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THE KATO SQUARE ROOT PROBLEM FOR MIXED BOUNDARY VALUE PROBLEMS

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ABSTRACT

We solve the Kato square root problem for second order elliptic systems in divergence form under mixed boundary conditions on Lipschitz domains. This answers a question posed by Lions in 1962. To do this we develop a general theory of quadratic estimates and functional calculi for complex perturbations of Dirac-type operators on Lipschitz domains.

1. *Introduction*

The Kato square root problem for elliptic operators on Lipschitz domains with mixed boundary conditions can be formulated as follows. Let $\Omega \subset \mathbb{R}^n$, $n \in \mathbb{N}$, be a Lipschitz domain, let Σ_1 be an open subset of the boundary Σ of Ω, and define

$$\mathcal{V} = \{u \in H^1(\Omega;\mathbb{C}) : \operatorname{supp}(\gamma u) \subset \overline{\Sigma_1}\}, \tag{1.1}$$

where γ is the trace operator from the Sobolev space $H^1(\Omega;\mathbb{C})$ to the boundary Sobolev space $H^{1/2}(\Sigma;\mathbb{C})$.

Given a matrix-valued function $A = (a_{jk})$, where $a_{jk} \in L_\infty(\Omega;\mathbb{C})$ for each $j,k = 0,1,\dots,n$, let $J_A : \mathcal{V} \times \mathcal{V} \to \mathbb{C}$ be given by

$$J_A[u,v] = \int_\Omega \sum_{j,k=1}^{n} \left(a_{jk} \frac{\partial u}{\partial x_k} \frac{\partial \overline{v}}{\partial x_j} + a_{j0} u \frac{\partial \overline{v}}{\partial x_j} + a_{0k} \frac{\partial u}{\partial x_k} \overline{v} + a_{00} u \overline{v} \right) dx \tag{1.2}$$

for every $u, v \in \mathcal{V}$.

Suppose that J_A satisfies the following coercivity condition: there exists $\kappa > 0$ such that

$$\operatorname{Re} J_A[u,u] \geqslant \kappa(\|\nabla u\|^2 + \|u\|^2) \tag{1.3}$$

for every $u \in \mathcal{V}$. Here and below $(\cdot,\cdot)$ and $\|\cdot\|$ denote the inner product and norm on $L_2(\Omega;\mathbb{C})$. Then J_A is a densely defined, closed, accretive sesquilinear form. Consequently, there exists an operator L_A on $L_2(\Omega;\mathbb{C})$ with $\mathsf{D}(L_A) \subset \mathcal{V}$ uniquely determined by the property that it is maximal accretive and satisfies $J_A[u,v] = (L_A u, v)$ for every $u \in \mathsf{D}(L_A)$ and $v \in \mathcal{V}$. Indeed, L_A is the divergence form operator

$$L_A u = -\sum \frac{\partial}{\partial x_j} \left(a_{jk} \frac{\partial u}{\partial x_k} \right) - \sum \frac{\partial}{\partial x_j} (a_{j0} u) + \sum a_{0k} \frac{\partial u}{\partial x_k} + a_{00} u$$

with Dirichlet boundary condition $u = 0$ on $\Sigma \setminus \overline{\Sigma_1}$ and natural boundary condition

$$\sum \nu_j a_{jk} \frac{\partial u}{\partial x_k} + \sum \nu_j a_{j0} u = 0 \quad \text{on } \Sigma_1,$$

defined in an appropriate weak sense.

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The square root $\sqrt{L_A}$ of L_A is the unique maximal accretive operator with $(\sqrt{L_A})^2 = L_A$. For an explanation of the terminology and results see [**9**, VI, Theorem 2.1, V, Theorem 3.35, VI, Remark 2.29]. Also see [**10**, Chapter II], [**15**, Chapter 1] and [**17**] for specific material on forms such as J_A and further references to mixed boundary value problems. The Kato square root problem is to determine whether the domain $\mathsf{D}(\sqrt{L_A}) = \mathcal{V}$.

The Kato square root problem for second order elliptic operators on $\Omega = \mathbb{R}^n$ was solved in [**3**] by Auscher, Hofmann, Lacey, McIntosh and Tchamitchian, and for higher order elliptic operators and systems on $\mathbb{R}^n$ in [**4**] by Auscher, Hofmann, McIntosh and Tchamitchian. The Kato square root problem for second order elliptic operators on strongly Lipschitz domains with Dirichlet or Neumann boundary conditions was solved in [**6**] by Auscher and Tchamitchian, who reduced the problem to the Kato problem on $\mathbb{R}^n$ by using extension maps. As different extensions are required for the Dirichlet and Neumann problems, their procedure does not work for mixed boundary value problems.

The following theorem solves the Kato square root problem for second order elliptic operators on Lipschitz domains with mixed boundary conditions. This result is new for both smooth and Lipschitz domains, and answers a question posed by Lions in 1962 [**11**, Remark 6.1]. We remark that, in the case when the coefficients are Hölder continuous, the Kato square root problem with mixed boundary conditions was solved in [**13**].

THEOREM 1. *Let $\Omega' \subset \mathbb{R}^n$, $n \in \mathbb{N}$, be a smooth domain which coincides with either the empty set $\emptyset$, the half space $\mathbb{R}^n_+$ or $\mathbb{R}^n$ on the complement of a bounded set. Let $\Sigma'_1 \subset \Sigma' = \partial\Omega'$ be a smooth open set which coincides with either the empty set $\emptyset$, the half space $\mathbb{R}^{n-1}_+ \subset \mathbb{R}^{n-1}$ or $\mathbb{R}^{n-1}$ on the complement of a bounded set.*

Let $\Omega \subset \mathbb{R}^n$ be a bi-Lipschitz image of Ω' and let $\Sigma_1 \subset \Sigma = \partial\Omega$ be the corresponding bi-Lipschitz image of Σ'_1.

Define $\mathcal{V}$, A, J_A with the properties specified in (1.1)–(1.3)*, and let L_A be the associated maximal accretive operator.*

Then $\mathsf{D}(\sqrt{L_A}) = \mathcal{V}$ with $\|\sqrt{L_A}\, u\| \approx \|\nabla u\| + \|u\|$ for every $u \in \mathcal{V}$. The comparability constant implicit in the use of '$\approx$' depends on $\|A\|_\infty$ and κ, as well as the constants implicit in the assumptions on Ω and Σ_1.

Indeed, a somewhat more general version is presented in Section 3, Theorem 3, concerning elliptic systems with local boundary conditions. This constitutes an application of results (Theorems 2 and Corollary 1) on homogenous first order systems Γ acting on $L_2(\Omega, \mathbb{C}^N)$ which satisfy $\Gamma^2 = 0$. We let $\Pi = \Gamma + \Gamma^*$, and consider perturbations of the type $\Pi_B = \Gamma + B_1\Gamma^* B_2$ where B_1 has positive real part on the range of Γ^*, B_2 has positive real part on the range of Γ, and $\Gamma^* B_2 B_1 \Gamma^* = 0$ and $\Gamma B_1 B_2 \Gamma = 0$. It is shown under certain hypotheses that Π_B satisfies quadratic estimates in $L_2(\Omega; \mathbb{C}^N)$, and hence that the estimate $\|\sqrt{\Pi_B^2}\, u\| \approx \|\Pi_B u\|$ holds.

Techniques developed in the current paper build upon ideas introduced by the authors in [**7**], where we prove quadratic estimates for complex perturbations of Dirac-type operators on $\mathbb{R}^n$ and show that such operators have a bounded functional calculus. This paper was in turn inspired by the proof of the Kato square root in [**3**]. The key idea employed from [**7**] is our utilization of only the first order structure of the operator, and subsequent exploitation of the algebra involved in the Hodge

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decomposition of the first order system. Duplicated arguments from [**7**] have been omitted, so the reader is advised to keep a copy of that paper handy.

2. *Quadratic estimates for perturbed Dirac operators*

In this section we expand on the comments made in the Introduction concerning first order elliptic systems.

For an unbounded linear operator $T : \mathsf{D}(T) \to \mathcal{H}_2$ from a domain $\mathsf{D}(T)$ in a Hilbert space $\mathcal{H}_1$ to another Hilbert space $\mathcal{H}_2$, denote its null space by $\mathsf{N}(T)$ and its range by $\mathsf{R}(T)$. The operator T is said to be *closed* when its graph is a closed subspace of $\mathcal{H}_1 \times \mathcal{H}_2$. The space of all bounded linear operators from $\mathcal{H}_1$ to $\mathcal{H}_2$ is denoted $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$, while $\mathcal{L}(\mathcal{H}) = \mathcal{L}(\mathcal{H}, \mathcal{H})$. See for example [**9**] for more details.

Consider three operators $\{\Gamma, B_1, B_2\}$ in a Hilbert space $\mathcal{H}$ with the following properties.

(H1) The operator $\Gamma : \mathsf{D}(\Gamma) \to \mathcal{H}$ is a *nilpotent* operator from $\mathsf{D}(\Gamma) \subset \mathcal{H}$ to $\mathcal{H}$, by which we mean that Γ is closed, densely defined and $\mathsf{R}(\Gamma) \subset \mathsf{N}(\Gamma)$. In particular, $\Gamma^2 = 0$ on $\mathsf{D}(\Gamma)$.

