Calderón Reproducing formulas and applications to Hardy spaces
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CALDERÓN REPRODUCING FORMULAS AND APPLICATIONS TO HARDY SPACES

PASCAL AUSCHER, ALAN MCINTOSH, AND ANDREW J. MORRIS

Abstract. We establish new Calderón reproducing formulas for self-adjoint operators $D$ that generate strongly continuous groups with finite propagation speed. These formulas allow the analysing function to interact with $D$ through holomorphic functional calculus whilst the synthesising function interacts with $D$ through functional calculus based on the Fourier transform. We apply these to prove the embedding $H^p_D(\wedge T^*M) \subseteq L^p(\wedge T^*M)$, $1 \leq p \leq 2$, for the Hardy spaces of differential forms introduced by Auscher, McIntosh and Russ, where $D = d + d^*$ is the Hodge–Dirac operator on a complete Riemannian manifold $M$ that has doubling volume growth. This fills a gap in that work. The new reproducing formulas also allow us to obtain an atomic characterisation of $H^1_D(\wedge T^*M)$. The embedding $H^p_L \subseteq L^p$ for divergence form elliptic operators, or a nonnegative self-adjoint operator that satisfies Davies–Gaffney estimates on a doubling metric measure space, is also established in the case when the semigroup generated by the adjoint $-L^*$ is ultracontractive.

Contents

1. Introduction and Main Results 1
2. Notation and Preliminaries 6
3. Sectorial Operators with Off-Diagonal Estimates 7
3.1. Molecular Theory 13
3.2. The Embedding $H^p_L \subseteq L^p$ for Divergence Form Elliptic Operators 15
4. Self-Adjoint Operators with Finite Propagation Speed 16
4.1. Atomic Theory 21
4.2. The Embedding $H^p_L \subseteq L^p$ for Smooth Differential Operators 22
5. The Embedding $H^p_L \subseteq L^p$ for Nonnegative Self-Adjoint Operators 24
6. Appendix: Off-Diagonal Estimates 27
Acknowledgements 30
References 30

1. Introduction and Main Results

The classical Hardy spaces $H^p(\mathbb{R}^n) \subseteq L^p(\mathbb{R}^n)$ provide a substitute for the $L^p(\mathbb{R}^n)$ scale of spaces on which homogeneous multipliers, such as the Riesz transforms $(R_j u)(\xi) = i\xi_j |\xi|^{-1} \hat{u}(\xi)$ for $j \in \{1, \ldots, n\}$, are bounded when $p \in [1, \infty)$. It is well

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known that $H^p(\mathbb{R}^n) = L^p(\mathbb{R}^n)$ when $p \in (1, \infty)$, whilst $H^1(\mathbb{R}^n) \subset L^1(\mathbb{R}^n)$, and that $H^1(\mathbb{R}^n)$ has an atomic characterisation and a molecular characterisation.

A variety of new Hardy spaces have been designed to obtain a similar theory for useful operators that do not belong to the standard Calderón–Zygmund class. We are primarily motivated by the Hardy spaces of differential forms $H^p_0(\wedge^* M)$ introduced by Auscher, McIntosh and Russ [9]. We temporarily restrict our attention to these spaces, although the main content of the paper contains a more general theory that can be applied to a variety of the contexts considered elsewhere.

The $H^p_0(\wedge^* M)$ spaces were designed for the analysis of the Hodge–Dirac operator $D = d + d^*$ and the Hodge–Laplacian $\Delta = D^2$, where $d$ and $d^*$ denote the exterior derivative and its adjoint, acting on the Hilbert space of square integrable differential forms $L^2(\wedge^* M)$ over a complete Riemannian manifold $M$. We will always assume that any such manifold $M$ is smooth and connected, and has doubling volume growth in the sense that there exist constants $A \geq 1$ and $\kappa \geq 0$ such that

$$(D_\kappa) \quad 0 < V(x, ar) \leq Aa^\kappa V(x, r) < \infty \quad \forall x \in M, \forall r > 0, \forall a \geq 1,$$

where $V(x, r)$ is the Riemannian measure of the geodesic ball $B(x, r)$ in $M$ with centre $x$ and radius $r$. These spaces were designed so that the geometric Riesz transform $D\Delta^{-1/2}$ is bounded on $H^p_0(\wedge^* M)$ when $p \in [1, \infty]$, and a molecular characterisation was obtained for $H^p_0(\wedge^* M)$.

One of the aims of this paper is to show that $H^p_0(\wedge^* M) \subseteq L^p(\wedge^* M)$ when $p \in [1, 2]$. This result was stated in [9] Corollary 6.3 but the proof contains a gap that we will fill here. Another aim is to show that $H^p_0(\wedge^* M)$ has an atomic characterisation, thus strengthening the result in [9] Theorem 6.2 that $H^1_0(\wedge^* M)$ has a molecular characterisation.

We now outline the main ideas. A function $f : S^0_\Theta \rightarrow \mathbb{C}$ is called nondegenerate when it is not identically zero on $\{z \in S^0_\Theta : \text{Re } z > 0\}$ nor on $\{z \in S^0_\Theta : \text{Re } z < 0\}$, where $S^0_\Theta$ is the open bisector in $\mathbb{C}$ of angle $\Theta \in (0, \pi/2)$ defined in (3.1). The space $H^p_0(\wedge^* M)$ is defined as a completion of a normed space $E^p_{D, \psi}(\wedge^* M)$ associated with a nondegenerate function $\psi$ from the set

$$\Psi^p_\sigma(S^0_\Theta) = \{\psi \in H^\infty(S^0_\Theta \cup \{0\}) : |\psi(z)| \lesssim \min\{|z|^\sigma, |z|^{-\tau}\}\},$$

for some $\sigma, \tau > 0$, where $H^\infty(S^0_\Theta \cup \{0\})$ denotes the algebra of bounded functions on $S^0_\Theta \cup \{0\}$ that are holomorphic on $S^0_\Theta$. We shall not define $E^p_{D, \psi}(\wedge^* M)$ precisely here except to mention that

$$(1.1) \quad u \in E^p_{D, \psi} \quad \text{if and only if} \quad u = \int_0^\infty \psi_t(D) U_t \frac{dt}{t} \quad \text{for some } U \in T^p \cap T^2,$$

where $T^p = T^p((\wedge^* M)_\perp)$ is an appropriate analogue of the tent space $T^p(\mathbb{R}^{n+1}_+)$ introduced by Coifman, Meyer and Stein [15], and $\psi_\tau(D) = \psi(tD)$ is defined by the holomorphic functional calculus of $D$ (see Definition 3.4).

There is an important distinction between a completion of $E^p_{D, \psi}$ and the completion of $E^p_{D, \psi}$ in $L^p$. The former is unique up to isometric isomorphism and can always be constructed as an abstract space, whereas the latter is a unique subspace of $L^p$ that may or may not exist. See Section 2 for further details. It was known previously that $E^p_{D, \psi} \subseteq L^p$ when $\psi$ has suitable decay at the origin and infinity, but this does not guarantee, nor was it proved, that the completion of $E^p_{D, \psi}$ in $L^p$ exists. Without this property, a completion of $E^p_{D, \psi}$ must be interpreted as an abstract space consisting
of, for example, equivalence classes of Cauchy sequences in $E_{D,\psi}^p$ or elements of the second dual space $(E_{D,\psi}^p)^{**}$. Although various realizations of such an abstract Hardy space were known, these were not shown to be contained in any function space. The approach of Hofmann, Mayorodera and McIntosh \cite{21 Appendix 2}, for instance, can be used to realize the abstract Hardy space as a space of distributions adapted to $D$.

We prove that the completion of $E_{D,\psi}^p(\wedge T^*M)$ in $L^p(\wedge T^*M)$ exists by utilizing the finite propagation speed of the $C_0$-group $(e^{itD})_{t\in\mathbb{R}}$ generated by the Hodge–Dirac operator $D$ on $L^2(\wedge T^*M)$. This provides a constant $c_D > 0$ such that for all geodesic balls $B(x,r) \subseteq M$, all $u \in L^2(\wedge T^*M)$ with $\text{sppt}(u) \subseteq B(x,r)$ and all $t \in \mathbb{R}$, it holds that $\text{sppt}(e^{itD}u) \subseteq B(x,r+c_D|t|)$.

The main ideas of the argument are as follows. We use nondegenerate Schwartz functions $\eta$ with compactly supported Fourier transform $\hat{\eta}$ from the set

$$\tilde{\Psi}_N^\delta(\mathbb{R}) = \{ \eta \in \mathcal{S}(\mathbb{R}) : \text{sppt} \hat{\eta} \subseteq [-\delta, \delta] \text{ and } \partial^k \eta(0) = 0 \text{ for all } k \in \{1, \ldots, N\} \},$$

for some $\delta > 0$ and $N \in \mathbb{N}$, to interact with the finite propagation speed of the group. We will see that for all $t > 0$, all $\eta \in \tilde{\Psi}_N^\delta(\mathbb{R})$ and all $u \in L^2(\wedge T^*M)$ with $\text{sppt}(u) \subseteq B(x,r)$, it holds that $\text{sppt}(\eta(D)u) \subseteq B(x,r+c_Dt)$, where $\eta(D) = \eta(tD)$ is defined by the Borel functional calculus of $D$. This is in contrast with a function $\psi \in \Psi((S^p_D)^*)$, for which $\psi(D)u$ may be supported everywhere on $M$.

We incorporate the finite propagation speed into the existing theory by choosing $\hat{\psi} \in \Psi((S^p_D)^*)$ and $\eta \in \tilde{\Psi}(\mathbb{R})$ so that the following Calderón reproducing formula holds:

$$\int_0^\infty \psi_t(D)\eta(D)u \frac{dt}{t} = \int_0^\infty \eta(D)\psi_t(D)u \frac{dt}{t} = u \quad \forall u \in E_{D,\psi}^p \cup E_{D,\eta}^p. \quad (1.2)$$

A comparison of (1.1) and (1.2) shows that if $u \in E_{D,\eta}^p$ and $\eta(D)u \in T^p \cap T^2$, then $u \in E_{D,\psi}^p$. This principle allows us to prove that $E_{D,\psi}^p = E_{D,\eta}^p$ when the family of operators $(\psi_t(D)\eta_s(D))_{s,t \in (0,\infty)}$ has enough $L^2$ off-diagonal decay to control volume growth on the manifold. We then use the Sobolev embedding theorem on geodesic balls and standard energy estimates for the group $(e^{itD})_{t \in \mathbb{R}}$ to prove that the completion of $E_{D,\eta}^p$ in $L^p$ exists, hence the completion of $E_{D,\psi}^p$ in $L^p$ exists as well.

Let us remark that the connection between the classical Hardy spaces $H^p(\mathbb{R}^n)$ and the tent spaces $T^p(\mathbb{R}^{n+1})_{0}$ was previously understood in terms of reproducing formulas analogous to (1.2) for convolution operators. In particular, Coifman, Meyer and Stein provided a short proof of the atomic characterisation of $H^p(\mathbb{R}^n)$ for $p \in (0,1]$ in \cite{15 Section 9b} by using the theory of tent spaces and constructing a function $\phi \in C_0^\infty(\mathbb{R}^n)$ satisfying $\int x^\gamma \phi(x) \, dx = 0$ for all $\gamma \in [0,N_p]$ and some $N_p \in \mathbb{N}$ depending on $p$ such that

$$\int_0^\infty \phi(t) * \partial_t P(t) * f \, dt = f \quad \forall f \in H^p(\mathbb{R}^n),$$

where $P$ is the Poisson kernel and $P(t)(x) = t^{-n}P(x/t)$. This is equivalent to

$$\int_0^\infty \phi_t(t\xi)(-2\pi t|\xi|) e^{-2\pi t|\xi|} \frac{dt}{t} = 1 \quad \forall \xi \in \mathbb{R}^n \setminus \{0\},$$

with $\phi_t(x) = \phi(x/t)$.
from which the analogy with \([1.2]\) is most apparent when \(n = 1\), since \(\eta(x) := \hat{\phi}(x)\)
is in \(\Psi^\delta_{N_\eta+1}(\mathbb{R})\) for some \(\delta > 0\), whilst \(\psi(z) := \begin{cases} -2\pi z e^{-2\pi z}, & \text{if } \text{Re}(z) \geq 0 \\ 2\pi z e^{2\pi z}, & \text{if } \text{Re}(z) < 0 \end{cases}\)
is in \(\Psi^\delta_1(S^\theta_\eta)\) for all \(\tau > 0\) and \(\theta \in (0, \pi/2)\).

After we establish the embedding \(H^1_D(\mathbb{T}^* M) \subseteq L^1(\mathbb{T}^* M)\), the finite propagation speed of the group \((e^{itD})_{t \in \mathbb{R}}\) also allows us to obtain an atomic characterisation of \(H^1_D(\mathbb{T}^* M)\). This builds on the molecular characterisation obtained in \([7]\). The molecular space \(H^1_{D,\text{mol}(N)}(\mathbb{T}^* M)\) and the atomic space \(H^1_{D,\text{at}(N)}(\mathbb{T}^* M)\) are introduced in Definition \(3.12\), where \(N \in \mathbb{N}\) is the number of moment conditions satisfied by the molecules and atoms in the respective spaces.

The following theorem summarizes our results for the Hodge–Dirac operator.

**Theorem 1.1.** Suppose that \(M\) is a complete Riemannian manifold satisfying \([D_3]\) and that \(D = d + d^*\) is the Hodge–Dirac operator on \(L^2(\mathbb{T}^* M)\). If \(p \in [1, 2]\), \(\theta \in (0, \pi/2)\), \(\beta > \kappa/3\) and \(\psi \in \Psi_\beta(S^\theta_\eta)\) is nondegenerate, then the completion \(H^p_{D,\psi}(\mathbb{T}^* M)\) of \(E^p_{D,\psi}(\mathbb{T}^* M)\) in \(L^p(\mathbb{T}^* M)\) exists. Moreover, if \(N \in \mathbb{N}\) and \(N > \kappa/2\), then \(H^p_{D,\psi}(\mathbb{T}^* M) = H^1_{D,\text{mol}(N)}(\mathbb{T}^* M) = H^1_{D,\text{at}(N)}(\mathbb{T}^* M)\).

The Hardy space \(H^p_{D,\psi}(\mathbb{T}^* M)\) in Theorem \ref{t:1.1} is thus the set of all \(u\) in \(L^p(\mathbb{T}^* M)\) for which there exists a Cauchy sequence \((u_n)_n\) in \(E^p_{D,\psi}(\mathbb{T}^* M)\) that converges to \(u\) in \(L^p(\mathbb{T}^* M)\), together with the norm \(\|u\|_{H^p_{D,\psi}} = \lim_n \|u_n\|_{E^p_{D,\psi}}\). The embedding \(H^p_{D,\psi}(\mathbb{T}^* M) \subseteq L^p(\mathbb{T}^* M)\) is then automatic. The comments below Definition \ref{d:2.1} contain more details.

The results obtained here can also be applied to Hardy spaces designed for higher order operators. In particular, consider the Hardy spaces \(H^p_{L,\psi}(\mathbb{R}^n)\) introduced by Hofmann, Mayboroda and McIntosh \([21]\) for the analysis of divergence form operators \(L = -\text{div} A\nabla = -\sum_{j,k=1}^n \partial_j A_{jk} \partial_k\), acting on \(L^2(\mathbb{R}^n)\) and interpreted in the usual weak sense via a sesquilinear form, where \(A = (A_{jk}) \in \mathbb{L}^\infty(\mathbb{R}^n, \mathbb{L}(\mathbb{C}^n))\) is elliptic in the sense that there exists \(\lambda > 0\) such that

\[
\text{Re}(A(x)\zeta, \zeta)_{\mathbb{C}^n} \geq \lambda |\zeta|^2 \quad \forall \zeta \in \mathbb{C}^n, \text{ a.e. } x \in \mathbb{R}^n.
\]

There exists \(\omega_L \in [0, \pi/2]\) such that \(L\) is \(\omega_L\)-sectorial, hence \(-L\) and \(-L^*\) generate analytic semigroups \((e^{-tL})_{t \geq 0}\) and \((e^{-tL^*})_{t \geq 0}\) on \(L^2(\mathbb{R}^n)\). In order to embed \(H^p_{L,\psi}(\mathbb{R}^n)\) in \(L^p(\mathbb{R}^n)\) when \(1 \leq p < 2\), we assume that there exists \(g \in L^2_{\text{loc}}((0, \infty))\) such that

\[
\|e^{-tL^*} u\|_\infty \leq g(t)\|u\|_2 \quad \forall u \in L^2(\mathbb{R}^n), \forall t > 0.
\]

Let us remark that \((1.4)\) is equivalent to the action of the semigroup \((e^{-tL})_{t \geq 0}\) from \(L^1(\mathbb{R}^n)\) to \(L^2(\mathbb{R}^n)\) (it is usually called ultracontractivity). Hence, this action of the semigroup on \(L^1(\mathbb{R}^n)\) suffices to obtain \(H^1_{L,\psi}(\mathbb{R}^n)\) as a subspace of \(L^1(\mathbb{R}^n)\) in Theorem \ref{t:1.2} below.

Let us also remark that \((1.4)\) is immediate when the semigroup \((e^{-tL^*})_{t \geq 0}\) has a kernel \((K_t(\cdot, \cdot))_{t \geq 0}\) defined pointwise almost everywhere on \(\mathbb{R}^n \times \mathbb{R}^n\) with the property that for each \(T > 0\), there exist constants \(C_T, c_T > 0\) such that

\[
|K_t(x, y)| \leq C_T t^{-n/2} e^{-c_T |x-y|^2/t} \quad \forall x, y \in \mathbb{R}^n, \forall t \in (0, T].
\]

In fact, property \((1.4)\) is usually obtained as a step toward proving \((1.5)\). For example, the local Gaussian estimates in \((1.5)\) hold when, in addition to having \(A\).
bounded and elliptic, $A$ is uniformly continuous (see [4, Theorem 4.8]) or belongs to $VMO$ or has small $BMO$ norm (see [10, Chapter 1]).

The following theorem is essentially known when \((1.5)\) holds (see the remark below Proposition 9.1 in [21]). We provide a short proof when \((1.4)\) holds as an application of our techniques.

**Theorem 1.2.** Suppose that $A \in L^\infty(\mathbb{R}^n, \mathcal{L}(\mathbb{C}^n))$ is elliptic and that $L = -\div A \nabla$ on $L^2(\mathbb{R}^n)$ satisfies \((1.4)\). If $p \in [1, 2]$, $\theta \in (\omega_L, \pi/2)$, $\beta > n/4$ and $\psi \in \Psi_\beta(S^2_0)$ is nondegenerate, then the completion $H^p_{L,\psi}(\mathbb{R}^n)$ of $E^p_{L,\psi}(\mathbb{R}^n)$ in $L^p(\mathbb{R}^n)$ exists. Moreover, if $N \in \mathbb{N}$ and $N > n/4$, then $H^1_{L,\psi}(\mathbb{R}^n) = H^1_{L,\text{mol}(N)}(\mathbb{R}^n)$, and when $A$ is self-adjoint, then also $H^1_{L,\psi}(\mathbb{R}^n) = H^1_{L,\text{af}(N)}(\mathbb{R}^n)$.

