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Hardy and BMO spaces associated to divergence form elliptic operators

Steve Hofmann · Svitlana Mayboroda

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Abstract Consider a second order divergence form elliptic operator L with complex bounded measurable coefficients. In general, operators based on L, such as the Riesz transform or square function, may lie beyond the scope of the Calderón–Zygmund theory. They need not be bounded in the classical Hardy, BMO and even some L^p spaces. In this work we develop a theory of Hardy and BMO spaces associated to L, which includes, in particular, a molecular decomposition, maximal and square function characterizations, duality of Hardy and BMO spaces, and a John–Nirenberg inequality.

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S. Hofmann (✉)
Department of Mathematics, University of Missouri at Columbia,
Columbia, MO 65211, USA
e-mail: hofmann@math.missouri.edu

S. Mayboroda
Department of Mathematics, The Ohio State University,
231 W 18th Avenue, Columbus, OH 43210, USA
e-mail: svitlana@math.ohio-state.edu

Present Address:
S. Mayboroda
Department of Mathematics, Purdue University, W. Lafayette, IN 47907-2067, USA
e-mail: svitlana@math.purdue.edu

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1 Introduction and statement of main results

Extensive study of classical real-variable Hardy spaces in $\mathbb{R}^n$ began in the early 1960s with the fundamental paper of Stein and Weiss [27]. Since then these classes of functions have played an important role in harmonic analysis, naturally continuing the scale of L^p spaces to the range of $p \leq 1$. Although many real-variable methods have been developed (see especially the work of Fefferman and Stein [17]), the theory of Hardy spaces is intimately connected with properties of harmonic functions and of the Laplacian.

For instance, Hardy space $H^1(\mathbb{R}^n)$ can be viewed as the collection of functions $f \in L^1(\mathbb{R}^n)$ such that the Riesz transform $\nabla\Delta^{-1/2} f$ belongs to $L^1(\mathbb{R}^n)$. One also has alternative characterizations of $H^1(\mathbb{R}^n)$ by the square function and the non-tangential maximal function associated to the Poisson semigroup generated by Laplacian. To be precise, fix a family of non-tangential cones $\Gamma(x) := \{(y,t) \in \mathbb{R}^n \times (0,\infty) : |x-y| < t\}$, $x \in \mathbb{R}^n$, and define

$$S^\Delta f(x) = \left(\iint_{\Gamma(x)} \left| t\nabla e^{-t\sqrt{\Delta}} f(y) \right|^2 \frac{dydt}{t^{n+1}} \right)^{1/2}, \tag{1.1}$$

$$\mathcal{N}^\Delta f(x) = \sup_{(y,t)\in\Gamma(x)} \left| e^{-t\sqrt{\Delta}} f(y) \right|. \tag{1.2}$$

Then $\|\mathcal{N}^\Delta f\|_{L^1(\mathbb{R}^n)}$ and $\|S^\Delta f\|_{L^1(\mathbb{R}^n)}$ give equivalent norms in the space $H^1(\mathbb{R}^n)$, that is

$$\|\mathcal{N}^\Delta f\|_{L^1(\mathbb{R}^n)} \approx \|S^\Delta f\|_{L^1(\mathbb{R}^n)} \approx \|f\|_{H^1(\mathbb{R}^n)}. \tag{1.3}$$

Consider now a general elliptic operator in divergence form with complex bounded coefficients. Let A be an $n \times n$ matrix with entries

$$a_{jk} : L^\infty(\mathbb{R}^n) \longrightarrow \mathbb{C}, \quad j = 1,\dots,n, \quad k = 1,\dots,n, \tag{1.4}$$

satisfying the ellipticity condition

$$\lambda|\xi|^2 \leq \Re e A\xi \cdot \bar{\xi} \quad \text{and} \quad |A\xi \cdot \bar{\zeta}| \leq \Lambda|\xi||\zeta|, \quad \forall \xi, \zeta \in \mathbb{C}^n, \tag{1.5}$$

for some constants $0 < \lambda \leq \Lambda < \infty$. Then the second order divergence form operator is given by

$$Lf := -\mathrm{div}(A\nabla f), \tag{1.6}$$

interpreted in the weak sense via a sesquilinear form.

Unfortunately, the classical Hardy spaces need not be applicable to problems connected with the general operator L defined in (1.4)–(1.6). For example, the corresponding Riesz transform $\nabla L^{-1/2}$ need not be bounded from $H^1(\mathbb{R}^n)$ to $L^1(\mathbb{R}^n)$. Indeed, by the solution of the Kato problem [5], we know that the Riesz transform is bounded in $L^2(\mathbb{R}^n)$. Thus, if it were also bounded from $H^1(\mathbb{R}^n)$ to $L^1(\mathbb{R}^n)$, then by interpolation we would have that $\nabla L^{-1/2} : L^p(\mathbb{R}^n) \to L^p(\mathbb{R}^n)$ for all $1 < p \leq 2$, which, in general, is not true. It *is* true that there exists p_L, $1 \leq p_L < 2n/(n+2)$, such that the Riesz transform is bounded on $L^p(\mathbb{R}^n)$ for $p_L < p \leq 2$ (see [3,9,19] and Sect. 2 for more details; see also [10] for related theory), but it is known that the best possible p_L may be strictly greater than 1. Similar statements apply to the heat semigroup e^{-tL} (for which L^p boundedness may fail also for p finite, but sufficiently large), as well as to the square function (see (1.15) below). This failure of L^p bounds for some $p \in (1,2)$ (and in $(2,\infty)$), which relies on counterexamples built in [4,14,23], along with some observations in [3], illustrates the significant difference between the operators associated to L and those arising in the classical Calderón–Zygmund theory. We note that it has been shown in [3] that the intervals of $p \leq 2$ such that the heat semigroup and Riesz transform are L^p-bounded have the same interior. In the sequel, we shall denote by $(p_L, \widetilde{p}_L)$ the interior of the interval of L^p boundedness of the semigroup, i.e.,

$$\begin{aligned} p_L &:= \inf\{p \geq 1 : \sup_{t>0} \|e^{-tL}\|_{L^p \to L^p} < \infty\} \quad \text{and} \\ \widetilde{p}_L &:= \sup\{p \leq \infty : \sup_{t>0} \|e^{-tL}\|_{L^p \to L^p} < \infty\}. \end{aligned} \tag{1.7}$$

We recall [3] that $\widetilde{p}_L > 2n/(n-2)$, and, as noted above, $p_L < 2n/(n+2)$.

In writing this paper we have two goals: (1) to generalize the classical theory of Hardy spaces in order to ameliorate the deficiencies described in the previous paragraph, and (2) to develop a corresponding BMO theory, which includes analogues of the $H^1 - BMO$ duality theorem [17] and of the John–Nirenberg Lemma [20].

We begin by discussing the first goal. Given an elliptic operator L as above, we construct an H^1 space adapted to L, which, for example, is mapped into L^1 by the Riesz transforms $\nabla L^{-1/2}$, and which serves as an endpoint of a complex interpolation scale which coincides in part with some range of L^p spaces. The utility of the Hardy space H^1 being due in part to its many useful characterizations, thus, we aim to provide analogues to most of these, including the atomic (or molecular) decomposition and characterizations by square and non-tangential maximal functions. We note that one problem which remains open is that of finding a Riesz transform characterization of the adapted H^1 space; i.e., we do not yet know (except in the low dimensional case $n \leq 4$) whether L^1 bounds for $\nabla L^{-1/2} f$, or some suitable substitute, imply that f

belongs to our Hardy space (as mentioned above, we do prove the converse). We plan to present the low dimensional results, as well as an analogous H^p theory, $p \neq 1$, in a forthcoming joint paper with McIntosh. We remark that, in contrast to the classical setting, even the case $p > 1$ may involve Hardy spaces which are strictly smaller than L^p, and for at least some such spaces, we do have a Riesz transform characterization. Finally, we remark that our Hardy spaces belong to a complex interpolation scale which includes L^p, $p_L < p < \widetilde{p}_L$. Indeed, this fact follows as in [12], using interpolation of the so-called "tent spaces", given the square function characterization of our H^1 space (cf. Theorem 1.1 below), and the fact that the square function S_h (cf. (1.15)) is bounded on L^p for $p_L < p < \widetilde{p}_L$ (cf. Lemma 2.6).

We now discuss the various characterizations of our Hardy space. Let us start with the matter of atomic/molecular decompositions. The decomposition into simple building blocks, atoms, originally proved by Coifman for $n = 1$ [11] and by Latter in higher dimensions [22], is a key feature of $H^1(\mathbb{R}^n)$. In this paper we work with an analogous molecular decomposition, in the spirit of the one introduced in the classical setting by Taibleson and Weiss [28].

Throughout the paper for cube $Q \subset \mathbb{R}^n$ we denote by $l(Q)$ the sidelength of Q and set

$$S_0(Q) := Q, \quad Q_i = 2^i Q \quad \text{and} \quad S_i(Q) := 2^i Q \backslash 2^{i-1} Q \quad \text{for } i = 1, 2, \dots \tag{1.8}$$

where $2^i Q$ is cube with the same center as Q and sidelength $2^i l(Q)$.

Let $1 \leq p_L < 2n/(n+2)$ and $\widetilde{p}_L > 2n/(n-2)$ retain the same significance as above (that is, they are the endpoints of the interval of L^p boundedness for the heat semigroup). A function $m \in L^p(\mathbb{R}^n)$, $p_L < p < \widetilde{p}_L$, is called a (p, ε, M)-*molecule*, $\varepsilon > 0$ and $M \in \mathbb{N}$, $M > n/4$, if there exists a cube $Q \subset \mathbb{R}^n$ such that

$$\text{(i)} \qquad \|m\|_{L^p(S_i(Q))} \leq 2^{-i(n-n/p+\varepsilon)} |Q|^{1/p-1}, \quad i = 0, 1, 2, \dots, \tag{1.9}$$

$$\text{(ii)} \qquad \|(l(Q)^{-2} L^{-1})^k m\|_{L^p(S_i(Q))} \leq 2^{-i(n-n/p+\varepsilon)} |Q|^{1/p-1}, \quad i=0, 1, 2, \dots, k=1, \dots, M. \tag{1.10}$$

Having fixed some p, ε and M, we will often use the term molecule rather than (p, ε, M)-molecule in the sequel. Then the adapted Hardy space can be defined as

$$H^1_L(\mathbb{R}^n) \equiv \left\{ \sum_{i=0}^{\infty} \lambda_j m_j \,:\, \{\lambda_j\}_{j=0}^{\infty} \in \ell^1 \text{ and } m_j \text{ are molecules} \right\}, \tag{1.11}$$

with the norm given by

$$\|f\|_{H^1_L(\mathbb{R}^n)} = \inf \left\{ \sum_{j=0}^{\infty} |\lambda_j| : f = \sum_{j=0}^{\infty} \lambda_j m_j, \{\lambda_j\}_{j=0}^{\infty} \in \ell^1 \text{ and } m_j \text{ are molecules} \right\}. \tag{1.12}$$

We shall prove in Sect. 4 that any fixed choice of p, ε and M within the allowable parameters stated above, will generate the same space.