(H2) The operators $B_1, B_2 : \mathcal{H} \to \mathcal{H}$ are bounded linear operators satisfying the following accretivity conditions for some $\kappa_1, \kappa_2 > 0$:

$$\begin{aligned} \operatorname{Re}(B_1 u, u) &\geqslant \kappa_1 \|u\|^2 \quad \text{for all } u \in \mathsf{R}(\Gamma^*), \\ \operatorname{Re}(B_2 u, u) &\geqslant \kappa_2 \|u\|^2 \quad \text{for all } u \in \mathsf{R}(\Gamma). \end{aligned}$$

Let the angles of accretivity be

$$\begin{aligned} \omega_1 &= \sup_{u \in \mathsf{R}(\Gamma^*) \setminus \{0\}} |\arg(B_1 u, u)| < \pi/2, \\ \omega_2 &= \sup_{u \in \mathsf{R}(\Gamma) \setminus \{0\}} |\arg(B_2 u, u)| < \pi/2, \end{aligned}$$

and set $\omega = \frac{1}{2}(\omega_1 + \omega_2)$.

(H3) The operators satisfy $\Gamma^* B_2 B_1 \Gamma^* = 0$ on $\mathsf{D}(\Gamma^*)$ and $\Gamma B_1 B_2 \Gamma = 0$ on $\mathsf{D}(\Gamma)$; that is, $B_2 B_1 : \mathsf{R}(\Gamma^*) \to \mathsf{N}(\Gamma^*)$ and $B_1 B_2 : \mathsf{R}(\Gamma) \to \mathsf{N}(\Gamma)$.

Definition 1. Let $\Pi = \Gamma + \Gamma^*$. Also let $\Gamma_B^* = B_1 \Gamma^* B_2$ and let $\Pi_B = \Gamma + \Gamma_B^*$.

Definition 2. Given $0 \leqslant \mu < \pi/2$, define the closed sectors and double sector in the complex plane by

$$\begin{aligned} S_{\mu+} &= \{z \in \mathbb{C} : |\arg z| \leqslant \mu\} \cup \{0\}, \quad S_{\mu-} = -S_{\mu+}, \\ S_\mu &= S_{\mu+} \cup S_{\mu-}. \end{aligned}$$

We now summarize consequences of the above hypotheses, proved in [**7**, Section 4]. The operator Γ_B^* is nilpotent, the operator Π_B is closed and densely defined, and the Hilbert space $\mathcal{H}$ has the following Hodge decomposition into closed subspaces:

$$\mathcal{H} = \mathsf{N}(\Pi_B) \oplus \overline{\mathsf{R}(\Gamma_B^*)} \oplus \overline{\mathsf{R}(\Gamma)}. \tag{2.1}$$

Moreover, $\mathsf{N}(\Pi_B) = \mathsf{N}(\Gamma_B^*) \cap \mathsf{N}(\Gamma)$ and $\overline{\mathsf{R}(\Pi_B)} = \overline{\mathsf{R}(\Gamma_B^*)} \oplus \overline{\mathsf{R}(\Gamma)}$. When $B_1 = B_2 = \mathrm{I}$ these decompositions are orthogonal, and in general the decompositions are topological.

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The spectrum $\sigma(\Pi_B)$ is contained in the double sector S_ω, and the operator Π_B satisfies resolvent bounds

$$\|(\mathrm{I}-\tau\Pi_B)^{-1}\| \leqslant \frac{C|\tau|}{\operatorname{dist}(\tau, S_\omega)}$$

for all $\tau \in \mathbb{C} \setminus S_\omega$, where $C = C(\|B_1\|, \|B_2\|, \kappa_1, \kappa_2)$. Such an operator is of type S_ω as defined in [**1**, **5**].

We now introduce further hypotheses which together with (H1)–(H3) summarize the properties of operators considered in this paper. These form an inhomogeneous version of hypotheses (H4)–(H8) of [**7**].

(H4) The Hilbert space is $\mathcal{H} = L_2(\Omega; \mathbb{C}^N)$, where $\Omega \subset \mathbb{R}^n$ and $n, N \in \mathbb{N}$. Here Ω is a bi-Lipschitz image of $\Omega' \subset \mathbb{R}^n$, where Ω' is a smooth domain which on the complement of a bounded set coincides with either the empty set $\emptyset$, the half space $\mathbb{R}^n_+$ or $\mathbb{R}^n$. (By a *domain* we mean a connected open set.)

(H5) The operators B_1 and B_2 denote multiplication by matrix-valued functions $B_1, B_2 \in L_\infty(\Omega; \mathcal{L}(\mathbb{C}^N))$.

(H6) (Localization) For every smooth, bounded $\eta : \mathbb{R}^n \to \mathbb{R}$ we have that $\eta \mathsf{D}(\Gamma) \subset \mathsf{D}(\Gamma)$, and the commutator $M_\eta = [\Gamma, \eta\,\mathrm{I}]$ is a multiplication operator. There exists $c > 0$ such that

$$|M_\eta(x)| \leqslant c|\nabla\eta(x)|$$

for all such η and for all $x \in \mathbb{R}^n$. (This implies that the same hypotheses hold with Γ replaced by Γ^*.)

(H7) (Cancellation) There exists $c > 0$ such that

$$\left|\int_\Omega \Gamma u\right| \leqslant c|B|^{1/2}\|u\| \quad \text{and} \quad \left|\int_\Omega \Gamma^* v\right| \leqslant c|B|^{1/2}\|v\|$$

for every open ball B centred in Ω, for all $u \in \mathsf{D}(\Gamma)$ with compact support in $B \cap \Omega$, and for all $v \in \mathsf{D}(\Gamma^*)$ with compact support in $B \cap \Omega$.

(H8) (Coercivity) There exists $\alpha, \beta, c > 0$ such that

$$\|u\|_{H^\beta(\Omega;\mathbb{C}^N)} \leqslant c\||\Pi|^\beta u\| \quad \text{and} \quad \|v\|_{H^\alpha(\Omega;\mathbb{C}^N)} \leqslant c\||\Pi|^\alpha v\|$$

for all $u \in \mathsf{R}(\Gamma^*) \cap \mathsf{D}(\Pi^2)$ and $v \in \mathsf{R}(\Gamma) \cap \mathsf{D}(\Pi^2)$. Here $|\Pi| = \sqrt{\Pi^2}$, and $H^\beta(\Omega; \mathbb{C}^N)$ denotes the Sobolev space of order β of $\mathbb{C}^N$-valued functions on Ω.

REMARK 1. In the following theorem and throughout the rest of the paper, the notation $a \approx b$ and $b \lesssim c$, for $a, b, c \geqslant 0$, means that there exists $C > 0$ that depends only on the hypothesis, so that $a/C \leqslant b \leqslant Ca$ and $b \leqslant Cc$ respectively.

THEOREM 2. *Consider the operator $\Pi_B = \Gamma + B_1\Gamma^* B_2$ acting in the Hilbert space $\mathcal{H} = L_2(\Omega; \mathbb{C}^N)$, where $\{\Gamma, B_1, B_2\}$ satisfies the hypotheses* (H1)–(H8). *Then Π_B satisfies the quadratic estimate*

$$\int_0^\infty \|\Pi_B(\mathrm{I}+t^2\Pi_B^2)^{-1}u\|^2\, t\, dt \approx \|u\|^2 \tag{2.2}$$

for all $u \in \mathsf{R}(\Pi_B) \subset L_2(\Omega; \mathbb{C}^N)$. The comparability constant implicit in the use of '$\approx$' depends only on the parameters quantified above including the bi-Lipschitz constants implicit in the definition of Ω, and on Ω'.

We defer the proof to Section 4.

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This result implies that, for every $\omega < \mu < \pi/2$, the operator Π_B has a bounded S°_μ holomorphic functional calculus in $\mathsf{R}(\Pi_B) \subset L_2(\Omega;\mathbb{C}^N)$, where S°_μ denotes the interior of S_μ. More to our purposes, it implies the following result. See [**7**, Section 2] for further discussion and proofs.

COROLLARY 1. *Assume the hypotheses of Theorem* 2. *Then* $\mathsf{D}(\Gamma) \cap \mathsf{D}(\Gamma^*_B) = \mathsf{D}(\Pi_B) = \mathsf{D}(\sqrt{\Pi_B^2})$ *with*

$$\|\Gamma u\| + \|\Gamma^*_B u\| \approx \|\Pi_B u\| \approx \|\sqrt{\Pi_B^2}u\|.$$

REMARK 2. This is equivalent to the statement that there is a (non-orthogonal) spectral decomposition

$$\mathcal{H} = \mathsf{N}(\Pi_B) \oplus \mathcal{H}^+_B \oplus \mathcal{H}^-_B$$

into spectral subspaces of Π_B corresponding to $\{0\}$, $S_{\omega+} \setminus \{0\}$ and $S_{\omega-} \setminus \{0\}$.