A theory of Hardy spaces was developed by Hofmann, Lu, Mitrea, Mitrea and Yan [20] for nonnegative self-adjoint operators $L$ satisfying Davies–Gaffney estimates (see \((5.1)\)) on doubling metric measure spaces $M$. For example, when $A$ is self-adjoint, then $L = -\div A \nabla$ has these properties. The framework developed here provides an embedding for these spaces when $L$ acts on a vector bundle $\mathcal{V}$ over $M$, as defined in Section 2 and there exists $g \in L^2_{\text{loc}}((0, \infty))$ such that
\[(1.6)\]
$$
\|e^{-tL}u\|_\infty \leq g(t)\|u\|_2 \quad \forall u \in L^2(\mathcal{V}), \forall t > 0.
$$

In this context, since $L$ is self-adjoint, it is well known that \((1.6)\) is equivalent to pointwise kernel estimates for the semigroup $\{e^{-tL}\}_{t > 0}$ (see [18, Lemma 2.1.2]).

**Theorem 1.3.** Suppose that $M$ is a doubling metric measure space satisfying \((D_n)\) and that $L$ is a nonnegative self-adjoint operator on $L^2(\mathcal{V})$ satisfying Davies–Gaffney estimates and \((1.6)\). If $p \in [1, 2]$, $\theta \in (0, \pi/2)$, $\beta > \kappa/4$ and $\psi \in \Psi_\beta(S^2_0)$ is nondegenerate, then the completion $H^p_{L,\psi}(\mathcal{V})$ of $E^p_{L,\psi}(\mathcal{V})$ in $L^p(\mathcal{V})$ exists. Moreover, if $N \in \mathbb{N}$ and $N > \kappa/4$, then $H^1_{L,\psi}(\mathcal{V}) = H^1_{L,\text{mol}(N)}(\mathcal{V}) = H^1_{L,\text{af}(N)}(\mathcal{V})$.

It remains an open question as to whether Theorems 1.2 and 1.3 hold in the absence of ultracontractivity estimates such as \((1.4)\) and \((1.6)\). The first-order methods developed here, however, provide a new proof of Theorem 1.2 that does not rely on ultracontractivity but instead requires that $\rho$ is self-adjoint with smooth coefficients. We present this proof at the conclusion of the paper as a basis for future work.

The structure of the paper is as follows. In Section 2, we fix notation and discuss when the completion of a normed space inside a given Banach space exists. In Section 3, we briefly recast the theory of Hardy spaces from [9] in the context of a vector bundle $\mathcal{V}$ over a doubling metric measure space $M$ for any operator $D$ on $L^2(\mathcal{V})$ that is bisectorial with a bounded holomorphic functional calculus and that satisfies polynomial off-diagonal estimates. We then introduce an additional hypothesis \((H4)\) on $D$, based on the $\Psi(S^2_0)$ class, that guarantees the embedding $H^p_D(\mathcal{V}) \subseteq L^p(\mathcal{V})$, when $p \in [1, 2]$, and the molecular characterisation of $H^1_D(\mathcal{V})$. This is the content of Theorems 3.10 and 3.13.

In Section 4, we restrict consideration to any operator $D$ that is self-adjoint on $L^2(\mathcal{V})$ and for which the associated $C_0$-group $(e^{itD})_{t \in \mathbb{R}}$ has finite propagation speed. This allows us to introduce an alternative hypothesis \((H4)\) on $D$, based on the $\Psi(\mathbb{R})$ class, that guarantees the embedding $H^p_D(\mathcal{V}) \subseteq L^p(\mathcal{V})$, when $p \in [1, 2]$, and the atomic characterisation of $H^1_D(\mathcal{V})$. This is the content of Theorems 4.7 and 4.9. In Theorem 4.11, we verify \((H4)\) when $M$ is a complete Riemannian manifold and
$D$ is a smooth-coefficient, self-adjoint, first-order, differential operator with bounded principal symbol

The results for the Hodge–Dirac operator $D = d + d^*$ and the divergence form operator $L = -\text{div} AV$ in Theorems 1.3 and 1.2 are deduced in Sections 3.2 and 4.2

In Section 5, we combine the techniques of the preceding two sections to prove Theorem 1.3. Section 6 is an appendix that contains the technical off-diagonal estimates used to prove Theorems 4.7 and 4.9

2. Notation and Preliminaries

Throughout the paper, let $M$ denote a metric measure space with a metric $\rho$ and a $\sigma$-finite measure $\mu$ that is Borel with respect to the $\rho$-topology. A ball in $M$ will always refer to an open $\rho$-ball. For $x \in M$ and $r > 0$, let $B(x, r)$ denote the ball in $M$ with centre $x$ and radius $r$, let $V(x, r) = \mu(B(x, r))$ and $(\alpha B)(x, r) = B(x, \alpha r)$. The metric measure space $M$ is called doubling when there exist constants $A \geq 1$ and $\kappa \geq 0$ such that

$$D_n \quad 0 < V(x, \alpha r) \leq A\alpha^n V(x, r) < \infty \quad \forall x \in M, \forall r > 0, \forall \alpha \geq 1.$$  

For any $E, F \subseteq M$, set $\rho(E, F) = \inf\{\rho(x, y) : x \in E, y \in F\}$.

A vector bundle $\mathcal{V}$ over $M$ refers to a complex vector bundle $\pi : \mathcal{V} \to M$ equipped with a Hermitian metric $\langle \cdot, \cdot \rangle_x$ that depends continuously on $x \in M$. For any vector bundle $\mathcal{V}$, there are naturally defined Banach spaces $L^p(\mathcal{V})$, $1 \leq p \leq \infty$, of measurable sections. The Hilbert space $L^2(\mathcal{V})$ of square integrable sections of $\mathcal{V}$ has the inner product $\langle u, v \rangle = \int_M \langle u(x), v(x) \rangle_x d\mu(x)$. For any linear operator $T$ on $L^2(\mathcal{V})$, the domain $\text{Dom}(T)$, range $\text{R}(T)$ and null space $\text{N}(T)$ are subspaces of $L^2(\mathcal{V})$, and the operator norm $\|T\| = \sup\{|Tu|_{L^2(\mathcal{V})}/|u|_{L^2(\mathcal{V})} : u \in \text{Dom}(T), u \neq 0\}$. The Banach algebra of all bounded linear operators on $L^2(\mathcal{V})$ is denoted by $L(L^2(\mathcal{V}))$.

For normed spaces $X$ and $Y$, we write $X \subseteq Y$ when $X$ is a subset of $Y$ with the property that there exists $C > 0$ such that $\|x\|_Y \leq C\|x\|_X$ for all $x \in X$, and we write $X = Y$ when $X \subseteq Y \subseteq X$. A completion $(\mathcal{X}, \iota)$ of a normed space $X$ consists of a Banach space $\mathcal{X}$ and an isometry $\iota : X \to \mathcal{X}$ such that $\iota(X)$ is dense in $\mathcal{X}$. Every normed space has a completion but this abstract construction is not sufficient for our purposes. It is convenient to formalise the following related notion.

Definition 2.1. Let $X$ be a normed space and suppose that $X \subseteq Y$ for some Banach space $Y$. A Banach space $\bar{X}$ is called the completion of $X$ in $Y$ when $X \subseteq \bar{X} \subseteq Y$, the set $X$ is dense in $\bar{X}$, and $\|x\|_X = \|x\|_{\bar{X}}$ for all $x \in X$.

It is easily checked that the completion $\bar{X}$ of $X$ in $Y$ is unique whenever it exists. Moreover, the set $\bar{X}$ consists of all $x$ in $Y$ for which there is a Cauchy sequence $(x_n)_n$ in $X$ such that $(x_n)_n$ converges to $x$ in $Y$, and with the norm $\|x\|_{\bar{X}} = \lim_{n \to \infty} \|x_n\|_X$, the space $(\bar{X}, \|\cdot\|_{\bar{X}})$ is complete. This can be deduced from the following necessary and sufficient conditions for the existence of a completion inside a given Banach space. The proof is left to the reader.

Proposition 2.2. Let $X$ be a normed space and suppose that $X \subseteq Y$ for some Banach space $Y$, so the identity $I : X \to Y$ is bounded. The following are equivalent:

1. The completion of $X$ in $Y$ exists;
(2) If \((X, i)\) is a completion of \(X\), then the unique operator \(\tilde{I}\) in \(\mathcal{L}(X, Y)\) defined by the commutative diagram below, is injective;

\[
\begin{array}{c}
X \\
\downarrow i
\end{array}
\xrightarrow{I}
\begin{array}{c}
Y
\end{array}
\]

(3) For each Cauchy sequence \((x_n)_n\) in \(X\) that converges to 0 in \(Y\), it follows that \((x_n)_n\) converges to 0 in \(X\).

We adopt the convention for estimating \(x, y \geq 0\) whereby \(x \lesssim y\) means that there exists a constant \(C \geq 1\), which only depends on constants specified in the relevant preceding hypotheses, such that \(x \leq Cy\). We write \(x \sim y\) when \(x \lesssim y \lesssim x\). The set of positive integers is denoted by \(\mathbb{N}\) whilst \(\mathbb{N}_0 = \mathbb{N} \cup \{0\}\) and \(\mathbb{R}_+ = (0, \infty)\). Finally, we apologise in advance for the excess of notation, but it is required to handle some delicate points.

### 3. Sectorial Operators with Off-Diagonal Estimates

Auscher, McIntosh and Russ \[9\] designed the Hardy spaces of differential forms \(H^p_T(\wedge T^*M)\), \(1 \leq p \leq \infty\), for the Hodge–Dirac operator \(D = d + d^*\) acting on \(L^2(\wedge T^*M)\) over a doubling Riemannian manifold \(M\). We briefly recast that theory in the context of a vector bundle \(\mathcal{V}\) over a doubling metric measure space \((M, \rho, \mu)\). Instead of the Hodge–Dirac operator, we consider any closed, densely defined operator \(\mathcal{D} : \text{Dom}(\mathcal{D}) \subseteq L^2(\mathcal{V}) \to L^2(\mathcal{V})\) that is bisectorial with a bounded holomorphic functional calculus (e.g. this holds when \(\mathcal{D}\) is self-adjoint) and satisfies polynomial off-diagonal estimates (e.g. these hold for suitable classes of differential operators \(\mathcal{D}\), not necessarily of first-order). The setup below allows us to define these properties.

For \(0 \leq \mu < \theta < \pi/2\), define the following bisectors in the complex plane:

\[
S_\mu = \{z \in \mathbb{C} : z = 0 \text{ or } |\arg z| \leq \mu \text{ or } |\pi - \arg z| \leq \mu\};
\]
\[
S_\theta^o = \{z \in \mathbb{C} \setminus \{0\} : |\arg z| < \theta \text{ or } |\pi - \arg z| < \theta\}.
\]

A function on \(S_\theta^o\) is called nondegenerate when it is not identically zero on each component of \(S_\theta^o\). The algebra of bounded complex-valued functions on \(S_\theta^o \cup \{0\}\) that are holomorphic on \(S_\theta^o\) is denoted by \(H^\infty(S_\theta^o \cup \{0\})\). For \(\sigma, \tau > 0\), define

\[
\Psi^\tau(S_\theta^o) = \{\psi \in H^\infty(S_\theta^o \cup \{0\}) : |\psi(z)| \lesssim \min\{|z|^{\sigma}, |z|^{-\tau}\}\},
\]

\[
\Psi_\sigma(S_\theta^o) = \bigcup_{\tau > 0} \Psi^\tau(S_\theta^o), \quad \Psi^\tau(S_\theta^o) = \bigcup_{\sigma > 0} \Psi^\tau(S_\theta^o) \quad \text{and} \quad \Psi(S_\theta^o) = \bigcup_{\sigma > 0} \bigcup_{\tau > 0} \Psi^\tau(S_\theta^o).
\]

For functions \(f : S_\theta^o \to \mathbb{C}\), define \(f^*(z) = \overline{f(z)}\), and for \(t > 0\), define \(f_t(z) = f(tz)\).

Consider the following hypotheses concerning a closed, densely defined operator \(\mathcal{D} : \text{Dom}(\mathcal{D}) \subseteq L^2(\mathcal{V}) \to L^2(\mathcal{V})\), where \(1_E\) denotes the characteristic function of a measurable set \(E \subseteq M\), and \(\langle \alpha \rangle = \min\{\alpha, 1\}\) and \(\langle \alpha \rangle = 1\) when \(\alpha > 0\).

(H1) There exists \(\omega \in [0, \pi/2]\) such that \(\mathcal{D}\) is type \(S_\omega\), which is defined to mean that the spectrum \(\sigma(\mathcal{D}) \subseteq S_\omega\) and that for each \(\theta \in (\omega, \pi/2)\), there exists \(C_\theta > 0\) such that \(||(zI - \mathcal{D})^{-1}u||_2 \leq C_\theta ||u||_2 / |z|\) for all \(z \in \mathbb{C} \setminus S_\theta\) and \(u \in L^2(\mathcal{V})\).

(H2) For each \(\theta \in (\omega, \pi/2)\), the operator \(\mathcal{D}\) has a bounded \(H^\infty(S_\theta^o \cup \{0\})\) functional calculus in \(L^2(\mathcal{V})\), which is defined to mean that there exists \(c_\theta > 0\) such that \(||\psi(\mathcal{D})u||_2 \leq c_\theta ||\psi||_\infty ||u||_2\) for all \(\psi \in \Psi(S_\theta^o)\) and \(u \in L^2(\mathcal{V})\).
(H3) There exists \( m \in \mathbb{N} \) such that for each \( \theta \in (\omega, \pi/2) \) and \( N \in \mathbb{N} \) it holds that
\[
\| 1_E(zI - D)^{-1} 1_F u \|_2 \leq C_{\theta, N} \left\| \frac{1}{\rho(E, F)^m} \right\|_2^N \| u \|_2
\]
for all \( z \in \mathbb{C} \setminus S_\theta, u \in L^2(V) \), measurable sets \( E, F \subseteq M \), and some \( C_{\theta, N} > 0 \).

Let us note that (H1) is implicit in (H2) and (H3). It is well known that (H1) and (H2) hold with \( \omega = 0 \), \( C_\theta = 1/\sin \theta \) and \( c_\theta = 1 \), whenever \( D \) is self-adjoint. The number \( m \) in (H3) indicates that the off-diagonal estimates associated with \( D \) resemble those associated with an \( m \)th-order differential operator.

The theory of type \( S_\omega \) operators is well known (see, for instance, [1, Lecture 2]). If (H1) holds, then for \( \theta \in (\omega, \pi/2) \) and \( \psi \in \Psi(S_\theta^0) \), define \( \psi(D) \in L(L^2(V)) \) by
\[
(3.2) \quad \psi(D)u = \frac{1}{2\pi i} \int_{\partial S_\theta} \psi(z)(zI - D)^{-1}u \, dz \quad \forall u \in L^2(V),
\]
where \( \mu \in (\omega, \theta) \) is arbitrary and \( \partial S_\mu^0 \) is the positively oriented boundary of \( S_\mu^0 \). It holds that \( L^2(V) = \mathbb{R}(D) \oplus N(D) \) when \( D \) is type \( S_\omega \) (see [16, Theorem 3.8]) and so
\[
(3.3) \quad \psi(D)u = P_{\mathbb{R}(D)} \psi(D)P_{\mathbb{R}(D)}u \quad \forall u \in L^2(V),
\]
where \( P_{\mathbb{R}(D)} \) denotes the projection from \( L^2(V) \) onto \( \mathbb{R}(D) \) (see [28, Lemma 4.5]).

It is well known (see [1, 25]) that (H2) holds if and only if the quadratic estimate
\[
(3.4) \quad \int_0^\infty \| \psi_t(D)u \|_2^2 \frac{dt}{t} \lesssim \| u \|^2 \quad \forall u \in \mathbb{R}(D)
\]
holds for all nondegenerate \( \psi \in \Psi(S_\theta^0) \), where \( \psi_t(z) = \psi(tz) \). If (H2) holds, then for \( f \in H^\infty(S_\theta^0 \cup \{0\}) \), define \( f(D) \in L(L^2(V)) \) satisfying \( \| f(D) \| \leq c_\theta \| f \|_\infty \) by
\[
(3.5) \quad f(D)u = \lim_{n \to \infty} (f\psi_{(n)})(D)u + f(0)P_{N(D)}u \quad \forall u \in L^2(V),
\]
where \( (\psi_{(n)})_{n \in \mathbb{N}} \) is an arbitrary sequence of uniformly bounded functions in \( \Psi(S_\theta^0) \) that converges to \( 1 \) uniformly on compact subsets of \( S_\theta^0 \). The mapping \( f \mapsto f(D) \) given by (3.5) is the unique algebra homomorphism from \( H^\infty(S_\theta^0 \cup \{0\}) \) into \( L(L^2(V)) \) with the following properties (see [1, Lecture 2]):

(3.6) If \( 1(z) = 1 \) on \( S_\theta^0 \cup \{0\} \), then \( 1(D) = I \) on \( L^2(V) \);

(3.7) If \( \lambda \in \mathbb{C} \setminus S_\theta \) and \( f(z) = (\lambda - z)^{-1} \) on \( S_\theta^0 \cup \{0\} \), then \( f(D) = (\lambda I - D)^{-1} \);

(3.8) If \( (f_n)_n \) is a sequence in \( H^\infty(S_\theta^0 \cup \{0\}) \) that converges uniformly on compact sets to a function \( f \) in \( H^\infty(S_\theta^0 \cup \{0\}) \), and \( \sup_n \| f_n \|_\infty < \infty \), then \( \lim_{n \to \infty} f_n(D)u = f(D)u \) for all \( u \in L^2(V) \).

Hypotheses (H1)–(H3) are sufficient to construct Hardy spaces \( H^p_D(V) \) as in [1]. To begin, we use (3.2) to obtain the following extension of [1, Lemma 3.6] (for the improved \( \Psi(S_\theta^0) \) class exponents presented here, see [23, Lemma 7.3]): if \( 0 < \delta < \sigma \), \( \theta \in (\omega, \pi/2) \) and \( \psi \in \Psi_\sigma(S_\theta^0) \), then there exists \( C > 0 \) such that
\[
(3.9) \quad \| 1_E(f\psi_t)(D)1_F u \|_2 \leq C \| f \|_\infty \left\| \frac{t}{\rho(E, F)^m} \right\|^{\sigma-\delta} \| u \|_2
\]
for all \( t > 0 \), \( f \in H^\infty(S_\theta^0 \cup \{0\}) \), \( u \in L^2(V) \), and measurable sets \( E, F \subseteq M \).