We remark that our molecules are, in particular, classical H^1 molecules, so that $H^1_L \subseteq H^1$ (and this containment is proper for some L, by our earlier observations concerning the failure of $H^1 \to L^1$ bounds). We also observe that one may construct examples of H^1_L molecules by hand: given a cube Q, let $f \in L^2(Q)$, with $\|f\|_2 \leq |Q|^{-1/2}$, and set

$$m = \left(\ell(Q)^2 L\right)^M e^{-\ell(Q)^2 L} f, \quad \tilde{m} = \left(I - (I + \ell(Q)^2 L)^{-1}\right)^M f. \tag{1.13}$$

One may then easily check, using the "Gaffney estimate" (2.8) below, that up to a suitable normalizing constant, $m, \tilde{m}$ are $(2, \varepsilon, M)$ molecules for every $\varepsilon > 0$.

Molecules have appeared in the H^1 theory as an analogue of atoms lacking compact support but decaying rapidly away from some cube Q [18]. However, the classical vanishing moment condition ($\int_{\mathbb{R}^n} m(x)\,dx = 0$) does not interact well with the operators we have in mind because it does not provide appropriate cancellation. Instead, we impose the requirement that the molecule "absorbs" properly normalized negative powers of the operator L—the condition made precise in (1.10). In such a setting it can be proved, for instance, that the Riesz transform

$$\nabla L^{-1/2} : H^1_L(\mathbb{R}^n) \longrightarrow L^1(\mathbb{R}^n), \tag{1.14}$$

as desired.

Next, given an operator L as above and function $f \in L^2(\mathbb{R}^n)$, consider the following quadratic and maximal operators associated to the heat semigroup generated by L

$$S_h f(x) := \left(\iint_{\Gamma(x)} |t^2 L e^{-t^2 L} f(y)|^2 \frac{dydt}{t^{n+1}} \right)^{1/2}, \tag{1.15}$$

$$\mathcal{N}_h f(x) := \sup_{(y,t)\in\Gamma(x)} \left(\frac{1}{t^n} \int_{B(y,t)} |e^{-t^2 L} f(z)|^2\, dz \right)^{1/2}, \tag{1.16}$$

where $B(y, t)$, $y \in \mathbb{R}^n$, $t \in (0, \infty)$, is a ball in $\mathbb{R}^n$ with center at y and radius t and $x \in \mathbb{R}^n$. These are the natural modifications of (1.1)–(1.2). We use an extra averaging in the space variable for the non-tangential maximal function in order to compensate for the lack of pointwise estimates on the heat semigroup (an idea originating in [21]).

Alternatively, one can consider the Poisson semigroup generated by the operator L and the operators

$$S_P f(x) := \left(\iint_{\Gamma(x)} |t \nabla e^{-t\sqrt{L}} f(y)|^2 \frac{dydt}{t^{n+1}} \right)^{1/2}, \tag{1.17}$$

$$\mathcal{N}_P f(x) := \sup_{(y,t)\in\Gamma(x)} \left(\frac{1}{t^n} \int\limits_{B(y,t)} |e^{-t\sqrt{L}} f(x)|^2 dx \right)^{1/2}, \tag{1.18}$$

with $x \in \mathbb{R}^n$, $f \in L^2(\mathbb{R}^n)$.

We define $H^1_{S_h}(\mathbb{R}^n)$ as the completion of $\{f \in L^2(\mathbb{R}^n) : S_h f \in L^1\}$, with respect to the norm

$$\|f\|_{H^1_{S_h}(\mathbb{R}^n)} \equiv \|S_h f\|_{L^1(\mathbb{R}^n)};$$

the spaces $H^1_{\mathcal{N}_h}(\mathbb{R}^n)$, $H^1_{S_P}(\mathbb{R}^n)$ and $H^1_{\mathcal{N}_P}(\mathbb{R}^n)$ are defined analogously. Then the following result holds.

Theorem 1.1 *Suppose that $p_L < p < \widetilde{p}_L$ (1.7), $\varepsilon > 0$ and $M > n/4$ in (1.9)–(1.10). For an operator L given by (1.4)–(1.6), the Hardy spaces $H^1_L(\mathbb{R}^n)$, $H^1_{S_h}(\mathbb{R}^n)$, $H^1_{\mathcal{N}_h}(\mathbb{R}^n)$, $H^1_{S_P}(\mathbb{R}^n)$, $H^1_{\mathcal{N}_P}(\mathbb{R}^n)$ coincide. Moreover,*

$$\|f\|_{H^1_L(\mathbb{R}^n)} \approx \|S_h f\|_{L^1(\mathbb{R}^n)} \approx \|\mathcal{N}_h f\|_{L^1(\mathbb{R}^n)} \approx \|S_P f\|_{L^1(\mathbb{R}^n)} \approx \|\mathcal{N}_P f\|_{L^1(\mathbb{R}^n)}, \tag{1.19}$$

for every $f \in H^1_L(\mathbb{R}^n)$.

The second half of the paper is to devoted to the study of the space of functions of bounded mean oscillation, adapted to L.

The BMO space originally introduced by John and Nirenberg in [20] in the context of partial differential equations, has been identified as the dual of classical H^1 in the work by Fefferman and Stein [17]. Analogous to the role of H^1 as a substitute for L^1, BMO substitutes for L^∞ as an endpoint of the L^p scale. For reasons similar to those discussed above in connection with H^1, the classical BMO may not be at all compatible with the operator L.

The second goal of this paper is to generalize the classical notion of BMO. We define a version of this space adapted to L, and prove that it is equipped with several characteristic properties of BMO; in particular, it is tied up with the Hardy space theory via duality. The adapted BMO theory (using a similar norm to our (1.22), but with $M = 1$) has previously been introduced by Duong and Yan [15,16], under the stronger assumption that the heat kernel associated to L satisfies a pointwise Gaussian upper bound. Much of their methodology seems inapplicable in the present setting; in particular, we have been forced to take a completely different approach to the John–Nirenberg Lemma, and to view our BMO space as a subspace, not of L^1_{loc}, but rather of a certain space of distributions as we shall describe momentarily. Moreover, the lack of pointwise kernel bounds renders the proof of the duality theorem significantly more problematic, and in addition seems to require the higher order cancellation inherent in the parameter M.

We define our adapted BMO space as follows. For $\varepsilon > 0$ and $M \in \mathbb{N}$ we introduce the norm

$$\|\mu\|_{\mathbf{M}_0^{2,\varepsilon,M}} \equiv \sup_{j\geq 0} 2^{j(n/2+\varepsilon)} \sum_{k=0}^{M} \|L^{-k}\mu\|_{L^2(S_j(Q_0))},$$

where Q_0 is the unit cube centered at 0, and set

$$\mathbf{M}_0^{2,\varepsilon,M} \equiv \{\mu \in L^2(\mathbb{R}^n) : \|\mu\|_{\mathbf{M}_0^{2,\varepsilon,M}} < \infty\}.$$

Implicitly, of course, this space depends upon L, and we shall write $\mathbf{M}_0^{2,\varepsilon,M}(L)$ when we need to indicate this dependence explicitly. We note that if $\mu \in \mathbf{M}_0^{2,\varepsilon,M}$ with norm 1, then μ is a $(2, \varepsilon, M)$ molecule adapted to Q_0. Conversely, if m is a $(2, \varepsilon, M)$ molecule adapted to any cube, then $m \in \mathbf{M}_0^{2,\varepsilon,M}$ (this follows from the fact that, given any two cubes Q_1 and Q_2, there exists integers K_1 and K_2, depending upon $\ell(Q_1)$, $\ell(Q_2)$ and $\mathrm{dist}(Q_1, Q_2)$, such that $2^{K_1}Q_1 \supseteq Q_2$ and $2^{K_2}Q_2 \supseteq Q_1$). Let $(\mathbf{M}_0^{2,\varepsilon,M})^*$ be the dual of $\mathbf{M}_0^{2,\varepsilon,M}$, and let A_t denote either $(I+t^2L)^{-1}$ or e^{-t^2L}. We claim that if $f \in (\mathbf{M}_0^{2,\varepsilon,M})^*$, then $(I - A_t^*)^M f$ is globally well defined in the sense of distributions, and belongs to L^2_{loc}. Indeed, if $\varphi \in L^2(Q)$ for some cube Q, it follows from the Gaffney estimate (2.8) below that $(I - A_t)^M\varphi \in \mathbf{M}_0^{2,\varepsilon,M}$ for every $\varepsilon > 0$. Thus,

$$\left\langle (I - A_t^*)^M f, \varphi\right\rangle \equiv \left\langle f, (I - A_t)^M\varphi\right\rangle \leq C_{t,\ell(Q),\mathrm{dist}(Q,0)}\|f\|_{(\mathbf{M}_0^{2,\varepsilon,M})^*}\|\varphi\|_{L^2(Q)}. \tag{1.20}$$

Since Q was arbitrary, the claim follows. Similarly, $(t^2L^*)^M A_t^* f \in L^2_{loc}$.

We are now ready to define our adapted BMO spaces. We suppose now and in the sequel that $M > n/4$. An element

$$f \in \cap_{\varepsilon>0}(\mathbf{M}_0^{2,\varepsilon,M})^* \equiv (\mathbf{M}_0^{2,M})^* \tag{1.21}$$

is said to belong to $BMO_{L^*}(\mathbb{R}^n)$ if

$$\|f\|_{BMO_{L^*}(\mathbb{R}^n)} := \sup_{Q\subset\mathbb{R}^n}\left(\frac{1}{|Q|}\int_Q \left|(I - e^{-l(Q)^2L^*})^M f(x)\right|^2 dx\right)^{1/2} < \infty, \tag{1.22}$$

where $M > n/4$ and Q stands for a cube in $\mathbb{R}^n$. Eventually, we shall see that this definition is independent of the choice of $M > n/4$ (up to "modding out" elements in the null space of the operator $(L^*)^M$, as these are annihilated by $(I - e^{-l(Q)^2L^*})^M$; we thank Lixin Yan for this observation). Clearly, we can define BMO_L by interchanging the roles of L and L^* in the preceding discussion. Using the "Gaffney" estimate (2.8) below, and the fact that $e^{-l(Q)^2L}1 = 1$, one may readily verify that $BMO \subseteq BMO_L$.

Compared to the classical definition, in (1.22) the heat semigroup $e^{-l(Q)^2L}$ plays the role of averaging over the cube, and an extra power $M > n/4$ provides the necessary cancellation.