2.1. *Sobolev spaces*

We take this opportunity to state some interpolation, trace and extension results for Sobolev spaces that we need in the next section.

Recall the complex interpolation method. Let $X \supset Y$ be Hilbert spaces and $S = \{z \in \mathbb{C} : 0 < \operatorname{Re} z < 1\}$. Let $\mathsf{H}[X,Y]$ denote the Banach space of bounded continuous functions $f : \overline{S} \to X$ holomorphic on S with $f(z) \in X$ if $\operatorname{Re} z = 0$ and $f(z) \in Y$ if $\operatorname{Re} z = 1$. Each *interpolation space* $[X,Y]_\theta$, $0 < \theta < 1$, is given by

$$[X,Y]_\theta = \{u(\theta) \in X : u \in \mathsf{H}[X,Y]\}$$

and inherits a Hilbert space topology from the quotient $\mathsf{H}[X,Y]/\{u : u(\theta) = 0\}$. A collection of Hilbert spaces $\{X_s\}_{s\in I}$, where $I \subset \mathbb{R}$ is an interval, is an *interpolation family* if $X_{(1-\theta)t_1+\theta t_2} = [X_{t_1}, X_{t_2}]_\theta$ for every $0 < \theta < 1$ and $t_1, t_2 \in I$. A good reference for complex interpolation spaces is [**12**].

Let Ω, Σ, Σ_1 and Ω' be as described in the Introduction.

For each $s \in \mathbb{R}$, let $H^s(\Omega;\mathbb{C}^m)$ denote the fractional order Sobolev space of order s of $\mathbb{C}^m$-valued functions on Ω. For each $-1 \leqslant s \leqslant 1$, let $H^s(\Sigma;\mathbb{C}^m)$ denote the fractional order Sobolev space of order s of $\mathbb{C}^m$-valued functions on Σ. This can be defined through localization arguments by utilizing bi-Lipschitz parametrizations of Σ. The spaces $H^s(\Sigma;\mathbb{C}^m)$, $-1 \leqslant s \leqslant 1$, form an interpolation family, as do the closed subspaces

$$H^s_0(\overline{\Sigma}_1;\mathbb{C}^m) = \{u \in H^s(\Sigma;\mathbb{C}^m) : \operatorname{supp} u \subset \overline{\Sigma}_1\}.$$

More generally, $H^s_0(\overline{\Sigma}_1;\mathbb{C}^m)$ interpolate whenever $\Sigma \setminus \overline{\Sigma}_1$ is an extension domain of Σ. By $\Sigma \setminus \overline{\Sigma}_1$ being an extension domain of Σ, we mean that the map R restricting distributions in $H^{-1}(\Sigma;\mathbb{C}^m)$ to $\Sigma \setminus \overline{\Sigma}_1$ has a right inverse E, such that $ER : H^s(\Sigma;\mathbb{C}^m) \to H^s(\Sigma;\mathbb{C}^m)$ is bounded for all $|s| \leqslant 1$.

In the case when Ω is smooth, that is, when $\Omega = \Omega'$, we also make use of the following facts.

(i) The trace operator γ is a bounded map $\gamma : H^s(\Omega;\mathbb{C}^m) \to H^{s-1/2}(\Sigma;\mathbb{C}^m)$ for $1/2 < s < 3/2$. There is a bounded extension operator $\varepsilon : H^{s-1/2}(\Sigma;\mathbb{C}^m) \to H^s(\Omega;\mathbb{C}^m)$ for $0 \leqslant s < 3/2$ which satisfies $\gamma\varepsilon = I$ on $H^{s-1/2}(\Sigma;\mathbb{C}^m)$ when $1/2 < s < 3/2$. In the case $\Omega = \mathbb{R}^n_+$, this map can be constructed as in [**2**, Section 2.8, Theorem 1b] with $\alpha = 1$.

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(ii) $H^s(\Omega;\mathbb{C}^m)$, $0 \leqslant s < 3/2$, is an interpolation family, as is $H^s_0(\Omega;\mathbb{C}^m) = \{u \in H^s(\Omega;\mathbb{C}^m) : \gamma u = 0\}$, $1/2 < s < 3/2$.

(iii) $H^s_0(\Omega;\mathbb{C}^m) = [L_2(\Omega;\mathbb{C}^m), H^1_0(\Omega;\mathbb{C}^m)]_s$ when $1/2 < s < 1$.

3. *A Kato square root estimate for systems on domains*

Let us now state a theorem which is somewhat more general than Theorem 1. We shall then prove that it is a consequence of Corollary 1, and thus of Theorem 2. Later, in Section 4, we shall prove Theorem 2.

Assumptions on Ω, $\mathcal{V}$ and S. For the remainder of this section, $n, m \in \mathbb{N}$, Ω is an open subset of $\mathbb{R}^n$ which satisfies hypothesis (H4) and has boundary Σ, and $\mathcal{V}$ is a closed subspace of $H^1(\Omega;\mathbb{C}^m)$ given by

$$\mathcal{V} = \{u \in H^1(\Omega;\mathbb{C}^m) : \gamma u \in B^{1/2}(\Sigma;\mathbb{C}^m)\}. \tag{3.1}$$

Here $B^s(\Sigma;\mathbb{C}^m)$, $-\frac{1}{2} \leqslant s < 1$, is a complex interpolation family of closed subspaces of $H^s(\Sigma;\mathbb{C}^m)$, and $B^{1/2}(\Sigma;\mathbb{C}^m)$ has the following localization property. Whenever $g \in B^{1/2}(\Sigma;\mathbb{C}^m)$ and $\eta : \overline{\Omega} \to \mathbb{R}$ is compactly supported and Lipschitz, then $\eta g \in B^{1/2}(\Sigma;\mathbb{C}^m)$ with

$$\|\eta g\|_{B^{1/2}} \leqslant c(\|\nabla\eta\|_\infty + \|\eta\|_\infty)\|g\|_{B^{1/2}}$$

for some c (independent of g and η). In the case when $\Omega = \mathbb{R}^n$, then $\mathcal{V} = H^1(\Omega;\mathbb{C}^m)$.

Further, S denotes the unbounded operator

$$S = \begin{bmatrix} \mathrm{I} \\ \nabla \end{bmatrix} : \mathsf{D}(S) \subset L_2(\Omega;\mathbb{C}^m) \to L_2(\Omega;\mathbb{C}^{m+nm})$$

with dense domain $\mathsf{D}(S) = \mathcal{V}$, and S^* is its adjoint:

$$S^* = \begin{bmatrix} \mathrm{I} & -\mathrm{div} \end{bmatrix} : \mathsf{D}(S^*) \subset L_2(\Omega;\mathbb{C}^{m+nm}) \to L_2(\Omega;\mathbb{C}^m).$$

Then S and S^* are closed and densely defined operators with $\mathsf{N}(S) = \{0\}$, $\mathsf{R}(S)$ closed in $L_2(\Omega;\mathbb{C}^{m+nm})$, and $\mathsf{R}(S^*) = L_2(\Omega;\mathbb{C}^m)$.

Assumptions on A_1 and A_2. Assume that $A_1 \in L_\infty(\Omega;\mathcal{L}(\mathbb{C}^m))$ and $A_2 \in L_\infty(\Omega;\mathcal{L}(\mathbb{C}^{m+nm}))$ satisfy, for some $\kappa_1, \kappa_2 > 0$, the accretivity conditions

$$\begin{aligned} &\mathrm{Re}(A_1 v, v) \geqslant \kappa_1 \|v\|^2 && \text{for all } v \in L_2(\Omega;\mathbb{C}^m), \\ &\mathrm{Re}(A_2 S u, S u) \geqslant \kappa_2 \|S u\|^2 && \text{for all } u \in \mathcal{V}. \end{aligned} \tag{3.2}$$

Set $\omega := \frac{1}{2}(\omega_1 + \omega_2)$ where

$$\begin{aligned} \omega_1 &:= \sup\{|\arg(A_1 v, v)| : v \in L_2(\Omega;\mathbb{C}^m), v \neq 0\} < \pi/2 \\ \omega_2 &:= \sup\{|\arg(A_2 S u, S u)| : u \in \mathcal{V} \setminus \{0\}\} < \pi/2. \end{aligned}$$

THEOREM 3. *Suppose that Ω, $\mathcal{V}$, S, A_1 and A_2 satisfy the above assumptions. Let $L_A = A_1 S^* A_2 S$ denote the unbounded operator in $L_2(\Omega;\mathbb{C}^m)$ with domain $\mathsf{D}(L_A) = \{u \in \mathcal{V} : A_2 S u \in \mathsf{D}(S^*)\}$. Then $\sigma(L_A) \subset S_{2\omega+}$ and L_A satisfies resolvent bounds*

$$\|(\mathrm{I} - \tau L_A)^{-1}\| \lesssim \frac{|\tau|}{\mathrm{dist}\,(\tau, S_{2\omega+})}$$

for all $\tau \in \mathbb{C} \setminus S_{2\omega+}$, so that L_A has a square root $\sqrt{L_A}$ with $\sigma(\sqrt{L_A}) \subset S_{\omega+}$.

