Q F\|_2,$$

which gives us

$$\|\mathbf{1}_Q(\gamma_t \mathcal{A}_t F)\|_2 \lesssim \left( \sum_{\ell=1}^{\infty} 2^{\frac{\ell n}{2}} e^{-c2^\ell} \right) \|\mathbf{1}_Q F\|_2 \lesssim \|\mathbf{1}_Q F\|_2.$$

Since the implicit constant is independent of  $Q$  and  $t$ , squaring the last bound and summing in  $Q$  yield the first assertion. Now, we can proceed with the second assertion. Since  $\Theta_t$  is bounded on  $L^2(\mathbf{O})^N$ , we have

$$\Theta_t F = \sum_{\ell=1}^{\infty} \Theta_t (\mathbf{1}_{C_\ell(Q)} F).$$

Taking the difference with  $\gamma_t \mathcal{A}_t F$  and again applying off-diagonal estimates, we have

$$\begin{aligned} \|\mathbf{1}_Q (\Theta_t - \gamma_t \mathcal{A}_t) F\|_2 &\leq \sum_{\ell=1}^{\infty} \|\mathbf{1}_Q \Theta_t (\mathbf{1}_{C_\ell(Q)} (F - (F)_Q))\|_2 \\ &\lesssim \sum_{\ell=1}^{\infty} e^{-c2^\ell} \|\mathbf{1}_{2^{\ell+1} Q^* \cap \mathbf{O}} (F - (F)_Q)\|_2. \end{aligned} \tag{15}$$

Now, we distinguish whether  $2^\ell t$  is small or large. More precisely, there is a natural number  $\ell_0$  such that the local Poincaré inequality from Remark 2.12 is applicable on  $2^\ell Q^* \cap \mathbf{O}$  if  $\ell \leq \ell_0$  (note that we tacitly use comparability between balls and “cubes” here). To the contrary, if  $\ell > \ell_0$ , we deduce that  $2^\ell t \geq \kappa$ , where  $\kappa$  is a constant depending on the geometry. In the first case, fix  $\ell \leq \ell_0$  and deduce by virtue of the local Poincaré inequality (Remark 2.12) the estimate

$$\begin{aligned} \|\mathbf{1}_{2^{\ell+1} Q^* \cap \mathbf{O}} (F - (F)_Q)\|_2 &\lesssim \ell 2^{n\ell/2} 2^\ell t \|\nabla F\|_{L^2(c2^{\ell+1} Q^* \cap \mathbf{O})} \\ &\leq \ell 2^{n\ell/2} 2^\ell t \|T_{\vec{D}} F\|_{L^2(c2^{\ell+1} Q^* \cap \mathbf{O})}. \end{aligned}$$

In the second case, for fixed  $\ell > \ell_0$ , estimate using Jensen’s inequality

$$\|\mathbf{1}_{2^{\ell+1} Q^* \cap \mathbf{O}} (F - (F)_Q)\|_2 \lesssim 2^{n\ell/2} \|F\|_{L^2(2^{\ell+1} Q^* \cap \mathbf{O})} \lesssim 2^{n\ell/2} 2^\ell t \|T_{\vec{D}} F\|_{L^2(2^{\ell+1} Q^* \cap \mathbf{O})}.$$

Plugging the last two bounds back into (15) and using the double exponential decay, we obtain

$$\|\mathbf{1}_Q (\Theta_t - \gamma_t \mathcal{A}_t) F\|_2 \lesssim t \sum_{\ell=1}^{\infty} e^{-c2^\ell} \|T_{\vec{D}} F\|_{L^2(c2^{\ell+1} Q^* \cap \mathbf{O})}.$$

To conclude the proof, we have to sum the last bound over all dyadic “cubes” on scale  $t$ . Due to the rapid decay in  $\ell$ , this follows by standard arguments, see, for instance, [20, Lem. 13.6] for details. □

*Remark 7.9.* Instead of using a local Poincaré inequality on small scales, there is another approach to obtain the aforementioned result in the literature based on a weighted (global) Poincaré inequality, see [22, Prop. 8.2]. For that approach, the existence of an (inhomogeneous) Sobolev extension operator is necessary. Even though our local Poincaré inequality was deduced by using a local and homogeneous Sobolev extension operator, there might be other settings in which local Poincaré inequalities are easier to obtain than a Sobolev extension operator.

**Proposition 7.10.** *There holds the quadratic estimate*

$$\int_0^1 \left\| (\Theta_t - \gamma_t \mathcal{A}_t) P_t T_{\vec{D}} u \right\|_2^2 \frac{dt}{t} \lesssim \left\| T_{\vec{D}} u \right\|_2^2, \quad u \in \mathbb{W}_{\vec{D}}^{1,2}(\mathbf{O}).$$

*Proof.* On the one hand,  $\Theta_t - \gamma_t \mathcal{A}_t$  is uniformly bounded in  $\mathcal{L}(L^2(\mathcal{O})^N, L^2(\mathcal{O})^m)$ , see Lemmas 6.2 and 7.8. On the other hand, the  $\mathcal{L}(\mathbb{W}_{\vec{D}}^{1,2}(\mathcal{O})^{n+1}, L^2(\mathcal{O})^m)$ -norm of  $\Theta_t - \gamma_t \mathcal{A}_t$  is controlled by  $t$  by virtue of Lemma 7.8. By interpolation, we obtain boundedness

$$\Theta_t - \gamma_t \mathcal{A}_t : (H_\alpha)^{n+1} \rightarrow L^2(\mathcal{O})^m, \quad \|\Theta_t - \gamma_t \mathcal{A}_t\|_{H_\alpha \rightarrow L^2(\mathcal{O})} \lesssim t^\alpha,$$

where  $H_\alpha$  denotes again the interpolation space  $[L^2(\mathcal{O})^m, \mathbb{W}_{\vec{D}}^{1,2}(\mathcal{O})]_\alpha$ . Therefore, in conjunction with the intertwining property and Proposition 5.1 (compare with the calculation in the proof of Proposition 7.7), we obtain that

$$\left\| (\Theta_t - \gamma_t \mathcal{A}_t) P_t T_{\vec{D}} u \right\|_2 \lesssim t^\alpha \left\| P_t T_{\vec{D}} u \right\|_{H_\alpha} \lesssim t^\alpha \| (M_{\vec{D}})^{\frac{\alpha}{2}} P_t T_{\vec{D}} u \|_2.$$