The theory of tent spaces \( T^p(\mathbb{R}^{n+1}) \) developed by Coifman, Meyer and Stein [15] has the following extension when \( \pi : V \to M \) is a vector bundle over a doubling
metric measure space $M$. Let $\mathcal{V}_+$ denote the vector bundle $\pi_+: \mathcal{V} \times \mathbb{R}_+ \to M \times \mathbb{R}_+$ over $M \times \mathbb{R}_+$ defined by $\pi_+(v,t) := (\pi(v), t)$ for all $v \in \mathcal{V}$, $t \in \mathbb{R}_+$. For $x \in M$, $t \in \mathbb{R}_+$ and sections $U, V$ of $\mathcal{V}_+$, suppose $U(x,t) \in \pi^{-1}({\{x\}}) \times \{t\}$, we let $U_i(x)$ denote the component of $U(x,t)$ in $\pi^{-1}(\{x\})$, and define the Hermitian metric on $\mathcal{V}_+$ by $\langle U(x,t), V(x,t) \rangle_{x,t} := \langle U_i(x), V_i(x) \rangle_x$. For $p \in [1, \infty)$, the tent space $T^p(\mathcal{V}_+)$ is the Banach space of all $U$ in $L^p_{\text{loc}}(\mathcal{V}_+)$ satisfying

$$
\|U\|_{T^p} := \left( \int_M \left( \int_{\Gamma(x)} |U_i(y)|^2 \frac{d\mu(y)}{V(y,t)} \frac{dt}{t} \right)^{p/2} d\mu(x) \right)^{1/p} < \infty,
$$

where the cone $\Gamma(x) = \{(y,t) \in M \times \mathbb{R}_+ \mid \rho(x,y) < t\}$. The tent space $T^\infty(\mathcal{V}_+)$ is the Banach space of all $U$ in $L^2_{\text{loc}}(\mathcal{V}_+)$ satisfying

$$
\|U\|_{T^\infty} := \sup_{x \in M} \sup_{B \subseteq M} \left( \frac{1}{\mu(B)} \int_{\Gamma(B)} |U_i(y)|^2 d\mu(y) \frac{dt}{t} \right)^{1/2} < \infty,
$$

where $B(x)$ denotes the set of all balls $B \subseteq M$ with the property that $x \in B$, and the tent $T(B) = \{(y,t) \in M \times \mathbb{R}_+ \mid \rho(y,M \setminus B) \geq t\}$.

We require the following properties, which can be proved as in the references cited when $M$ is a doubling metric measure space:

(3.10) If $p \in [1, \infty)$ and $1/p + 1/p' = 1$, then $T^{p'}$ is realized as the dual of $T^p$ by the pairing $\langle U, V \rangle_{T^2} := \int_0^\infty \int_M (U_i(x), V_i(x))_x d\mu(x) dt/t$ (see [15]);

(3.11) If $\theta \in (0, 1)$, $1 \leq p_0 < p_1 \leq \infty$ and $1/p_0 = (1 - \theta)/p_0 + \theta/p_1$, then the complex interpolation space $[T^{p_0}, T^{p_1}]_\theta = T^{p_\theta}$ (see [22] [11] [14] [2]).

There is also the following atomic characterisation of $T^1(\mathcal{V}_+)$, for which a section $A \in L^2(\mathcal{V}_+)$ is called a $T^1$-atom when there is a ball $B \subseteq M$ such that $A$ is supported on the tent $T(B)$ and the norm $\|A\|_{T^2} \leq \mu(B)^{-1/2}$.

**Theorem 3.1.** Suppose that $\mathcal{V}$ is a vector bundle over a doubling metric measure space $M$ and that $p \in [1, \infty)$. For each $U$ in $T^1(\mathcal{V}_+) \cap T^p(\mathcal{V}_+)$, there exist a sequence $(\lambda_j)_j$ in $\ell^1$ and a sequence $(A_j)_j$ of $T^1$-atoms such that $\sum_j \lambda_j A_j$ converges to $U$ in $T^1(\mathcal{V}_+)$, in $T^p(\mathcal{V}_+)$ and almost everywhere in $M \times \mathbb{R}_+$, such that $\|U\|_{T^1} \approx \|(\lambda_j)_j\|_{\ell^1}$.

**Proof.** This follows the proof in [20] Theorem 1.1, which is based on [15] Theorem 1. The convergence in $T^p$ is not explicit in those references, but it follows by dominated convergence, as in [21] Proposition 3.25 or [12] Theorem 3.6. $\square$

We follow [9] to begin the development of Hardy spaces $H^p_\omega(\mathcal{V})$ in earnest.

**Definition 3.2.** Suppose that $\mathcal{D}$ satisfies [H1]–[H3] on $L^2(\mathcal{V})$ for some $\omega \in [0, \pi/2)$ and $m \in \mathbb{N}$. For $\theta \in (\omega, \pi/2)$ and $\psi \in \Psi(S^m_\omega)$, define $Q^\omega_\psi$ in $\mathcal{L}(L^2, T^2)$ by

$$(Q^\omega_\psi u)_t = \psi(t^m \mathcal{D}) u \quad \forall t > 0, \forall u \in L^2(\mathcal{V})$$

and $S^\omega_\psi$ in $\mathcal{L}(T^2, L^2)$ by

$$S^\omega_\psi U = \int_0^\infty \psi(s^m \mathcal{D}) U_s \frac{ds}{s} \quad \forall U \in T^2(\mathcal{V}_+).$$

The operator $Q^\omega_\psi$ is bounded because [H2] is equivalent to the quadratic estimate in (3.4). The operator $S^\omega_\psi$ is bounded because $S^\omega_\psi = (Q^\omega_\psi)^*$ and the adjoint $\mathcal{D}^*$ satisfies [H2] if and only if $\mathcal{D}$ satisfies [H2] (see, for instance, [1] Lecture 3). These operators provide the following Calderón reproducing formula (see [9] Remark 2.1).
Proposition 3.3. Suppose that $\mathcal{D}$ satisfies (H1)–(H3) for some $\omega \in [0, \pi/2)$ and $m \in \mathbb{N}$. If $\sigma, \tau > 0$, $\theta \in (\omega, \pi/2)$ and $\psi \in \Psi(S_\theta^p)$ is nondegenerate, then there exists a nondegenerate $\tilde{\psi} \in \Psi_\sigma^r(S_\theta^p)$ such that $S^D_\psi \tilde{Q}^D u = S^D_\tilde{\psi} Q^D u = P_{R(\mathcal{D})} u$ for all $u \in L^2(\mathcal{V})$.

In preparation for defining the Hardy space $H^p_{D,\psi}(\mathcal{V})$, we now define a possibly incomplete space $E^p_{D,\psi}(\mathcal{V})$.

Definition 3.4. Suppose that $\mathcal{D}$ satisfies (H1)–(H3) on $L^2(\mathcal{V})$ for some $\omega \in [0, \pi/2)$ and $m \in \mathbb{N}$. For each $\theta \in (\omega, \pi/2)$, $\psi \in \Psi(S_\theta^p)$ and $p \in [1, \infty]$, the space $E^p_{D,\psi}(\mathcal{V})$ consists of the set $S^D_\psi (T^p \cap T^2)$ together with the seminorm

$$
\|u\|_{E^p_{D,\psi}} := \inf \{ \|U\|_{T^p} : U \in T^p \cap T^2 \text{ and } u = S^D_\psi U \}
$$

equation{3.12}
for all $u \in S^D_\psi (T^p \cap T^2)$.

In $\mathcal{E}$, the Hardy space $H^p_{D,\psi}(\mathcal{V})$ is defined to be an abstract completion of $E^p_{D,\psi}(\mathcal{V})$. Our question here is whether we can define $H^p_{D,\psi}(\mathcal{V})$ to be the completion of $E^p_{D,\psi}(\mathcal{V})$ in $L^p(\mathcal{V})$. So does the completion of $E^p_{D,\psi}(\mathcal{V})$ in $L^p(\mathcal{V})$ exist? This is immediate when (H2) holds and $p = 2$, since for each $\theta \in (\omega, \pi/2)$ and nondegenerate $\tilde{\psi} \in \Psi(S_\theta^p)$, we have by (3.3), (3.4) and Proposition 3.3 that $S^D_\psi (T^2) = R(\mathcal{D})$ with

$$
\|u\|_{E^p_{D,\psi}} \sim \|Q^D u\|_{T^2} \sim \|u\|_2 \quad \forall u \in \overline{R(\mathcal{D})}.
$$

equation{3.12}
This motivates the following definition.

Definition 3.5. Suppose that $\mathcal{D}$ satisfies (H1)–(H3) on $L^2(\mathcal{V})$ for some $\omega \in [0, \pi/2)$ and $m \in \mathbb{N}$. For each $\theta \in (\omega, \pi/2)$ and nondegenerate $\psi \in \Psi(S_\theta^p)$, let $H^p_{D,\psi}(\mathcal{V})$ denote the set $\overline{R(\mathcal{D})}$ together with the norm $\|u\|_{H^p_{D,\psi}} := \|u\|_{E^p_{D,\psi}}$.

When $p \in [1, 2)$, we do not know whether or not the completion of $E^p_{D,\psi}(\mathcal{V})$ in $L^p(\mathcal{V})$ always exists, so we proceed under additional hypotheses on $\mathcal{D}$. We begin by recording a routine extension of $\mathcal{E}$, Theorem 4.9 and Lemma 5.2). In particular, the improved $\Psi(S_\theta^p)$ class exponents in the theorem below follow from $\mathcal{E}$ (for details, see [23] Proposition 7.5) or $\mathcal{Z}$ (Theorem 6.2).

Theorem 3.6. Suppose that $\mathcal{M}$ is a doubling metric measure space satisfying (D3) and that $\mathcal{D}$ satisfies (H1)–(H3) on $L^2(\mathcal{V})$ for some $\omega \in [0, \pi/2)$ and $m \in \mathbb{N}$. If $\rho \in [1, 2]$, $\theta \in (\omega, \pi/2)$, $\beta > \kappa/2m$, $\varphi \in \Psi_\beta(S_\theta^p)$, $\psi \in \Psi_\beta(S_\theta^p)$ and $\tilde{\psi} \in \Psi_\beta(S_\theta^p)$, then

$$
\|Q^D S^D_\psi U\|_{T^p} \lesssim \|U\|_{T^p} \quad \forall U \in T^p \cap T^2
$$

equation{3.13}
If, in addition, all of $\varphi, \psi$ and $\tilde{\psi}$ are nondegenerate, then

$$
S^D_\varphi (T^p \cap T^2) = S^D_\psi (T^p \cap T^2) = \{ u \in \overline{R(\mathcal{D})} : Q^D u \in T^p \}
$$

with the norm equivalence

$$
\|u\|_{E^p_{D,\psi}} \sim \|u\|_{E^p_{D,\tilde{\psi}}} \sim \|Q^D u\|_{T^p} \quad \forall u \in E^p_{D,\psi} = S^D_\varphi (T^p \cap T^2).
$$

equation{3.14}
If, in addition, the completion $H^p_{D,\varphi}$ of $E^p_{D,\varphi}$ in $L^p$ exists, then there are unique extensions $\hat{S}^D_\varphi \in L(T^p, H^p_{D,\varphi})$ and $\hat{Q}^D_\varphi \in L(H^p_{D,\varphi}, T^p)$ such that $\hat{S}^D_\psi = S^D_\psi$ on $T^p \cap T^2$ and $\hat{Q}^D_\psi = Q^D_\psi$ on $E^p_{D,\psi}$. It also holds that $H^p_{D,\psi} = \hat{S}^D_\psi (T^p)$ with the norm equivalence

$$
\|u\|_{H^p_{D,\psi}} \sim \inf \{ \|U\|_{T^p} : U \in T^p \text{ and } u = \hat{S}^D_\psi U \} \sim \|Q^D_\psi u\|_{T^p} \quad \forall u \in H^p_{D,\psi}.
$$

equation{3.15}
Moreover, if $E^p_{D,\psi}$ is dense in $H^p_{D,\varphi} \cap L^2$, then also $\widetilde{Q}^D_{\psi} = Q^D_{\psi}$ on $H^p_{D,\varphi} \cap L^2$.

**Proof.** As explained in the remarks preceding the theorem, properties $\eqref{3.13}$–$\eqref{3.15}$ are a routine extension of $\eqref{9}$. Theorem 4.9 and Lemma 5.2. Now suppose that all of $\varphi, \psi$ and $\tilde{\psi}$ are nondegenerate and that the completion $H^p_{D,\varphi}$ of $E^p_{D,\varphi}$ in $L^p$ exists. The existence of the completion in $L^p$ is used here to ensure that the space $H^p_{D,\varphi} \cap L^2$ is a well-defined subspace of, for example, $L^1_{loc}$. It follows from $\eqref{3.15}$ that $\|S^D_{\psi}U\|_{E^p_{D,\varphi}} \leq \|U\|_{T^p}$ for all $U \in T^p \cap T^2$, and so the operator $S^D_{\psi}$ in $L(T^2, L^2)$ extends by density to a unique operator $\widetilde{S}^D_{\psi}$ in $L(T^p, H^p_{D,\varphi})$. It follows from $\eqref{3.15}$ that the operator $Q^D_{\psi}$ in $L(L^2, T^2)$ restricts to an operator in $L(E^p_{D,\varphi}, T^p)$, and so the density of $E^p_{D,\varphi}$ in $H^p_{D,\varphi}$ provides the unique operator $\widetilde{Q}^D_{\psi}$ in $L(H^p_{D,\varphi}, T^p)$ such that $\widetilde{Q}^D_{\psi} = Q^D_{\psi}$ on $E^p_{D,\varphi}$. We obtain $H^p_{D,\varphi} = \widetilde{S}^D_{\psi}(T^p)$ and $\eqref{3.16}$ by using $\widetilde{S}^D_{\psi}$ and $\widetilde{Q}^D_{\psi}$ to extend Proposition 3.3 and properties $\eqref{3.13}$–$\eqref{3.15}$. Finally, if $E^p_{D,\varphi}$ is dense in $H^p_{D,\varphi} \cap L^2$, then for each $u$ in $H^p_{D,\varphi} \cap L^2$, there exists a sequence $(u_n)_n$ in $E^p_{D,\varphi}$ such that $u_n$ converges to $u$ in both $H^p_{D,\varphi}$ and $L^2$, so by writing

$$\|\widetilde{Q}^D_{\psi}u - Q^D_{\psi}u\|_{T^p + T^2} \leq \|\widetilde{Q}^D_{\psi}u - Q^D_{\psi}u_n\|_{T^p} + \|Q^D_{\psi}u_n - Q^D_{\psi}u\|_{T^2} \lesssim \|u_n\|_{H^p_{D,\varphi} \cap L^2},$$

we conclude that $\widetilde{Q}^D_{\psi}u = Q^D_{\psi}u$. This completes the proof. \hfill \Box

**Remark 3.7.** In the context of Theorem 3.6, if the completion $H^p_{D,\varphi}(\mathcal{V})$ of $E^p_{D,\varphi}(\mathcal{V})$ in $L^p(\mathcal{V})$ exists for some nondegenerate $\varphi \in \Psi_\beta(S^p_\theta)$, then $\eqref{3.16}$ implies that the completion $H^p_{D,\psi}(\mathcal{V})$ of $E^p_{D,\psi}(\mathcal{V})$ in $L^p(\mathcal{V})$ exists for all nondegenerate $\psi \in \Psi_\beta(S^p_\theta)$. Therefore, we could adopt the notation in $\eqref{9}$ whereby $H^p_{D,\psi}(\mathcal{V})$ denotes any of the equivalent Banach spaces $H^p_{D,\psi}(\mathcal{V})$. We found it convenient not to do this, however, given the technical nature of this article.

We now introduce atoms and molecules in order to show that $E^p_{D,\psi}(\mathcal{V}) \subseteq L^p(\mathcal{V})$.

**Definition 3.8.** Suppose that $\mathcal{D}$ satisfies $\eqref{H1}$ and $\eqref{H3}$ on $L^2(\mathcal{V})$ for some $m \in \mathbb{N}$. For $N \in \mathbb{N}$, a section $a \in L^2(\mathcal{V})$ is called an $H^1_{D}(\mathcal{V})$-molecule of type $N$ when there exist a section $b \in \text{Dom}(D^N)$ and a ball $B \subseteq M$ of radius $r(B) > 0$ such that $a = D^N b$ and the following hold for all $k \in \mathbb{N}_0$:

1. $\|1_k(B)a\|_2 \leq 2^{-k} \mu(2^k B)^{-1/2}$;
2. $\|1_k(B)b\|_2 \leq r(B)^{mN} 2^{-k} \mu(2^k B)^{-1/2}$,

where $1_0(B) = 1_B$ and $1_k(B) = 1_{2^kB \setminus 2^{k-1}B}$ for all $k \in \mathbb{N}$. An $H^1_{D}(\mathcal{V})$-atom of type $N$ is defined in the same way, except that $a$ and $b$ are required to be supported on the ball $B$, which obviates (1) and (2) when $k \geq 1$.

The following proof uses a molecular characterisation obtained in $\eqref{9}$ Section 6.1.

**Lemma 3.9.** Suppose that $\mathcal{D}$ is a doubling metric measure space satisfying $\eqref{D_1}$ and that $\mathcal{D}$ satisfies $\eqref{H1}$–$\eqref{H3}$ on $L^2(\mathcal{V})$ for some $\omega \in [0, \pi/2)$ and $m \in \mathbb{N}$. If $p \in [1, 2]$, $\theta \in (\omega, \pi/2)$, $\beta > \kappa/2m$ and $\psi \in \Psi_\beta(S^p_\theta)$ is nondegenerate, then $E^p_{D,\psi}(\mathcal{V}) \subseteq L^p(\mathcal{V})$.

**Proof.** When $p = 2$, the result holds by $\eqref{3.12}$. When $p \in [1, 2)$, it suffices to prove the result for a fixed nondegenerate $\psi \in \Psi_\beta(S^p_\theta)$ by $\eqref{3.15}$. Therefore, we fix $N \in \mathbb{N}$ and use the construction in $\eqref{9}$ Lemma 6.7 to fix a nondegenerate $\psi \in \Psi_\beta(S^p_\theta)$ such that $S^p_{\psi}(A)$ is an $H^1_D$-molecule of type $N$ whenever $A$ is a $T^1$-atom.
Now consider when $p = 1$. For all $H^1_D$-molecules $a$ of type $N$, note that

$$
\|a\|_1 \leq \sum_{k=0}^{\infty} \mu(2^kB)^{1/2}\|1_k(B)a\|_2 \leq 2.
$$

(3.17)

Suppose that $u \in E^1_{D,\psi}$ and $V \in T^1 \cap T^2$ such that $u = S^D_{\psi}V$ and $\|V\|_{T^1} \leq 2\|u\|_{E^1_{D,\psi}}$.

The atomic characterisation of $T^1$ in Theorem 3.1 provides a sequence $(\lambda_j)_j$ in $l^1$ and a sequence $(A_j)_j$ of $T^1$-atoms such that $\sum_j \lambda_j A_j$ converges to $V$ in $T^1$ and $T^2$, and $\|V\|_{T^1} \lesssim \|\psi\|_{T^1}$. The operator $S^D_{\psi}$ in $L(T^2, L^2)$ is bounded from $(T^1 \cap T^2, \|\cdot\|_{T^1})$ into $E^1_{D,\psi}$, by the definition of $E^1_{D,\psi}$, so $\sum_j \lambda_j S^D_{\psi} A_j$ converges to $u$ in $E^1_{D,\psi}$ and $L^2$.

Now recall that $\psi$ has the property whereby each $S^D_{\psi} A_j$ is an $H^1_D$-molecule of type $N$, so in accordance with (3.17), the sequence $(S^D_{\psi} A_j)_j$ is uniformly bounded in $L^1$, and as such, there exists $\tilde{u}$ in $L^1$ such that $\sum_j \lambda_j S^D_{\psi} A_j$ converges to $\tilde{u}$ in $L^1$. We must have $u = \tilde{u}$ in $L^1$, since $L^1$ and $L^2$ are embedded in $L^1_{\text{loc}}$, and so $\sum_j \lambda_j S^D_{\psi} A_j$ converges to $u$ in $L^1$ with $\|u\|_1 = \lim_{n \to \infty} \sum_{j=1}^n \lambda_j S^D_{\psi} A_j \|1 \lesssim \|\lambda_j\|_{l^1} \lesssim \|V\|_{T^1} \lesssim \|u\|_{E^1_{D,\psi}}$.