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This square root has the Kato square root property $\mathsf{D}(\sqrt{L_A}) = \mathcal{V}$ *with*

$$\|\sqrt{L_A}\, u\| \approx \|Su\| \approx \|\nabla u\| + \|u\| \tag{3.3}$$

for all $u \in \mathcal{V}$. *The comparability constant implicit in the use of '*$\approx$*' depends on* m, c, $\|A_1\|_\infty$, $\|A_2\|_\infty$, κ_1, κ_2 *and* Ω', *the bi-Lipschitz constant implicit in the definition of* Ω, *and constants of interpolation for* $B^s(\Sigma;\mathbb{C}^m)$.

We first deduce that Theorem 1 is a consequence of this one.

Proof of Theorem 1. Apply Theorem 3 with $m = 1$, $A_1 = I$, $A_2 = A$ and $B^s(\Sigma;\mathbb{C}) = H^s_0(\overline{\Sigma}_1;\mathbb{C})$, noting that these spaces satisfy the above hypotheses, and that the sesquilinear form defined in the Introduction is $J_A[u,v] = (ASu, Sv)$, $u, v \in \mathcal{V}$, with associated operator $L_A = S^*AS$. □

We now express Theorem 3 in terms of the first order systems presented in Section 2. Consider the operators

$$\Gamma = \begin{bmatrix} 0 & 0 \\ S & 0 \end{bmatrix}, \quad \Gamma^* = \begin{bmatrix} 0 & S^* \\ 0 & 0 \end{bmatrix}, \quad B_1 = \begin{bmatrix} A_1 & 0 \\ 0 & 0 \end{bmatrix}, \quad B_2 = \begin{bmatrix} 0 & 0 \\ 0 & A_2 \end{bmatrix}$$

in the Hilbert space $\mathcal{H} = L_2(\Omega;\mathbb{C}^m) \oplus L_2(\Omega;\mathbb{C}^{m+nm})$. They satisfy hypotheses (H1)–(H3), and so have the properties listed in Section 2. Moreover

$$\Gamma^*_B = B_1\Gamma^* B_2 = \begin{bmatrix} 0 & A_1S^*A_2 \\ 0 & 0 \end{bmatrix}, \quad \Pi_B = \Gamma + \Gamma^*_B = \begin{bmatrix} 0 & A_1S^*A_2 \\ S & 0 \end{bmatrix}$$
$$\Pi_B^2 = \begin{bmatrix} A_1S^*A_2S & 0 \\ 0 & SA_1S^*A_2 \end{bmatrix} = \begin{bmatrix} L_A & 0 \\ 0 & SA_1S^*A_2 \end{bmatrix}.$$

We remark that Γ, Γ^*, Γ^*_B, Π_B and Π_B^2 all have closed range, and that

$$\mathsf{R}(\Gamma) \subset L_2(\Omega;\mathbb{C}^{m+nm}) = \mathsf{N}(\Gamma)$$

and

$$\mathsf{R}(\Gamma^*) = \mathsf{R}(\Gamma^*_B) = L_2(\Omega;\mathbb{C}^m) \subset \mathsf{N}(\Gamma^*), \mathsf{N}(\Gamma^*_B).$$

Moreover $\sigma(\Pi_B) \subset S_\omega$ and $\sigma(\Pi_B^2) \subset S_{2\omega+}$ with resolvent bounds

$$\|(\mathrm{I} - \tau\Pi_B)^{-1}\| \lesssim \frac{|\tau|}{\operatorname{dist}(\tau, S_\omega)}$$

and

$$\|(\mathrm{I} - \tau^2\Pi_B^2)^{-1}\| \lesssim \frac{|\tau^2|}{\operatorname{dist}(\tau^2, S_{2\omega+})}$$

for all $\tau \in \mathbb{C} \setminus S_\omega$.

Proposition 1. *Under the above assumptions, the operator* Π_B *satisfies the quadratic estimate* (2.2) *for all* $u \in \mathsf{R}(\Pi_B)$, *and thus* $\mathsf{D}(\Gamma) \cap \mathsf{D}(\Gamma^*_B) = \mathsf{D}(\Pi_B) = \mathsf{D}(\sqrt{\Pi_B^2})$ *with*

$$\|\Gamma u\| + \|\Gamma^*_B u\| \approx \|\Pi_B u\| \approx \|\sqrt{\Pi_B^2}\, u\|.$$

We first deduce that Theorem 3 and hence Theorem 1 is a consequence of Proposition 1.

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Proof of Theorem 3. On restricting the above result to $u \in L_2(\Omega;\mathbb{C}^m)$ we conclude that $\mathsf{D}(\sqrt{L_A}) = \mathsf{D}(S) = \mathcal{V}$ with the Kato square root estimate

$$\|\sqrt{L_A}\, u\| \approx \|Su\| = \|\nabla u\| + \|u\|$$

for all $u \in \mathcal{V}$. □

REMARK 3. It is also a consequence of the quadratic estimate (2.2) that Π_B has a bounded S°_μ holomorphic functional calculus in $\mathsf{R}(\Pi_B) \subset \mathcal{H}$ for $\omega < \mu < \pi/2$. Therefore L_A has a bounded $S^\circ_{2\mu+}$ holomorphic functional calculus in $L_2(\Omega;\mathbb{C}^m)$. This is a generalization of results in [**14**] and [**8**].

Our task now is to prove Proposition 1. We do this in two stages. In the first, we show that, when the domain Ω is smooth, then hypotheses (H4)–(H8) are satisfied, and so Theorem 2 and Corollary 1 can be applied. This in itself is a new result. In the second stage, we show that the full result is a consequence of the result for smooth domains.

Proof of Proposition 1 *when* $\Omega = \Omega'$. Our aim is to verify that $\{\Gamma, B_1, B_2\}$ satisfies hypotheses (H4)–(H8) in $\mathcal{H} = L_2(\Omega;\mathbb{C}^m) \oplus L_2(\Omega;\mathbb{C}^{m+nm}) = L_2(\Omega;\mathbb{C}^N)$ with $N = 2m + nm$.

(i) Hypothesis (H4) is already assumed, while (H5) follows immediately from the assumptions on A_1 and A_2.

(ii) The localization hypothesis (H6) follows directly from the definition (3.1) of $\mathcal{V}$, and the fact that $B^{1/2}(\Sigma;\mathbb{C}^m)$ satisfies a localization property.

(iii) Hypothesis (H7) follows from the fact that $\int_\Omega \nabla u = 0$ and $\int_\Omega \operatorname{div} v = 0$ for u and v with compact support in Ω, and the use of the Cauchy–Schwarz inequality on the zero order terms.

(iv) To prove (H8), first assume $u \in \mathsf{R}(\Gamma^*) \cap \mathsf{D}(\Gamma)$. Then

$$\|u\|_{H^1(\Omega;\mathbb{C}^N)} = \|\Gamma u\| = \|\Pi u\| = \||\Pi| u\|,$$

so we can choose $\beta = 1$. Next assume $v = \Gamma u \in \mathsf{R}(\Gamma) \cap \mathsf{D}(\Pi^2)$, where $u \in L_2(\Omega;\mathbb{C}^m)$. From Proposition 2 below it follows that

$$\|v\|_{H^\alpha(\Omega;\mathbb{C}^N)} = \|u\|_{H^{1+\alpha}(\Omega;\mathbb{C}^N)} \lesssim \||\Pi|^{1+\alpha} u\| = \||\Pi|^\alpha \Pi u\| = \||\Pi|^\alpha v\|,$$

since $L^{1/2} = |\Pi|$ on $L_2(\Omega;\mathbb{C}^m)$.

The result now follows on applying Corollary 1. Proposition 1 is proved in this case. □

We are left with the task of proving the following result.

PROPOSITION 2. *Under the above assumptions on* $\mathcal{V}$ *and* S, *and the smoothness assumption* $\Omega = \Omega'$, *consider the positive operator* $L = S^*S$ *in* $L_2(\Omega;\mathbb{C}^m)$. *Then there exists* $\alpha > 0$ *such that* $\mathsf{D}(L^{(1+\alpha)/2}) \subset H^{1+\alpha}(\Omega;\mathbb{C}^m)$ *with*

$$\|u\|_{H^{1+\alpha}(\Omega;\mathbb{C}^m)} \lesssim \|L^{(1+\alpha)/2} u\|.$$

REMARK 4. Note that $L = -\Delta + I$ with $\mathsf{D}(L) = \{u \in \mathcal{V} : Su \in \mathsf{D}(S^*)\}$. When $m = 1$, $\mathcal{V}$ is defined as in the Introduction, and the boundary of Σ_1 in Σ is smooth, then this result can be derived for any $0 < \alpha < 1/2$ as a consequence of

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results on mixed boundary value problems proved by Pryde in [**16**]. The proof of Lemma 1 is an adaptation of an interpolation argument in [**16**].

We prove Proposition 2 with an interpolation and duality argument using the family

$$\mathcal{V}^s = \{u \in H^s(\Omega;\mathbb{C}^m) : \gamma u \in B^{s-1/2}(\Sigma;\mathbb{C}^m)\}$$

for $1/2 < s < 3/2$ and the following three lemmas.