With the  $H^\infty$ -function  $f : z \mapsto z^{\alpha/2}(1+z)^{-1}$ , quadratic estimates for  $M_{\vec{D}}$  give

$$\int_0^1 \left\| (\Theta_t - \gamma_t \mathcal{A}_t) P_t T_{\vec{D}} u \right\|_2^2 \frac{dt}{t} \lesssim \int_0^1 \| f(t^2 M_{\vec{D}}) T_{\vec{D}} u \|_2^2 \frac{dt}{t} \lesssim \left\| T_{\vec{D}} u \right\|_2^2.$$

□

#### 7.4. Reduction to a Carleson measure estimate

So far, we have reduced (QE) to the quadratic estimate

$$\int_0^1 \left\| \gamma_t \mathcal{A}_t P_t T_{\vec{D}} u \right\|_2^2 \frac{dt}{t} \lesssim \left\| T_{\vec{D}} u \right\|_2^2, \quad u \in \mathbb{W}_{\vec{D}}^{1,2}(\mathcal{O}).$$

To eliminate the smoothing via the resolvents  $P_t$  and to reduce this to a Carleson measure estimate, we split again

$$\int_0^1 \left\| \gamma_t \mathcal{A}_t P_t T_{\vec{D}} u \right\|_2^2 \frac{dt}{t} \lesssim \int_0^1 \left\| \gamma_t \mathcal{A}_t (P_t - 1) T_{\vec{D}} u \right\|_2^2 \frac{dt}{t} + \int_0^1 \left\| \gamma_t \mathcal{A}_t T_{\vec{D}} u \right\|_2^2 \frac{dt}{t}. \tag{16}$$

The second term can be dominated by

$$\int_0^1 \int_{\mathbb{R}^d} \left| \gamma_t(x) (\mathcal{A}_t T_{\vec{D}} u)(x) \right|^2 \frac{dx dt}{t} \leq \int_0^1 \int_{\mathbb{R}^d} \left| (\mathcal{A}_t T_{\vec{D}} u)(x) \right|^2 \|\gamma_t(x)\|^2 \frac{dx dt}{t},$$

where  $\|\gamma_t(x)\|$  denotes the operator norm of  $\gamma_t(x) \in \mathcal{L}(\mathbb{C}^N, \mathbb{C}^m)$ . By Proposition 4.8, this integral is controlled by  $\|T_{\vec{D}} u\|_2^2$ , provided  $d\sigma = \|\gamma_t\|^2 \frac{dx dt}{t}$  is a Carleson measure, which we are going to prove in Sect. 8. To treat the first term on the right-hand side of (16), we need the following interpolation inequality, which is useful again in Sect. 8.

Recall the notation  $Tu = [u, \nabla u]^t$  for  $u \in \mathbb{W}^{1,2}(\mathcal{O})$ . Later, we apply the subsequent results with  $u \in \mathbb{W}_{\vec{D}}^{1,2}(\mathcal{O})$ , so that  $Tu = T_{\vec{D}}u$  as usual.

**Lemma 7.11** (Interpolation inequality). *Let  $\eta$  be as in Proposition 4.1. We have the bound*

$$\left| \int_Q \nabla u \right|^2 \lesssim \frac{1}{t^\eta} \left( \int_Q |u|^2 \right)^{\frac{\eta}{2}} \left( \int_Q |\nabla u|^2 \right)^{1-\frac{\eta}{2}}$$

for all  $t \in (0, 1]$ ,  $Q \in \square_t$  and  $u \in \mathbb{W}^{1,2}(\mathbf{O})$ .

*Proof.* Fix  $t \in (0, 1]$ ,  $Q \in \square_t$  and  $u \in \mathbb{W}^{1,2}(\mathbf{O})$ . Write the estimate above as

$$X \lesssim t^{-\eta} Y^{\eta/2} Z^{1-\eta/2}.$$

First, observe that  $X \leq Z$  by Jensen’s inequality and that  $Y = 0$  implies  $Z = 0$ . Thus, we can safely assume  $Y, Z > 0$ . Put  $\tau := Y^{1/2} Z^{-1/2} > 0$  and note that, for  $\tau \geq t$ , we have

$$X \leq Z \leq \tau^\eta t^{-\eta} Z = t^{-\eta} Y^{\eta/2} Z^{1-\eta/2}.$$

Hence, we can suppose  $\tau < t$ , which circumvents awkward cases. Let  $Q_r = \{x \in Q : d(x, \mathbb{R}^n \setminus Q) \leq r\}$  for  $r > 0$ , and note that, by Proposition 4.1 (5), we have the estimate

$$|Q_r| \leq Cr^\eta \ell(Q)^{-\eta} |Q| \leq Cr^\eta t^{-\eta} |Q|. \tag{17}$$

Convolve  $\mathbf{1}_{Q \setminus Q_{\tau/2}}$  by a suitable kernel to obtain  $\varphi \in C_c^\infty(Q)$  with range in  $[0, 1]$ , equal to 1 on  $Q \setminus Q_\tau$  and satisfying  $\|\nabla \varphi\|_\infty \leq \frac{c}{\tau}$  for  $c > 0$  depending only on  $n$ . Now, write

$$\nabla u = \varphi \nabla u + (1 - \varphi) \nabla u,$$

and apply integration by parts (here, we use that  $\varphi$  is compactly supported in  $Q$ ) to see that

$$\int_Q \nabla u = - \int_Q u \nabla \varphi + \int_Q (1 - \varphi) \nabla u.$$

From here, apply the inequality  $(x + y)^2 \leq 2(x^2 + y^2)$  as well as Hölder’s inequality, noting that both  $\nabla \varphi$  and  $1 - \varphi$  vanish on  $Q \setminus Q_\tau$  and using (17), to achieve

$$\begin{aligned} \left| \int_Q \nabla u \right|^2 &\leq 2 \left( \int_Q \mathbf{1}_{Q_\tau} |\nabla \varphi|^2 \right) \left( \int_Q |u|^2 \right) + 2 \left( \int_Q \mathbf{1}_{Q_\tau} |1 - \varphi|^2 \right) \left( \int_Q |\nabla u|^2 \right) \\ &\lesssim |Q_\tau| \left( \tau^{-2} \int_Q |u|^2 + \int_Q |\nabla u|^2 \right) \\ &\lesssim \tau^\eta t^{-\eta} |Q| \left( \tau^{-2} \int_Q |u|^2 + \int_Q |\nabla u|^2 \right). \end{aligned}$$

Translating back in terms of  $X, Y$  and  $Z$ , the above says

$$\begin{aligned} |Q|^2 X &\lesssim \tau^{\eta-2} t^{-\eta} |Q|^2 Y + \tau^\eta t^{-\eta} |Q|^2 Z \\ &= 2 |Q|^2 t^{-\eta} Y^{\eta/2} Z^{1-\eta/2}. \end{aligned}$$

Now, the claim follows when dividing the last inequality by  $|Q|^2$ . □

The following inhomogeneous version of Lemma 7.11 is an easy consequence.