This completes the proof when $p = 1$.

Now consider when $p \in (1, 2)$. We have shown that $E^1_{D,\psi} \subseteq L^1$, so by the definition of $E^p_{D,\psi}$, it follows that $\|S^D_{\psi} U\|_1 \lesssim \|S^D_{\psi} U\|_{E^1_{D,\psi}} \lesssim \|U\|_{T^1}$ for all $U \in T^1 \cap T^2$.

Therefore, the operator $S^D_{\psi}$ in $L(T^2, L^2)$ has an extension in $L(T^1, L^1)$, and then by the interpolation of tent spaces in (3.11), this extension is also in $L(T^p, L^p)$. It follows that $E^p_{D,\psi} \subseteq L^p$, for since each $u \in E^p_{D,\psi}$, there exists $V \in T^p \cap T^2$ such that $u = S^D_{\psi} V$ and $\|V\|_{T^p} \leq 2\|u\|_{E^p_{D,\psi}}$, hence $\|u\|_p = \|S^D_{\psi} V\|_p \lesssim \|V\|_{T^p} \lesssim \|u\|_{E^p_{D,\psi}}$.

The proof of Lemma 3.9 shows that for each $N \in \mathbb{N}$ and $u \in E^1_{D,\psi}(\mathcal{V})$, there exist a sequence $(\lambda_j)_j$ in $l^1$ and a sequence $(a_j)_j$ of $H^1_D(\mathcal{V})$-molecules of type $N$ such that $\sum_j \lambda_j a_j$ converges to $u$ in $E^1_{D,\psi}(\mathcal{V})$ and $L^1(\mathcal{V})$ with $\|\lambda_j\|_{l^1} \lesssim \|u\|_{E^1_{D,\psi}}$. Although this characterisation extends to completions of $E^1_{D,\psi}(\mathcal{V})$ (see Theorem 3.13), it does not seem to guarantee that the completion of $E^1_{D,\psi}(\mathcal{V})$ in $L^1(\mathcal{V})$ exists. We introduce hypothesis (H4)ψ on $\mathcal{D}$ in the next theorem for this reason.

Theorem 3.10. Suppose that $M$ is a doubling metric measure space satisfying [Dₙ] and that $\mathcal{D}$ satisfies (H1)–(H₃) on $L^2(\mathcal{V})$ for some $\omega \in [0, \pi/2)$ and $m \in \mathbb{N}$. If $1 \leq q < p \leq 2$, $\theta \in ([\omega, \pi/2), \beta > \kappa/2m$, $\psi \in \Psi_\beta(S^\omega_\psi)$ is nondegenerate and

$$
\text{(H4)ψ} \quad \text{there exists a nondegenerate function } \tilde{\psi} \in \Psi_\beta(S^\omega_\psi) \text{ such that the set } \\
\{ F \in T^2 \cap T^{q'} : S^D_{\psi} F \in L^{q'}(\mathcal{V}) \} \text{ is weak-star dense in } T^{q'}(\mathcal{V}),
$$

where $1/q + 1/q' = 1$, then the completion $H^p_{D,\psi}(\mathcal{V})$ of $E^p_{D,\psi}(\mathcal{V})$ in $L^p(\mathcal{V})$ exists. Moreover, it holds that $H^p_{D,\psi}(\mathcal{V}) \cap L^2(\mathcal{V}) = E^p_{D,\psi}(\mathcal{V})$.

Proof. Lemma 3.9 shows that $E^p_{D,\psi} \subseteq L^p$, so the existence of the completion of $E^p_{D,\psi}$ in $L^p$ will follow by proving (3) in Proposition (2.2) with $X = E^p_{D,\psi}$ and $Y = L^p$. To this end, let $(u_n)_n$ denote a Cauchy sequence in $E^p_{D,\psi}$ that converges to 0 in $L^p$. We claim that $(u_n)_n$ converges to 0 in $E^p_{D,\psi}$. To see this, fix $\tilde{\psi} \in \Psi_\beta(S^\omega_\psi)$ satisfying (H4)ψ so that $\mathcal{E} := \{ F \in T^2 \cap T^{q'} : S^D_{\psi} F \in L^{q'} \}$ is weak-star dense in $T^{q'}$. For all $n \in \mathbb{N}$, we have by (3.15) that

$$
\|u_n\|_{E^p_{D,\psi}} \simeq \|Q^D_{\psi} u_n\|_{T^p},
$$

(3.18)
and since \((u_n)_n\) is Cauchy in \(E^p_{D,\psi}\), there exists \(U\) in \(T^p\) such that \(Q^D\psi u_n\) converges to \(U\) in \(T^p\). Using the duality pairing in (3.10), for all \(n \in \mathbb{N}\) and \(F \in \mathcal{E}\), we have
\[
\langle U, F \rangle_{T^2} \leq \langle U - Q^D\psi u_n, F \rangle_{T^2} + \langle Q^D\psi u_n, F \rangle_{T^2} \leq \|U - Q^D\psi u_n\|_{T^p} \|F\|_{T^2} + \|u_n\|_{L^p} \|S^D\psi F\|_{L^{p'}},
\]
since \(2 \leq p' \leq q'\) ensures that \(L^2 \cap L^{q'} \subseteq L^{p'}\) and \(T^2 \cap T^{q'} \subseteq T^{p'}\). Moreover, since (3.18) holds and (3.17) holds, the preceding convergence results imply that
\[
\langle U, F \rangle_{T^2} = 0 \quad \forall F \in \mathcal{E}.
\]

Then, since \(U \in T^p\) and \(\mathcal{E}\) is weak-star dense in \(T^{p'}\), it follows that \(\langle U, F \rangle_{T^2} = 0\) for all \(F \in T^{p'}\), hence \(U = 0\) and \((u_n)_n\) converges to 0 in \(E^p_{D,\psi}\), as claimed. This proves that the completion \(H^p_{D,\psi}\) of \(E^p_{D,\psi}\) in \(L^p\) exists.

The inclusion \(E^p_{D,\psi} \subseteq H^p_{D,\psi} \cap L^2\) holds by (3.14). To prove the reverse inclusion, suppose that \(u \in H^p_{D,\psi} \cap L^2\). The density of \(E^p_{D,\psi}\) in \(H^p_{D,\psi}\) provides a sequence \((u_n)_n\) in \(E^p_{D,\psi}\) that converges to \(u\) in \(H^p_{D,\psi}\). This sequence also converges in \(L^p\) because \(H^p_{D,\psi} \subseteq L^p\). Moreover, since (3.18) holds and \((u_n)_n\) is Cauchy in \(E^p_{D,\psi}\), there exists \(U\) in \(T^p\) such that \(Q^D\psi u_n\) converges to \(U\) in \(T^p\). For all \(n \in \mathbb{N}\) and \(F \in \mathcal{E}\), we have
\[
\langle U - Q^D\psi u, F \rangle_{T^2} \leq \langle U - Q^D\psi u_n, F \rangle_{T^2} + \langle Q^D\psi u_n - Q^D\psi u, F \rangle_{T^2} \leq \|U - Q^D\psi u_n\|_{T^p} \|F\|_{T^2} + \|u_n - u\|_{L^p} \|S^D\psi F\|_{L^{p'}}.
\]

The preceding convergence arguments then show that \(U = Q^D\psi u \in T^p \cap T^2\), and since \(\|Q^D\psi u\|_{T^p} \asymp \|u\|_{E^p_{D,\psi}}\), we conclude that \(u \in E^p_{D,\psi}\), as required. \(\Box\)

Remark 3.11. In the context of Theorem 3.10, since \(M\) is \(\sigma\)-finite, hypothesis \((H4)_\psi\) holds whenever \(S^D\psi(T_0^2(\mathcal{V}_+)) \subseteq L^q(\mathcal{V})\), where \(T_0^2(\mathcal{V}_+)\) denotes the set of all \(U\) in \(T^2(\mathcal{V}_+)\) for which there exists some ball \(B\) in \(M\) and some constants \(b > a > 0\) such that \(\text{sppt}(U) \subseteq B \times [a, b]\). This is because \(T_0^2(\mathcal{V}_+)\) is weak-star dense in \(T^{p'}(\mathcal{V}_+)\) for all \(p \in [1, 2]\). To see this, let \((B_n)_n\) denote an increasing sequence of balls that exhaust \(M\). For all \(F \in T^p(\mathcal{V}_+)\) and all \(G \in T^{p'}(\mathcal{V}_+)\), we have
\[
\int_0^\infty \int_M |\langle F(x, G(x))_x \rangle_{d\mu(x)} dt|/t \leq \|F\|_{T^p} \|G\|_{T^{p'}}
\]
by the duality in (3.10). The dominated convergence theorem then implies that \(\langle F, 1_{B_n \times [1/n, n]} G \rangle_{T^2} \) converges to \(\langle F, G \rangle_{T^2}\), which proves the asserted weak-star density, since \(1_{B_n \times [1/n, n]} G \in T_0^2(\mathcal{V}_+)\).

3.1. Molecular Theory. We defined \(H^1_D(\mathcal{V})\)-molecules and atoms in Definition 3.8. The molecular characterisation of \(H^1_{D,\psi}(\mathcal{V})\) below is based on the characterisation obtained in [9, Theorem 6.2]. It is convenient to first introduce the following spaces.

Definition 3.12. Suppose that \(\mathcal{D}\) satisfies \((H1)\) and \((H3)\) on \(L^2(\mathcal{V})\) for some \(m \in \mathbb{N}\). For \(N \in \mathbb{N}\), the Banach space \(H^1_{D,\text{mol}(N)}(\mathcal{V})\) is the set of all \(u\) in \(L^1(\mathcal{V})\) for which there exist a sequence \((\lambda_j)_j\) in \(l^1\) and a sequence \((a_j)_j\) of \(H^1_D\)-molecules of type \(N\) such that \(\sum_j \lambda_j a_j\) converges to \(u\) in \(L^1(\mathcal{V})\), together with the norm
\[
\|u\|_{H^1_{D,\text{mol}(N)}} := \inf \{\|\lambda_j\|_{l^1} : \sum_j \lambda_j a_j\text{ converges to }u\text{ in }L^1\}.
\]
The Banach space \(H^1_{D,\text{at}(N)}(\mathcal{V})\) is defined by replacing molecules with atoms.
The $L^1(\mathcal{V})$ convergence required in the above definition ensures that $H^1_{D,\text{mol}(N)}(\mathcal{V})$ and $H^1_{D,\text{at}(N)}(\mathcal{V})$ are complete. This is because molecules and atoms are uniformly bounded in $L^1(\mathcal{V})$. In particular, if $(u_n)_n$ is a sequence in $H^1_{D,\text{mol}(N)}(\mathcal{V})$ such that $\sum_n \|u_n\|_{H^1_{D,\text{mol}(N)}}$ is finite, then the uniform $L^1(\mathcal{V})$ bound for molecules and the dominated convergence theorem imply that $\sum_n u_n$ converges in the $H^1_{D,\text{mol}(N)}(\mathcal{V})$ norm to some $u \in H^1_{D,\text{mol}(N)}(\mathcal{V})$, hence $H^1_{D,\text{mol}(N)}(\mathcal{V})$ is complete. The $L^1(\mathcal{V})$ convergence requirement also distinguishes these spaces from those in the literature that are defined as an abstract completion of a molecular or atomic space on which $L^2(\mathcal{V})$ convergence is required. This is discussed further in Remark 3.13.

The embedding $H^1_{D,\psi}(\mathcal{V}) \subseteq L^1(\mathcal{V})$ is not required to define the molecular space nor the atomic space, since $H^1_{D,\text{at}(N)}(\mathcal{V}) \subseteq H^1_{D,\text{mol}(N)}(\mathcal{V}) \subseteq L^1(\mathcal{V})$ is automatic. It is only when the embedding of $H^1_{D,\psi}(\mathcal{V})$ in $L^1(\mathcal{V})$ holds, however, that we can establish the following connection.

**Theorem 3.13.** Suppose that $M$ is a doubling metric measure space satisfying (D$_1$) and that $\mathcal{D}$ satisfies (H$_1$)–(H$_3$) on $L^2(\mathcal{V})$ for some $\omega \in [0, \pi/2)$ and $m \in \mathbb{N}$. Also, assume that for some $\theta \in (\omega, \pi/2)$, $\beta > \kappa/2m$ and nondegenerate $\psi \in \Psi_{\beta}(S^d_\theta)$, the completion $H^1_{D,\psi}(\mathcal{V})$ of $E^1_{\mathcal{V}}(\mathcal{V})$ in $L^1(\mathcal{V})$ exists. It follows that if $N \in \mathbb{N}$ and $N > \kappa/2m$, then $H^1_{D,\psi}(\mathcal{V}) = H^1_{D,\text{mol}(N)}(\mathcal{V})$.

**Proof.** Suppose that $N \in \mathbb{N}$. The proof that $H^1_{D,\psi} \subseteq H^1_{D,\text{mol}(N)}$ follows that of Lemma 3.9 except we need to replace $L^2$ convergence with $H^1_{D,\psi}$ convergence. We use the construction in [9] Lemma 6.7] to fix a nondegenerate $\tilde{\psi} \in \Psi_{\beta}(S^d_\theta)$ such that $S^d_\psi A$ is an $H^1_D$-molecule of type $N$ whenever $A$ is a $T^1$-atom. The existence of the completion $H^1_{D,\psi}(\mathcal{V})$ of $E^1_{\mathcal{V}}(\mathcal{V})$ in $L^1$ allows us to apply (3.16) and ensures that $H^1_{D,\psi} \subseteq L^1$.

Suppose that $u \in H^1_{D,\psi}$, and use (3.16) to choose $V$ in $T^1$ such that $u = \tilde{S}^d_\psi V$ and $\|V\|_{T^1} \leq 2\|u\|_{H^1_{D,\psi}}$. The atomic characterisation of $T^1$ in Theorem 3.1 provides a sequence $(\lambda_j)_j$ in $\ell^1$ and a sequence $(A_j)_j$ of $T^1$-atoms such that $\sum_j \lambda_j A_j$ converges to $V$ in $T^1$ and $\|\lambda_j\|_{\ell^1} \lesssim \|V\|_{T^1}$. It follows that $\sum_j \lambda_j S^d_\psi A_j$ converges to $u$ in $H^1_{D,\psi}$, and in $L^1$, because $\tilde{S}^d_\psi \in \mathcal{L}(T^1, H^1_{D,\psi})$ and $\tilde{S}^d_\psi = S^d_\psi$ on $T^1 \cap T^2$ by (3.16), and because $H^1_{D,\psi} \subseteq L^1$. Now recall that $\tilde{\psi}$ has the property whereby each $S^d_\psi A_j$ is an $H^1_D$-molecule of type $N$, so that $u \in H^1_{D,\text{mol}(N)}$ and $\|u\|_{H^1_{D,\text{mol}(N)}} \leq \|(\lambda_j)\|_{\ell^1} \lesssim \|V\|_{T^1} \lesssim \|u\|_{H^1_{D,\psi}}$, hence $H^1_{D,\psi} \subseteq H^1_{D,\text{mol}(N)}$.

Now suppose that $N \in \mathbb{N}$, $N > \kappa/2m$ and $u \in H^1_{D,\text{mol}(N)}$. Then $u \in L^1$ and there is a sequence $(\lambda_j)_j$ in $\ell^1$ and a sequence $(a_j)_j$ of $H^1_D$-molecules of type $N$ such that $\sum_j \lambda_j a_j$ converges to $u$ in $L^1$ with $\|(\lambda_j)\|_{\ell^1} \leq 2\|u\|_{H^1_{D,\text{mol}(N)}}$. The construction in [9] Lemma 6.8] allows us to fix $\hat{\psi} \in \Psi_{\beta}(S^d_\theta)$ such that $Q^d_\psi$ is uniformly bounded in $T^1$ on all $H^1_D$-molecules of type $N$ (this requires $N > \kappa/2m$), so by (3.15) we have

$$\left\| \sum_{j=1}^l \lambda_j a_j - \sum_{j=1}^k \lambda_j a_j \right\|_{H^1_{D,\psi}} \lesssim \sum_{j=k+1}^l |\lambda_j||Q^d_\psi a_j|_{T^1} \lesssim \sum_{j=k+1}^l |\lambda_j|.$$
whenever \( l > k > 0 \). Therefore, there exists \( v \) in \( H^1_{D,\psi} \) such that \( \sum_j \lambda_j a_j \) converges to \( v \) in \( H^1_{D,\psi} \), and hence in \( L^1 \) because \( H^1_{D,\psi} \subseteq L^1 \). It follows that \( u = v \in H^1_{D,\psi} \) with 
\[ \|u\|_{H^1_{D,\psi}} \lesssim \lim_{k \to \infty} \sum_{j=1}^k |\lambda_j| \|\nabla^j \psi a_j\|_{T^1} \lesssim \|\lambda_j\|_{\varepsilon} \lesssim \|u\|_{H^1_{D,\psi}}. \]
so \( H^1_{D,\psi} \subseteq H^1_{D,\psi} \) and the proof is complete. \( \square \)

**Remark 3.14.** The proof of Theorem 3.13 shows that the same result holds when the \( L^1(V) \) convergence required in Definition 3.12 is replaced with \( H^1_{D,\psi}(V) \) convergence.

**Remark 3.15.** If we define \( E^1_{D,\psi}(V) \) to be the normed space obtained by replacing \( L^1(V) \) convergence with \( L^2(V) \) convergence in Definition 3.12 then we can prove that 
\( E^1_{D,\psi}(V) = E^1_{D,\psi}(V) \) without assuming that the embedding \( H^1_{D,\psi}(V) \subseteq L^1(V) \) holds. This was known previously (see [21, Theorem 3.5]). In particular, the proof of Lemma 3.9 shows that \( E^1_{D,\psi}(V) \subseteq E^1_{D,\psi}(V) \), whilst the reverse inclusion is proved in a manner similar to that of Theorem 3.13. This means that we can identify any completion of \( E^1_{D,\psi}(V) \) with any completion of \( E^1_{D,\psi}(V) \), but both are still abstract spaces and it is not known whether either can be embedded in \( L^1(V) \), or in any function space, without the extra hypotheses on \( D \) in Theorem 3.10 (or Theorem 4.7).

### 3.2. The Embedding \( H^p_L \subseteq L^p \) for Divergence Form Elliptic Operators

It is a simple matter to verify the hypotheses of Theorem 3.10 for an operator that generates a semigroup satisfying pointwise kernel estimates. We demonstrate this by obtaining Theorem 1.2 as a special case of the more general result below.

Let \( M = \mathbb{R}^n \) and consider the divergence form operator \( L = -\text{div} AV \) acting on \( L^2(\mathbb{R}^n) \) and interpreted in the usual weak sense via a sesquilinear form, where \( A \in L^\infty(\mathbb{R}^n, L(\mathbb{C}^n)) \) is elliptic in the sense that there exists \( \lambda > 0 \) such that 
\[ \text{Re} \langle A(x)\zeta, \zeta \rangle_{\mathbb{C}^n} \geq \lambda |\zeta|^2 \quad \forall \zeta \in \mathbb{C}^n, \text{ a.e. } x \in \mathbb{R}^n \]
There exists \( \omega_L \in [0, \pi/2) \), depending on \( \lambda \) and \( \|A\|_\infty \), such that \( L \) is \( \omega_L \)-sectorial (see, for instance, [5, Chapter 2]), hence \( L : \text{Dom}(L) \subseteq L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n) \) satisfies (H1), (H2) with \( \omega = \omega_L \). Note that \( \text{Dom}(L) = \{u \in W^{1,2}(\mathbb{R}^n) : AVu \in \text{Dom}(\nabla^*)\} \).
It is also known that \( L \) satisfies (H3) with \( m = 2 \) (see [6, Lemma 2.1]).