LEMMA 1. *If $1/2 < s \leqslant 1$, then $\mathcal{V}^s \subset \mathsf{D}(L^{s/2})$ with $\|L^{s/2}u\| \lesssim \|u\|_{H^s}$.*

Proof. By [**9**, VI, Theorem 2.23] we have $\mathcal{V} = \mathcal{V}^1 = \mathsf{D}(L^{1/2})$. It follows that

$$[L_2(\Omega;\mathbb{C}^m), \mathcal{V}]_s = [L_2(\Omega;\mathbb{C}^m), \mathsf{D}(L^{1/2})]_s = \mathsf{D}(L^{s/2}).$$

Thus it suffices to prove that $\mathcal{V}^s \subset [L_2(\Omega;\mathbb{C}^m), \mathcal{V}]_s$. To this end, let $u \in \mathcal{V}^s$. It suffices to show that there exists $F \in \mathsf{H}[L_2(\Omega;\mathbb{C}^m), \mathcal{V}]$ with $F(s) = u$. By definition $g = \gamma u \in B^{s-1/2}(\Sigma;\mathbb{C}^m)$. Therefore there exists

$$G \in \mathsf{H}[B^{-1/2}(\Sigma;\mathbb{C}^m), B^{1/2}(\Sigma;\mathbb{C}^m)] \subset \mathsf{H}[H^{-1/2}(\Sigma;\mathbb{C}^m), H^{1/2}(\Sigma;\mathbb{C}^m)]$$

with $G(s) = g$. Let $F_1 = EG$ where E is the extension operator mentioned in Section 2.1, and note that $F_1 \in \mathsf{H}[L_2(\Omega;\mathbb{C}^m), \mathcal{V}]$. Since $\gamma F_1(s) = \gamma EG(s) = g = \gamma u$, it follows that $u - F_1(s) \in H_0^s(\Omega;\mathbb{C}^m)$. Therefore, there exists

$$F_2 \in \mathsf{H}[L_2(\Omega;\mathbb{C}^m), H_0^1(\Omega;\mathbb{C}^m)] \subset \mathsf{H}[L_2(\Omega;\mathbb{C}^m), \mathcal{V}]$$

with $F_2(s) = u - F_1(s)$. Thus $F = F_1 + F_2 \in \mathsf{H}[L_2(\Omega;\mathbb{C}^m), \mathcal{V}]$ and $F(s) = u$. This completes the proof of Lemma 1. □

LEMMA 2. *The spaces $\{\mathcal{V}^s\}_{1/2<s<3/2}$ form an interpolation family.*

Proof. We need to prove that $\mathcal{V}^s = [\mathcal{V}^{t_1}, \mathcal{V}^{t_2}]_\theta$ for $1/2 < t_1 < s < t_2 < 3/2$ and $s = (1-\theta)t_1 + \theta t_2$. The inclusion $\subset$ is proved in the same way as in the proof of Lemma 1. To prove the inclusion $\supset$, let $u = F(\theta)$, where

$$F \in \mathsf{H}[\mathcal{V}^{t_1}, \mathcal{V}^{t_2}] \subset \mathsf{H}[H^{t_1}(\Omega;\mathbb{C}^m), H^{t_2}(\Omega;\mathbb{C}^m)].$$

Thus $u \in H^s(\Omega;\mathbb{C}^m)$. Furthermore, since $\gamma F \in \mathsf{H}[B^{t_1-1/2}(\Sigma;\mathbb{C}^m), B^{t_2-1/2}(\Sigma;\mathbb{C}^m)]$ we obtain from the interpolation assumptions on $B^s(\Sigma;\mathbb{C}^m)$ that $\gamma u \in B^{s-1/2}(\Sigma;\mathbb{C}^m)$. This proves that $u \in \mathcal{V}^s$ and completes the proof of Lemma 2. □

LEMMA 3. *There exists $0 < c_0 < 1/2$ that depends only on m and the constants implicit in the definition of Ω such that, for $|\alpha| < c_0$, the form $J : \mathcal{V} \times \mathcal{V} \to \mathbb{C}$ extends to a duality $J : \mathcal{V}^{1+\alpha} \times \mathcal{V}^{1-\alpha} \to \mathbb{C}$. In particular, we have the estimate*

$$\|u\|_{H^{1+\alpha}} \lesssim \sup_{v \in \mathcal{V}^{1-\alpha}} \frac{|J[u,v]|}{\|v\|_{H^{1-\alpha}}}, \quad u \in \mathcal{V}^{1+\alpha}.$$

Proof. Using the fact that $H^\alpha(\Omega;\mathbb{C}^m)$ is the dual of $H^{-\alpha}(\Omega;\mathbb{C}^m)$ when $-1/2 < \alpha < 1/2$ we get

$$|J[u,v]| = |(Su, Sv)| \lesssim \|Su\|_{H^\alpha(\Omega;\mathbb{C}^{m+nm})} \|Sv\|_{H^{-\alpha}(\Omega;\mathbb{C}^{m+nm})} \lesssim \|u\|_{H^{1+\alpha}} \|v\|_{H^{1-\alpha}}.$$

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Thus we have an associated bounded operator $L_\alpha : \mathcal{V}^{1+\alpha} \to (\mathcal{V}^{1-\alpha})' : u \mapsto J[u,\cdot]$ when $|\alpha| < 1/2$ which is invertible for $\alpha = 0$. By Lemma 2 and the stability result of Šneĭberg [**18**], there exists a constant $c_0 > 0$ such that $L_\alpha : \mathcal{V}^{1+\alpha} \to (\mathcal{V}^{1-\alpha})'$ is an isomorphism when $|\alpha| < c_0$, which completes the proof of Lemma 3. □

Proof of Proposition 2. Let c_0 be the constant from Lemma 3 and let $0 < \alpha < c_0$. For $u \in \mathsf{D}(L^{(1+\alpha)/2})$ we get from Lemmas 3 and 1, that

$$\|u\|_{H^{1+\alpha}} \lesssim \sup_{v\in\mathcal{V}^{1-\alpha}} \frac{|J[u,v]|}{\|v\|_{H^{1-\alpha}}} \lesssim \sup_{v\in\mathsf{D}(L^{(1-\alpha)/2})} \frac{|(L^{(1+\alpha)/2}u, L^{(1-\alpha)/2}v)|}{\|L^{(1-\alpha)/2}v\|}$$
$$\lesssim \sup_{w\in L_2(\Omega;\mathbb{C}^m)} \frac{|(L^{(1+\alpha)/2}u, w)|}{\|w\|} = \|L^{(1+\alpha)/2}u\|.$$

This completes the proof of Proposition 2. □

We have now completed the proof of Proposition 1 in the case of smooth domains. It remains for us to consider bi-Lipschitz images of smooth domains. In doing so, we use the following operator theoretic lemma. The proof is straightforward and we omit it.

LEMMA 4. *Let $T : \mathcal{H} \to \mathcal{H}'$ be an isomorphism between Hilbert spaces, let $\{\Gamma, B_1, B_2\}$ be operators in $\mathcal{H}$ satisfying* (H1)–(H3). *Assume that Γ' satisfies* (H1) *in $\mathcal{H}'$ and that $\Gamma' T = T\Gamma$ with $\mathsf{D}(\Gamma') = T\mathsf{D}(\Gamma)$.*

Then $\Pi_B = T^{-1}\Pi'_{B'}T$ with $\mathsf{D}(\Pi'_{B'}) = T\mathsf{D}(\Pi_B)$, where $\Pi'_{B'} = \Gamma' + B_1'(\Gamma')^* B_2'$,

$$B_1' := TB_1T^*, \quad B_2' := (T^{-1})^* B_2 T^{-1},$$

and $\{\Gamma', B_1', B_2'\}$ satisfies (H1)–(H3). *Consequently, if $\Pi'_{B'}$ satisfies quadratic estimates, then so does Π_B.*

Proof of Proposition 1. Suppose that $\Omega, \mathcal{V}$ and S have the properties specified at the beginning of this section, and denote the bi-Lipschitz map from the smooth domain Ω' with boundary Σ' to the domain Ω with boundary Σ by $\rho : \overline{\Omega'} \to \overline{\Omega}$.

The map ρ_0^* defined by $\rho_0^* u = u \circ \rho$ is an isomorphism from $L_2(\Omega;\mathbb{C}^m)$ to $L_2(\Omega';\mathbb{C}^m)$, from $H^1(\Omega;\mathbb{C}^m)$ to $H^1(\Omega';\mathbb{C}^m)$ and from $H^s(\Sigma;\mathbb{C}^m)$ to $H^s(\Sigma';\mathbb{C}^m)$ when $|s| \leqslant 1$, and it commutes with the trace map γ. On defining $\mathcal{V}' = \rho_0^*(\mathcal{V})$, we deduce that $\mathcal{V}$ satisfies the same assumptions on Ω' as $\mathcal{V}$ does on Ω. Next define S' to be the unbounded operator

$$S' = \begin{bmatrix} \mathrm{I} \\ \nabla \end{bmatrix} : \mathsf{D}(S') \subset L_2(\Omega';\mathbb{C}^m) \to L_2(\Omega';\mathbb{C}^{m+nm})$$

with dense domain $\mathsf{D}(S') = \mathcal{V}'$, and let

$$\Gamma' = \begin{bmatrix} 0 & 0 \\ S' & 0 \end{bmatrix}.$$

The operator

$$\rho_{01}^* = \begin{bmatrix} \rho_0^* & 0 \\ 0 & \rho_1^* \end{bmatrix}$$

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is an isomorphism from $L_2(\Omega;\mathbb{C}^{m+nm})$ to $L_2(\Omega';\mathbb{C}^{m+nm})$, where ρ_1^* denotes the pullback $\rho_1^* v := (d\rho)^t v \circ \rho : L_2(\Omega;\mathbb{C}^{nm}) \to L_2(\Omega';\mathbb{C}^{nm})$. By the chain rule, $S'\rho_0^* = \rho_{01}^* S$.