As usual, we have some flexibility in the choice of BMO norm, by virtue of an appropriate version of the John–Nirenberg inequality (see [20] for the case of usual BMO), although in our case we obtain a more restricted range of equivalence. To be more precise, let us denote by $BMO_L^p(\mathbb{R}^n)$, $1 < p < \infty$, the set of elements of $(\mathbf{M}_0^{2,M})^*$ with the property that

$$\|f\|_{BMO_L^p(\mathbb{R}^n)} := \sup_{Q\subset\mathbb{R}^n} \left(\frac{1}{|Q|} \int_Q \left|(I - e^{-l(Q)^2L})^M f(x)\right|^p \, dx \right)^{1/p} \tag{1.23}$$

is finite. By definition, $BMO_L^2(\mathbb{R}^n) = BMO_L(\mathbb{R}^n)$. We have a "John–Nirenberg Lemma":

Theorem 1.2 *For all p such that $p_L < p < \widetilde{p}_L$ the spaces $BMO_L^p(\mathbb{R}^n)$ coincide.*

Another important feature of classical BMO is its Carleson measure characterization. Roughly speaking, we shall establish the following analogue of the Fefferman–Stein criterion:

$$f \in BMO_L(\mathbb{R}^n) \quad \Longleftrightarrow \quad \left|(t^2L)^M e^{-t^2L} f(y)\right|^2 \frac{dydt}{t} \quad \text{is a Carleson measure;} \tag{1.24}$$

see Theorem 9.1 for the precise statement, in which, as in the classical case, a certain "controlled growth" hypothesis is needed to prove the $\Leftarrow$ direction.

And finally, we prove the desired duality with the Hardy spaces.

Theorem 1.3 *Suppose $p_L < p < \widetilde{p}_L$, $\varepsilon > 0$ and $M > n/4$ in* (1.9)–(1.10), (1.22). *Then for an operator L given by* (1.4)–(1.6)

$$\left(H_L^1(\mathbb{R}^n)\right)^* = BMO_{L^*}(\mathbb{R}^n). \tag{1.25}$$

As we have mentioned, our results lie beyond the classical Calderón–Zygmund setting. Moreover, the methods we have at our disposal are substantially restricted. For instance, no analogue of the subaveraging property of harmonic functions, no maximum principle, no regularity or pointwise bounds for the kernel of the heat or Poisson semigroup are available. The operators we work with do not even possess a kernel in the regular sense. In fact, we employ only certain estimates in L^2 and L^p with p close to 2, controlling the growth of the heat semigroup and the resolvent.

The layout of the paper is as follows: Section 2 contains a few preliminary results, regarding general square functions and properties of the operator L. Section 3 is devoted to the behavior of sublinear operators, in particular, Riesz transform, acting on

$H^1_L(\mathbb{R}^n)$. Sections 4, 5, 6 and 7 cover the characterizations of Hardy space announced in Theorem 1.1. Finally, in Sects. 8, 9 and 10 we discuss the spaces $BMO_L(\mathbb{R}^n)$, duality, connection with Carleson measures and John–Nirenberg inequality.

While this work was in preparation, we learned that much of the Hardy space theory that we present here has also been treated independently by Auscher et al. [7]. Their results are stated in the context of a Dirac operator on a Riemannian manifold, but their arguments carry over to the present setting as well. To the best of our knowledge, the theory of $BMO_L(\mathbb{R}^n)$ spaces, in the absence of pointwise heat kernel bounds, is unique to this paper. As mentioned above, some of this material has been developed previously, assuming pointwise kernel bounds (see [8,15,16]).

2 Notation and preliminaries

Let Γ^α, $\alpha > 0$, be the cone of aperture α, i.e. $\Gamma^\alpha(x) := \{(y,t) \in \mathbb{R}^n \times (0,\infty) : |x-y| < \alpha t\}$ for $x \in \mathbb{R}^n$. Then for a closed set $F \in \mathbb{R}^n$ we define a saw-tooth region $\mathcal{R}^\alpha(F) := \bigcup_{x\in F} \Gamma^\alpha(x)$. For simplicity we will often write Γ in place of Γ^1 and $\mathcal{R}(F)$ instead of $\mathcal{R}^1(F)$.

Suppose F is a closed set in $\mathbb{R}^n$ and $\gamma \in (0,1)$ is fixed. We set

$$F^* := \left\{x \in \mathbb{R}^n : \text{ for every } B(x), \text{ ball in } \mathbb{R}^n \text{ centered at } x, \quad \frac{|F \cap B(x)|}{|B(x)|} \geq \gamma\right\}, \tag{2.1}$$

and every x as above is called a point having global γ-density with respect to F. One can see that F^* is closed and $F^* \subset F$. Also,

$${}^cF^* = \{x \in \mathbb{R}^n : \mathcal{M}(\chi_{{}^cF})(x) > 1-\gamma\}, \tag{2.2}$$

which implies $|{}^cF^*| \leq C|{}^cF|$ with C depending on γ and the dimension only.

Here and throughout the paper we denote by ${}^cF$ the complement of F, χ_F is the characteristic function of F, and $\mathcal{M}$ is the Hardy-Littlewood maximal operator, i.e.

$$\mathcal{M}f(x) := \sup_{r>0} \frac{1}{|B(x,r)|} \int\limits_{B(x,r)} |f(y)|\, dy, \tag{2.3}$$

where f is a locally integrable function and $B(x,r)$ stands for the ball with radius r centered at $x \in \mathbb{R}^n$.

Lemma 2.1 [12] *Fix some* $\alpha > 0$. *There exists* $\gamma \in (0,1)$, *sufficiently close to 1, such that for every closed set* F *whose complement has finite measure and every non-negative function* Φ *the following inequality holds*:

$$\int\limits_{\mathcal{R}^\alpha(F^*)} \Phi(x,t)\, t^n\, dxdt \le C(\alpha,\gamma) \int\limits_F \left[\int\limits_{\Gamma(x)} \Phi(y,t)\, dydt \right] dx, \tag{2.4}$$

where F^* denotes the set of points of global γ-density with respect to F.

Conversely,

$$\int\limits_F \left[\int\limits_{\Gamma^\alpha(x)} \Phi(y,t)\, dydt \right] dx \le C(\alpha) \int\limits_{\mathcal{R}^\alpha(F)} \Phi(x,t)\, t^n\, dxdt, \tag{2.5}$$

for every closed set $F \subset \mathbb{R}^n$ and every non-negative function Φ.

Lemma 2.2 [12] *Consider the operator*

$$S^\alpha F(x) := \left(\int\int\limits_{\Gamma^\alpha(x)} |F(y,t)|^2 \frac{dydt}{t^{n+1}} \right)^{1/2}, \tag{2.6}$$

where $\alpha > 0$. There exists a constant $C > 0$ depending on the dimension only such that

$$\|S^\alpha F\|_{L^1(\mathbb{R}^n)} \le C \|S^1 F\|_{L^1(\mathbb{R}^n)}. \tag{2.7}$$

Both lemmas above are proved in [12].

Turning to the properties of the differential operator L we start with the off-diagonal estimates. We say that the family of operators $\{S_t\}_{t>0}$ satisfies L^2 off-diagonal estimates (Gaffney estimates) if there exist some constants $c, C, \beta > 0$ such that for arbitrary closed sets $E, F \subset \mathbb{R}^n$

$$\|S_t f\|_{L^2(F)} \le C\, e^{-\left(\frac{\operatorname{dist}(E,F)^2}{ct}\right)^\beta} \|f\|_{L^2(E)}, \tag{2.8}$$

for every $t > 0$ and every $f \in L^2(\mathbb{R}^n)$ supported in E.

Lemma 2.3 [19] *If two families of operators, $\{S_t\}_{t>0}$ and $\{T_t\}_{t>0}$, satisfy Gaffney estimates (2.8) then so does $\{S_t T_t\}_{t>0}$. Moreover, there exist $c, C > 0$ such that for arbitrary closed sets $E, F \subset \mathbb{R}^n$*

$$\|S_s T_t f\|_{L^2(F)} \le C\, e^{-\left(\frac{\operatorname{dist}(E,F)^2}{c \max\{t,s\}}\right)^\beta} \|f\|_{L^2(E)}, \tag{2.9}$$

for all $t, s > 0$ and all $f \in L^2(\mathbb{R}^n)$ supported in E.

Lemma 2.4 [5,19] *The families*

$$\{e^{-tL}\}_{t>0}, \quad \{tLe^{-tL}\}_{t>0}, \quad \{t^{1/2}\nabla e^{-tL}\}_{t>0}, \tag{2.10}$$

as well as

$$\{(1+tL)^{-1}\}_{t>0}, \quad \{t^{1/2}\nabla(1+tL)^{-1}\}_{t>0}, \tag{2.11}$$

satisfy Gaffney estimates with $c, C > 0$ *depending on* n, λ *and* Λ *only. For the operators in* (2.10), $\beta = 1$, *and in* (2.11), $\beta = 1/2$.

We remark that it is well known from functional calculus and ellipticity (accretivity) that the operators in (2.10)–(2.11) are bounded from $L^2(\mathbb{R}^n)$ to $L^2(\mathbb{R}^n)$ uniformly in t.

Lemma 2.5 *There exist* p_L, $1 \le p_L < \frac{2n}{n+2}$ *and* $\widetilde{p}_L$, $\frac{2n}{n-2} < \widetilde{p}_L \le \infty$, *such that for every* p *and* q *with* $p_L < p \le q < \widetilde{p}_L$, *the family* $\{e^{-tL}\}_{t>0}$ *satisfies* $L^p - L^q$ *off-diagonal estimates, i.e. for arbitrary closed sets* $E, F \subset \mathbb{R}^n$

$$\|e^{-tL} f\|_{L^q(F)} \le C t^{\frac{1}{2}\left(\frac{n}{q}-\frac{n}{p}\right)} e^{-\frac{\operatorname{dist}(E,F)^2}{ct}} \|f\|_{L^p(E)}, \tag{2.12}$$

for every $t > 0$ *and every* $f \in L^p(\mathbb{R}^n)$ *supported in* E. *The operators* e^{-tL}, $t > 0$, *are bounded from* $L^p(\mathbb{R}^n)$ *to* $L^q(\mathbb{R}^n)$ *with the norm* $Ct^{\frac{1}{2}\left(\frac{n}{q}-\frac{n}{p}\right)}$ *and from* $L^p(\mathbb{R}^n)$ *to* $L^p(\mathbb{R}^n)$ *with the norm independent of* t.

In the case $p = q$, *the statement of the Lemma remains valid with* $\{e^{-tL}\}_{t>0}$ *replaced by* $\{(1+tL)^{-1}\}_{t>0}$, *and with exponent* $\beta = 1/2$ *in the exponential decay expression.*

Proof For the heat semigroup the proof of the Lemma can be found in [3] and the result for the resolvent can be obtained following similar ideas. □

Remark It has been shown in [3] that the interval of p such that the heat semigroup is L^p-bounded, and the interval of p, q such that it enjoys the off-diagonal bound (2.12), have the same interior. In particular, there is no inconsistency between the definitions of p_L in (1.7) and in Lemma 2.5. We will preserve this notation for p_L and $\widetilde{p}_L$ throughout the paper.

Lemma 2.6 *The operator*

$$S_h^K f(x) := \left(\iint_{\Gamma(x)} |(t^2L)^K e^{-t^2L} f(y)|^2 \frac{dydt}{t^{n+1}} \right)^{1/2}, \quad x \in \mathbb{R}^n, \quad K \in \mathbb{N}, \tag{2.13}$$

is bounded in $L^p(\mathbb{R}^n)$ *for* $p \in (p_L, \widetilde{p}_L)$.