In order to embed \( H^p_{L,\psi}(\mathbb{R}^n) \) in \( L^p(\mathbb{R}^n) \) when \( 1 \leq p \leq 2 \) and \( 1/q' + 1/q = 1 \), we assume that there exists \( g \in L^2_{\text{loc}}((0, \infty)) \) such that the analytic semigroup \( (e^{-tL^*})_{t>0} \) generated by the adjoint \(-L^* \) on \( L^2(\mathbb{R}^n) \) satisfies
\[ \|e^{-tL^*} u\|_p \lesssim g(t)\|u\|_2 \quad \forall u \in L^2(\mathbb{R}^n), \forall t > 0. \]
This assumption is always satisfied when \( 2n/(n+2) \leq q \leq 2 \) in dimension \( n \geq 3 \) (see [5, Proposition 3.2] and [21, Lemma 2.25]). It remains an open question, however, as to whether the following theorem holds in the absence of estimates such as (3.20).

**Theorem 3.16.** Suppose that \( A \in L^\infty(\mathbb{R}^n, L(\mathbb{C}^n)) \) is elliptic and \( L = -\text{div} AV \) on \( L^2(\mathbb{R}^n) \) satisfies (3.20) for some \( q \in [1, 2] \). If \( g \leq p \leq 2 \), \( \theta \in (\omega_L, \pi/2) \), \( \beta > n/4 \) and \( \psi \in \Psi_\beta(S_\theta^p) \) is nondegenerate, then the completion \( H^p_{L,\psi}(\mathbb{R}^n) \) of \( E^p_{L,\psi}(\mathbb{R}^n) \) in \( L^p(\mathbb{R}^n) \) exists and \( H^p_{L,\psi}(\mathbb{R}^n) \cap L^2(\mathbb{R}^n) = E^p_{L,\psi}(\mathbb{R}^n) \). Moreover, if \( q = 1 \), \( N \in \mathbb{N} \) and \( N > n/4 \), then \( H^1_{L,\psi}(\mathbb{R}^n) = H^1_{L,\psi}(\mathbb{R}^n) \), and when \( A \) is self-adjoint, then also \( H^1_{L,\psi}(\mathbb{R}^n) = H^1_{L,\psi}(\mathbb{R}^n) \).
Proof. We will use (3.20) to show that (H4)$_q$ holds with $\kappa = n$. The hypotheses of Theorem 3.10 will then be satisfied, since it was noted above that $L$ satisfies (H1)–(H3) with $\omega = \omega_L$ and $m = 2$. To this end, choose $\theta \in (\omega_L, \pi/2)$, define the nondegenerate function $\psi(z) = ze^{-z^2}$ on $S^0_\theta \cup \{0\}$ and note that $\psi \in \Psi^\beta(S^0_\theta)$ for any $\beta > n/4$. For each $F \in T^2_\theta(\mathbb{R}^{n+1}_+)$, as defined in Remark 3.11 there is a ball $B \subseteq M$ and $r > 1$ such that $\text{sppt}(F) \subseteq B \times [1/r, r]$, and so we have

$$\|S^{L^*}_{\psi^*} F\|_{q'} = \left\| \int_{1/r}^r t^2 L^* e^{-t^2 L^*} F_t \frac{dt}{t} \right\|_{q'}$$

$$\leq \int_{1/r}^r \left\| e^{-(t^2/2)L^*} t^2 L^* e^{-(t^2/2)L^*} F_t \right\|_{q'} \frac{dt}{t}$$

$$\leq \left( \int_{1/r}^r (g(t^2/2))^2 \frac{dt}{t} \right)^{1/2} \left( \int_0^{\infty} \| F_t \|_2^2 \frac{dt}{t} \right)^{1/2}$$

$$\leq \| F \|_{T^2},$$

where the third line uses (3.20), and the fourth line uses the analyticity of the semigroup $(e^{-tL^*})_{t>0}$ (see, for instance, [19, Theorem II.4.6]) followed by the Cauchy–Schwarz inequality. This shows that $S^{L^*}_{\psi^*}(T^2_\theta(\mathbb{R}^{n+1}_+)) \subseteq L^{q'}(\mathbb{R}^n)$, so Remark 3.11 implies that (H4)$_q$ holds with $\kappa = n$, as required.

We have now shown that the hypotheses of Theorem 3.10 hold. Moreover, when $q = 1$, the hypotheses of Theorem 3.11 follow. The conclusions of those two theorems complete the proof, except for the atomic characterisation in the case when $q = 1$ and $A$ is self-adjoint, but then $L = -\text{div} \, A \nabla$ satisfies the requirements of Theorem 1.3 (see [3, Proposition 3.2] for a proof of the Davies–Gaffney estimates (5.1)), so we refer the reader to the proof of that theorem in Section 5.

Theorem 1.2 is a special case of the above result.

Proof of Theorem 1.2. This is a special case of Theorem 3.16 since property (1.4) corresponds to property (3.20) with $q = 1$. □

4. Self-Adjoint Operators with Finite Propagation Speed

We now restrict the theory of the previous section to the context of any self-adjoint operator $D : \text{Dom}(D) \subseteq L^2(\mathcal{V}) \to L^2(\mathcal{V})$ for which the associated unitary $C_0$-group $(e^{itD})_{t \in \mathbb{R}}$ has finite propagation speed. The existence of this group is guaranteed by Stone’s Theorem because $D$ is self-adjoint. The defining features of such a group are that the mapping $t \mapsto e^{itD}$ is strongly continuous from $\mathbb{R}$ to $\mathcal{L}(L^2(\mathcal{V}))$ with $e^{i(s+t)D} = e^{isD}e^{itD}$, $e^{itD}|_{t=0} = I$ and $\frac{d}{dt}(e^{itD}u)|_{t=0} = iDu$ for all $u \in \text{Dom}(D) = \{u \in L^2(\mathcal{V}) : \frac{d}{dt}(e^{itD}u)|_{t=0} \text{ exists in } L^2(\mathcal{V})\}$. An introduction to the theory of such groups can be found in [24, 19]. The group $(e^{itD})_{t \in \mathbb{R}}$ is said to have finite propagation speed when there exists a finite constant $c_D > 0$ such that for all $u \in L^2(\mathcal{V})$ satisfying $\text{sppt}(u) \subseteq F \subseteq M$ and all $t \in \mathbb{R}$, it holds that $\text{sppt}(e^{itD}u) \subseteq \{x \in M : \rho(\{x\}, F) \leq c_D |t|\}$. We begin by establishing that these assumptions allow us to apply the theory from the previous section with $\mathcal{D} = D$, $\omega = 0$ and $m = 1$. 
Lemma 4.1. If $D$ is a self-adjoint operator on $L^2(\mathcal{V})$ and the group $(e^{itD})_{t \in \mathbb{R}}$ has finite propagation speed $c_D > 0$, then $D$ satisfies (H1)–(H3) with $\omega = 0$ and $m = 1$.

Proof. Since $D$ is self-adjoint, it satisfies (H1) and (H2) with $\omega = 0$, $C_\theta = 1/\sin \theta$ and $c_\theta = 1$. It remains to prove (H3). Let $E$ and $F$ denote measurable subsets of $M$. The finite propagation speed implies that $1_E e^{itD} 1_F = 0$ whenever $\rho(E, F) > c_D |t|$. For all $z \in \mathbb{C}$ with $\text{Im}(\pm z) > 0$, we use the integral representation of the resolvent $(zI - D)^{-1} = \mp i \int_0^\infty e^{\mp izt} e^{itD} dt$ to obtain

$$\|1_E(zI - D)^{-1} 1_F\| \leq \int_{\rho(E,F)/c_D}^\infty |e^{\mp izt}| \|1_E e^{\mp izt} 1_F\| dt \leq \int_{\rho(E,F)/c_D}^\infty e^{-|\text{Im}(\pm z)t|} dt.$$ 

For each $\theta \in (0, \pi/2)$, it follows that

$$\|1_E(zI - D)^{-1} 1_F\| \leq \frac{C_\theta}{|z|} \exp \left( -\frac{\rho(E, F) |z|}{c_D C_\theta} \right) \quad \forall z \in \mathbb{C} \setminus S_\theta,$$

which implies (H3) with $m = 1$. \qed

The algebra of complex-valued bounded Borel measurable functions on $\mathbb{R}$ is denoted by $B^\infty(\mathbb{R})$. The Spectral Theorem for self-adjoint operators provides $D$ with a bounded $B^\infty(\mathbb{R})$ functional calculus such that $\|f(D)\| \leq \|f\|_\infty$ for all $f \in B^\infty(\mathbb{R})$. This coincides with the holomorphic functional calculus defined by (3.2) and (3.5) when $f \in H^\infty(S_\theta^c \cup \{0\})$ because the holomorphic functional calculus is unique with respect to (3.6)–(3.8). In particular, it is well known (see [25, Chapter XX, §1]) that the Borel functional calculus is an algebra homomorphism from $B^\infty(\mathbb{R})$ into $L(L^2(\mathcal{V}))$ that satisfies (3.6) and (3.7), with $\mathbb{R}$ in place of $S_\theta^c \cup \{0\}$, as well as the following convergence lemma, which is related to (3.8):

If $(f_n)_n$ is a sequence in $B^\infty(\mathbb{R})$ that converges pointwise to a function $f$ in $B^\infty(\mathbb{R})$, and $\sup_n \|f_n\|_\infty < \infty$, then $\lim_{n \to \infty} f_n(D)u = f(D)u$ for all $u \in L^2(\mathcal{V})$.

The orthogonal decomposition $L^2(\mathcal{V}) = \mathbb{R}(D) \oplus N(D)$ and the properties of the Borel functional calculus allow us to prove the following Calderón reproducing formula.

Proposition 4.2. Suppose that $D$ is self-adjoint on $L^2(\mathcal{V})$. If $f$ and $g$ in $B^\infty(\mathbb{R})$ satisfy $f(0)g(0) = 0$, $\int_0^\infty |f(\pm t)g(\pm t)| \frac{dt}{t} < \infty$ and $\int_0^\infty f(\pm t)g(\pm t) \frac{dt}{t} = 1$, then

$$\int_0^\infty f_t(D)g_t(D)u \frac{dt}{t} = P_{\mathbb{R}(D)} u \quad \forall u \in L^2(\mathcal{V}),$$

where $P_{\mathbb{R}(D)}$ denotes the projection from $L^2(\mathcal{V})$ onto $\mathbb{R}(D)$.

Proof. Suppose that $f$ and $g$ in $B^\infty(\mathbb{R})$ satisfy the hypotheses of the proposition. For each $n \in \mathbb{N}$, we have

$$h_n(x) := \int_0^n f_t(x)g_t(x) \frac{dt}{t} = \begin{cases} \int_0^n f(t)g(t) \frac{dt}{t}, & \text{if } x > 0; \\ 0, & \text{if } x = 0; \\ \int_{-n}^{-1} f(t)g(-t) \frac{dt}{-t}, & \text{if } x < 0. \end{cases}$$

The sequence $(h_n)_n$ converges pointwise on $\mathbb{R}$ to the characteristic function $1_{\mathbb{R} \setminus \{0\}}$, and $\sup_n \|h_n\|_\infty \leq \int_0^\infty |f(\pm t)g(\pm t)| \frac{dt}{t} < \infty$, so it follows from (4.1) that

$$\int_0^\infty f_t(D)g_t(D)u \frac{dt}{t} = \lim_{n \to \infty} h_n(D)u = 1_{\mathbb{R} \setminus \{0\}}(D)u = P_{\mathbb{R}(D)} u \quad \forall u \in L^2(\mathcal{V}),$$

where $P_{\mathbb{R}(D)}$ denotes the projection from $L^2(\mathcal{V})$ onto $\mathbb{R}(D)$. \qed
where the final equality relies on the fact that $1_{\mathbb{R}}(D) = I$ and $1_{(0)}(D) = P_{\mathbb{N}(D)}$. \hfill \Box

We now require a class of functions that interact well with finite propagation speed. To this end, a function on $\mathbb{R}$ is called nondegenerate when it is not identically zero on $(0, \infty)$ nor on $(-\infty, 0)$. The Fourier transform of any Schwartz function $f \in \mathcal{S}(\mathbb{R})$ is denoted by $\hat{f}$. For $\delta > 0$ and $N \in \mathbb{N}$, define

$$\tilde{\Theta}(\mathbb{R}) = \{ \varphi \in \mathcal{S}(\mathbb{R}) : \text{sppt } \hat{\varphi} \subseteq [-\delta, \delta] \},$$

$$\tilde{\Psi}_N(\mathbb{R}) = \{ \eta \in \tilde{\Theta}(\mathbb{R}) : \partial^k\eta(0) = 0 \text{ for all } k \in \{1, \ldots, N\} \},$$

$$\tilde{\Theta}(\mathbb{R}) = \bigcup_{\delta > 0} \tilde{\Theta}(\mathbb{R}), \tilde{\Psi}_N(\mathbb{R}) = \bigcup_{\delta > 0} \tilde{\Psi}_N(\mathbb{R}) \text{ and } \tilde{\Psi}(\mathbb{R}) = \tilde{\Psi}_1(\mathbb{R}).$$

For $\varphi \in \tilde{\Theta}(\mathbb{R})$, the Fourier inversion formula and the $B^\infty(\mathbb{R})$ functional calculus imply that

$$\varphi(D)u = \frac{1}{2\pi} \int_{\mathbb{R}} \varphi(t)e^{itD}u \, dt \quad \forall u \in L^2(\mathcal{V}). \tag{4.3}$$

For $\eta \in \tilde{\Psi}(\mathbb{R})$, using the $B^\infty(\mathbb{R})$ functional calculus, define $Q^D_{\eta}$ in $\mathcal{L}(L^2, T^2)$ by $(Q^D_{\eta}u)_t = \eta(tD)u$, and $S^D_{\eta}$ in $\mathcal{L}(T^2, L^2)$ by $S^D_{\eta}u = \int_0^\infty \eta(sD)U_sds$, as well as the space $E^p_{D,\eta}(\mathcal{V}) = S^D_{\eta}(T^2 \cap T^2)$. This extends Definitions 3.2 and 3.4, which use the $H^\infty(S^t_0 \cup \{0\})$ functional calculus. Also, note that

$$\eta(D)u = \frac{P_{\mathbb{R}(D)}^2}{P_{\mathbb{R}(D)}} \eta(D) \frac{P_{\mathbb{R}(D)}}{P_{\mathbb{R}(D)}} u \quad \forall u \in L^2(\mathcal{V}), \tag{4.4}$$

since $\eta(0) = 0$ and $1_{(0)}(D) = P_{\mathbb{N}(D)}$.

The following corollary of Proposition 4.2 extends the Calderón reproducing formula in Proposition 3.3 and allows us to incorporate $\tilde{\Psi}(\mathbb{R})$ class functions into the theory of Section 3.

**Corollary 4.3.** Suppose that $D$ is a self-adjoint operator on $L^2(\mathcal{V})$. If $\sigma, \tau > 0$, $\theta \in (0, \pi/2)$ and $\eta \in \tilde{\Psi}(\mathbb{R})$ is nondegenerate, then there exists a nondegenerate $\psi \in \Psi^*_\sigma(S^t_0)$ such that $S^D_{\psi}Q^D_{\eta}u = S^D_{\eta}Q^D_{\psi}u = \frac{P_{\mathbb{R}(D)}}{P_{\mathbb{R}(D)}} u$ for all $u \in L^2(\mathcal{V})$.

**Proof.** Suppose that $\eta \in \tilde{\Psi}_N(\mathbb{R})$ for some $\delta > 0$ and $N \in \mathbb{N}$. It follows by the Paley–Wiener Theorem that $\eta$ extends to an entire function satisfying $|\eta(z)| \leq Ce^{\delta|z|}$ for some constant $C > 0$ and all $z \in \mathbb{C}$. Now consider $\sigma, \tau > 0$ and $\theta \in (0, \pi/2)$. When $\text{Re}(z) > 0$, define $\psi(z) = \alpha_+ z^\sigma e^{-2\delta t \sec \theta} \eta^*(z)$, and when $\text{Re}(z) < 0$, define $\psi(z) = \alpha_- (-z)^\sigma e^{2\delta t \sec \theta} \eta^*(z)$, where $\alpha_\pm$ are the normalising constants defined by

$$\alpha_+ \int_0^\infty t^\sigma e^{-2\delta t \sec \theta} |\eta(t)|^2 \frac{dt}{t} = 1 \quad \text{and} \quad \alpha_- \int_0^\infty t^\sigma e^{-2\delta t \sec \theta} |\eta(-t)|^2 \frac{dt}{t} = 1.$$

The integrals above are positive, so the normalising constants exist, and for all $z \in \mathbb{C}$ with $\text{Re}(z) \neq 0$, we have

$$\int_0^\infty \psi(tz) \eta(tz) \frac{dt}{t} = 1.$$

Finally, define $\psi(0) = 0$ so that $\psi \in \Psi^*_\sigma(S^t_0)$, and since $\psi$ is clearly nondegenerate, the result follows from Proposition 4.2. \hfill \Box

The next result shows how $\tilde{\Theta}(\mathbb{R})$ functions interact with finite propagation speed. In particular, the off-diagonal estimate in (4.5) is much sharper than that in (3.9).
Lemma 4.4. Suppose that $D$ is a self-adjoint operator on $L^2(\mathcal{V})$ and the group $(e^{itD})_{t \in \mathbb{R}}$ has finite propagation speed $c_D > 0$. If $\delta > 0$ and $\varphi \in \tilde{\Theta}^1(\mathbb{R})$, then

$$
\|1_E \varphi(D) 1_F\| \leq \frac{1}{\pi} \|\hat{\varphi}\|_{\infty} \max \left\{ \delta - \frac{\rho(E,F)}{c_D t}, 0 \right\} \leq C e^{-\rho(E,F)t/t}
$$

for all $t > 0$, all measurable sets $E, F \subseteq M$, and some $C > 0$.

Proof. Suppose that $\varphi \in \tilde{\Theta}(\mathbb{R})$ with $\text{sppt } \varphi \subseteq [-\delta, \delta]$. It follows from (4.3) that

$$
\varphi(D) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{\varphi}(s) e^{isD} u ds = \frac{1}{2\pi} \int_{|s| \leq \delta t} \hat{\varphi}\left(\frac{s}{t}\right) e^{isD} u ds \quad \forall t > 0, \forall u \in L^2(\mathcal{V}).
$$

Suppose that $E$ and $F$ are measurable subsets of $M$. The finite propagation speed implies $1_E e^{isD} 1_F = 0$ whenever $\rho(E,F) > c_D |s|$, hence $1_E \varphi(D) 1_F = 0$ whenever $\rho(E,F)/c_D > \delta t$ by the preceding formula. In addition, if $\rho(E,F)/c_D \leq \delta t$, then

$$
\|1_E \varphi(D) 1_F u\|_2 \leq \frac{1}{2\pi} \int_{\rho(E,F)/c_D \leq |s| \leq \delta t} \|\hat{\varphi}\left(\frac{s}{t}\right)\|_2 \|1_E e^{isD} 1_F u\|_2 \frac{ds}{t}
$$

$$
\leq \frac{1}{2\pi} \int_{\rho(E,F)/c_D \leq |s| \leq \delta} \|\hat{\varphi}(\sigma)\| d\sigma \|u\|_2
$$

$$
\leq \frac{1}{\pi} \|\hat{\varphi}\|_{\infty} \left(\delta - \frac{\rho(E,F)}{c_D t}\right) \|u\|_2
$$

$$
\leq \frac{1}{\pi} \|\hat{\varphi}\|_{\infty} \delta c_D e^{-\rho(E,F)/t} \|u\|_2
$$

for all $u \in L^2(\mathcal{V})$, which completes the proof. \qed

The next two results show that $E^p_{\delta,D,\psi}(\mathcal{V}) = E^p_{\delta,\eta}(\mathcal{V})$ for suitable $\psi$ in $\Psi(S^0_\eta)$ and $\eta$ in $\tilde{\Psi}(\mathbb{R})$. The results rely on some technical off-diagonal estimates that we postpone until Section 6. The first result is an extension of [9, Theorem 4.9].