We can apply the above lemma with

$$\mathcal{H} = L_2(\Omega;\mathbb{C}^m) \oplus L_2(\Omega;\mathbb{C}^{m+nm}), \quad \mathcal{H}' = L_2(\Omega';\mathbb{C}^m) \oplus L_2(\Omega';\mathbb{C}^{m+nm})$$

and

$$T = \begin{bmatrix} \rho_0^* & 0 \\ 0 & \rho_{01}^* \end{bmatrix},$$

as $\Gamma' T = T\Gamma$. Now $\Omega', \mathcal{V}', S', B_1' = TB_1T^*$ and $B_2' = (T^{-1})^* B_2 T^{-1}$ satisfy the hypotheses of Proposition 1, and we have already proved that $\Pi'_{B'} = \Gamma' + B_1'(\Gamma')^* B_2'$ satisfies the quadratic estimate (2.2) on $\mathsf{R}(\Pi'_{B'})$. Thus Π_B satisfies the quadratic estimate (2.2) on $\mathsf{R}(\Pi_B)$ as required. Thus the proof of Proposition 1 is complete. □

4. *Proof of Theorem 2*

The proof here is an adaption of our previous work in [**7**]. The main novelty is the inhomogeneity in hypotheses (H7) and (H8).

Definition 3. Define bounded operators in $\mathcal{H}$ for each $t \in \mathbb{R}$ by

$$\begin{aligned} R_t^B &= (\mathrm{I} + it\Pi_B)^{-1}, \\ P_t^B &= (\mathrm{I} + t^2\Pi_B^2)^{-1} = \tfrac{1}{2}(R_t^B + R_{-t}^B) = R_t^B R_{-t}^B \\ Q_t^B &= t\Pi_B(\mathrm{I} + t^2\Pi_B^2)^{-1} = \frac{1}{2i}(-R_t^B + R_{-t}^B), \\ \Theta_t^B &= t\Gamma_B^*(\mathrm{I} + t^2\Pi_B^2)^{-1}. \end{aligned}$$

In the unperturbed case $B_1 = B_2 = \mathrm{I}$, we write R_t, P_t and Q_t for R_t^B, P_t^B and Q_t^B.

To prove Theorem 2 it suffices by the Hodge decomposition (2.1) and duality considerations as in [**7**, Proposition 4.8] to prove that the square function estimate

$$\int_0^\infty \|\Theta_t^B P_t u\|^2 \, \frac{dt}{t} \lesssim \|u\|^2 \tag{4.1}$$

holds for every $u \in \mathsf{R}(\Gamma)$ under the hypotheses (H1)–(H8) stated in Section 2, together with the three similar estimates obtained on replacing $\{\Gamma, B_1, B_2\}$ by $\{\Gamma^*, B_2, B_1\}$, $\{\Gamma^*, B_2^*, B_1^*\}$ and $\{\Gamma, B_1^*, B_2^*\}$. As the hypotheses are preserved under these replacements, it suffices to consider (4.1).

We now introduce a *dyadic decomposition* $\triangle$ of Ω that is better suited to our circumstance than the standard dyadic decomposition. It can easily be constructed using hypothesis (H4). The decomposition is given by $\triangle = \bigcup_{j \leqslant j_0} \triangle_{2^j}$ for some $j_0 \leqslant 0$, where each $\triangle_{2^j}$ is a collection of Borel subsets Q of Ω (each of which we refer to as a *dyadic cube*) such that the following holds.

(i) We have $\Omega = \bigcup_{Q \in \triangle_{2^j}} Q$ for every integer $j \leqslant j_0$.
(ii) We have $Q \cap R = \varnothing$ whenever $Q, R \in \triangle_{2^j}$ with $Q \neq R$.
(iii) If $R \in \triangle_{2^k}$ and $Q \in \triangle_{2^j}$ for some $k \leqslant j$, then either $R \subset Q$ or $R \cap Q = \varnothing$.

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(iv) There exists $c \geqslant 1$ such that, for each $j \leqslant j_0$ and each $Q \in \triangle_{2^j}$, the closure of Q is bi-Lipschitz equivalent to a closed ball of radius 2^j, with bi-Lipschitz constants bounded by c.

Set $t_0 := 2^{j_0} \leqslant 1$, and for $0 < t \leqslant t_0$ let $\triangle_t := \triangle_{2^j}$ when $2^{j-1} < t \leqslant 2^j$. Note that $|Q| \approx t^n$, where $|Q|$ denotes the Lebesgue measure of $Q \in \triangle_t$. The *dyadic averaging operator* $A_t : \mathcal{H} \to \mathcal{H}$ is given by

$$A_t u(x) = u_{Q(x,t)} = \frac{1}{|Q(x,t)|} \int_{Q(x,t)} u(y)\, dy$$

for every $x \in \Omega$ and $0 < t \leqslant t_0$, where $Q(x,t)$ is specified by $x \in Q(x,t) \in \triangle_t$.

4.1. *Estimates for inequality* (4.1)

To prove the square function estimate (4.1), we begin by observing that (H8) implies $\|P_t u\| \leqslant \||\Pi|^\alpha P_t u\|$ for every $u \in \mathsf{R}(\Gamma)$, and therefore by spectral theory (because Π is self-adjoint) that

$$\int_{t_0}^\infty \|\Theta_t^B P_t u\|^2 \frac{dt}{t} \lesssim \int_{t_0}^\infty \|(t|\Pi|)^\alpha P_t u\|^2 \frac{dt}{t^{1+2\alpha}} \lesssim \|u\|^2 \int_{t_0}^\infty \frac{dt}{t^{1+2\alpha}} \lesssim \|u\|^2,$$

where $t_0 = 2^{j_0}$. Thus to prove (4.1) it suffices to show that

$$\int_0^{t_0} \|\Theta_t^B P_t u\|^2 \frac{dt}{t} \lesssim \|u\|^2 \tag{4.2}$$

for every $u \in \mathsf{R}(\Gamma)$.

Definition 4. By the *principal part* of the operator family Θ_t^B under consideration, we mean the multiplication operators γ_t defined by

$$\gamma_t(x) w = (\Theta_t^B w)(x)$$

for every $w \in \mathbb{C}^N$. Here we view w on the right-hand side as the constant function defined on Ω by $w(x) = w$. It will be proven in Corollary 2 that $\gamma_t \in L_2^{\mathrm{loc}}(\Omega; \mathcal{L}(\mathbb{C}^N))$.

To establish (4.2), we estimate each of the following three terms separately

$$\begin{aligned}\int_0^{t_0} \|\Theta_t^B P_t u\|^2 \frac{dt}{t} \lesssim{}& \int_0^{t_0} \|\Theta_t^B P_t u - \gamma_t A_t P_t u\|^2 \frac{dt}{t} \\ &+ \int_0^{t_0} \|\gamma_t A_t (P_t - \mathrm{I}) u\|^2 \frac{dt}{t} + \int_0^{t_0} \int_\Omega |A_t u(x)|^2 |\gamma_t(x)|^2 \frac{dx\, dt}{t}\end{aligned} \tag{4.3}$$

when $u \in \mathsf{R}(\Gamma)$.

We estimate the first two terms in Section 4.3, and the last term in Section 4.4. In the next section we introduce crucial off-diagonal estimates for various operators involving Π_B, and also prove local L_2 estimates for γ_t.

4.2. *Off-diagonal estimates*

We require off-diagonal estimates for the following class of operators. Denote $\langle x \rangle = 1 + |x|$, and $\operatorname{dist}(E,F) = \inf\{|x-y| : x \in E, y \in F\}$ for every $E, F \subset \Omega$.

Proposition 3 [**7**, Section 5.1]. *Let U_t be given by P_t^B, Q_t^B or Θ_t^B for every $t > 0$ (see Definition 3). Then for every $M \in \mathbb{N}$ there exists $C_M > 0$ (that depends*

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only on M and the hypotheses (H1)–(H8)) *such that*

$$\|U_t u\|_{L_2(E)} \leqslant C_M \langle \operatorname{dist}(E,F)/t\rangle^{-M} \|u\| \tag{4.4}$$

whenever $E, F \subset \Omega$ are Borel sets, and $u \in \mathcal{H}$ satisfies $\operatorname{supp} u \subset F$.