**Corollary 7.12.** *With  $\eta$  as in Proposition 4.1, we have*

$$\left| \int_Q Tu \right|^2 \lesssim \frac{1}{t^\eta} \left( \int_Q |u|^2 \right)^{\frac{\eta}{2}} \left( \int_Q |Tu|^2 \right)^{1-\eta/2}$$

for all  $t \in (0, 1]$ ,  $Q \in \square_t$  and  $u \in \mathbb{W}^{1,2}(\mathcal{O})$ .

*Proof.* We use Jensen’s inequality, Lemma 7.11,  $t \leq 1$  and  $a^{1-\eta/2} + b^{1-\eta/2} \leq 2(a + b)^{1-\eta/2}$  for  $a, b > 0$ , to estimate

$$\begin{aligned} \left| \int_Q Tu \right|^2 &= \left| \int_Q u \right|^2 + \left| \int_Q \nabla u \right|^2 \\ &\lesssim \int_Q |u|^2 + \frac{1}{t^\eta} \left( \int_Q |u|^2 \right)^{\frac{\eta}{2}} \left( \int_Q |\nabla u|^2 \right)^{1-\frac{\eta}{2}} \\ &\lesssim \frac{1}{t^\eta} \left( \int_Q |u|^2 \right)^{\frac{\eta}{2}} \left( \left( \int_Q |u|^2 \right)^{1-\frac{\eta}{2}} + \left( \int_Q |\nabla u|^2 \right)^{1-\frac{\eta}{2}} \right) \\ &\lesssim \frac{1}{t^\eta} \left( \int_Q |u|^2 \right)^{\frac{\eta}{2}} \left( \int_Q |Tu|^2 \right)^{1-\frac{\eta}{2}}. \end{aligned}$$

□

We can now control the first term on the right-hand side of (16).

**Proposition 7.13.** *There holds the square function estimate*

$$\int_0^1 \left\| \gamma_t \mathcal{A}_t (1 - P_t) T_{\vec{D}} u \right\|_2^2 \frac{dt}{t} \lesssim \left\| T_{\vec{D}} u \right\|_2^2, \quad u \in \mathbb{W}_{\vec{D}}^{1,2}(\mathcal{O}).$$

*Proof.* Recall from Proposition 4.7 that the averaging operator  $\mathcal{A}_t$  is a projection, that is,  $\mathcal{A}_t^2 = \mathcal{A}_t$ . By the uniform boundedness of  $\gamma_t \mathcal{A}_t$  from Lemma 7.8, we have

$$\left\| \gamma_t \mathcal{A}_t (1 - P_t) T_{\vec{D}} u \right\|_2 = \left\| (\gamma_t \mathcal{A}_t) \mathcal{A}_t (1 - P_t) T_{\vec{D}} u \right\|_2 \lesssim \left\| \mathcal{A}_t (1 - P_t) T_{\vec{D}} u \right\|_2.$$

So, we are left to prove

$$\int_0^1 \left\| \mathcal{A}_t (1 - P_t) T_{\vec{D}} u \right\|_2^2 \frac{dt}{t} \lesssim \left\| T_{\vec{D}} u \right\|_2^2.$$

To establish this estimate, let us assume for the moment that there is a non-negative function  $\zeta \in L^1((0, \infty), d\tau/\tau)$  such that for all  $s \in (0, 1], t > 0$ , we have the bound

$$\left\| \mathcal{A}_s (1 - P_s) \mathcal{Q}_t^* v \right\|_2 \lesssim \zeta(s/t) \|v\|_2, \quad v = T_{\vec{D}}^* F \text{ for some } F \in D(M_{\vec{D}}), \quad (18)$$

uniformly in  $v$ . Since  $\mathcal{A}_s (1 - P_s)$  is a bounded operator on  $L^2(\mathcal{O})^N$ , the Calderón reproducing formula in Lemma 7.5 with  $F = T_{\vec{D}} u$  gives

$$\mathcal{A}_s (1 - P_s) T_{\vec{D}} u = 2 \int_0^\infty \mathcal{A}_s (1 - P_s) \mathcal{Q}_t^* \mathcal{Q}_t T_{\vec{D}} u \frac{dt}{t}.$$

Hence, as  $v := \mathcal{Q}_t T_{\vec{D}} u = t T_{\vec{D}}^* (1 + t^2 M_{\vec{D}})^{-1} T_{\vec{D}} u$  is admissible for (18), Young’s convolution inequality with indices  $1 + \frac{1}{2} = \frac{1}{1} + \frac{1}{2}$  on the multiplicative group  $(0, \infty)$  with measure  $\frac{dt}{t}$  gives

$$\begin{aligned} \int_0^1 \|\mathcal{A}_s(1 - P_s)T_{\vec{D}}u\|_2^2 \frac{ds}{s} &\lesssim \int_0^1 \left( \int_0^\infty \|\mathcal{A}_s(1 - P_s)\mathcal{Q}_t^* \mathcal{Q}_t T_{\vec{D}}u\|_2 \frac{dt}{t} \right)^2 \frac{ds}{s} \\ &\lesssim \int_0^\infty \left( \int_0^\infty \zeta(s/t) \|\mathcal{Q}_t T_{\vec{D}}u\|_2 \frac{dt}{t} \right)^2 \frac{ds}{s} \\ &\lesssim \left( \int_0^\infty \zeta(\tau) \frac{d\tau}{\tau} \right)^2 \int_0^\infty \|\mathcal{Q}_t T_{\vec{D}}u\|_2^2 \frac{dt}{t} \lesssim \|T_{\vec{D}}u\|_2^2, \end{aligned}$$

where the last step above follows from the quadratic estimate in Lemma 7.4.