Proposition 4.5. Suppose that $M$ is a doubling metric measure space satisfying [D], that $D$ is a self-adjoint operator on $L^2(\mathcal{V})$, and the group $(e^{itD})_{t \in \mathbb{R}}$ has finite propagation speed. If $\rho \in [1, 2], \theta \in (0, \pi/2), N \in \mathbb{N}, N > \kappa/2, \psi \in \Psi_{2N+1}(S^0_\eta)$, $\eta \in \tilde{\Psi}_N(\mathbb{R})$ and $\tilde{\eta} \in \tilde{\Psi}(\mathbb{R})$, then

$$
\|Q_{\eta}^D S_{\psi}^D U\|_{T^p} \lesssim \|U\|_{T^p} \quad \text{and} \quad \|Q_{\psi}^D S_{\eta}^D U\|_{T^p} \lesssim \|U\|_{T^p}
$$

for all $U \in T^p \cap T^2$.

Proof. The proof follows [9, Theorem 4.9]. When $p = 2$, the result is immediate. When $p = 1$, it suffices to show that there exists $C > 0$ such that

$$
\|Q_{\eta}^D S_{\psi}^D (A)\|_{T^1} \leq C \quad \text{and} \quad \|Q_{\psi}^D S_{\eta}^D (A)\|_{T^1} \leq C
$$

for all $A$ that are $T^1$-atoms, since Theorem 3.1 applies. When $p \in (1, 2)$, the result then follows by the interpolation in (3.11). Therefore, it remains to prove (4.6).

Lemma 6.3 applied with $(m, n, N, \sigma, \tau, \delta) = (1, N, 1, 2N+1, N + 1, 1)$ shows that

$$
\|1_E (\tilde{\eta}_r \psi_s)(D) 1_F\| \leq C \left\{ \begin{array}{ll}
(s/t)^N (t/\rho(E,F))^N, & \text{if } 0 < s \leq t; \\
(t/s) (s/\rho(E,F))^{2N+1}, & \text{if } 0 < t \leq s,
\end{array} \right.
$$

for all $t > 0$, all measurable sets $E, F \subseteq M$, and some $C > 0$. \qed
for all measurable sets $E, F \subseteq M$. Since $(\psi \eta_s)(D) = (\eta_s \psi_t)(D)$, Lemma 6.3 applied with $(m, n, N, \sigma, \tau, \delta) = (N, 1, N, 2N + 1, N + 1, 1)$ also shows that
\[
\|1_E(\psi \eta_s)(D)1_F\| \leq C \begin{cases} (s/t)^N(t/p(E, F))^{3N}, & \text{if } 0 < s \leq t; \\ (t/s)(s/p(E, F))^{2N-1}, & \text{if } 0 < t \leq s, \end{cases}
\]
for all measurable sets $E, F \subseteq M$. These estimates combined with \([D_\alpha]\) prove (4.6) as in Step 2 of the proof of Theorem 4.9 in \([9]\). This completes the proof.

The second result is an extension of \([9]\) Lemma 5.2.

**Proposition 4.6.** Suppose that $M$ is a doubling metric measure space satisfying $[D_\alpha]$, that $D$ is a self-adjoint operator on $L^2(V)$, and the group $(e^{itD})_{t \in \mathbb{R}}$ has finite propagation speed. If $p \in [1, 2]$, $\theta \in (0, \pi/2)$, $\beta > \kappa/2$, $N \in \mathbb{N}$, $N > \kappa/2$, and all of $\psi \in \Psi_\beta(S^\theta_\eta)$, $\eta \in \overline{\Psi}_N(\mathbb{R})$ and $\tilde{\eta} \in \overline{\Psi}(\mathbb{R})$ are nondegenerate, then
\[
S^D_\psi(T^p \cap T^2) = S^D_\eta(T^p \cap T^2) = \{u \in \overline{R}(D) : Q^D_\eta u \in T^p\}
\]
with the norm equivalence
\[
\|u\|_{E^p_{D, \psi}} \simeq \|u\|_{E^p_{D, \eta}} \simeq \|Q^D_\eta u\|_{T^p} \quad \forall u \in E^p_{D, \psi} = S^D_\psi(T^p \cap T^2).
\]
If, in addition, the completion $H^p_{D, \psi}$ of $E^p_{D, \psi}$ in $L^p$ exists, then there are unique extensions $\tilde{S}^D_\eta \in \mathcal{L}(T^p, H^p_{D, \psi})$ and $\tilde{Q}^D_\eta \in \mathcal{L}(H^p_{D, \psi}, T^p)$ such that $\tilde{S}^D_\eta = S^D_\eta$ on $T^p \cap T^2$ and $\tilde{Q}^D_\eta = Q^D_\eta$ on $E^p_{D, \psi}$. It also holds that $H^p_{D, \psi} = \tilde{S}^D_\psi(T^p)$ with the norm equivalence
\[
\|u\|_{H^p_{D, \psi}} \simeq \inf \{\|U\|_{T^p} : U \in T^p \text{ and } u = \tilde{S}^D_\eta U\} \simeq \|\tilde{Q}^D_\eta u\|_{T^p} \quad \forall u \in H^p_{D, \psi}.
\]
Moreover, if $E^p_{D, \psi}$ is dense in $H^p_{D, \psi} \cap L^2$, then also $\tilde{Q}^D_\eta = Q^D_\eta$ on $H^p_{D, \psi} \cap L^2$.

**Proof.** It suffices, by Theorem 3.6, to prove the result for a fixed nondegenerate $\psi$ in $\Psi_\beta(S^\theta_\eta)$, so we select $\psi \in \Psi_\beta(S^\theta_\eta)$ satisfying $\int_0^\infty \psi(t^2)\frac{dt}{t^\theta} = 1$. Suppose that both $\eta \in \overline{\Psi}_N(\mathbb{R})$ and $\tilde{\eta} \in \overline{\Psi}(\mathbb{R})$ are nondegenerate, and then use Corollary 4.3 to obtain $\varphi$ and $\tilde{\varphi}$ in $\Psi^N_{2N+1}(S^\theta_\eta)$ such that $S^D_\varphi Q^D_\varphi = S^D_\tilde{\varphi} Q^D_\tilde{\varphi} = P_{R(D)} = S^D_\varphi Q^D_\varphi$. The proof of (4.7) and (4.8) proceeds in three parts corresponding to the set inclusions
\[
S^D_\psi(T^p \cap T^2) \subseteq S^D_{\tilde{\varphi}}(T^p \cap T^2) \subseteq \{u \in \overline{R}(D) : Q^D_\eta u \in T^p\} \subseteq S^D_\varphi(T^p \cap T^2)
\]
and the related norm estimates.

(i) If $u \in S^D_\psi(T^p \cap T^2)$, then (3.14) implies that $u \in \overline{R}(D)$ and $Q^D_\eta u \in T^p \cap T^2$, so $u = S^D_\eta(Q^D_\varphi S^D_\psi Q^D_\varphi u)$ and (3.13) followed by (3.15) imply that
\[
\|u\|_{E^p_{D, \eta}} \leq \|Q^D_\eta S^D_\psi (Q^D_\psi u)\|_{T^p} \lesssim \|Q^D_\eta u\|_{T^p} \simeq \|u\|_{E^p_{D, \psi}}.
\]

(ii) If $u \in S^D_\eta(T^p \cap T^2)$, then $u \in \overline{R}(D)$ by (4.4), and there exists $V \in T^p \cap T^2$ such that $u = S^D_\eta(V)$ and $\|V\|_{T^p} \leq 2\|u\|_{E^p_{D, \eta}}$, so by applying Proposition 4.5 twice we obtain
\[
\|Q^D_\eta u\|_{T^p} = \|Q^D_\eta S^D_\psi (Q^D_\psi S^D_\eta u)\|_{T^p} \lesssim \|V\|_{T^p} \lesssim \|u\|_{E^p_{D, \eta}}.
\]

(iii) If $u \in \overline{R}(D)$ and $Q^D_\eta u \in T^p$, then $u = S^D_\eta(Q^D_\varphi S^D_\psi Q^D_\varphi u)$, so (3.13) implies that
\[
\|u\|_{E^p_{D, \psi}} \leq \|Q^D_\psi S^D_\varphi (Q^D_\eta u)\|_{T^p} \lesssim \|Q^D_\eta u\|_{T^p}.
\]
We obtain (4.9) and the related properties by the arguments used to prove (3.16) and the related properties. This completes the proof.
We now introduce hypothesis \([H4]\) on \(D\) in order to prove that the completion of \(E_{D,\psi}^p(V)\) in \(L^p(V)\) exists. This provides an alternative to hypothesis \([H4]\) from Theorem 3.10 when \(D\) is self-adjoint and \((e^{itD})_{t \in \mathbb{R}}\) has finite propagation speed. The advantage of hypothesis \([H4]\) is that \(S_n^D F\) has compact support whenever \(F\) has compact support, and as such, it is more easily verified that \(S_n^D F \in L^q(V)\).

**Theorem 4.7.** Suppose that \(M\) is a doubling metric measure space satisfying \([D_m]\), that \(D\) is a self-adjoint operator on \(L^2(V)\), and \((e^{itD})_{t \in \mathbb{R}}\) has finite propagation speed. If \(1 \leq q \leq p \leq 2\), then \(D,\psi\) is nondegenerate and

\[
\text{there exists a nondegenerate function } \eta \in \tilde{\Psi}(\mathbb{R}) \text{ such that the set } \{F \in T^2 \cap \mathcal{T'} : S_n^D F \in L^q(V)\} \text{ is weak-star dense in } T^p(V_+),
\]

where \(1/q + 1/q' = 1\), then the completion \(H_{D,\psi}^p(V)\) of \(E_{D,\psi}^p(V)\) in \(L^p(V)\) exists. Moreover, it holds that \(H_{D,\psi}^p(V) \cap L^2(V) = E_{D,\psi}^p(V)\).

**Proof.** Following the proof of Theorem 3.10, let \((u_n)_n\) denote a Cauchy sequence in \(E_{D,\psi}^p(V)\) that converges to 0 in \(L^p\). We need to show that \((u_n)_n\) converges to 0 in \(E_{D,\psi}^p(V)\). To see this, fix \(\eta \in \tilde{\Psi}(\mathbb{R})\) satisfying \([H4]\). For all \(n \in \mathbb{N}\), we have by (4.10) that

\[
\|u_n\|_{E_{D,\psi}^p} \sim \|Q_{n}^D u_n\|_{T^p}.
\]

We conclude by repeating the proof of Theorem 3.10 with (3.18) replaced by (4.10) and \(Q_{\psi}^p\) replaced by \(Q_{n}^D\).

**Remark 4.8.** In the context of Theorem 4.7, when \(M\) is a complete Riemannian manifold, hypothesis \([H4]\) holds whenever \(S_{\eta}^D(C^\infty_c(\mathcal{V}_+)) \subseteq L^q(V)\), where \(C^\infty_c(\mathcal{V}_+)\) denotes the space of smooth compactly supported sections in \(T^2(\mathcal{V}_+)\). This is because \(C^\infty_c(\mathcal{V}_+)\) is weak-star dense in \(T^p(\mathcal{V}_+)\) for all \(p \in [1, 2]\). To see this, a mollification argument can be applied in combination with Remark 3.11.

### 4.1. Atomic Theory

We obtain a characterisation of \(H_{D,\psi}^1(V)\) in terms of the atoms from Definition 3.8 and the space \(H_{D,\text{at}(N)}^1(V)\) from Definition 3.12.

**Theorem 4.9.** Suppose that \(M\) is a doubling metric measure space satisfying \([D_\kappa]\), that \(D\) is a self-adjoint operator on \(L^2(V)\), and \((e^{itD})_{t \in \mathbb{R}}\) has finite propagation speed. Also, assume that for some \(\theta \in (0, \pi/2)\), \(\beta > \kappa/2\) and nondegenerate \(\psi \in \Psi(\mathbb{R})\), the completion \(H_{D,\psi}^1(V)\) of \(E_{D,\psi}^1(V)\) in \(L^1(V)\) exists. It follows that if \(N \in \mathbb{N}\) and \(N > \kappa/2\), then \(H_{D,\psi}^1(V) = H_{D,\text{at}(N)}^1(V)\).

**Proof.** Suppose that \(N \in \mathbb{N}\) and \(N > \kappa/2\). Theorem 3.13 and Lemma 4.1 show that \(H_{D,\psi}^1(V) = H_{D,\text{mol}(N)}^1(V) \geq H_{D,\text{at}(N)}^1(V)\). It remains to prove that \(H_{D,\psi}^1(V) \subseteq H_{D,\text{at}(N)}^1(V)\). To do this, fix a nondegenerate \(\eta \in \tilde{\Psi}_N(\mathbb{R})\). We claim that there exists \(c > 0\) such that \(cS_{\eta}^D A\) is an \(H_{D,\psi}^1\)-atom of type \(N\) whenever \(A\) is a \(T^1\)-atom. The claim allows us to prove that \(H_{D,\psi}^1(V) \subseteq H_{D,\text{at}(N)}^1(V)\) by repeating the proof of Theorem 3.13 with \(\psi\) replaced by \(\eta\) and then relying on (4.8) and (4.9) instead of (3.15) and (3.16).

To prove the claim, let \(A\) denote a \(T^1\)-atom and let \(B\) denote a ball in \(M\) with radius \(r(B) > 0\) such that \(A\) is supported in the tent \(T(B)\) and \(\|A\|_{T^2} \leq \mu(B)^{-1/2}\). Note that \(A_t\) is supported in \(B\) when \(t \in (0, r(B))\), and that \(\eta_t(D)A_t = 0\) when \(t > r(B)\). The finite propagation speed, in particular (4.5), then implies that there exists \(\alpha > 0\), which only depends on \(\eta\) and \(D\), such that \(\eta_t(D)A_t\) is supported in \(\alpha B\) for all \(t > 0\), hence \(S_{\eta}^D A\) is supported in \(\alpha B\).
Now set \( \tilde{\eta}(x) = x^{-N} \eta(x) \) for all \( x \in \mathbb{R} \setminus \{0\} \), and \( \tilde{\eta}(0) = \partial^N \eta(0)/N! \), which equals \( \lim_{x \to 0} x^{-N} \eta(x) \). Lemma 6.1 shows that \( \tilde{\eta} \in \Theta(\mathbb{R}) \), and so the properties of the \( B^\infty(\mathbb{R}) \) functional calculus imply that the putative atom \( a := S^D_\eta A \) has the form

\[
a = S^D_\eta A = D^N \left( \int_0^\infty t^N \tilde{\eta}(D) A_t \frac{dt}{t} \right) =: D^N b.
\]

It remains to verify that \( a \) and \( b \) above satisfy the atomic bounds in Definition 3.8. We use the doubling property to obtain

\[
\|a\|_2 = \|S^D_\eta A\|_2 \lesssim \|A\|_{T^2} \leq \mu(B)^{-1/2} \lesssim \mu(\alpha B)^{-1/2},
\]

and since \( A_t = 0 \) for all \( t > r(B) \), we also have

\[
\|b\|_2 = \left\| \int_0^\infty t^N \tilde{\eta}(D) A_t \frac{dt}{t} \right\|_2 = \|S^D_\eta (t^N A_t)\|_2 \lesssim r(B)^N \|A\|_{T^2} \lesssim (\alpha r(B))^N \mu(\alpha B)^{-1/2}.
\]

Therefore, there exists \( c > 0 \), which does not depend on \( A \), such that \( c S^D_\eta (A) \) is an \( H^1_D \)-atom of type \( N \). This proves the claim and completes the proof. \( \square \)

**Remark 4.10.** The proof of Theorem 4.9 shows that the same result holds when the \( L^1(\mathcal{V}) \) convergence required in Definition 3.12 is replaced with \( H^1_D\)-atom of type \( N \) convergence.

### 4.2. The Embedding \( H^p_D \subseteq L^p \) for Smooth Differential Operators.

We now consider the case when \( M \) is a complete Riemannian manifold, which is assumed to be smooth (infinitely differentiable) and connected, with geodesic distance \( \rho \) and Riemannian measure \( \mu \). The vector bundle \( \mathcal{V} \) is also assumed to be smooth, which means that the complex vector bundle \( \pi : \mathcal{V} \to M \) is equipped with a Hermitian metric \( \langle \cdot, \cdot \rangle_x \) that is infinitely differentiable with respect to \( x \in M \). Let \( \dim(M) \) denote the dimension of \( M \) and let \( \dim(\mathcal{V}) \) denote the fibre dimension of \( \mathcal{V} \). We prove a general result for a class of first-order differential operators on \( L^2(\mathcal{V}) \). The results for the Hodge–Dirac operator in Theorem 4.1 are deduced afterwards.

A smooth-coefficient, first-order, differential operator \( D_c \) is a linear operator on \( L^2(\mathcal{V}) \) with domain \( \text{Dom}(D_c) = C^\infty_c(\mathcal{V}) \) such that on any coordinate patch over which \( \mathcal{V} \) is trivial, there are smooth, matrix-valued \( \mathcal{L}(C^{\dim(\mathcal{V})}) \)-valued) functions \( (A_j)_{j=0}^{\dim(M)} \) such that the action of \( D_c \) on that coordinate patch is given by the Euclidean operator \( \sum_{j=1}^{\dim(M)} A_j \partial_j + A_0 \). For each \( x \in M \) in such a coordinate patch and each \( \xi \in T^*_x M \) given by \( \xi = \sum_{j=1}^{\dim(M)} \xi_j dx^j \), the principal symbol \( \sigma_{D_c}(x, \xi) \) is the endomorphism on the fibre \( \mathcal{V}_x \) given by \( \sum_{j=1}^{\dim(M)} A_j \xi_j \). A full account of these standard facts, including a coordinate-free definition of the principal symbol, is in [22, Chapter IV, Section 2]. Moreover, for any \( \eta \in C^\infty_c(M) \), the principal symbol is given by the commutator \( [D_c, \eta I]u = D_c(\eta u) - \eta D_c u \), since

\[
(\sigma_{D_c}(x, d\eta(x))) (u(x)) = ([D_c, \eta I]u)(x) \quad \forall x \in M, \forall u \in C^\infty_c(\mathcal{V}),
\]

where \( d \) is the exterior derivative.