The proof is omitted as it is essentially the same as [**7**, Proposition 5.2]. The key hypothesis used in the proof is (H6). A simple consequence is that

$$\|U_s u\|_{L_2(Q)} \leqslant \sum_{R\in\triangle_t} \|U_s(\chi_R u)\|_{L_2(Q)} \lesssim \sum_{R\in\triangle_t} \langle \operatorname{dist}(R,Q)/s\rangle^{-M} \|u\|_{L_2(R)} \tag{4.5}$$

whenever $0 < s \leqslant t$ and $Q \in \triangle_t$, where U_s is as specified in Proposition 3. We also note that the dyadic cubes satisfy

$$\sup_{Q\in\triangle_t} \sum_{R\in\triangle_t} \langle \operatorname{dist}(R,Q)/t\rangle^{-(n+1)} \lesssim 1, \tag{4.6}$$

and therefore, choosing $M \geqslant n+1$, we see that U_t extends to an operator $U_t : L_\infty(\Omega) \to L_2^{\mathrm{loc}}(\Omega)$. The following corollary is a consequence of the above results with $U_t = \Theta_t^B$.

Corollary 2. *The functions $\gamma_t \in L_2^{\mathrm{loc}}(\Omega; \mathcal{L}(\mathbb{C}^N))$ satisfy the boundedness conditions*

$$\frac{1}{|Q|}\int_Q |\gamma_t(y)|^2\, dy \lesssim 1$$

for all $Q \in \triangle_t$, $0 < t \leqslant t_0$. Moreover $\|\gamma_t A_t\| \lesssim 1$ uniformly in t.

4.3. *Principal part approximation*

In this section we prove the principal part approximation $\Theta_t^B \approx \gamma_t$ in the sense that we estimate the first two terms on the right-hand side of (4.3). The following lemma is used in estimating the first term.

Lemma 5. *If $0 < t \leqslant t_0$, $Q \in \triangle_t$ and $M > 2n$, then we have*

$$\int_\Omega |u(x) - u_Q|^2 \langle \operatorname{dist}(x,Q)/t\rangle^{-M}\, dx \lesssim \int_\Omega (|t\nabla u(x)|^2 + |tu(x)|^2)\langle \operatorname{dist}(x,Q)/t\rangle^{2n-M}\, dx$$

for every u in the Sobolev space $H^1(\Omega;\mathbb{C}^N)$.

Proof. In the case when Ω is a smooth domain one can use reflection techniques to construct an extension operator $\mathcal{E} : H^1(\Omega;\mathbb{C}^N) \to H^1(\mathbb{R}^n;\mathbb{C}^N)$ such that

$$\begin{aligned}\int_{\mathbb{R}^n} |\nabla(\mathcal{E}u)(x)|^2 \langle \operatorname{dist}(x,Q)/t\rangle^{2n-M}\, dx \\ \lesssim \int_\Omega (|\nabla u(x)|^2 + |u(x)|^2)\langle \operatorname{dist}(x,Q)/t\rangle^{2n-M}\, dx.\end{aligned}$$

The desired estimate then follows from the corresponding result on $\mathbb{R}^n$ [**7**, Lemma 5.4], noting that the set Q used there does not need to be a Euclidean cube, but merely satisfy $|Q| \approx t^n$.

In the general case of a domain which is bi-Lipschitz equivalent to a smooth domain, the bi-Lipschitz parametrization of Ω gives the required inequality, except for the fact that u_Q is replaced by a constant $c = c(u,Q)$. However, this suffices,

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because

$$\int_\Omega |u_Q - c|^2 \langle \operatorname{dist}(x,Q)/t\rangle^{-M}\,dx \lesssim t^n |u_Q - c|^2 \lesssim \int_\Omega |u(x)-c|^2 \langle \operatorname{dist}(x,Q)/t\rangle^{-M}\,dx.$$

□

We now estimate the first term in the right-hand side of (4.3).

PROPOSITION 4. *For all $u \in \mathsf{R}(\Gamma)$, we have*

$$\int_0^{t_0} \|\Theta_t^B P_t u - \gamma_t A_t P_t u\|^2 \,\frac{dt}{t} \lesssim \|u\|^2.$$

Proof. Using Proposition 3, Lemma 5 and estimate (4.6) we get, as in [**7**], that

$$\|\Theta_t^B v - \gamma_t A_t v\| \lesssim t \|v\|_{H^1(\Omega;\mathbb{C}^N)}$$

for every v in the Sobolev space $H^1(\Omega;\mathbb{C}^N)$. Since $\Theta_t^B - \gamma_t A_t$ is bounded on $\mathcal{H}$, we have by interpolation and then (H8) that

$$\|\Theta_t^B v - \gamma_t A_t v\| \lesssim t^\alpha \|v\|_{H^\alpha(\Omega;\mathbb{C}^N)} \lesssim \|(t|\Pi|)^\alpha v\|$$

for every $v \in \mathsf{R}(\Gamma) \cap \mathsf{D}(\Pi^2)$.

Taking $v = P_t u$, we then have

$$\int_0^{t_0} \|\Theta_t^B P_t u - \gamma_t A_t P_t u\|^2 \,\frac{dt}{t} \lesssim \int_0^{t_0} \|(t|\Pi|)^\alpha P_t u\|^2 \,\frac{dt}{t} \lesssim \|u\|^2.$$

The last inequality above follows from spectral theory. This completes the proof. □

We use the following lemma to estimate the second term on the right-hand side of (4.3), and also in the proof of Lemma 7 (cf. Lemma 5.15 of [**3**]).

LEMMA 6. *Let Υ be either Π, Γ or Γ^*. Then we have the estimate*

$$\left|\frac{1}{|Q|}\int_Q \Upsilon u\right|^2 \lesssim \frac{1}{t}\left(\frac{1}{|Q|}\int_Q |u|^2\right)^{1/2}\left(\frac{1}{|Q|}\int_Q |\Upsilon u|^2\right)^{1/2} + \frac{1}{|Q|}\int_Q |u|^2 \tag{4.7}$$

for all $Q \in \triangle_t$ and $u \in \mathsf{D}(\Upsilon)$.

Proof. Let

$$\tau = \left(\int_Q |u|^2\right)^{1/2}\left(\int_Q |\Upsilon u|^2\right)^{-1/2}.$$

If $\tau \geqslant t$, then (4.7) follows directly from the Cauchy–Schwarz inequality. If $\tau \leqslant t$, let $\eta \in C_0^\infty(Q)$ be a real-valued bump function with $|\nabla \eta| \lesssim 1/\tau$ such that $\eta(x) = 1$ whenever $x \in Q$ satisfies $d(x, \mathbb{R}^n \setminus Q) \geqslant \tau$. Then by hypothesis (H7), the Cauchy–Schwarz inequality, and the fact that $|\{x \in Q : \operatorname{dist}(x, \mathbb{R}^n \setminus Q) \leqslant \tau\}| \lesssim \tau t^{n-1}$,

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we obtain

$$\begin{aligned}\left|\int_Q \Upsilon u\right| &= \left|\int_Q (1-\eta)\Upsilon u + \int_Q \eta\Upsilon u\right| \\ &= \left|\int_Q (1-\eta)\Upsilon u + \int_Q [\eta,\Upsilon]u + \int_Q \Upsilon(\eta u)\right| \\ &\lesssim (\tau t^{n-1})^{1/2}\left(\int_Q |\Upsilon u|^2\right)^{1/2} \\ &\quad + \|\nabla\eta\|_\infty(\tau t^{n-1})^{1/2}\left(\int_Q |u|^2\right)^{1/2} + |Q|^{1/2}\left(\int_Q |u|^2\right)^{1/2},\end{aligned}$$

which leads to (4.7) on substituting the chosen value of τ. □

We now estimate the second term on the right-hand side of (4.3).

PROPOSITION 5. *For all $u \in \mathcal{H}$, we have*

$$\int_0^{t_0} \|\gamma_t A_t (P_t - \mathrm{I})u\|^2 \,\frac{dt}{t} \lesssim \|u\|^2.$$

Proof. Corollary 2 shows that $\|\gamma_t A_t\| \lesssim 1$ and since $A_t^2 = A_t$ it suffices to prove the square function estimate with integrand $\|A_t(P_t - \mathrm{I})u\|^2$. If $u \in \mathsf{N}(\Pi)$ then this is zero. If $u \in \mathsf{R}(\Pi)$ then by spectral theory we can write

$$u = 2\int_0^\infty Q_s^2 u \,\frac{ds}{s}.$$

The result will follow from a Schur estimate and the spectral theory estimate

$$\int_0^\infty \|Q_t u\|^2 \,\frac{dt}{t} \leqslant \|u\|^2$$

once we have obtained the bound

$$\|A_t(P_t - \mathrm{I})Q_s\| \lesssim \min\left\{\frac{s}{t}, \frac{t}{s}\right\}^{1/2}$$

for all $s > 0$ and $0 < t \leqslant t_0$.