We turn our attention to proving (18). By Definition 7.3, one readily checks the relations

$$P_s \mathcal{Q}_t^* = \frac{t}{s} P_t \mathcal{Q}_s^*, \quad (1 - P_s) \mathcal{Q}_t^* = \frac{s}{t} (1 - P_t) \mathcal{Q}_s^*.$$

Indeed, this is proved by commuting resolvents of  $M_{\vec{D}}$ . For instance, to see the second identity, calculate on the dense subset  $\mathbb{W}_{\vec{D}}^{1,2}(\mathcal{O})$  of  $L^2(\mathcal{O})^m$  that

$$\begin{aligned} (1 - P_s) \mathcal{Q}_t^* &= s^2 M_{\vec{D}} (1 + s^2 M_{\vec{D}})^{-1} t (1 + t^2 M_{\vec{D}})^{-1} T_{\vec{D}} \\ &= \frac{s}{t} t^2 M_{\vec{D}} (1 + t^2 M_{\vec{D}})^{-1} s (1 + s^2 M_{\vec{D}})^{-1} T_{\vec{D}} \\ &= \frac{s}{t} (1 - P_t) \mathcal{Q}_s^*. \end{aligned}$$

This identity extends to  $L^2(\mathcal{O})^m$  by continuity. Next, let  $F \in D(M_{\vec{D}})$  and  $v = T_{\vec{D}}^* F$ . For  $s \leq t$ , uniform  $L^2$ -bounds (see Proposition 4.7 and Lemma 7.4) give

$$\|\mathcal{A}_s(1 - P_s) \mathcal{Q}_t^* v\|_2 = \frac{s}{t} \|\mathcal{A}_s(1 - P_t) \mathcal{Q}_s^* v\|_2 \lesssim \frac{s}{t} \|v\|_2.$$

For  $t \leq s$ , we have

$$\|\mathcal{A}_s(1 - P_s) \mathcal{Q}_t^* v\|_2 \lesssim \|\mathcal{A}_s \mathcal{Q}_t^* v\|_2 + \|P_s \mathcal{Q}_t^* v\|_2 \lesssim \|\mathcal{A}_s \mathcal{Q}_t^* v\|_2 + \frac{t}{s} \|v\|_2.$$

So, we are left with estimating the first term on the right-hand side. Since  $F \in D(M_{\vec{D}})$ , we have  $v = T_{\vec{D}}^* F \in D(T_{\vec{D}})$ , so  $\mathcal{Q}_t^* v = t(1 + t^2 M_{\vec{D}})^{-1} T_{\vec{D}} v$ . Writing out the averaging operator at scale  $s$ , we have

$$\|\mathcal{A}_s \mathcal{Q}_t^* v\|_2^2 = \sum_{R \in \square_s} |R| \left| \int_R t P_t T_{\vec{D}} T_{\vec{D}}^* F \right|^2. \tag{19}$$

Combining  $T_{\vec{D}}$  and  $T_{\vec{D}}^*$  to  $M_{\vec{D}}$ , we can “commute”  $P_t M_{\vec{D}} \subseteq M_{\vec{D}} P_t$ , which yields

$$\left| \int_R t P_t T_{\vec{D}} T_{\vec{D}}^* F \right|^2 = \left| \int_R t M_{\vec{D}} P_t F \right|^2 = \left| \int_R t T_{\vec{D}} T_{\vec{D}}^* P_t F \right|^2.$$

Using Corollary 7.12 and Hölder’s inequality (in the sequence space  $\ell^2$ ), we can thus estimate the right-hand side of (19) by

$$\begin{aligned} & \frac{1}{s^\eta} \sum_{R \in \square_s} |R| \left( \int_R |t T_{\vec{D}}^* P_t F|^2 \right)^{\eta/2} \left( \int_R |t T_{\vec{D}} T_{\vec{D}}^* P_t F|^2 \right)^{1-\eta/2} \\ & \leq \frac{t^\eta}{s^\eta} \left( \sum_{R \in \square_s} \int_R |T_{\vec{D}}^* P_t F|^2 \right)^{\eta/2} \left( \sum_{R \in \square_s} \int_R |t T_{\vec{D}} T_{\vec{D}}^* P_t F|^2 \right)^{1-\eta/2} \\ & = \frac{t^\eta}{s^\eta} \|T_{\vec{D}}^* P_t F\|_2^\eta \|t M_{\vec{D}} P_t F\|_2^{2-\eta}. \end{aligned}$$

Now, since  $t M_{\vec{D}} P_t F = t P_t M_{\vec{D}} F = Q_t^* T_{\vec{D}}^* F = Q_t^* v$ , Lemma 7.4 gives  $\|t M_{\vec{D}} P_t F\|_2 \lesssim \|v\|_2$ . Similarly, the square root property for  $M_{\vec{D}}$  applied twice, the fact that  $F \in D(M_{\vec{D}}) \subseteq D(\sqrt{M_{\vec{D}}})$  and uniform boundedness of  $\{P_t\}_{t>0}$  give

$$\|T_{\vec{D}}^* P_t F\|_2 = \|\sqrt{M_{\vec{D}}} P_t F\|_2 = \|P_t \sqrt{M_{\vec{D}}} F\|_2 \lesssim \|\sqrt{M_{\vec{D}}} F\|_2 = \|T_{\vec{D}}^* F\|_2 = \|v\|_2.$$

Putting things together, we arrive at (18) with  $\zeta(\tau) = \min\{\tau, \tau^{-1} + \tau^{-\eta}\}$ , which belongs to  $L^1((0, \infty), d\tau/\tau)$ . □

### 7.5. Full principal part approximation

Let us summarize the different estimates of the previous sections in a single result for future reference.

**Proposition 7.14.** *There holds the quadratic estimate for the principal part approximation*

$$\int_0^1 \left\| (\Theta_t - \gamma_t \mathcal{A}_t) T_{\vec{D}} u \right\|_2^2 \frac{dt}{t} \lesssim \|T_{\vec{D}} u\|_2^2, \quad u \in \mathbb{W}_{\vec{D}}^{1,2}(\mathcal{O}).$$

*Proof.* Write

$$\Theta_t - \gamma_t \mathcal{A}_t = (\Theta_t - \gamma_t \mathcal{A}_t) P_t + \Theta_t(1 - P_t) - \gamma_t \mathcal{A}_t(1 - P_t).$$

Each term is treated separately in Propositions 7.6, 7.10 and 7.13, respectively. □

## 8. Carleson measure estimate and a first conclusion

In Sect. 7, we have reduced the proof of the quadratic estimate (QE) (and hence of the Kato square root conjecture on the interior thick set  $\mathcal{O}$ ) to proving that the measure  $\|\gamma_t(x)\|^2 \frac{dx dt}{t}$  is a Carleson measure on  $(0, 1] \times \mathcal{O}$ , that is,

$$\iint_{R(Q)} \|\gamma_t(x)\|^2 \frac{dx dt}{t} \lesssim |Q|, \quad Q \in \square. \tag{20}$$

Here,  $R(Q)$  denotes the Carleson box over  $Q$  and is given by  $R(Q) = (0, \ell(Q)] \times Q \subseteq (0, 1] \times \mathcal{O}$ . The estimate (20) follows from the subsequent lemma, whose proof amounts to covering the unit sphere in  $\mathbb{C}^{m \times N}$  by finitely many sectors.