An operator \( D_c \) is called symmetric when \( \langle D_c u, v \rangle = \langle u, D_c v \rangle \) for all \( u, v \in C^\infty_c(\mathcal{V}) \). A symmetric first-order operator has a skew-symmetric principal symbol. Chernoff proved in [13] that if the principal symbol of a symmetric, smooth-coefficient, first-order, differential operator satisfies a certain bound, then the operator is essentially self-adjoint and generates a group with finite propagation speed (related results are discussed in Remark 4.12). This allows us to prove the following result.
Theorem 4.11. Suppose that $M$ is a complete Riemannian manifold satisfying $[D]$, and that $V$ is a smooth vector bundle over $M$. Let $D$ denote the unique self-adjoint extension of a symmetric, smooth-coefficient, first-order, differential operator $D_c$ on $L^2(V)$ for which there exists $c_D > 0$ such that the principal symbol $\sigma_D$ satisfies

\begin{equation}
\|\sigma_D(x, \xi)\|_{L^\infty(\xi \cdot \xi)} \leq c_D \|\xi\|_{T^*_xM} \quad \forall x \in M, \forall \xi \in T^*_xM.
\end{equation}

If $p \in [1, 2]$, $\theta \in (0, \pi/2)$, $\beta > \kappa/2$ and $\psi \in \Psi_\beta(S^\theta_p)$ is nondegenerate, then the completion $H^p_{0, \psi}(V)$ of $E^p_{D, \psi}(V)$ in $L^p(V)$ exists and $H^p_{D, \psi}(V) \cap L^2(V) = E^p_{D, \psi}(V)$. Moreover, if $\alpha \in \mathbb{N}$ and $\alpha > \kappa/2$, then $H^1_{D, \psi}(V) = H^1_{D, \rho(N)}(V) = H^1_{D, \rho(N)}(V)$.

Proof. Assumption (4.11) implies that $D_c$ is essentially self-adjoint on $L^2(V)$ by the result of Chernoff in [13, Theorem 2.2]. The results in [13, Theorem 1.3 and Corollary 1.4] also show that the group $(e^{itD})_{t \in \mathbb{R}}$ has finite propagation speed $c_D$. Therefore, by Theorems 4.7 and 4.9 it suffices to prove that (H4) holds with $q = 1$.

First, we require a known estimate for the Sobolev spaces $W^{k,2}(V)$, where $k \in \mathbb{N}$. If $k > 1 + \dim(M)/2$ and $B$ is a ball in $M$, then there exists $C_B > 0$ such that, for all $u \in W^{k,2}(V)$ with sppt$(u) \subseteq B$,

\begin{equation}
\|u\|_\infty \leq C_B \|u\|_{W^{k,2}(V)}.
\end{equation}

This Sobolev embedding theorem can be found in [32, Chapter IV, Proposition 1.1].

Second, we require a known energy estimate. If $k \in \mathbb{N}$, $T > 0$, and $B$ is a ball in $M$, then there exists $C_{T,B} > 0$ such that, for all $u \in C^\infty_0(V)$ with sppt$(u) \subseteq B$,

\begin{equation}
\|e^{itD}u\|_{W^{k,2}(V)} \leq C_{T,B} \|u\|_{W^{k,2}(V)} \quad \forall t \in [-T, T].
\end{equation}

This can be proved by the methods in [31, Chapter IV, Section 2], since $v(t) = e^{itD}u$ solves the initial value problem $\frac{dv}{dt} = iv$ with $v(0) = u$.

Now choose a nondegenerate $\eta$ in $\tilde{\Psi}(\mathbb{R})$ and $\delta > 0$ such that $\text{sppt} \tilde{\eta} \subseteq [-\delta, \delta]$. Fix $k \in \mathbb{N}$ such that $k > 1 + \dim(M)/2$ and set $\alpha = 1 + c_D \delta$. For each $F \in C^\infty_0(V_+)$, there is a ball $B \subseteq M$ and $r > 1$ such that sppt$(F) \subseteq B \times [1/r, r]$. It follows that sppt$(e^{itD}F_t) \subseteq (1 + c_D |s|t/r)B \subseteq \alpha B$ for all $s \in [-\delta, \delta]$ and $t \in [1/r, r]$. Hence

\begin{align*}
\|S^D_\eta F\|_\infty &= \left\| \int_{1/r}^r \left( \frac{1}{2\pi} \int_{-\delta}^\delta \tilde{\eta}(s) e^{i\xi D} F_t ds \right) \frac{dt}{t} \right\|_\infty \\
&\lesssim \int_{1/r}^r \int_{-\delta}^\delta \|e^{i\xi D} F_t\|_\infty ds dt \\
&\lesssim \int_{1/r}^r \int_{-\delta}^\delta \|e^{i\xi D} F_t\|_{W^{k,2}(V)} ds dt \\
&\lesssim \int_{1/r}^r \|F_t\|_{W^{k,2}(V)} dt \\
&< \infty,
\end{align*}

where the first line uses (4.3), the third line uses (4.12) with $B = \alpha B$, the fourth line uses (4.13) with $B = B$, and the fifth line uses the continuity of $F$ (recall that $F \in C^\infty_0(V_+)$). This shows that $S^D_\eta(C^\infty_0(V_+)) \subseteq L^\infty(V)$, so Remark 4.8 implies that (H4) holds with $q = 1$. This completes the proof. \qed

Remark 4.12. McIntosh and Morris [27, Theorem 1.1] proved recently that any $C_0$-group $(e^{itD})_{t \in \mathbb{R}}$ generated by a first-order system $D$ satisfying (4.11) has finite
propagation speed. In particular, finite propagation speed for such groups is not restricted to smooth-coefficient nor self-adjoint systems.

We now prove Theorem 1.1, which fills a gap in the theory of Hardy spaces of differential forms developed by Auscher, McIntosh and Russ [9].

**Proof of Theorem 1.1.** Let $\rho T$ be a symmetric, smooth-coefficient, first-order, differential operator on $M$ by the Riemannian metric. The Hodge–Dirac operator $D = d + d^*$ is defined initially on $C_c^\infty(\Lambda T^*M)$, where $d$ and $d^*$ denote the exterior derivative and its adjoint. This is a symmetric, first-order, differential operator on $L^2(\Lambda T^*M)$ with principal symbol

$$\sigma_D(x, \xi)\zeta = \xi \wedge \zeta - \xi \downarrow \zeta \quad \forall x \in M, \forall \xi \in T^*_x M, \forall \zeta \in \Lambda T^*_x M,$$

where $\wedge$ and $\downarrow$ denote the exterior and (left) interior products on $\Lambda T^*_x M$. These properties of the Hodge–Dirac operator are well known, and in particular, we have

$$|\sigma_D(x, \xi)\zeta|_{\Lambda T^*_x M} = |\xi|_{T^*_x M}|\zeta|_{T^*_x M} \quad \forall x \in M, \forall \xi \in T^*_x M, \forall \zeta \in \Lambda T^*_x M,$$

so the hypotheses of Theorem 4.11 hold, and its conclusions imply Theorem 1.1. □

5. **The Embedding $H^p_L \subseteq L^p$ for Nonnegative Self-Adjoint Operators**

We now combine the theory of the previous two sections to prove Theorem 1.3. The atomic characterisation in Theorem 1.2 is then an immediate corollary. A new proof of Theorem 1.2 for smooth coefficient operators is also presented.

We return to the context of a vector bundle $\mathcal{V}$ over a doubling metric measure space $M$. A nonnegative self-adjoint operator $L : \text{Dom}(L) \subseteq L^2(\mathcal{V}) \rightarrow L^2(\mathcal{V})$ is said to satisfy *Davies–Gaffney estimates* when there exist constants $C, c > 0$ such that

$$\|1_E e^{-tL}1_F u\|_2 \leq Ce^{-ct \|E,F\|/t}\|u\|_2$$

for all $t > 0$, all $u \in L^2(\mathcal{V})$ and all measurable sets $E, F \subseteq M$, where $(e^{-tL})_{t \geq 0}$ is the analytic semigroup generated by $-L$. The following builds on the theory of Hardy spaces developed for such operators by Hofmann, Lu, Mitrea, Mitrea and Yan [20].

**Proof of Theorem 1.3.** Since $L$ is self-adjoint, it satisfies ([H1] and [H2]) with $\omega = 0$, $C_0 = 1/\sin \theta$ and $c_0 = 1$. We now prove that $L$ satisfies ([H3]) with $m = 2$. Let $E$ and $F$ denote measurable subsets of $M$. Since $L$ is nonnegative and self-adjoint, the Davies–Gaffney estimate ([5.1]) is equivalent to the property that the cosine group

$$\cos(t\sqrt{L}) := \frac{1}{2}(e^{it\sqrt{L}} + e^{-it\sqrt{L}})$$

has finite propagation speed (see [30, Theorem 2] and [17, Theorem 3.4]), where $(e^{it\sqrt{L}})_{t \in \mathbb{R}}$ is the $C_0$-group generated by the skew-adjoint operator $i\sqrt{L}$. Therefore, there exists $c_L > 0$ such that $1_E \cos(t\sqrt{L})1_F = 0$ whenever $\rho(E, F) > c_L |t|$. For all $z \in \mathbb{C}$ with Im$(\pm z) > 0$, we use the integral representation

$$(zI - L)^{-1} = \frac{1}{i\sqrt{2}} \int_0^\infty e^{\pm i\sqrt{2}t} \cos(t\sqrt{L}) \, dt$$

(see [3, Example 3.14.15]) to obtain

$$\|1_E(zI - L)^{-1}1_F\| \leq \frac{1}{|z|^{1/2}} \int_0^\infty \rho(E, F)/c_L e^{\pm i\sqrt{2}t}|1_E \cos(t\sqrt{L})1_F| \, dt$$

$$\leq \frac{1}{|z|^{1/2}} \int_0^\infty e^{-(\text{Im}(\pm \sqrt{2}))t} \, dt.$$
It is understood here that $\sqrt{z} = |z|^{1/2}\exp \frac{\pi i}{2} \arg(z)$ with $\arg(z) \in (-\pi, \pi]$, so then $\text{Im}(\sqrt{z}) = |z|^{1/2} \sin(\arg(z)/2)$, and for each $\theta \in (0, \pi/2)$, it follows that

$$
\|1_{E}(zI - L)^{-1}1_{F}\| \leq \frac{C_{\theta}/2}{|z|} \exp \left( -\frac{\rho(E, F)|z|^{1/2}}{c_{L}C_{\theta}/2} \right) \quad \forall z \in \mathbb{C} \setminus S_{\theta},
$$

which implies $[H3]$ with $m = 2$.

We have now shown that $L$ satisfies $[H1]$–$[H3]$ with $\omega = 0$ and $m = 2$, and since $L$ satisfies $[L0]$, hypothesis $[H4]_\psi$ holds with $q = 1$ by (3.21). Therefore, except for

the atomic characterisation, Theorems 3.10 and 3.13 complete the proof.

It thus remains to prove that $H_{L, \psi}^1 \subseteq H_{L, \text{at}(N)}^1$ when $\psi \in \Psi_{\beta}(S_{\theta})$ and $N > \kappa/4$.

Let $\tilde{\psi}(z) = ze^{-z}$ on $S_{\theta}$ and fix a nondegenerate even function $\eta$ in $\tilde{\Psi}^0_{2N}(\mathbb{R})$ such that

$$
\int_{0}^{\infty} \eta(tz)\tilde{\psi}(t^2z^2) \frac{dt}{t} = 1 \quad \forall z \in S_{\theta}/2.
$$

For example, choose any nondegenerate, even, real-valued function $\varphi \in C^\infty_c(\mathbb{R})$ supported on $[-\delta/2, \delta/2]$ and let $\eta(x) = \alpha |xN\hat{\varphi}(x)|^2$ for all $x \in \mathbb{R}$, where $\alpha$ is the normalizing constant defined by $\alpha \int_{0}^{\infty} t^{2N}\hat{\varphi}(t)^2 t^2 e^{-t^2} dt = 1$.

Applying Proposition 4.2 with $D = \sqrt{L}$, we obtain

$$
S_{\eta}^{\sqrt{L}} Q_{\tilde{\psi}} u := \int_{0}^{\infty} \eta(t\sqrt{L})\tilde{\psi}(t^2L)u \frac{dt}{t} = u \quad \forall u \in R(L).
$$

The operator $Q_{\tilde{\psi}}$ has an extension $Q_{\tilde{\psi}} \in \mathcal{L}(H_{L, \psi}^1, T^1)$ by (3.16), since we have already established the embedding $H_{L, \psi}^1 \subseteq L^1$ and that $H_{L, \psi}^1 \cap L^2 = E_{D, \psi}$ by Theorem 3.10.

It is also the case that $S_{\eta}^{\sqrt{L}}$ has an extension $S_{\eta}^{\sqrt{L}} \in \mathcal{L}(T^1, H_{L, \psi}^1)$, but to prove this we must modify the theory in Section 4 to incorporate the finite propagation of the cosine group $\cos(t\sqrt{L})$. To this end, the fact that $\eta$ is an even function allows us to write

$$
\eta(\sqrt{L})u = \frac{1}{\pi} \int_{0}^{\infty} \tilde{\eta}(s) \cos(s\sqrt{L})u \frac{ds}{s} \quad \forall t > 0, \forall u \in L^2(\mathcal{N}).
$$

We then follow the proof of Lemma 4.4, but instead use the finite propagation of the cosine group, to deduce that

$$
\|1_{E} \eta(\sqrt{L})1_{F}\| \leq \frac{1}{\pi} \|\tilde{\eta}\|_\infty \max \left\{ \delta - \frac{\rho(E, F)}{c_{L}t}, 0 \right\} \quad \forall t > 0, \forall E, F \subseteq M.
$$

The extension $S_{\eta}^{\sqrt{L}} \in \mathcal{L}(T^1, H_{L, \psi}^1)$ is then obtained as in Propositions 4.5 and 4.6.

Now let $u \in H_{L, \psi}^1$. It follows from above that $u = S_{\eta}^{\sqrt{L}} U$, where $U := Q_{\tilde{\psi}}^{\eta} u \in T^1$.

Therefore, in order to show that $u \in H_{L, \text{at}(N)}^1$, it suffices to show that $S_{\eta}^{\sqrt{L}} A$ is an $H_{L}^1$-atom of type $N$ whenever $A$ is a $T^1$-atom (see the reasoning in the proof of the atomic characterisation in Theorem 4.9). To do this, note that when $A$ is supported in the tent $T(B)$ over a ball $B \subseteq M$, then (5.2) implies that $\eta(t\sqrt{L})A_t$ is supported in $\alpha B$ for all $t > 0$, where $\alpha > 0$ only depends on $\eta$ and $L$. Following the proof of Theorem 4.9, we write $\alpha := S_{\eta}^{\sqrt{L}} A = (\sqrt{L})^{2N} \left( \int_{0}^{\infty} t^{2N}\tilde{\eta}(t\sqrt{L})A_t^{\eta} \right) =: L^N b$ for a suitable $\tilde{\eta} \in \Theta(\mathbb{R})$, and then verify that $a$ and $b$ satisfy the atomic bounds in Definition 3.8. This proves that $H_{L, \psi}^1 \subseteq H_{L, \text{at}(N)}^1$, which completes the proof.
We conclude by presenting a new proof of the results in Theorem 1.2 that does not rely explicitly on the ultracontractivity estimate (1.4) but instead requires that $A$ is self-adjoint with smooth coefficients.

Proof of Theorem 1.2 when $A$ is self-adjoint with smooth coefficients. Let $M = \mathbb{R}^n$ and consider $L = -\text{div} A \nabla$ on $L^2(V) = L^2(\mathbb{R}^n)$, where $A \in L^\infty(\mathbb{R}^n, \mathcal{L}(\mathbb{C}^n))$ has $C^\infty(\mathbb{R}^n)$ coefficients and is elliptic in the sense that there exists $\lambda > 0$ such that

$$\langle A(x)\zeta, \zeta \rangle_{\mathbb{C}^n} \geq \lambda |\zeta|^2 \quad \forall \zeta \in \mathbb{C}^n, \forall x \in \mathbb{R}^n.$$ 

This ellipticity condition, which is stronger than (1.3), implies that the matrix $A(x)$ is strictly positive and Hermitian. We proceed by introducing a first-order system $D$, a multiplication operator $B$, and a vector bundle $\mathcal{V}_B$, such that $L$ is a component of $(BD)^2$, and $BD$ satisfies the hypotheses of Theorem 4.11 on $L^2(\mathcal{V}_B)$.

Let $D_c : C^\infty_c(\mathbb{R}^n, \mathbb{C}^{1+n}) \to C^\infty_c(\mathbb{R}^n, \mathbb{C}^{1+n})$ denote the symmetric, smooth-coefficient, first-order, differential operator on $L^2(\mathbb{R}^n, \mathbb{C}^{1+n})$ defined by

$$D_c = \begin{bmatrix} 0 & -\text{div} \\ \nabla & 0 \end{bmatrix} : C^\infty_c(\mathbb{R}^n, \mathbb{C}^n) \to C^\infty_c(\mathbb{R}^n, \mathbb{C}^n),$$

where $\nabla f = (\partial_1 f, \ldots, \partial_n f)$ and $\text{div}(u_1, \ldots, u_n) = \sum_{j=1}^n \partial_j u_j$. The principal symbol

$$\sigma_{D_c}(x, \xi) = \begin{bmatrix} 0 & -\xi^T \\ \xi & 0 \end{bmatrix} \quad \forall x \in \mathbb{R}^n, \forall \xi \in \mathbb{C}^n$$

satisfies (4.11), so the unique self-adjoint extension of $D_c$ is the operator

$$D = \begin{bmatrix} 0 & -\text{div} \\ \nabla & 0 \end{bmatrix} : W^{1,2}(\mathbb{R}^n) \subseteq L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n),$$

where $\nabla$ denotes the gradient extended to $W^{1,2}(\mathbb{R}^n)$ and $\text{div} := -\nabla^*$. Let $B(x) = \begin{bmatrix} 1 & 0 \\ 0 & A(x) \end{bmatrix}$, so $B \in L^\infty(\mathbb{R}^n, \mathcal{L}(\mathbb{C}^{1+n})) \cap C^\infty(\mathbb{R}^n, \mathcal{L}(\mathbb{C}^{1+n}))$ and

$$BD = \begin{bmatrix} 0 & -\text{div} \\ A \nabla & 0 \end{bmatrix} \quad \text{and} \quad (BD)^2 = \begin{bmatrix} L & 0 \\ 0 & \tilde{L} \end{bmatrix},$$

where $\tilde{L} := -A \nabla \text{div}$.