Proof The proof closely follows an analogous argument for vertical square function [3]. We omit the details. □

Finally, the solutions of strongly parabolic and elliptic systems satisfy the following versions of Caccioppoli inequality.

Lemma 2.7 *Suppose* $Lu = 0$ *in* $B_{2r}(x_0) = \{x \in \mathbb{R}^n : |x - x_0| < 2r\}$. *Then there exists* $C = C(\lambda, \Lambda) > 0$ *such that*

$$\int\limits_{B_r(x_0)} |\nabla u(x)|^2 \, dx \leq \frac{C}{r^2} \int\limits_{B_{2r}(x_0)} |u(x)|^2 \, dx. \tag{2.14}$$

Lemma 2.8 *Suppose* $\partial_t u = -Lu$ *in* $I_{2r}(x_0, t_0)$, *where* $I_r(x_0, t_0) = B_r(x_0) \times [t_0 - cr^2, t_0]$, $t_0 > 4cr^2$ *and* $c > 0$. *Then there exists* $C = C(\lambda, \Lambda, c) > 0$ *such that*

$$\int\int\limits_{I_r(x_0,t_0)} |\nabla u(x,t)|^2 \, dxdt \leq \frac{C}{r^2} \int\int\limits_{I_{2r}(x_0,t_0)} |u(x,t)|^2 \, dxdt. \tag{2.15}$$

3 Sublinear operators in Hardy spaces

To begin, let us note that the space H^1_L, defined by means of molecular decompositions, is complete. We learned the following proof of this fact from E. Russ. We first require a well known completeness criterion from functional analysis.

Lemma 3.1 *Let X be a normed space which enjoys the property that* $\sum x_k$ *converges in X, whenever* $\sum \|x_k\| < \infty$. *Then, X is complete.*

The lemma is well known, and we omit the proof.

Let us now use the lemma to establish completeness of H^1_L. To this end, we suppose that $f_k \in H^1_L$, and that $\sum \|f_k\|_{H^1_L} < \infty$. Given the former fact, there exists for each k a molecular decomposition $f_k = \sum_{i=0}^{\infty} \lambda_i^k m_i^k$, with $\sum_{i=0}^{\infty} |\lambda_i^k| \approx \|f_k\|_{H^1_L}$. Thus,

$$\sum_{i,k} |\lambda_i^k| \approx \sum_k \|f_k\|_{H^1_L} < \infty.$$

Consequently, the sum $\sum f_k = \sum_{k,i} \lambda_i^k m_i^k$ converges in H^1_L, as desired. □

For certain technical reasons, we shall need to work also with a modified version of the molecular representations. Given $p \in (p_L, \widetilde{p}_L)$, $\varepsilon > 0$, $M > n/4$, and $\delta > 0$, we say that $f = \sum \lambda_j m_j$ is a δ-representation of f if $\{\lambda_j\}_{j=0}^{\infty} \in \ell^1$ and each m_j is a (p, ε, M)-molecule adapted to a cube Q_j of side length **at least** δ. We set

$$H^1_{L,\delta}(\mathbb{R}^n) \equiv \{f \in L^1(\mathbb{R}^n) : f \text{ has a } \delta\text{-representation}\}.$$

Observe that a δ-representation is also a δ'-representation for all $\delta' < \delta$. Thus, $H^1_{L,\delta} \subseteq H^1_{L,\delta'}$ for $0 < \delta' < \delta$. Set

$$\widehat{H}^1_L(\mathbb{R}^n) \equiv \cup_{\delta > 0} H^1_{L,\delta}(\mathbb{R}^n),$$

and define

$$\|f\|_{\widehat{H}^1_L(\mathbb{R}^n)} \equiv \inf\left\{\sum_{j=0}^{\infty}|\lambda_j| : f = \sum_{j=0}^{\infty}\lambda_j m_j \text{ is a } \delta\text{-representation for some } \delta > 0\right\}. \tag{3.1}$$

We note that for $f \in \widehat{H}^1_L$, $\|f\|_{L^1} \le C\|f\|_{\widehat{H}^1_L}$, since in particular, $\|m\|_{L^1} \le C$ for every molecule m (of course, a similar statement is true for H^1_L). Now for $f \in \widehat{H}^1_L$, set

$$\|f\|_{\widetilde{H}^1_L(\mathbb{R}^n)} \equiv \|f\|_{\widehat{H}^1_L(\mathbb{R}^n)} + \|f\|_{L^1(\mathbb{R}^n)} \approx \|f\|_{\widehat{H}^1_L(\mathbb{R}^n)}, \tag{3.2}$$

and define $\widetilde{H}^1_L$ as the completion of $\widehat{H}^1_L$ with respect to this norm. We now show that

$$H^1_L = \widetilde{H}^1_L, \tag{3.3}$$

for any choice of p, ε and M, within the allowable parameters. By definition, and the completeness of H^1_L, we have

$$\widetilde{H}^1_L \subseteq H^1_L \quad \text{and} \quad \|f\|_{H^1_L} \le \|f\|_{\widetilde{H}^1_L} \tag{3.4}$$

whenever $f \in \widetilde{H}^1_L$. Let us now verify that these statements can be reversed (up to a multiplicative constant). We learned the following argument from P. Auscher. Let $f \in H^1_L$, $f = \sum \lambda_i m_i$, with $\|f\|_{H^1_L} \approx \sum|\lambda_i|$. Set $f_k = \sum_{i=1}^k \lambda_i m_i$. Note in particular that $f_k \to f$ in L^1. Moreover, $f_k \in \widehat{H}^1_L$, so that

$$\|f_k\|_{\widetilde{H}^1_L} \le \sum_{i=1}^{k}|\lambda_i| \le C\|f\|_{H^1_L}.$$

Also,

$$\|f_k - f_{k'}\|_{\widetilde{H}^1_L} \le \sum_{i=k'}^{k}|\lambda_i| \to 0,$$

so that $\{f_k\}$ is a Cauchy sequence in $\widetilde{H}^1_L$. Consequently, there exists $\tilde{f}$ such that $f_k \to \tilde{f}$ in $\widetilde{H}^1_L$ and thus also in L^1. Therefore, $\tilde{f} = f$ a.e., so $f \in \widetilde{H}^1_L$.

The advantage to working with $\widetilde{H}^1_L$ is that, if $f = \sum \lambda_i m_i$ is a δ-representation with (p, ϵ, M)-molecules, for some $\delta > 0$, then the partial sums $f_k \equiv \sum_{i \le k}\lambda_i m_i$ converge to f in L^p, since the L^p norms of the molecules are uniformly bounded (with a constant depending upon δ).

Theorem 3.2 *Let $p_L < p \le 2$ and assume that the sublinear operator*

$$T : L^p(\mathbb{R}^n) \longrightarrow L^p(\mathbb{R}^n) \tag{3.5}$$

satisfies the following estimates. There exists $M \in \mathbb{N}$, $M > n/4$, such that for all closed sets E, F in $\mathbb{R}^n$ with $\operatorname{dist}(E, F) > 0$ *and every $f \in L^p(\mathbb{R}^n)$ supported in E*

$$\|T(I - e^{-tL})^M f\|_{L^p(F)} \le C\left(\frac{t}{\operatorname{dist}(E, F)^2}\right)^M \|f\|_{L^p(E)}, \quad \forall t > 0, \tag{3.6}$$

$$\|T(tLe^{-tL})^M f\|_{L^p(F)} \le C\left(\frac{t}{\operatorname{dist}(E, F)^2}\right)^M \|f\|_{L^p(E)}, \quad \forall t > 0. \tag{3.7}$$

Then

$$T : H^1_L(\mathbb{R}^n) \longrightarrow L^1(\mathbb{R}^n). \tag{3.8}$$

Remark Of course, the estimates (3.5)–(3.7) are of interest only when $t \le \operatorname{dist}(E, F)^2$. The proof below shows that (3.5)–(3.7) imply (3.8) with the Hardy space $H^1_L(\mathbb{R}^n)$ defined by linear combinations of (p, ε, M)-molecules for the same values of p and M as in (3.5)–(3.7). We do not emphasize this fact as the space $H^1_L(\mathbb{R}^n)$ does not depend on the choice (within the stated allowable parameters) of p, ε and M in (1.9)–(1.12)—see Corollary 4.3.

Proof Suppose that $T : L^p \to L^p$ is sublinear. We claim that for every (p, ε, M) molecule m, we have

$$\|Tm\|_{L^1(\mathbb{R}^n)} \le C \tag{3.9}$$

with constant C independent of m. Let us take this statement for granted momentarily. The conclusion of the theorem is then an immediate consequence of the following lemma.

Lemma 3.3 *Fix p, ϵ, M within the allowable parameters, with $p_L < p \le 2$. Suppose that T is either a linear operator, or a positive sublinear operator, bounded on L^p, which satisfies* (3.9) *for all (p, ϵ, M) molecules. Then T extends to a bounded operator on H^1_L, and*

$$\|Tf\|_{L^1} \le C\|f\|_{H^1_L}.$$

Proof By our previous observations, it is enough to work with the space $\widetilde{H}^1_L$. By density, it is enough to show that

$$\|Tf\|_1 \le C\|f\|_{\widetilde{H}^1_L}$$

for $f \in \widehat{H}^1_L$. Choose such an f, so that $f = \sum_{i=1}^{\infty} \lambda_i m_i$ is a δ-representation, where the m_i are $(p, \epsilon, M)-$molecules and

$$\|f\|_{\widetilde{H}^1_L} \approx \sum |\lambda_i|.$$

Set $f_k = \sum_{i=1}^{k} \lambda_i m_i$. Then $f_k \to f$ in $L^p \cap L^1$. By hypothesis, $|Tf_k - Tf| \leq |T(f_k - f)| \to 0$ in L^p. On the other hand, by (3.9),

$$\|Tf_k - Tf_{k'}\|_1 \leq \|T(f_k - f_{k'})\|_1 \leq C \sum_{i=k'}^{k} |\lambda_i| \to 0,$$

as $k, k' \to \infty$. Consequently, $\{Tf_k\}$ is a Cauchy sequence in L^1 so there exists $h \in L^1$ such that $Tf_k \to h$ in L^1. Taking subsequences, we see that $Tf = h$ a.e.. Hence,

$$\|Tf\|_1 = \lim_{k\to\infty} \|Tf_k\|_1 \leq C \sum |\lambda_i| \leq \|f\|_{\widetilde{H}^1_L}.$$

□

We now turn to the proof of (3.9). To begin, we write

$$\begin{aligned}\|Tm\|_{L^1(\mathbb{R}^n)} \leq{}& \left\| T\left(I - e^{-l(Q)^2 L}\right)^M m \right\|_{L^1(\mathbb{R}^n)} \\ &+ \left\| T\left[I - \left(I - e^{-l(Q)^2 L}\right)^M\right] m \right\|_{L^1(\mathbb{R}^n)} := \mathbf{I} + \mathbf{II},\end{aligned}$$

and we further split $\mathbf{I}$ so that

$$\mathbf{I} \leq \sum_{i=0}^{\infty} \left\| T(I - e^{-l(Q)^2 L})^M (m\chi_{S_i(Q)}) \right\|_{L^1(\mathbb{R}^n)}.$$