**Lemma 8.1.** *Suppose that there is an  $\varepsilon > 0$  such that, for each “sector”*

$$\Gamma_v^\varepsilon = \left\{ \mu \in \mathbb{C}^{m \times N} \setminus \{0\} : \left\| \frac{\mu}{\|\mu\|} - v \right\| \leq \varepsilon \right\}, \quad v \in \mathbb{C}^{m \times N}, \quad \|v\| = 1,$$

in  $\mathbb{C}^{m \times N}$ , there holds the estimate

$$\iint_{R(Q)} \|\gamma_t(x) \mathbf{1}_{\Gamma_v^\varepsilon}(\gamma_t(x))\|^2 \frac{dx dt}{t} \lesssim |Q|, \quad Q \in \square. \tag{21}$$

Then  $\|\gamma_t(x)\|^2 \frac{dx dt}{t}$  is a Carleson measure.

It remains to establish the bound (21).

### 8.1. Construction of Tb-type test functions

The proof of the key estimate (21) relies on a  $T(b)$ -argument and the construction of test functions adapted to a “cube”  $Q \in \square$  and a vector direction  $\xi = \xi_v \in \mathbb{C}^N$ . This vector direction  $\xi$  is related to a matrix direction  $v \in \mathbb{C}^{m \times N}$  appearing in the definition of the “sector”  $\Gamma_v^\varepsilon$ . Indeed, later on in Proposition 8.3, we will see that the vector direction  $\xi$  provides sufficient information to obtain an estimate for the matrix direction  $v$ .

**Proposition 8.2.** *There is a constant  $\varepsilon_0 \in (0, 1)$  such that, for all  $0 < \varepsilon < \varepsilon_0$ , all unit vectors  $\xi \in \mathbb{C}^N$  and each dyadic “cube”  $Q \in \square$ , we can find a “ $T(b)$ -type test function”  $b = b^{\xi, Q, \varepsilon} \in L^2(\mathbf{O})^N$  with the following properties:*

- (a)  $\|b^{\xi, Q, \varepsilon}\|^2 \lesssim |Q|$ ,
- (b)  $\operatorname{Re}(\xi \cdot f_Q b^{\xi, Q, \varepsilon}) \geq 1$ ,
- (c)  $\iint_{R(Q)} |\gamma_t(x) \mathcal{A}_t b^{\xi, Q, \varepsilon}(x)|^2 \frac{dx dt}{t} \lesssim |Q|/\varepsilon^2$ .

*Proof.* Fix a unit vector  $\xi \in \mathbb{C}^N$  and  $Q \in \square$ , and denote by  $\ell = \ell(Q)$  the “sidelength” of  $Q$ . For  $\varepsilon > 0$  subject to further constraints below, define

$$b := b^{\xi, Q, \varepsilon} := 2(1 + \varepsilon^2 \ell^2 M_{\vec{D}} \mathbf{B})^{-1} (\mathbf{1}_{2Q} \bar{\xi}), \tag{22}$$

where the set  $2Q$  was defined in Sect. 4. Recall also the bound  $|2Q| \lesssim |Q|$  from that section. Owing to Lemma 3.13,  $M_{\vec{D}} \mathbf{B}$  is sectorial, and hence  $b$  is well defined. We are going to verify that, upon choosing  $\varepsilon \in (0, 1)$  sufficiently small,  $b$  satisfies the three properties listed above. Write  $\tau = \varepsilon \ell$  for brevity.

**Proof of (a):** Since  $M_{\vec{D}} \mathbf{B}$  is sectorial, the resolvents  $(1 + \tau^2 M_{\vec{D}} \mathbf{B})^{-1}$  are uniformly bounded in  $\mathcal{L}(L^2(\mathbf{O})^N)$ , so we have

$$\|b\|_2 = 2\|(1 + \tau^2 M_{\vec{D}} \mathbf{B})^{-1} \mathbf{1}_{2Q} \bar{\xi}\|_2 \lesssim \|\mathbf{1}_{2Q} \bar{\xi}\|_2 \lesssim |Q|^{\frac{1}{2}}.$$

**Proof of (b)** The underlying heuristic of (b) is that the average of  $b$  over  $Q$  points roughly in the direction  $\bar{\xi}$ . To exploit this, we estimate the difference

$$\frac{1}{2}b - \mathbf{1}_{2Q} \bar{\xi} = -\tau^2 M_{\vec{D}} \mathbf{B} (1 + \tau^2 M_{\vec{D}} \mathbf{B})^{-1} \mathbf{1}_{2Q} \bar{\xi} = \tau^2 T_{\vec{D}} v, \tag{23}$$

where  $v := -T_{\vec{D}}^* \mathbf{B}(1 + \tau^2 M_{\vec{D}} \mathbf{B})^{-1} \mathbf{1}_{2Q} \bar{\xi}$ , with the hope that this difference becomes small in the end. Since this difference is a “gradient field”, Corollary 7.12 yields

$$\begin{aligned} \left| \int_Q T_{\vec{D}} v \right|^2 &\lesssim \frac{1}{\ell^\eta} \left( \int_Q |v|^2 \right)^{\frac{\eta}{2}} \left( \int_Q |T_{\vec{D}} v|^2 \right)^{1-\frac{\eta}{2}} \\ &\leq \frac{1}{\ell^\eta} \frac{1}{|Q|} \|v\|_2^\eta \|T_{\vec{D}} v\|_2^{2-\eta}. \end{aligned}$$

By (23) and (a), we have

$$\left\| T_{\vec{D}} v \right\|_2 = \tau^{-2} \left\| \frac{1}{2} b - \mathbf{1}_{2Q} \bar{\xi} \right\|_2 \lesssim \tau^{-2} |Q|^{1/2}.$$

Similarly, by the uniform boundedness from Lemma 3.13 and the doubling property for dyadic “cubes”, we can control

$$\|v\|_2 = \|T_{\vec{D}}^* \mathbf{B}(1 + \tau^2 M_{\vec{D}} \mathbf{B})^{-1} \mathbf{1}_{2Q} \bar{\xi}\|_2 \lesssim \tau^{-1} \|\mathbf{1}_{2Q} \bar{\xi}\|_2 \approx \tau^{-1} |Q|^{\frac{1}{2}}.$$

Collecting the powers, we arrive at

$$\left| \int_Q \frac{1}{2} b - \mathbf{1}_{2Q} \bar{\xi} \right|^2 = \tau^4 \left| \int_Q T_{\vec{D}} v \right|^2 \lesssim \frac{\tau^{4-\eta-4+2\eta}}{\ell^\eta} = \varepsilon^\eta.$$

Write  $C^2$  for the implicit constant in the preceding bound. Now, assertion (b) follows from

$$\operatorname{Re} \left( \xi \cdot \int_Q b \right) = 2 + 2 \operatorname{Re} \left( \xi \cdot \int_Q \frac{1}{2} b - \mathbf{1}_{2Q} \bar{\xi} \right) \geq 2 - 2C\varepsilon^{\frac{\eta}{2}},$$

if we choose  $\varepsilon$  small enough so that  $2C\varepsilon^{\eta/2} \leq 1$ .