Note that

$$(\mathrm{I} - P_t)Q_s = \frac{t}{s}Q_t(\mathrm{I} - P_s) \quad \text{and} \quad P_t Q_s = \frac{s}{t}Q_t P_s \quad \text{for every } s, t > 0.$$

Thus, if $t \leqslant \min(s, t_0)$, then

$$\|A_t(P_t - \mathrm{I})Q_s\| \lesssim \|(P_t - \mathrm{I})Q_s\| \lesssim t/s,$$

while if $s < t \leqslant t_0$, then

$$\|A_t(P_t - \mathrm{I})Q_s\| \lesssim \|P_t Q_s\| + \|A_t Q_s\| \lesssim s/t + \|A_t Q_s\|.$$

To estimate $\|A_t Q_s\|$, we use Lemma 6 with (4.5) and (4.6) to obtain

$$\begin{aligned}\|A_t Q_s u\|^2 &= \sum_{Q\in\triangle_t} \frac{1}{|Q|}\left|\int_Q s\Pi(\mathrm{I} + s^2\Pi^2)^{-1}u\right|^2 \\ &\lesssim \frac{s}{t}\sum_{Q\in\triangle_t}\left(\int_Q |P_s u|^2\right)^{1/2}\left(\int_Q |Q_s u|^2\right)^{1/2} + s^2\int_Q |P_s u|^2\end{aligned}$$

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$$\lesssim \frac{s}{t}\sum_{Q\in\triangle_t}\Bigg(\sum_{R\in\triangle_t}\langle d(R,Q)/t\rangle^{-(n+1)}\|u\|_{L_2(R)}\Bigg)^2+\left(\frac{s}{t}\right)^2\|u\|^2$$
$$\lesssim \frac{s}{t}\sum_{Q\in\triangle_t}\Bigg(\sum_{R'\in\triangle_t}\langle d(R',Q)/t\rangle^{-(n+1)}\Bigg)\Bigg(\sum_{R\in\triangle_t}\langle d(R,Q)/t\rangle^{-(n+1)}\|u\|^2_{L_2(R)}\Bigg)$$
$$+\left(\frac{s}{t}\right)^2\|u\|^2\lesssim\frac{s}{t}\|u\|^2,$$

which completes the proof. □

We have now estimated the first two terms on the right-hand side of (4.3).

4.4. *Carleson measure estimate*

In this subsection we estimate the third term on the right-hand side of (4.3). To do this we reduce the problem to a Carleson measure estimate. Recall that a measure μ on $\Omega\times(0,t_0)$ is said to be *Carleson* if $\|\mu\|_{\mathcal{C}}=\sup_{Q\in\triangle}|Q|^{-1}\mu(R_Q)<\infty$. Here and below, $R_Q=Q\times(0,2^j)$ denotes the *Carleson box* over $Q\in\triangle_{2^j}$. For such Q we define $\lambda Q=\{x\in\mathbb{R}^n:\operatorname{dist}(x,Q)\leqslant(\lambda-1)2^j\}$ when $\lambda\geqslant 1$.

We now recall the following theorem of Carleson.

THEOREM 4 [**19**, p. 59]. *If μ is a Carleson measure on $\Omega\times(0,t_0)$ then*

$$\int\!\!\int_{\Omega\times(0,t_0)}|A_tu(x)|^2\,d\mu(x,t)\leqslant C\|\mu\|_{\mathcal{C}}\|u\|^2$$

for every $u\in\mathcal{H}$. Here $C>0$ is a constant that depends only on n.

Thus, in order to prove (4.3) it suffices to show that

$$\int\!\!\int_{R_Q}|\gamma_t(x)|^2\,\frac{dx\,dt}{t}\lesssim|Q| \tag{4.8}$$

for every dyadic cube $Q\in\triangle$.

Define a measure ν on $\Omega\times(0,t_0)$ by

$$d\nu=\chi(x,t)\frac{dx\,dt}{t},$$

where χ is the characteristic function defined by $\chi(x,t)=1$ if there is $x\in Q\in\triangle_t$ with $4Q\setminus\Omega\neq\emptyset$; otherwise let $\chi(x,t)=0$. It follows from (H4) that ν is a Carleson measure. From Corollary 2 we then see that $|\gamma_t(x)|^2\,d\nu(x,t)$ is a Carleson measure. Now, the sum of two Carleson measures is again Carleson. Therefore, to prove (4.8) it remains to consider the case when $Q\in\triangle$ with $4Q\subset\Omega$.

Fix such a cube Q and set $\sigma>0$; its value is to be chosen later. Let $\mathcal{F}$ be a finite set consisting of $\nu\in\mathcal{L}(\mathbb{C}^N)$ with $|\nu|=1$, such that $\bigcup_{\nu\in\mathcal{F}}K_\nu=\mathcal{L}(\mathbb{C}^N)\setminus\{0\}$, where

$$K_\nu=\left\{\nu'\in\mathcal{L}(\mathbb{C}^N)\setminus\{0\}:\left|\frac{\nu'}{|\nu'|}-\nu\right|\leqslant\sigma\right\}.$$

To prove (4.8) it suffices to show that

$$\int\!\!\int_{\substack{(x,t)\in R_Q\\ \gamma_t(x)\in K_\nu}}|\gamma_t(x)|^2\,\frac{dx\,dt}{t}\lesssim|Q| \tag{4.9}$$

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for every $\nu \in \mathcal{F}$. By a standard stopping time argument as used in [**3**, Section 5], in order to prove (4.9) it suffices to prove the following claim.

PROPOSITION 6. *There exists $\beta > 0$ such that for every dyadic cube $Q \in \triangle$ with $4Q \subset \Omega$, and for every $\nu \in \mathcal{L}(\mathbb{C}^N)$ with $|\nu| = 1$, there is a collection $\{Q_k\}_k \subset \triangle$ of disjoint subcubes of Q such that $|E_{Q,\nu}| > \beta|Q|$ where $E_{Q,\nu} = Q \setminus \bigcup_k Q_k$, and such that*

$$\int\int_{\substack{(x,t)\in E^*_{Q,\nu}\\ \gamma_t(x)\in K_\nu}} |\gamma_t(x)|^2 \,\frac{dx\,dt}{t} \lesssim |Q|,$$

where $E^*_{Q,\nu} = R_Q \setminus \bigcup_k R_{Q_k}$.

Let $Q \in \triangle_\tau$ and ν be as in the above proposition. Choose $\hat{w}, w \in \mathbb{C}^N$ with $|\hat{w}| = |w| = 1$ and $\nu^*(\hat{w}) = w$. Let η_Q be a smooth cut-off function with range $[0,1]$, equal to 1 on $2Q$, with support in $4Q$, and such that $\|\nabla\eta_Q\|_\infty \leqslant 1/\tau$. Define $w_Q = \eta_Q w$, and for each $\epsilon > 0$ let

$$f^w_{Q,\epsilon} = w_Q - \epsilon\tau i\Gamma(1+\epsilon\tau i\Pi_B)^{-1}w_Q = (1+\epsilon\tau i\Gamma^*_B)(1+\epsilon\tau i\Pi_B)^{-1}w_Q.$$

LEMMA 7. *We have $\|f^w_{Q,\epsilon}\| \lesssim |Q|^{1/2}$,*

$$\int\int_{R_Q} |\Theta^B_t f^w_{Q,\epsilon}|^2 \,\frac{dx\,dt}{t} \lesssim \frac{1}{\epsilon^2}|Q| \quad \text{and} \quad \left|\frac{1}{|Q|}\int_Q f^w_{Q,\epsilon} - w\right| \leqslant C\epsilon^{1/2}$$

for every $\epsilon > 0$. Here C is a constant that depends only on hypotheses (H1)–(H8).

Proof. The first and second estimates follow as in [**7**]. To obtain the last estimate, we use the fact that $\tau \leqslant 1$ and also Lemma 6 with $\Upsilon = \Gamma$ and $u = (\mathrm{I}+\epsilon\tau i\Pi_B)^{-1}w_Q$ to show that

$$\begin{aligned}
&\left|\frac{1}{|Q|}\int_Q f^w_{Q,\epsilon} - w\right| \\
&\quad= \left|\frac{1}{|Q|}\int_Q \epsilon\tau\Gamma(\mathrm{I}+\epsilon\tau i\Pi_B)^{-1}w_Q\right| \\
&\quad\lesssim \epsilon^{1/2}\left(\frac{1}{|Q|}\int_Q |(\mathrm{I}+\epsilon\tau i\Pi_B)^{-1}w_Q|^2\right)^{1/4}\left(\frac{1}{|Q|}\int_Q |\epsilon\tau\Gamma(\mathrm{I}+\epsilon\tau i\Pi_B)^{-1}w_Q|^2\right)^{1/4} \\
&\qquad+ \epsilon\tau\left(\frac{1}{|Q|}\int_Q |(\mathrm{I}+\epsilon\tau i\Pi_B)^{-1}w_Q|^2\right)^{1/2} \\
&\quad\lesssim \epsilon^{1/2}.
\end{aligned}$$

This completes the proof. □

The proof of Proposition 6 can now be completed exactly as in [**7**]. Therefore the last term in (4.3) is bounded by a constant times $\|u\|^2$. This proves the square function estimate (4.1) and thus Theorem 2.

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