Here, the family of annuli $\{S_i(Q)\}_{i=0}^{\infty}$ is taken with respect to the cube Q associated with m. Going further,

$$\begin{aligned}&\left\| T(I - e^{-l(Q)^2 L})^M (m\chi_{S_i(Q)}) \right\|_{L^1(\mathbb{R}^n)} \\ &\quad\leq C \sum_{j=0}^{\infty} \left(2^{i+j} l(Q)\right)^{n-\frac{n}{p}} \left\| T(I - e^{-l(Q)^2 L})^M (m\chi_{S_i(Q)}) \right\|_{L^p(S_j(Q_i))} \\ &\quad\leq C \sum_{j=2}^{\infty} \left(2^{i+j} l(Q)\right)^{n-\frac{n}{p}} \left(\frac{l(Q)^2}{\mathrm{dist}\,(S_j(Q_i), S_i(Q))^2} \right)^M \|m\|_{L^p(S_i(Q))} \\ &\qquad+ C\left(2^i l(Q)\right)^{n-\frac{n}{p}} \|m\|_{L^p(S_i(Q))}, \end{aligned} \tag{3.10}$$

where the last inequality follows from (3.5)–(3.6) and uniform boundedness of $\{e^{-tL}\}_{t>0}$ in $L^p(\mathbb{R}^n)$. Then by the properties of (p, ε, M)-molecules the expression above is bounded by

$$C\sum_{j=2}^{\infty} 2^{i(-2M-\varepsilon)} 2^{j(n-n/p-2M)} + C\,2^{-i\varepsilon} \leq C\,2^{-i\varepsilon}, \tag{3.11}$$

so that $\mathbf{I} \leq C$.

As for the remaining part,

$$I - \left(I - e^{-l(Q)^2 L}\right)^M = \sum_{k=1}^{M} C_k^M (-1)^{k+1} e^{-kl(Q)^2 L}, \tag{3.12}$$

where $C_k^M = \frac{M!}{(M-k)!k!}$, $k = 1, \ldots, M$, are binomial coefficients. Therefore,

$$\begin{aligned} \left\| T[I - (I - e^{-l(Q)^2 L})^M] m \right\|_{L^1(\mathbb{R}^n)} &\leq C \sup_{1\leq k\leq M} \left\| T e^{-kl(Q)^2 L} m \right\|_{L^1(\mathbb{R}^n)} \\ &\leq C \sup_{1\leq k\leq M} \left\| T \left(\frac{k}{M} l(Q)^2 L e^{-\frac{k}{M} l(Q)^2 L} \right)^M (l(Q)^{-2} L^{-1})^M m \right\|_{L^1(\mathbb{R}^n)}. \end{aligned} \tag{3.13}$$

At this point we proceed as in (3.10)–(3.11) with $(l(Q)^{-2}L^{-1})^M m$ in place of m, $\left(\frac{k}{M} l(Q)^2 L e^{-\frac{k}{M} l(Q)^2 L}\right)^M$ in place of $(I - e^{-l(Q)^2 L})^M$, and using (3.7) and (1.10) to obtain that

$$\sup_{1\leq k\leq M} \left\| T \left(\frac{k}{M} l(Q)^2 L e^{-\frac{k}{M} l(Q)^2 L} \right)^M \left(\left[(l(Q)^{-2} L^{-1})^M m \right] \chi_{S_i(Q)} \right) \right\|_{L^1(\mathbb{R}^n)} \leq C 2^{-i\varepsilon}. \tag{3.14}$$

Summing in i, we obtain that $\mathbf{II} \leq C$, as desired. □

Remark The result of Theorem 3.2 holds for $p \in (2, \widetilde{p}_L)$ as well. However, in that case one has to take $M > \frac{1}{2}\left(n - \frac{n}{p}\right)$.

For $f \in L^2(\mathbb{R}^n)$ consider the following vertical version of square function:

$$g_h f(x) := \left(\int_0^{\infty} |t^2 L e^{-t^2 L} f(y)|^2 \, \frac{dt}{t} \right)^{1/2}. \tag{3.15}$$

Theorem 3.4 *The operators g_h and $\nabla L^{-1/2}$ satisfy (3.6)–(3.7) for $p = 2$, $M > n/4$, and map $H^1_L(\mathbb{R}^n)$ to $L^1(\mathbb{R}^n)$.*

Proof The proof rests on ideas of similar estimates for the Riesz transform (cf. Lemma 2.2 in [19]) and Theorem 3.2. By the L^p bounds, $p_L < p < \widetilde{p}_L$, for g_h [3], it is enough to treat the case $t < \operatorname{dist}(E, F)^2$ in (3.6)–(3.7).

First of all, the operators under consideration are obviously sublinear. Further, L^2 boundedness of the Riesz transform has been proved in [5] and boundedness of g_h in $L^2(\mathbb{R}^n)$ follows from the quadratic estimates for operators having bounded holomorphic calculus [1].

Let us now address the inequalities (3.6)–(3.7) for $p = 2$ and the operator $T = g_h$. An argument for the Riesz transform, viewed as

$$\nabla L^{-1/2} = C \int_0^\infty \nabla e^{-sL} f \, \frac{ds}{\sqrt{s}}, \tag{3.16}$$

is completely analogous [19]. Write

$$\begin{aligned}
\left\| g_h (I - e^{-tL})^M f \right\|_{L^2(F)} &= C \left\| \left(\int_0^\infty |sLe^{-sL}(I - e^{-tL})^M f|^2 \, \frac{ds}{s} \right)^{1/2} \right\|_{L^2(F)} \\
&\leq C \left\| \left(\int_0^\infty |sLe^{-s(M+1)L}(I - e^{-tL})^M f|^2 \, \frac{ds}{s} \right)^{1/2} \right\|_{L^2(F)} \\
&\leq C \left(\int_0^t \left\| sLe^{-s(M+1)L}(I - e^{-tL})^M f \right\|_{L^2(F)}^2 \frac{ds}{s} \right)^{1/2} \\
&\quad + C \left(\int_t^\infty \left\| sLe^{-s(M+1)L}(I - e^{-tL})^M f \right\|_{L^2(F)}^2 \frac{ds}{s} \right)^{1/2} =: I_1 + I_2
\end{aligned} \tag{3.17}$$

We will analyze I_1 and I_2 separately. Expanding $(I - e^{-tL})^M$ by the binomial formula, one can see that

$$\begin{aligned}
I_1 &\leq C \left(\int_0^t \left\| sLe^{-s(M+1)L} f \right\|_{L^2(F)}^2 \frac{ds}{s} \right)^{1/2} \\
&\quad + C \sup_{1 \leq k \leq M} \left(\int_0^t \left\| sLe^{-s(M+1)L} e^{-ktL} f \right\|_{L^2(F)}^2 \frac{ds}{s} \right)^{1/2} \\
&\leq C \left(\int_0^t \left\| sLe^{-s(M+1)L} f \right\|_{L^2(F)}^2 \frac{ds}{s} \right)^{1/2} \\
&\quad + C \sup_{1 \leq k \leq M} \left(\int_0^t \left\| e^{-s(M+1)L} ktLe^{-ktL} f \right\|_{L^2(F)}^2 \frac{s\,ds}{t^2} \right)^{1/2}
\end{aligned}$$

$$\leq C\left(\int_0^t e^{-\frac{\operatorname{dist}(E,F)^2}{cs}}\,\frac{ds}{s}\right)^{1/2}\quad \|f\|_{L^2(E)}$$

$$+C\sup_{1\leq k\leq M}\left(\frac{1}{t^2}\,e^{-\frac{\operatorname{dist}(E,F)^2}{ct}}\int_0^t s\,ds\right)^{1/2}\quad \|f\|_{L^2(E)},$$

where we used Lemma 2.4 and a variant of Lemma 2.3 in the last step. One may readily check that the expression above is bounded by $C\left(\frac{t}{\operatorname{dist}(E,F)^2}\right)^M \|f\|_{L^2(E)}$, as desired.

Turning to the second integral,

$$I_2\leq C\left(\int_t^\infty \left\|sLe^{-sL}(e^{-sL}-e^{-(s+t)L})^M f\right\|_{L^2(F)}^2\frac{ds}{s}\right)^{1/2}. \tag{3.18}$$

It was observed in [19] that

$$\begin{aligned}\left\|\frac{s}{t}(e^{-sL}-e^{-(s+t)L})g\right\|_{L^2(F)} &= \left\|\frac{s}{t}\int_0^t \partial_r e^{-(s+r)L}g\,dr\right\|_{L^2(F)}\\ &\leq C\frac{s}{t}\int_0^t \left\|(s+r)Le^{-(s+r)L}g\right\|_{L^2(F)}\frac{dr}{s+r}\\ &\leq C\,\|g\|_{L^2(E)}\left(\frac{s}{t}\int_0^t e^{-\frac{\operatorname{dist}(E,F)^2}{c(s+r)}}\,\frac{dr}{s+r}\right).\end{aligned} \tag{3.19}$$

But $s+r\approx s$ for $s\geq t$ and $r\in(0,t)$, therefore the expression above does not exceed

$$C\,\|g\|_{L^2(E)}e^{-\frac{\operatorname{dist}(E,F)^2}{cs}}\left(\frac{s}{t}\int_0^t\frac{dr}{s+r}\right)\leq Ce^{-\frac{\operatorname{dist}(E,F)^2}{cs}}\|g\|_{L^2(E)}. \tag{3.20}$$

Now we multiply and divide the integrand in (3.18) by $\left(\frac{s}{t}\right)^{2M}$ and use Lemma 2.3 for sLe^{-sL} and M copies of $\frac{s}{t}(e^{-sL}-e^{-(s+t)L})$ to get

$$
\begin{aligned}
I_2 &\le C \left(\int_t^\infty e^{-\frac{\operatorname{dist}(E,F)^2}{cs}} \left(\frac{t}{s}\right)^{2M} \frac{ds}{s} \right)^{1/2} \|f\|_{L^2(E)} \\
&\le C \left(\int_0^\infty e^{-r} \left(\frac{tr}{\operatorname{dist}(E,F)^2}\right)^{2M} \frac{dr}{r} \right)^{1/2} \|f\|_{L^2(E)} \\
&\le C \left(\frac{t}{\operatorname{dist}(E,F)^2}\right)^{M} \|f\|_{L^2(E)}, \qquad (3.21)
\end{aligned}
$$

as desired, where in the second inequality we have made the the change of variables $r := \frac{\operatorname{dist}(E,F)^2}{cs}$.