**Proof of (c)** Our choice of  $T(b)$ -type test function  $b$  is not in the range of  $T_{\vec{D}}$ , so we cannot directly apply the principal part approximation estimate from Proposition 7.14 to it. However, recalling (23), we split the integral as follows

$$\begin{aligned} \iint_{R(Q)} |\gamma_t(x)(\mathcal{A}_t b)(x)|^2 \frac{dx dt}{t} &\lesssim \iint_{R(Q)} |(\gamma_t \mathcal{A}_t - \Theta_t) b|^2 + |\Theta_t b|^2 \frac{dx dt}{t} \\ &\lesssim \iint_{R(Q)} \left| (\gamma_t \mathcal{A}_t - \Theta_t) \left( \frac{1}{2} b - \mathbf{1}_{2Q} \bar{\xi} \right) \right|^2 + |(\gamma_t \mathcal{A}_t - \Theta_t) \mathbf{1}_{2Q} \bar{\xi}|^2 + |\Theta_t b|^2 \frac{dx dt}{t} \\ &=: I + II + III. \end{aligned}$$

Since  $\frac{1}{2} b - \mathbf{1}_{2Q} \bar{\xi}$  is in the range of  $T_{\vec{D}}$ , Proposition 7.14 and property (a) above control the first term as

$$I \lesssim \int_0^1 \|(\gamma_t \mathcal{A}_t - \Theta_t) (\frac{1}{2} b - \mathbf{1}_{2Q} \bar{\xi})\|_2^2 \frac{dt}{t} \lesssim \|b\|_2^2 + \|\mathbf{1}_{2Q} \bar{\xi}\|_2^2 \lesssim |Q|.$$

Since we have  $|Q| \lesssim |Q|/\varepsilon^2$ , this completes the treatment of the first term. The second term can be estimated via off-diagonal estimates and the definition of the principal part approximation, similar to the proof of Lemma 7.8. Recall that we seek to control

$$\int_0^\ell \|\mathbf{1}_Q (\gamma_t \mathcal{A}_t - \Theta_t) \mathbf{1}_{2Q} \bar{\xi}\|_2^2 \frac{dt}{t}.$$

On the “cube”  $Q$ ,  $\mathbf{1}_{2Q}\bar{\xi}$  is constant, so we have  $\mathcal{A}_t\mathbf{1}_{2Q}\bar{\xi}(x) = \bar{\xi}$  for almost every  $x \in Q$ . This yields  $\mathcal{Y}_t\mathcal{A}_t\mathbf{1}_{2Q}\bar{\xi} = \Theta_t\bar{\xi}$  on  $Q$ . With the notation from the proof of Lemma 7.8, this leads to

$$\mathbf{1}_Q(\mathcal{Y}_t\mathcal{A}_t - \Theta_t)\mathbf{1}_{2Q}\bar{\xi} = \mathbf{1}_Q\Theta_t(\bar{\xi} - \mathbf{1}_{2Q}\bar{\xi}) = \sum_{j \geq 1} \mathbf{1}_Q\Theta_t(\mathbf{1}_{C_j(Q)\setminus 2Q}\bar{\xi}), \tag{24}$$

where we split  $\mathbf{O}$  into truncated annuli  $C_j(Q)$ . Observe that, for  $j \geq 1$  and  $t \leq 1$ , we have

$$e^{-c\frac{2^j}{t}} = e^{-c\frac{2^{j-1}}{t}} e^{-c\frac{2^{j-1}}{t}} \leq e^{-c2^{j-1}} e^{-\frac{c}{t}}.$$

Then,  $L^2$  off-diagonal estimates (see Proposition 3.12) control the  $L^2(\mathbf{O})$ -norm of (24) by

$$\begin{aligned} \sum_{j \geq 1} e^{-c\frac{d(C_j(Q)\setminus 2Q, Q)}{t}} \|\mathbf{1}_{C_j(Q)\setminus 2Q}\bar{\xi}\|_2 &\lesssim \sum_{j \geq 1} e^{-c\frac{2^j}{t}} 2^{\frac{jn}{2}} |Q|^{1/2} \\ &\leq \left( \sum_{j \geq 1} e^{-c2^{j-1}} 2^{\frac{jn}{2}} \right) e^{-c/t} |Q|^{1/2} \\ &\lesssim t |Q|^{1/2}, \end{aligned}$$

where the last step follows from convergence of the series and estimating  $e^{-s} \lesssim \frac{1}{s}$  for  $s \geq 0$ . It follows that

$$\int_0^\ell \|\mathbf{1}_Q(\mathcal{Y}_t\mathcal{A}_t - \Theta_t)\mathbf{1}_{2Q}\bar{\xi}\|_2^2 \frac{dt}{t} \lesssim \int_0^1 t^2 |Q| \frac{dt}{t} \lesssim |Q|.$$

For the last term  $III$ , observe that resolvents of  $M_{\vec{D}}\mathbf{B}$  map into  $D(M_{\vec{D}}\mathbf{B}) \subseteq D(T_{\vec{D}}^*\mathbf{B})$ , so we have

$$\begin{aligned} \Theta_t b &= 2t(1 + t^2\mathcal{L})^{-1}T_{\vec{D}}^*\mathbf{B}(1 + \tau^2M_{\vec{D}}\mathbf{B})^{-1}\mathbf{1}_{2Q}\bar{\xi} \\ &= 2t(1 + t^2\mathcal{L})^{-1}T_{\vec{D}}^*\mathbf{B}(1 + \tau^2M_{\vec{D}}\mathbf{B})^{-1}\mathbf{1}_{2Q}\bar{\xi} \\ &= t(1 + t^2\mathcal{L})^{-1}T_{\vec{D}}^*\mathbf{B}b. \end{aligned}$$

By Lemma 3.13, we have  $\|T_{\vec{D}}^*\mathbf{B}b\|_2 \lesssim \tau^{-1}\|\mathbf{1}_{2Q}\bar{\xi}\|_2 \lesssim \tau^{-1}|Q|^{1/2}$ . Hence, uniform boundedness of the resolvents  $(1 + t^2\mathcal{L})^{-1}$  in  $\mathcal{L}(L^2(\mathbf{O})^m)$  gives

$$III \lesssim \varepsilon^{-2}\ell^{-2} \int_0^\ell t^2|Q| \frac{dt}{t} = \frac{|Q|}{\varepsilon^2}.$$

□

### 8.2. Stopping time argument

We can now exploit the dyadic structure on  $\mathbf{O}$  and the properties of the  $T(b)$ -test functions constructed in Proposition 8.2 to derive the key estimate (21). For this, fix

a matrix  $v \in \mathcal{L}(\mathbb{C}^N, \mathbb{C}^m)$  with  $\|v\| = 1$ . As the adjoint matrix  $v^* \in \mathcal{L}(\mathbb{C}^m, \mathbb{C}^N)$  also has norm 1, we find unit vectors  $\xi = \xi_v \in \mathbb{C}^N$  and  $\eta = \eta_v \in \mathbb{C}^m$  with  $\bar{\xi} = v^*\eta$ . To prove (21), the main point is to deduce from property (b) in Proposition 8.2 that  $\mathcal{A}_t b^{\xi, Q, \varepsilon}(x)$  points roughly in direction  $\bar{\xi}$ , so that  $\mu \mathcal{A}_t b^{\xi, Q, \varepsilon}(x)$  is not too small whenever  $\mu \in \Gamma_v^\varepsilon$ , at least for all  $x$  in a “substantial subset” of  $Q$ .