Let $\mathcal{V}_B$ denote the trivial bundle over $\mathbb{R}^n$ that has $\mathbb{C}^{1+n}$-valued sections and the smooth Hermitian metric $\langle \xi, \zeta \rangle_{\mathcal{V}_B} := \langle B^{-1}x, \xi, \zeta \rangle_{\mathbb{C}^{1+n}}$ for $x \in \mathbb{R}^n$ and $\xi, \zeta \in \mathbb{C}^{1+n}$ (since $B(x)$ is strictly positive and Hermitian, $B(x)^{-1}$ and $B(x)^{-1/2}$ are Hermitian; also $B^{-1}, B^{-1/2} \in L^\infty(\mathbb{R}^n, \mathcal{L}(\mathbb{C}^{1+n})) \cap C^\infty(\mathbb{R}^n, \mathcal{L}(\mathbb{C}^{1+n}))$). For $p \in [1, 2]$, the space $L^p(\mathcal{V}_B)$ is then the set $L^p(\mathbb{R}^n, \mathbb{C}^{1+n})$ together with the norm

$$\|u\|_{L^p(\mathcal{V}_B)} := \left( \int_{\mathbb{R}^n} |B(x)^{-1/2} u(x)|_{\mathbb{C}^{1+n}}^p \, dx \right)^{1/p} \approx \|u\|_{L^p(\mathbb{R}^n, \mathbb{C}^{1+n})} \quad \forall u \in L^p(\mathbb{R}^n, \mathbb{C}^{1+n}).$$

We now verify the hypotheses of Theorem 4.11 for the system $BD_c$ on $L^2(\mathcal{V}_B)$. The inner product on $L^2(\mathcal{V}_B)$ is given by $\langle B^{-1}u, v \rangle_{L^2(\mathbb{R}^n, \mathbb{C}^{1+n})}$, so $BD_c$ is symmetric on $L^2(\mathcal{V}_B)$. The principal symbol satisfies $\sigma_{BD_c}(x, \xi) = B(x) \sigma_{D_c}(x, \xi)$ and

$$|\sigma_{BD_c}(x, \xi)\zeta|_{\mathcal{V}_B} = |B(x)^{1/2}\sigma_{D_c}(x, \xi)\zeta|_{\mathbb{C}^n} \leq \|B\|_{L^1(\mathbb{R}^n, \mathbb{C}^{1+n})} \leq \|B\|_{L^\infty(\mathbb{R}^n, \mathbb{C}^{1+n})} \leq \|B\|_{L^\infty(\mathbb{R}^n, \mathbb{C}^{1+n})} \|\zeta\|_{\mathcal{V}_B}$$

for all $x \in \mathbb{R}^n$, $\xi \in \mathbb{C}^n$ and $\zeta \in \mathbb{C}^{1+n}$, so $BD_c$ satisfies (4.11) on $\mathcal{V}_B$, as required.
We can now apply Theorem 4.11. In particular, consider $p \in [1, 2]$, $\theta \in (0, \pi/2)$ and $\beta > n/4$. Fix a nondegenerate $\psi \in \Psi(\beta(S^0_n))$, and let $\tilde{\psi}(z) = \psi(z^2)$ on $S^0_{\beta/2}$ (thus $\tilde{\psi} \in \Psi(2\beta(S^0_{\beta/2}))$ and $2\beta > n/2$). The completion $H^p_{BD,\tilde{\psi}}(V_B)$ of $E^p_{BD,\tilde{\psi}}(V_B)$ in $L^p(V_B)$ then exists (and $H^p_{BD,\tilde{\psi}}(V_B) \cap L^2(V_B) = E^p_{BD,\tilde{\psi}}(V_B)$) by Theorem 4.11.

We now use the fact that $L$ is a component of $(BD)^2$ to complete the proof. Note that $L$ satisfies (H1) with $m = 2$ (see Section 3.2), so $E^p_{BD,\psi}(\mathbb{R}^n)$ is defined with $m = 2$, whereas $E^p_{BD,\tilde{\psi}}(V_B)$ is defined with $m = 1$ (see Lemma 4.1). Let $\varphi(z) = e^{-z^2}$ on $S^0_n$, and let $\tilde{\varphi}(z) = \varphi(z^2)$ on $S^0_{\beta/2}$. We use (5.3) to write

$$\tilde{\varphi}(tBD) = t^2(\beta^2 - t^2(\beta^2)^2 = \begin{bmatrix} t^2Le^{-t^2L} & 0 \\ 0 & t^2\tilde{L}e^{-t^2\tilde{L}} \end{bmatrix} = \begin{bmatrix} \varphi(t^2L) & 0 \\ 0 & \varphi(t^2\tilde{L}) \end{bmatrix}$$

and then apply (3.15) to obtain

$$\|u\|_{E^p_{BD,\tilde{\psi}}(\mathbb{R}^n)} \leq \|\varphi(t^2L)u\|_{T^p(\mathbb{R}^n+1)} \leq \|\tilde{\varphi}(tBD)\|_{T^p(V_B^+)} \leq \|u\|_{E^p_{BD,\tilde{\psi}}(V_B)}$$

for all $u \in E^p_{BD,\tilde{\psi}}(\mathbb{R}^n)$. The equivalence $L^p(V_B) \approx L^p(\mathbb{R}^n)$ and the results above for $H^p_{BD,\tilde{\psi}}(V_B)$ then imply that the completion $H^p_{L,\tilde{\psi}}(\mathbb{R}^n)$ of $E^p_{L,\tilde{\psi}}(\mathbb{R}^n)$ in $L^p(\mathbb{R}^n)$ exists (and $H^p_{L,\tilde{\psi}}(\mathbb{R}^n) \cap L^2(\mathbb{R}^n) = E^p_{L,\tilde{\psi}}(\mathbb{R}^n)$). Theorem 3.13 then provides the molecular characterisation of $H^1_{L,\tilde{\psi}}(\mathbb{R}^n)$. Moreover, if $N \in \mathbb{N}$ and $N > n/4$, then $H^1_{BD,\tilde{\psi}}(\mathbb{R}^n) = H^1_{BD,\tilde{\psi}}(\mathbb{R}^n)$ by Theorem 4.9, which implies that $H^1_{L,\tilde{\psi}}(\mathbb{R}^n) = H^1_{L,\tilde{\psi}}(\mathbb{R}^n)$, since when $(a, \tilde{a}) = (BD)^2N(b, \tilde{b})$ in $L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n, \mathbb{C}^n)$ is an $H^1_{BD}(\mathbb{R}^n)$-atom of type $2N$, then $a = L^N b$ is an $H^1_{L}(\mathbb{R}^n)$-atom of type $N$ by (5.3). This completes the proof. □

6. Appendix: Off-Diagonal Estimates

This section contains technical estimates used to prove Propositions 4.5 and 4.6. We begin with the following lemma, which allows us to manipulate $\Psi(\mathbb{R})$ class functions in a manner analogous to $\Psi(S^0_n)$ class functions.

**Lemma 6.1.** Suppose that $N \in \mathbb{N}$. The following hold.

1. For $n \in \mathbb{N}$ and $\varphi \in \widetilde{\Theta}(\mathbb{R})$, the function $\tilde{\varphi}(x) := x^n \varphi(x)$ for all $x \in \mathbb{R}$, is in $\widetilde{\Psi}_n(\mathbb{R})$.

2. If $\varphi \in \Psi_N(\mathbb{R})$ and $\eta \in \Psi_N(\mathbb{R})$, then $\tilde{\varphi}(x) := x^{-m} \eta(x)$ for all $x \in \mathbb{R} \setminus \{0\}$, with $\tilde{\eta}(0) := \lim_{x \to 0} x^{-m} \eta(x) = \partial^m \eta(0)/m!$, is in $\widetilde{\Theta}(\mathbb{R})$.

3. For $m \in \{1, \ldots, N - 1\}$, then $\tilde{\varphi}(x) \in \Psi_{N-m}(\mathbb{R})$ (and so $\tilde{\eta}(0) = 0$).

**Proof.** Suppose that $n \in \mathbb{N}$ and $\varphi \in \widetilde{\Theta}(\mathbb{R})$. The function $\tilde{\varphi}$ defined in (1) belongs to $S(\mathbb{R})$ because $\varphi \in S(\mathbb{R})$. The Fourier transform $\hat{\tilde{\varphi}}$ is compactly supported because $\hat{\varphi}$ is compactly supported and $\hat{\tilde{\varphi}} = \hat{\varphi}^n \hat{\partial^n \varphi}$. For each $k \in \mathbb{N}$, there exist constants $c_{k,0}, c_{k,1}, \ldots, c_{k,k}$ such that

$$\partial^k \tilde{\varphi}(x) = \sum_{j=0}^{\min\{n-k, 1\}} c_{k,j} x^{n-j} \partial^{k-j} \varphi(x) + \sum_{j=n}^{k} c_{k,j} x^{n-j} \partial^{k-j} \varphi(x), \quad \forall x \in \mathbb{R}.$$
Now suppose that \( m \in \{1, \ldots, N\} \) and \( \eta \in \tilde{\Psi_d}(\mathbb{R}) \). The function \( \hat{\eta} \) defined in (2) satisfies the requirements of a Schwartz function, except possibly in a neighbourhood of the origin, because \( \eta \in \mathcal{S}(\mathbb{R}) \). The Paley–Wiener Theorem guarantees that \( \eta \) has a holomorphic extension to the entire complex plane, since \( \hat{\eta} \) is compactly supported. Therefore, there exist \( \epsilon > 0 \) and a sequence \((a_j)_{j \in \mathbb{N}_0}\) such that the power series \( a_0 + \sum_{j=1}^{\infty} a_j x^j \) converges to \( \eta(x) \) for all \( x \in [-\epsilon, \epsilon] \). The assumption that \( \eta \in \tilde{\Psi_d}(\mathbb{R}) \) implies that \( a_j = 0 \) for all \( j \in \{0, \ldots, N-1\} \), hence \( a_N x^{-m} + \sum_{j=N+1}^{\infty} a_j x^{j-m} \) converges to \( \hat{\eta}(x) \) for all \( x \in [-\epsilon, \epsilon] \), and \( \hat{\eta} \in \mathcal{S}(\mathbb{R}) \). Moreover, if \( m \in \{1, \ldots, N-1\} \), then this also shows that \( \partial^k \hat{\eta}(0) = 0 \) for all \( k \in \{0, \ldots, N-m-1\} \). This proves (2) provided that \( \hat{\eta} \) is compactly supported.

To show that \( \hat{\eta} \) is compactly supported when \( m \in \{1, \ldots, N\} \), choose \( \delta > 0 \) such that \( \hat{\eta} \) is supported in \([0, \delta]\). It is enough to show that for each \( k \in \{1, \ldots, m\} \), there exist constants \( c_{k,0}, c_{k,1}, \ldots, c_{k,k-1} \) such that

\[
\partial^m \hat{\eta}(y) = \left\{ \begin{array}{ll}
\sum_{j=0}^{k-1} c_{k,j} y^{k-1-j} \int_{-\delta}^{y} x^j \hat{\eta}(x) \, dx, & \text{if } |y| \leq \delta; \\
0, & \text{if } |y| > \delta,
\end{array} \right.
\]

since this proves that \( \hat{\eta} \) is compactly supported in \([-\delta, \delta]\) by setting \( k = m \).

We prove (6.1) by induction. For \( k = 1 \), since \( \eta(x) = x^m \hat{\eta}(x) \), we have \( \hat{\eta} = \partial^m \hat{\eta} \), and so \( \partial^{m-1} \hat{\eta}(y) = \int_{-\delta}^{y} \hat{\eta}(x) \, dx \). This shows that (6.1) holds for \( k = 1 \), since \( \hat{\eta} \) is supported in \([-\delta, \delta]\) and \( \int_{-\delta}^{\infty} \hat{\eta}(x) \, dx = \eta(0) = 0 \). Next, assume that (6.1) holds for some \( k = l \in \{1, \ldots, m-1\} \). Note that \( \partial^{m-(l+1)} \hat{\eta}(y) = \int_{-\delta}^{y} \partial^{m-l} \hat{\eta}(x) \, dx \). When \( y < -\delta \), then \( \partial^{m-(l+1)} \hat{\eta}(y) = 0 \) by (6.1). When \( y \geq -\delta \), then we use (6.1) to obtain

\[
\partial^{m-(l+1)} \hat{\eta}(y) = \int_{-\delta}^{\min\{y, \delta\}} \left( \sum_{j=0}^{l-1} c_{l,j} x^{l-1-j} \int_{-\delta}^{x} w^j \hat{\eta}(w) \, dw \right) \, dx \\
= \sum_{j=0}^{l-1} c_{l,j} \int_{-\delta}^{\min\{y, \delta\}} \left( \int_{w}^{\min\{y, \delta\}} x^{l-1-j} \, dx \right) w^j \hat{\eta}(w) \, dw \\
= \sum_{j=0}^{l-1} \frac{c_{l,j}}{l-j} \left( \min\{y, \delta\} \right)^{l-j} \int_{-\delta}^{y} w^{l-j} \hat{\eta}(w) \, dw - \int_{-\delta}^{\min\{y, \delta\}} w^{l-j} \hat{\eta}(w) \, dw.
\]

This shows that (6.1) holds for \( k = l + 1 \), since \( \hat{\eta} \) is supported in \([-\delta, \delta]\) and \( \int_{-\delta}^{\infty} w^{l-j} \hat{\eta}(w) \, dw = \partial^l \hat{\eta}(0) = 0 \) for all \( j \in \{0, \ldots, N-1\} \). We then conclude that (6.1) holds for each \( k \in \{1, \ldots, m\} \). This completes the proof.

We use a proof of Auscher and Martell [17, Theorem 2.3(b)] to show that polynomial off-diagonal estimates are stable under composition. This allows us to combine the off-diagonal estimates for the \( \Psi_s(\mathcal{S}_d^0) \) class in (3.9) with those for the \( \tilde{\Psi}_d(\mathbb{R}) \) class in (4.5). We use the notation \( \langle \alpha \rangle = \min\{\alpha, 1\} \) and \( \langle \alpha \rangle^\alpha \) when \( \alpha > 0 \).

**Lemma 6.2.** Suppose that \( C, \alpha > 0 \). If \( \{T_t\}_{t>0} \) and \( \{S_t\}_{t>0} \) are collections of operators in \( L(L^2(\mathcal{V})) \) such that

\[
\|1_E T_t 1_F\| \leq C \langle t/\rho(E, F) \rangle^\alpha \quad \text{and} \quad \|1_E S_t 1_F\| \leq C \langle t/\rho(E, F) \rangle^\alpha
\]
for all $t > 0$ and all measurable sets $E, F \subseteq M$, then there exists $\widetilde{C} > 0$ such that

$$
\|1_E T_s S_x 1_F \| \leq \widetilde{C} \langle \max \{s, t \} / \rho(E, F) \rangle^\alpha
$$

for all $s, t > 0$ and all measurable sets $E, F \subseteq M$.

**Proof.** Let $E, F \subseteq M$ denote measurable sets. The measure on $M$ is Borel with respect to the metric topology, so the set $\widetilde{E} = \{ x \in M : \rho(x, E) \leq \rho(E, F)/2 \}$ is closed and hence measurable. The result follows by writing

$$
\|1_E T_s S_x 1_F \| = \|1_E T_s (\widetilde{E} + 1_M \backslash \widetilde{E}) S_x 1_F \| \leq \|T_s\| \|1_E S_x 1_F \| + \|1_E T_s 1_M \backslash \widetilde{E}\| \|S_x\|
$$

for all $s, t > 0$, since $\rho(\widetilde{E}, F) \geq \rho(E, F)/2$ and $\rho(E, M \backslash \widetilde{E}) \geq \rho(E, F)/2$. \hfill \Box

The following off-diagonal estimates are used to prove Propositions 4.3 and 4.6.

**Lemma 6.3.** Suppose that $D$ is a self-adjoint operator on $L^2(\mathcal{V})$ and the group $(e^{iD})_{t \in \mathbb{R}}$ has finite propagation speed. If $m, n, N \in \mathbb{N}$ and $\delta, \sigma, \tau > 0$ satisfy

$$
m \leq N, \quad m < \tau, \quad n < \sigma \quad \text{and} \quad \delta \in (0, \sigma - n),
$$

then for each $\eta \in \Psi_N(\mathbb{R})$ and $\psi \in \Psi^\sigma(S^\delta_\theta)$, there exists $C > 0$ such that

$$
\|1_E (\eta \psi_\sigma) (D) 1_F \| \leq C \begin{cases} 
(s/t)^m (t/\rho(E, F))^\sigma - n - \delta, & \text{if } 0 < s \leq t; \\
(t/s)^n (s/\rho(E, F))^\sigma + m - \delta, & \text{if } 0 < t \leq s,
\end{cases}
$$

for all measurable sets $E, F \subseteq M$.

**Proof.** Let $E, F \subseteq M$ denote measurable sets. Suppose that $0 < s \leq t$ and define

$$
\tilde{\eta}(x) = x^m \eta(x) \quad \forall x \in \mathbb{R}, \quad \tilde{\psi}(z) = z^{-n} \psi(z) \quad \forall z \in S^\delta_\theta \quad \text{and} \quad \tilde{\psi}(0) = 0.
$$

The function $\tilde{\eta}$ is in $\Psi_{N+m}(\mathbb{R})$ by Lemma 6.1, so Lemma 4.4 implies that

$$
\|1_E \tilde{\eta} (D) 1_F \| \lesssim e^{-\rho(E, F)/t} \lesssim \langle t/\rho(E, F) \rangle^{\sigma - n - \delta}.
$$

The function $\tilde{\psi}$ is in $\Psi^\sigma_{\sigma-n}(S^\delta_\theta)$, so (3.9) implies that

$$
\|1_E \tilde{\psi}_\sigma (D) 1_F \| \lesssim \langle s/\rho(E, F) \rangle^{\sigma - n - \delta}.
$$

We combine (6.3) and (6.4) using Lemma 6.2 to obtain

$$
\|1_E \tilde{\eta} (D) \tilde{\psi}_\sigma (D) 1_F \| \lesssim \langle t/\rho(E, F) \rangle^{\sigma - n - \delta}
$$

when $0 < s \leq t$. The $B^\infty(\mathbb{R})$ functional calculus is an algebra homomorphism and $\tilde{\eta} \psi_{\sigma} = (s/t)^m \tilde{\eta} \tilde{\psi}_{\sigma}$ on $\mathbb{R}$, where both $\tilde{\eta}$ and $\tilde{\psi}_\sigma$ are in $B^\infty(\mathbb{R})$. Therefore, we have

$$
(\eta \psi_{\sigma})(D) = (s/t)^m \tilde{\eta} \tilde{\psi}_\sigma (D),
$$

so (6.5) implies (6.2) when $0 < s \leq t$.

Now suppose that $0 < t \leq s$ and define

$$
\tilde{\eta}(x) = x^{-m} \eta(x) \quad \forall x \in \mathbb{R} \backslash \{0\}, \quad \tilde{\eta}(0) = \lim_{x \to 0} x^{-m} \eta(x) \quad \text{and} \quad \tilde{\psi}(z) = z^m \psi(z) \quad \forall z \in S^\delta_\theta \cup \{0\}.
$$

The function $\tilde{\eta}$ is in $\tilde{\Theta}(\mathbb{R})$ by Lemma 6.1 since $m \leq N$ (note that $\tilde{\eta}(0) = \partial^m \eta(0)/m!$ and so we may have $\tilde{\eta}(0) \neq 0$ when $m = N$). Lemma 4.4 then implies that

$$
\|1_E \tilde{\eta} (D) 1_F \| \lesssim e^{-\rho(E, F)/t}. \quad \text{The function $\tilde{\psi}$ is in $\Psi^\sigma_{\sigma+m}(S^\delta_\theta)$, so (3.9) implies that}
$$

$$
\|1_E \tilde{\psi}_\sigma (D) 1_F \| \lesssim \langle s/\rho(E, F) \rangle^{\sigma + m - \delta}. \quad \text{We also have $\eta \psi_{\sigma} = (t/s)^m \tilde{\eta} \tilde{\psi}_\sigma$ on $\mathbb{R}$, so by writing $(\eta \psi_{\sigma})(D) = (t/s)^m \tilde{\eta} \tilde{\psi}_\sigma (D)$ and using Lemma 6.2 to combine the two preceding estimates, we obtain (6.2) when $0 < t \leq s$. \hfill \Box}
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REFERENCES


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