This finishes the proof of (3.6) for the operator g_h. The argument for (3.7) follows essentially the same path. More precisely, one needs to estimate the integrals I_1 and I_2 with $(I - e^{-tL})^M$ replaced by $(tLe^{-tL})^M$. As for the first one,

$$
\begin{aligned}
&\left(\int_0^t \left\| sLe^{-s(M+1)L} (tLe^{-tL})^M f \right\|_{L^2(F)}^2 \frac{ds}{s} \right)^{1/2} \\
&\le C \left(\frac{1}{t^2} \int_0^t \left\| e^{-s(M+1)L} (tLe^{-tL})^{M-1} \left(\frac{t}{2} Le^{-\frac{t}{2}L}\right)^2 f \right\|_{L^2(F)} sds \right)^{1/2} \\
&\le Ce^{-\frac{\operatorname{dist}(E,F)^2}{ct}} \|f\|_{L^2(E)} \le C \left(\frac{t}{\operatorname{dist}(E,F)^2}\right)^{M} \|f\|_{L^2(E)}, \qquad (3.22)
\end{aligned}
$$

by Lemma 2.3. Concerning to the analogue of I_2, one can write

$$
\begin{aligned}
&\left(\int_t^\infty \left\| sLe^{-s(M+1)L} (tLe^{-tL})^M f \right\|_{L^2(F)}^2 \frac{ds}{s} \right)^{1/2} \\
&\le \left(\int_t^\infty \left(\frac{t}{s}\right)^{2M} \left\| sLe^{-sL} (sLe^{-(t+s)L})^M f \right\|_{L^2(F)}^2 \frac{ds}{s} \right)^{1/2}. \qquad (3.23)
\end{aligned}
$$

At this stage, similarly to (3.19),

$$
\begin{aligned}
\left\| sLe^{-(s+t)L} g \right\|_{L^2(F)} &= \left\| \frac{s}{t} e^{-sL} \int_0^t \partial_r (rLe^{-rL}) g \, dr \right\|_{L^2(F)} \\
&\le C \left\| \frac{s}{t} e^{-sL} \int_0^t (Le^{-rL} - rL^2 e^{-rL}) g \, dr \right\|_{L^2(F)}
\end{aligned}
$$

$$\leq C\frac{s}{t}\int_0^t \|(r+s)Le^{-(r+s)L}g\|_{L^2(F)}\,\frac{dr}{r+s}$$

$$+C\frac{s}{t}\int_0^t \|(r+s)^2L^2e^{-(r+s)L}g\|_{L^2(F)}\,\frac{rdr}{(r+s)^2}$$

$$\leq C\,\|g\|_{L^2(E)}\left(\frac{s}{t}\int_0^t e^{-\frac{\mathrm{dist}\,(E,F)^2}{c(s+r)}}\,\frac{dr}{s+r}\right)$$

$$\leq Ce^{-\frac{\mathrm{dist}\,(E,F)^2}{cs}}\,\|g\|_{L^2(E)}, \tag{3.24}$$

and following (3.21) we complete the proof. □

Remark Using the same line of reasoning and $L^p - L^2$ off-diagonal estimates ($p_L < p \leq 2$) one can show for all closed sets E, F in $\mathbb{R}^n$ with $\mathrm{dist}(E,F) > 0$ and every $f \in L^p(\mathbb{R}^n)$ supported in E

$$\left\|g_h(I-e^{-tL})^M f\right\|_{L^2(F)} \leq C\,t^{\frac{1}{2}\left(\frac{n}{2}-\frac{n}{p}\right)}\left(\frac{t}{\mathrm{dist}\,(E,F)^2}\right)^M \|f\|_{L^p(E)}, \quad \forall t>0, \tag{3.25}$$

$$\left\|g_h(tLe^{-tL})^M f\right\|_{L^2(F)} \leq C\,t^{\frac{1}{2}\left(\frac{n}{2}-\frac{n}{p}\right)}\left(\frac{t}{\mathrm{dist}\,(E,F)^2}\right)^M \|f\|_{L^p(E)}, \quad \forall t>0. \tag{3.26}$$

4 Characterization by the square function associated to the heat semigroup

Theorem 4.1 *The spaces H^1_L and $H^1_{S_h}$ are the same; in particular,*

$$\|f\|_{H^1_L(\mathbb{R}^n)} \approx \|S_h f\|_{L^1(\mathbb{R}^n)}. \tag{4.1}$$

In light of (3.3), the theorem is an immediate consequence of the following lemma.

Lemma 4.2 *We have the containments $H^1_L \subseteq H^1_{S_h} \subseteq \widetilde{H}^1_L$. Moreover,*

(i) *If $f \in L^2 \cap H^1_{S_h}$, then f is the limit in $\widetilde{H}^1_L$ of $f_N \in \widehat{H}^1_L$. Furthermore, for every $\varepsilon > 0$, $M \in \mathbb{N}$, $p_L < p < \widetilde{p}_L$ there exists a family of (p,ε,M)-molecules $\{m_i\}_{i=0}^{\infty}$ and a sequence of numbers $\{\lambda_i\}_{i=0}^{\infty}$ such that f can be represented in the form $f = \sum_{i=0}^{\infty}\lambda_i m_i$, with*

$$\|f\|_{\widetilde{H}^1_L(\mathbb{R}^n)} \leq C\sum_{i=0}^{\infty}|\lambda_i| \leq C\|f\|_{H^1_{S_h}(\mathbb{R}^n)}. \tag{4.2}$$

(ii) *Conversely, given* $\varepsilon > 0$, $M > n/4$ *and* $p_L < p < \widetilde{p}_L$, *let* $f \equiv \sum_{i=0}^{\infty} \lambda_i m_i$, *where* $\{m_i\}_{i=0}^{\infty}$ *is a family of* (p, ε, M)*-molecules and* $\sum_{i=0}^{\infty} |\lambda_i| < \infty$. *Then the series* $\sum_{i=0}^{\infty} \lambda_i m_i$ *converges in* $H^1_{S_h}(\mathbb{R}^n)$ *and*

$$\left\| \sum_{i=0}^{\infty} \lambda_i m_i \right\|_{H^1_{S_h}(\mathbb{R}^n)} \leq C \sum_{i=0}^{\infty} |\lambda_i|.$$

In particular, we have that

$$\|f\|_{H^1_{S_h}(\mathbb{R}^n)} \leq C\|f\|_{H^1_L(\mathbb{R}^n)}. \tag{4.3}$$

The proof follows that of [12], and is based on the tent space decomposition of that paper, as well as on the ideas of the proof of the atomic decomposition of the classical Hardy spaces (as in [29]).

Proof *Step I.* Let $f \in H^1_{S_h}(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$. We shall construct a family $\{f_N\}_{N=1}^{\infty} \subseteq \widehat{H}^1_L$ such that $f_N \to f$ in $\widetilde{H}^1_L$ and in $H^1_{S_h}$, with

$$\sup_N \|f_N\|_{\widetilde{H}^1_L(\mathbb{R}^n)} \leq C\|f\|_{H^1_{S_h}(\mathbb{R}^n)}.$$

In particular, this will show that $f \in \widetilde{H}^1_L$, with norm controlled by $\|f\|_{H^1_{S_h}}$. The claimed molecular decomposition will be established in the course of the proof.

We start with a suitable version of the Calderón reproducing formula. By L^2 functional calculus, for every $f \in L^2(\mathbb{R}^n)$ one can write

$$\begin{aligned} f &= C_M \int_0^{\infty} (t^2 L e^{-t^2 L})^{M+2} f \, \frac{dt}{t} \\ &= C_M \lim_{N\to\infty} \int_{1/N}^{N} (t^2 L e^{-t^2 L})^{M+2} f \, \frac{dt}{t} \equiv \lim_{N\to\infty} f_N, \end{aligned} \tag{4.4}$$

with the integral converging in $L^2(\mathbb{R}^n)$.

Now define the family of sets $O_k := \{x \in \mathbb{R}^n : S_h f(x) > 2^k\}$, $k \in \mathbb{Z}$, and consider $O_k^* := \{x \in \mathbb{R}^n : \mathcal{M}(\chi_{O_k}) > 1 - \gamma\}$ for some fixed $0 < \gamma < 1$. Then $O_k \subset O_k^*$ and $|O_k^*| \leq C(\gamma)|O_k|$ for every $k \in \mathbb{Z}$. Next let $\{Q_k^j\}_j$ be a Whitney decomposition of O_k^* and $\widehat{O}_k^*$ be a tent region, that is

$$\widehat{O}_k^* := \{(x,t) \in \mathbb{R}^n \times (0,\infty) : \operatorname{dist}(x, {}^c O_k^*) \geq t\}. \tag{4.5}$$

For every $k, j \in \mathbb{Z}$ we define

$$T_k^j := \left(Q_k^j \times (0,\infty)\right) \cap \widehat{O}_k^* \cap {}^c \widehat{O}_{k+1}^*, \tag{4.6}$$

and then recall the formula (4.4) to write

$$f_N = C_M \sum_{j,k\in\mathbb{Z}} \int_{1/N}^{N} (t^2Le^{-t^2L})^{M+1} \left(\chi_{T_k^j} t^2Le^{-t^2L}\right) f \,\frac{dt}{t} =: \sum_{j,k\in\mathbb{Z}} \lambda_k^j m_k^j(N), \tag{4.7}$$

where $\lambda_k^j = C_M 2^k |Q_k^j|$ and

$$m_k^j(N) = \frac{1}{\lambda_k^j} \int_{1/N}^{N} (t^2Le^{-t^2L})^{M+1} \left(\chi_{T_k^j} t^2Le^{-t^2L}\right) f \,\frac{dt}{t}. \tag{4.8}$$

We claim that, up to a normalization by a harmless multiplicative constant, the $m_k^j(N)$ are molecules. Assuming the claim, we note that by definition of T_k^j, $m_k^j(N) = 0$ if $C\ell(Q_k^j) < 1/N$, so that (4.7) is a δ-representation with $\delta \approx 1/N$. Thus, once the claim is established, we shall have

$$\begin{aligned}\sup_N \|f_N\|_{\widetilde{H}_L^1(\mathbb{R}^n)} &\leq C \sum_{j,k\in\mathbb{Z}} \lambda_k^j = C \sum_{j,k\in\mathbb{Z}} 2^k |Q_k^j| \leq C \sum_{k\in\mathbb{Z}} 2^k |O_k^*| \\ &\leq C \sum_{k\in\mathbb{Z}} 2^k |O_k| \leq C \|S_h f\|_{L^1(\mathbb{R}^n)},\end{aligned} \tag{4.9}$$

as desired. Let us now prove the claim: that is, we will show that for every $j, k \in \mathbb{Z}$, and $N \in \mathbb{N}$ the function $C^{-1} m_k^j(N)$ is a (p, ε, M)- molecule associated with the cube Q_k^j, $2 \leq p < \widetilde{p}_L$, for some harmless constant C. The case $p \leq 2$ follows from this one by Hölder's inequality.