**Proposition 8.3.** *There is some  $\varepsilon \in (0, \varepsilon_0)$  and some  $\kappa > 0$  such that, for all matrices  $v \in \mathcal{L}(\mathbb{C}^m, \mathbb{C}^N)$  of unit norm and all  $Q \in \square$ , there exist pairwise disjoint dyadic children  $Q_j \subseteq Q$  such that for the sets*

$$E(Q) = Q \setminus \bigcup_j Q_j \subseteq Q, \quad E^*(Q) = R(Q) \setminus \bigcup_j R(Q_j), \quad (25)$$

there hold the following properties:

- (a)  $|E(Q)| \geq \kappa |Q|$ ,
- (b)  $|\mu(\mathcal{A}_t b^{\xi, Q, \varepsilon})(x)| \geq \frac{1}{2} \|\mu\|$  for all  $(x, t) \in E^*(Q)$  and  $\mu \in \Gamma_v^\varepsilon$ .

*Proof.* Having Proposition 8.2 at hand, we can follow the Euclidean proof (for instance in [20, Lem. 14.8]) almost verbatim. Hence, we are only going to present the necessary changes.

The selection of the dyadic children  $Q_j \subseteq Q$  and the proof of part (a) is completely analogous to the Euclidean case. Hence, we concentrate on (b). Let  $(x, t) \in E^*(Q)$  and  $\mu \in \Gamma_v^\varepsilon$ . For brevity, set  $v := (\mathcal{A}_t b^{\xi, Q, \varepsilon})(x) \in \mathbb{C}^N$ . As in the Euclidean case, the construction of  $E^*(Q)$  implies the bounds  $|v| \leq \frac{1}{4\varepsilon}$  and  $\text{Re}(\xi \cdot v) \geq \frac{3}{4}$ . Using the triangle inequality, the definition of  $\Gamma_v^\varepsilon$  and the upper bound for  $|v|$ , deduce

$$\left| \frac{\mu}{\|\mu\|} v \right| \geq |vv| - \left\| \frac{\mu}{\|\mu\|} - v \right\| |v| \geq |vv| - \varepsilon |v| \geq |vv| - \frac{1}{4}. \quad (26)$$

Next, by the Cauchy–Schwarz inequality in  $\mathbb{C}^m$  and the relation  $\bar{\xi} = v^*\eta$ , we obtain the lower bound

$$|vv| \geq \text{Re}\langle \eta, vv \rangle = \text{Re}\langle v^*\eta, v \rangle = \text{Re}\langle \bar{\xi}, v \rangle = \text{Re}(\xi \cdot v),$$

where the brackets denote the inner products in either  $\mathbb{C}^m$  or  $\mathbb{C}^N$ . Plugging this bound back into (26) and using the lower bound for  $\text{Re}(\xi \cdot v)$  deduce

$$\left| \frac{\mu}{\|\mu\|} v \right| \geq \text{Re}(\xi \cdot v) - \frac{1}{4} \geq \frac{1}{2}.$$

Multiplying this bound by  $\|\mu\|$  yields the claim. □

To conclude the proof of the key estimate (21), we cite the John–Nirenberg lemma for Carleson measures. The result is well known and a detailed proof using the dyadic “cubes” from Definition 4.2 is presented in [18, p. 191].

**Lemma 8.4** (John–Nirenberg lemma for Carleson measures). *Let  $\sigma$  be a Borel measure on  $\mathbf{O} \times (0, 1]$  such that there are  $K, \kappa > 0$  with the following property: Each dyadic “cube”  $Q \in \square$  has pairwise disjoint dyadic children  $Q_j \in \square$  such that the sets  $E(Q) \subseteq Q$  and  $E^*(Q)$  defined in (25) satisfy*

- (a)  $|E(Q)| \geq \kappa |Q|$ .
- (b)  $\sigma(E^*(Q)) \leq K |Q|$ .

Then  $\sigma$  is a Carleson measure with norm at most  $K/\kappa$ .

*Proof of the key estimate (21).* Fix a unit matrix  $v \in \mathcal{L}(\mathbb{C}^m, \mathbb{C}^N)$  and set  $\xi = \xi_v \in \mathbb{C}^N$ . By Propositions 8.3 (b) and 8.2 (c), we compute

$$\begin{aligned} \iint_{E^*(Q)} \left\| \boldsymbol{y}_t(x) \mathbf{1}_{\Gamma_v^\varepsilon}(\boldsymbol{y}_t(x)) \right\|^2 \frac{dx dt}{t} &\leq 4 \iint_{E^*(Q)} \left| \boldsymbol{y}_t(x) (\mathcal{A}_t b^{\xi, Q, \varepsilon})(x) \mathbf{1}_{\Gamma_v^\varepsilon}(\boldsymbol{y}_t(x)) \right|^2 \frac{dx dt}{t} \\ &\leq 4 \iint_{R(Q)} \left| \boldsymbol{y}_t(x) (\mathcal{A}_t b^{\xi, Q, \varepsilon})(x) \right|^2 \frac{dx dt}{t} \lesssim \frac{|Q|}{\varepsilon^2}. \end{aligned}$$

By Lemma 8.4, this and Proposition 8.3 (a) ensure that  $d\sigma = \|\boldsymbol{y}_t(x) \mathbf{1}_{\Gamma_v^\varepsilon}(\boldsymbol{y}_t(x))\|^2 \frac{dx dt}{t}$  is a Carleson measure, which yields the asserted estimate (21). □

We are now done with the proof of the quadratic estimate (QE), and hence of Theorem 1.1, under the additional assumption that  $\mathbf{O}$  is interior thick. To convince the reader, we give below a short proof summarizing the different reduction steps of our proof.

*Proof of Theorem 1.1 when  $\mathbf{O}$  is interior thick.* In Proposition 6.1, we have seen that the Kato square root property is equivalent to (QE). The integral on the left-hand side can be split as

$$\begin{aligned} \int_0^\infty \|\Theta_t T_{\vec{D}} u\|_2^2 \frac{dt}{t} &\lesssim \int_1^\infty \|\Theta_t (1 - P_t) T_{\vec{D}} u\|_2^2 \frac{dt}{t} + \int_1^\infty \|\Theta_t P_t T_{\vec{D}} u\|_2^2 \frac{dt}{t} \\ &\quad + \int_0^1 \|(\Theta_t - \boldsymbol{y}_t \mathcal{A}_t) T_{\vec{D}} u\|_2^2 \frac{dt}{t} + \int_0^1 \|\boldsymbol{y}_t \mathcal{A}_t T_{\vec{D}} u\|_2^2 \frac{dt}{t}. \end{aligned}$$

The first and second terms are controlled by Propositions 7.6 and 7.7, respectively, and the third one is estimated in Proposition 7.14. The last integral is bounded by

$$\int_0^1 \int_{\mathbf{O}} \left| (\mathcal{A}_t T_{\vec{D}} u)(x) \right|^2 \|\boldsymbol{y}_t(x)\|^2 \frac{dx dt}{t}.$$

By Proposition 4.8, it then suffices to prove that  $d\sigma = \|\boldsymbol{y}_t(x)\|^2 \frac{dx dt}{t}$  is a Carleson measure on  $\mathbf{O} \times (0, 1]$ , that is, the validity of (20). Splitting over angular sectors  $\Gamma_v^\varepsilon$  in  $\mathcal{L}(\mathbb{C}^m, \mathbb{C}^N)$  reduces this to finding an  $\varepsilon > 0$  such that (21) holds true for all (matrix) directions  $v \in \mathcal{L}(\mathbb{C}^m, \mathbb{C}^N)$ . The latter was accomplished right above via the usage of  $T(b)$ -type test functions and a stopping time argument. □

### 9. Removing the thickness condition

In this final section, we remove the interior thickness condition imposed in the approach performed throughout Sects. 6–8, thereby completing the proof of Theorem 1.1 in the general case. To do so, we employ the transference strategy pioneered in [15, Sec. 6]. If the Dirichlet parts were the same for all components, their argument would apply out of the box. For the reader’s convenience, and since we want to extend their result to varying Dirichlet parts for different components of the system, we recap their argument and comment on the necessary changes.

Let  $O \subseteq \mathbb{R}^n$  be open and  $D_j \subseteq \partial O$  be closed, and assume that  $O$  is locally uniform near  $\partial O \setminus D_j$  for every  $j = 1, \dots, m$ . Put  $\vec{D} := (D_j)_{j=1}^m$ . Now, fix a decomposition of  $O$  into pairwise disjoint open sets  $O_i$ . Define the array  $\vec{D}_i$  via  $(\vec{D}_i)_j := D_j \cap \partial O_i$  and consider elliptic operators  $L_i$  on  $O_i$  subject to a vanishing trace condition on  $\vec{D}_i \subseteq (\partial O_i)^m$  and whose coefficients are the restriction of the coefficients of  $L$  to  $O_i$ . Then, the following correspondence holds [15, Prop. 6.8].

**Proposition 9.1** (Transference principle). *The following are equivalent:*

- (i)  $D(\sqrt{L}) = \mathbb{W}_{\vec{D}}^{1,2}(O)^m$  with  $\|\sqrt{L}u\|_2 \approx \|u\|_{\mathbb{W}^{1,2}(O)}$ ,
- (ii)  $D(\sqrt{L_i}) = \mathbb{W}_{\vec{D}_i}^{1,2}(O_i)$  with  $\|\sqrt{L_i}u\|_2 \approx \|u\|_{\mathbb{W}^{1,2}(O_i)}$  for all  $i$ , where the implicit constants are independent of  $i$ .

Now, the central idea in [15] is as follows: Starting with a triple  $(O, \vec{D}, L)$  as in Theorem 1.1, they construct a new triple  $(O, \vec{D}, L)$  that satisfies all assumptions of Theorem 1.1, contains  $(O, \vec{D}, L)$  as a “component” in the sense explained above, and such that  $O$  is in addition interior thick. Then, since we have proved Theorem 1.1 under the additional assumption that  $O$  is interior thick, item (i) of Proposition 9.1 is verified. Therefore, Proposition 9.1 provides the square root property for all triples quantified in (ii), including the triple  $(O, \vec{D}, L)$ , which completes the proof of Theorem 1.1 in the general case.

Hence, it only remains to clarify the construction of the triple  $(O, \vec{D}, L)$ . By assumption,  $O$  is locally an  $(\varepsilon, \delta)$ -domain near  $\partial O \setminus D_j =: N_j$  for all  $j = 1, \dots, m$ . Let  $\Sigma$  denote a grid of open axis-parallel cubes of diameter  $\delta/8$  in  $\mathbb{R}^n$ . Let  $\Sigma'$  contain those cubes  $Q$  from  $\Sigma$  for which  $\bar{Q}$  intersects  $D$  but which have empty intersection with the tube of size  $\delta/4$  around  $N^* := \cup_{j=1}^m N_j$ . Now, put

$$O := O \cup \bigcup_{Q \in \Sigma'} (Q \setminus \partial O) \quad \text{and} \quad (\vec{D})_j := \partial O \setminus N_j.$$

In [15], all components were subject to the same Dirichlet boundary conditions, so that  $N^* = N$  in that paper. In our more general setting, all desired properties for  $(O, \vec{D})$  except the interior thickness condition immediately follow by the same proof as in [15, Sec. 6.3].

To show the interior thickness condition for  $\mathcal{O}$ , the authors of [15] argue first that only balls centered in  $x \in \mathcal{O}$  have to be considered. Now, we need to distinguish cases: First, if  $x$  is in the  $\delta/2$ -tube around  $N^*$ , then  $x$  is in the  $\delta/2$ -tube around  $N_j$  for *some* index  $j = 1, \dots, m$ , and thickness in  $x$  is provided by the corkscrew condition in Proposition 2.7. Otherwise, as in [15], it follows that  $x \in \overline{Q}$  for some  $Q \in \Sigma'$ , so that thickness is guaranteed by the respective property of the cube  $Q$ . Thus,  $\mathcal{O}$  is indeed interior thick. Finally, the operator  $L$  can be extended to  $\mathcal{O}$  by setting it equal to  $-\Delta_{\vec{D}} + 1$  on  $\mathcal{O} \setminus \mathcal{O}$ . This completes the proof.  $\square$

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