To this end, fix $j, k \in \mathbb{Z}$ and $i \in \mathbb{N} \cup \{0\}$ and consider some $h \in L^{p'}(S_i(Q_k^j))$ such that $\|h\|_{L^{p'}(S_i(Q_k^j))} = 1$, $\frac{1}{p} + \frac{1}{p'} = 1$. Set

$$\chi_k^j := \chi_{\left(Q_k^j \times (0,\infty)\right) \cap \widehat{O}_k^*}. \tag{4.10}$$

Then

$$\begin{aligned}\left|\int_{\mathbb{R}^n} m_k^j(N)(x)\overline{h(x)}\,dx\right| &\leq \frac{1}{\lambda_k^j} \iint_{T_k^j} \left|t^2Le^{-t^2L} f(x) \left((t^2Le^{-t^2L})^{M+1}\right)^* h(x)\right| \frac{dt}{t}\,dx \\ &\leq \frac{C}{\lambda_k^j} \int_{{}^cO_{k+1}} \iint_{\Gamma(x)} \chi_k^j(y,t) \left|t^2Le^{-t^2L} f(y) \left((t^2Le^{-t^2L})^{M+1}\right)^* h(y)\right| \frac{dtdy}{t^{n+1}}\,dx\end{aligned}$$

$$\leq \frac{C}{\lambda_k^j}\left(\int\limits_{{}^cO_{k+1}\cap cQ_k^j}\left(\iint\limits_{\Gamma(x)}\left|t^2Le^{-t^2L}f(y)\right|^2\frac{dydt}{t^{n+1}}\right)^{\frac{p}{2}}dx\right)^{\frac{1}{p}}$$

$$\times\left(\int\limits_{{}^cO_{k+1}\cap cQ_k^j}\left(\int\limits_{\Gamma(x)\cap\left(Q_k^j\times(0,\infty)\right)\cap\widehat{O}_k^*}\left|\left((t^2Le^{-t^2L})^{M+1}\right)^*h(y)\right|^2\frac{dydt}{t^{n+1}}\right)^{\frac{p'}{2}}dx\right)^{\frac{1}{p'}}$$

$$=: I_1\times I_2. \tag{4.11}$$

Some comments are in order here. For the second inequality we used Lemma 2.1 with $F = {}^cO_{k+1}$ (so that $F^* = {}^cO_{k+1}^*$ and $\mathcal{R}^1(F^*) = {}^c\widehat{O}_{k+1}^*$) and

$$\Phi(x,t) := \chi_k^j(y,t)\left|t^2Le^{-t^2L}f(x)\left((t^2Le^{-t^2L})^{M+1}\right)^*h(x)\right|t^{-n-1}. \tag{4.12}$$

The third estimate above is based on Hölder's inequality and the fact that whenever $y\in\Gamma(x)\cap\left(Q_k^j\times(0,\infty)\right)\cap\widehat{O}_k^*$ we have $x\in c\,Q_k^j$, where the constant c is related to the implicit constant in Whitney decomposition. Without loss of generality we will assume that $c\leq 3$.

Observe now that

$$I_1\leq C\frac{1}{\lambda_k^j}\left(\int\limits_{cQ_k^j\cap{}^cO_{k+1}}(S_hf(x))^p\,dx\right)^{1/p}, \tag{4.13}$$

and $S_hf(x)$ is bounded by 2^{k+1} for every $x\in{}^cO_{k+1}$. Therefore

$$I_1\leq C\frac{1}{\lambda_k^j}2^{k+1}|Q_k^j|^{\frac{1}{p}}\leq C\,|Q_k^j|^{\frac{1}{p}-1}. \tag{4.14}$$

Turning to I_2, recall that supp $h\subset S_i(Q_k^j)$. Then to handle $i\leq 4$ it is enough to notice that

$$I_2\leq C\left\|S_h^{M+1}h\right\|_{L^{p'}(\mathbb{R}^n)}\leq C\|h\|_{L^{p'}(S_i(Q_k^j))}\leq C, \tag{4.15}$$

using Lemma 2.6. Then

When $i\geq 5$, we proceed as follows. We invoke Hölder's inequality to estimate $L^{p'}$ norm by L^2 norm and then apply (2.5) with $F = {}^cO_{k+1}\cap c\,Q_k^j$ and

$$\Phi(y,t)=\chi_{(0,\,c\,l(Q_k^j))}(t)\left|\left((t^2Le^{-t^2L})^{M+1}\right)^*h(y)\right|^2t^{-n-1}. \tag{4.16}$$

Then

$$I_2 \le C|Q_k^j|^{\frac{1}{p'}-\frac{1}{2}} \left(\int\limits_{3c\,Q_k^j} \int\limits_0^{c\,l(Q_k^j)} \left| \left((t^2 L e^{-t^2 L})^{M+1} \right)^* h(x) \right|^2 \frac{dxdt}{t} \right)^{\frac{1}{2}} \tag{4.17}$$

By Lemmas 2.5 and 2.3 applied to the operator L^* the expression in (4.17) is bounded by

$$\begin{aligned} &C|Q_k^j|^{\frac{1}{p'}-\frac{1}{2}} \left(\int\limits_0^{c\,l(Q_k^j)} e^{-\frac{\operatorname{dist}(3cQ_k^j, S_i(Q_k^j))^2}{ct^2}} t^{2\left(\frac{n}{2}-\frac{n}{p'}\right)} \frac{dt}{t} \right)^{1/2} \|h\|_{L^{p'}(S_i(Q_k^j))} \\ &\quad \le C|Q_k^j|^{\frac{1}{p'}-\frac{1}{2}} \left(\int\limits_0^{c\,l(Q_k^j)} \left(\frac{t}{2^i l(Q_k^j)} \right)^{2\left(\frac{n}{p'}+\varepsilon\right)} t^{2\left(\frac{n}{2}-\frac{n}{p'}\right)} \frac{dt}{t} \right)^{1/2} \le C 2^{-i\left(n-\frac{n}{p}+\varepsilon\right)}. \end{aligned} \tag{4.18}$$

All in all,

$$\left| \int\limits_{\mathbb{R}^n} m_k^j(N)(x)\overline{h(x)}\,dx \right| \le C2^{-i(n-n/p+\varepsilon)} |Q_k^j|^{1/p-1} \tag{4.19}$$

for every $h \in L^{p'}(S_i(Q_k^j))$ with $\|h\|_{L^{p'}(S_i(Q_k^j))} = 1$. Taking the supremum over all such h we arrive at (1.9).

The condition (1.10) can be verified directly applying $(l(Q_k^j)^{-2}L^{-1})^k$, $1 \le k \le M$, to the molecule and arguing along the lines (4.11)–(4.19). A few modifications relate solely to I_2 which is majorized by

$$\left(\int\limits_{{}^cO_{k+1}\cap cQ_k^j} \left(\iint\limits_{\Gamma(x)} \chi_k^j \left| \left(e^{-kt^2 L} (t^2 L e^{-t^2 L})^{M+1-k} \right)^* h(y) \right|^2 \frac{dydt}{t^{n+1}} \right)^{\frac{p'}{2}} dx \right)^{\frac{1}{p'}}$$

(cf. (4.10)), and the rest of the argument follows verbatim. We have therefore established that $f_N \in \widehat{H}_L^1$, and that f_N satisfies the desired bounds in $\widetilde{H}_L^1$, uniformly in N. It remains to verify that $f_N \to f$ in $\widetilde{H}_L^1$ and in $H_{S_h}^1$, and also that $f = \sum \lambda_k^j m_k^j$, where the $m_k^j = \lim_{N\to\infty} m_k^j(N)$ exist and are molecules (up to a harmless normalization). We defer consideration of this matter for the moment, and proceed to:

Step II. Let us now move to part (ii) of the lemma. To begin, observe that it is enough to consider the case $p \le 2$.

The proof follows that of Theorem 3.2 above. We recall that $S_h : L^p \to L^p$, $p_L < p < \tilde{p}_L$ (Lemma 2.6). By Lemma 3.3, it will therefore be enough to show that S_h maps allowable (p, ε, M) molecules uniformly into L^1. To this end, we show that S_h satisfies certain estimates arising in the proof of Theorem 3.2, which may be inserted directly into the appropriate places in the argument to establish (3.9). More precisely, the combination of estimates (3.10) and (3.11) amounts to showing that

$$\left\| S_h(I - e^{-l(Q)^2 L})^M (m\chi_{S_i(Q)}) \right\|_{L^1(\mathbb{R}^n)} \le C2^{-i\varepsilon}, \tag{4.20}$$

while (3.14), with $T = S_h$, becomes

$$\sup_{1\le k\le M} \left\| S_h \left(\frac{k}{M}\, l(Q)^2 L e^{-\frac{k}{M} l(Q)^2 L} \right)^M \left(\chi_{S_i(Q)} (l(Q)^{-2} L^{-1})^M m \right) \right\|_{L^1(\mathbb{R}^n)} \le C2^{-i\varepsilon}. \tag{4.21}$$

Given the latter two estimates, the remainder of the proof of Theorem 3.2 carries over verbatim.

We begin with (4.20). We first note that since S_h and $(I - e^{-l(Q)^2 L})^M$ are bounded in L^p (in the latter case with constant independent of $l(Q)$), we have for $j = 0, 1, 2$,

$$\| S_h(I - e^{-l(Q)^2 L})^M (m\chi_{S_i(Q)}) \|_{L^p(S_j(Q_i))} \le C \|m\|_{L^p(S_i(Q))}. \tag{4.22}$$

Assume now that $j \ge 3$. By Hölder's inequality and Lemma 2.1

$$\begin{aligned}
&\left\| S_h(I - e^{-l(Q)^2 L})^M (m\chi_{S_i(Q)}) \right\|^2_{L^p(S_j(Q_i))} \\
&\le C(2^{i+j} l(Q))^{2\left(\frac{n}{p} - \frac{n}{2}\right)} \int\int_{\mathcal{R}(S_j(Q_i))} \left| t^2 L e^{-t^2 L} (I - e^{-l(Q)^2 L})^M (m\chi_{S_i(Q)})(x) \right|^2 \frac{dt\,dx}{t} \\
&\le C(2^{i+j} l(Q))^{2\left(\frac{n}{p} - \frac{n}{2}\right)} \int_{\mathbb{R}^n \setminus Q_{j-2+i}} \int_0^\infty \left| t^2 L e^{-t^2 L} (I - e^{-l(Q)^2 L})^M (m\chi_{S_i(Q)})(x) \right|^2 \frac{dt\,dx}{t} \\
&\quad + C(2^{i+j} l(Q))^{2\left(\frac{n}{p} - \frac{n}{2}\right)} \\
&\quad \times \sum_{k=0}^{j-2} \int_{S_k(Q_i)} \int_{(2^{j-1} - 2^k) 2^i l(Q)}^\infty | t^2 L e^{-t^2 L} (I - e^{-l(Q)^2 L})^M (m\chi_{S_i(Q)})(x) |^2 \frac{dt\,dx}{t} \\
&=: I + \sum_{k=0}^{j-2} I_k.
\end{aligned} \tag{4.23}$$

We observe that

$$
\begin{aligned}
I &\leq C(2^{i+j}l(Q))^{2\left(\frac{n}{p}-\frac{n}{2}\right)} \|g_h(I-e^{-l(Q)^2L})^M(m\chi_{S_i(Q)})\|^2_{L^2(\mathbb{R}^n\setminus Q_{j-2+i})} \\
&\leq C(2^{i+j}l(Q))^{2\left(\frac{n}{p}-\frac{n}{2}\right)} l(Q)^{2\left(\frac{n}{2}-\frac{n}{p}\right)} \left(\frac{l(Q)^2}{\operatorname{dist}(S_i(Q),\mathbb{R}^n\setminus Q_{j-2+i})^2}\right)^{2M} \|m\|^2_{L^p(S_i(Q))} \\
&\leq C\left(\frac{1}{2^{i+j}}\right)^{4M+2\left(\frac{n}{2}-\frac{n}{p}\right)} \|m\|^2_{L^p(S_i(Q))}, \qquad (4.24)
\end{aligned}
$$

where the second inequality follows from (3.25). Turning to I_k, $k=0,1,\dots,j-2$, we make a change of variables $s:=t^2/(m+1)$, so that $s\geq[(2^{j-1}-2^k)2^il(Q)]^2/(m+1)\approx[2^{i+j}l(Q)]^2$ and

$$
\begin{aligned}
I_k &\leq C(2^{i+j}l(Q))^{2\left(\frac{n}{p}-\frac{n}{2}\right)} \\
&\quad\times \int_{c[2^{i+j}l(Q)]^2}^{\infty} \left\| sLe^{-(m+1)sL}(I-e^{-l(Q)^2L})^M(m\chi_{S_i(Q)})\right\|^2_{L^2(S_k(Q_i))} \frac{ds}{s} \\
&\leq C(2^{i+j}l(Q))^{2\left(\frac{n}{p}-\frac{n}{2}\right)} \times \int_{c\,[2^{i+j}l(Q)]^2}^{\infty} \left(\frac{l(Q)^2}{s}\right)^{2M} \\
&\quad\times \left\| sLe^{-sL}\left[\frac{s}{l(Q)^2}(e^{-sL}-e^{-(l(Q)^2+s)L})\right]^M (m\chi_{S_i(Q)})\right\|^2_{L^2(S_k(Q_i))} \frac{ds}{s}. \qquad (4.25)
\end{aligned}
$$

At this point we apply (3.19)–(3.20) with $t=l(Q)^2$ combined with L^p-L^2 off-diagonal estimates for sLe^{-sL} and obtain

$$
\begin{aligned}
I_k &\leq C(2^{i+j}l(Q))^{2\left(\frac{n}{p}-\frac{n}{2}\right)} \|m\|^2_{L^2(S_i(Q))} \\
&\quad\times \int_{c\,[2^{i+j}l(Q)]^2}^{\infty} s^{\left(\frac{n}{2}-\frac{n}{p}\right)} e^{-\frac{\operatorname{dist}(S_i(Q),S_k(Q_i))^2}{cs}} \left(\frac{l(Q)^2}{s}\right)^{2M} \frac{ds}{s} \\
&\leq C\left(\int_{c\,[2^{i+j}l(Q)]^2}^{\infty} \left(\frac{l(Q)^2}{s}\right)^{2M} \frac{ds}{s}\right) \|m\|^2_{L^p(S_i(Q))} \\
&\leq C\left(\frac{1}{2^{i+j}}\right)^{4M} \|m\|^2_{L^p(S_i(Q))}. \qquad (4.26)
\end{aligned}
$$

Combining (4.24) and (4.26), one can see that

$$\left\| S_h(I - e^{-l(Q)^2 L})^M (m\chi_{S_i(Q)}) \right\|^2_{L^p(S_j(Q_i))} \leq Cj \left(\frac{1}{2^{i+j}} \right)^{4M+2\left(\frac{n}{2}-\frac{n}{p}\right)} \|m\|^2_{L^p(S_i(Q))}. \tag{4.27}$$

Finally, using (4.22) and (4.27) we obtain (4.20) as follows:

$$\begin{aligned}
&\left\| S_h(I - e^{-l(Q)^2 L})^M (m\chi_{S_i(Q)}) \right\|_{L^1(\mathbb{R}^n)} \\
&\leq C \sum_{j=3}^{\infty} (2^{i+j} l(Q))^{n-\frac{n}{p}} \sqrt{j} \left(\frac{1}{2^{i+j}} \right)^{2M+\left(\frac{n}{2}-\frac{n}{p}\right)} \|m\|_{L^p(S_i(Q))} \\
&\quad + C(2^i l(Q))^{n-\frac{n}{p}} \|m\|_{L^p(S_i(Q))} \\
&\leq C 2^{i\left(\frac{n}{p}-\frac{n}{2}-2M-\varepsilon\right)} \sum_{j=3}^{\infty} \sqrt{j}\, 2^{j(n/2-2M)} + C\, 2^{-i\varepsilon} \leq C\, 2^{-i\varepsilon}.
\end{aligned}$$

A similar argument establishes (4.21). This time we use (3.26) to control an analogue of (4.24), and (3.24) instead of (3.19) at the step corresponding to (4.25)–(4.26). This completes the proof of part (ii) of the lemma.

To finish part (i), it remains to show that $f_N \to f$ in $\widetilde{H}^1_L$ and in $H^1_{S_h}$, and that f has the claimed molecular decomposition. To this end, we recall that $f_N \to f$ in L^2. We claim that $\{f_N\}$ is a Cauchy sequence in $\widetilde{H}^1_L$. Let us postpone establishing this claim until the end of the proof. Assuming the claim, we see that there exists $g \in \widetilde{H}^1_L$ such that $f_N \to g$ in $\widetilde{H}^1_L$, and, in particular, in L^1. By taking subsequences which converge a.e., we see that the L^1 and L^2 limits are the same, i.e., $g = f$, and $f_N \to f$ in $\widetilde{H}^1_L$.

Since we have already established part (ii), we may use (4.3) to extend S_h to all of H^1_L (thus in particular by (3.4) to $\widetilde{H}^1_L$) by continuity. Let us momentarily call this extension $\widetilde{S}_h$. Then by (4.3) and (3.4), we have

$$\|\widetilde{S}_h(f_N - f)\|_{L^1(\mathbb{R}^n)} \to 0.$$

Thus, by sublinearity, $S_h f_N \to \widetilde{S}_h f$ in L^1. But also, $S_h f_N \to S_h f$ in L^2, so $S_h f = \widetilde{S}_h f$ almost everywhere. Therefore, using (4.9), we have that

$$\begin{aligned}
\|f\|_{\widetilde{H}^1_L(\mathbb{R}^n)} &= \lim_{N\to\infty} \|f_N\|_{\widetilde{H}^1_L(\mathbb{R}^n)} \leq C \sum \lambda_k^j \leq \|S_h f\|_{L^1(\mathbb{R}^n)} \\
&= \|\widetilde{S}_h f\|_{L^1(\mathbb{R}^n)} \leq C\|f\|_{H^1_L(\mathbb{R}^n)}.
\end{aligned}$$

Next, we show that $m_k^j(N)$ converges weakly in each L^p, $p_L < p < \widetilde{p}_L$, and that the limits are molecules (up to a harmless multiplicative constant). Indeed, let

$h \in L^{p'} \cap L^2$. Then

$$\begin{aligned}\langle m_k^j(N), h\rangle &= \frac{1}{\lambda_k^j}\int\limits_{\mathbb{R}^n}\left(\int\limits_{1/N}^{N}(t^2Le^{-t^2L})^{M+1}\chi_{T_k^j}t^2Le^{-t^2L}f(x)\frac{dt}{t}\right)\overline{h(x)}\,dx\\ &= \frac{1}{\lambda_k^j}\int\limits_{1/N}^{N}\left\langle\chi_{T_k^j}t^2Le^{-t^2L}f, (t^2L^*e^{-t^2L^*})^{M+1}h\right\rangle\frac{dt}{t}\\ &\to \frac{1}{\lambda_k^j}\int\limits_{0}^{\infty}\left\langle\chi_{T_k^j}t^2Le^{-t^2L}f, (t^2L^*e^{-t^2L^*})^{M+1}h\right\rangle\frac{dt}{t},\end{aligned}$$

by dominated convergence, since the square functions

$$\left(\int\limits_0^\infty|t^2Le^{-t^2L}f|^2\frac{dt}{t}\right)^{1/2}, \quad \left(\int\limits_0^\infty|(t^2L^*e^{-t^2L^*})^{M+1}h|^2\frac{dt}{t}\right)^{1/2},$$

belong, in particular, to L^2. Similarly, but even more crudely, we may obtain existence of

$$\lim_{N\to\infty}\langle(\ell(Q_k^j)^2L)^{-i}m_k^j(N), h\rangle, \quad 1 \le i \le M,$$

since $t \le C\ell(Q_k^j)$ in T_k^j. On the other hand, we have shown that, up to a multiplicative constant, the $m_k^j(N)$ are molecules, i.e., the bounds (1.9) and (1.10) hold uniformly in N, for $m_k^j(N)$, with $Q = Q_k^j$. In particular,

$$\sup_N \|m_k^j(N)\|_{L^p(\mathbb{R}^n)} \le C|Q_k^j|^{1/p-1}.$$

Taking a supremum over $h \in L^{p'}(\mathbb{R}^n)$, with norm 1, we therefore obtain by the Riesz representation theorem that the weak limit m_k^j belongs to L^p. The desired bounds (1.9) and (1.10) follow by taking $h \in L^{p'}(S_i(Q_k^j))$, and using the corresponding uniform bounds for $m_k^j(N)$. Thus, up to a multiplicative constant, the m_k^j are molecules.

We now show that $f = \sum\lambda_k^j m_k^j$. Let $\varphi \in C_0^\infty$. Then, using absolute convergence, and the fact that $m_k^j(N) \to m_k^j$ weakly in L^p, we obtain

$$\begin{aligned}\int\varphi\left(\sum\lambda_k^j m_k^j\right) &= \sum\lambda_k^j\int\varphi\, m_k^j\\ &= \sum\lambda_k^j\lim_{N\to\infty}\int\varphi\, m_k^j(N)\end{aligned}$$

$$
\begin{aligned}
&= \lim_{N\to\infty} \sum \lambda_k^j \int \varphi\, m_k^j(N) \quad \text{(by dominated convergence)}\\
&= \lim_{N\to\infty} \int \varphi \left(\sum \lambda_k^j m_k^j(N) \right)\\
&\equiv \lim_{N\to\infty} \int \varphi f_N = \int \varphi f.
\end{aligned}
$$

Since this equality holds for all $\varphi \in C_0^\infty$, we have that $f = \sum \lambda_k^j m_k^j$ almost everywhere.

To complete the proof of the lemma, it remains to show that $\{f_N\}$ is a Cauchy sequence in $\widetilde{H}_L^1$. We recall that $f_N = \sum \lambda_k^j m_k^j(N)$ where $\lambda_k^j = C2^k|Q_k^j|$, and

$$
m_k^j(N) \equiv \frac{1}{\lambda_k^j} \int_{1/N}^{N} \left(t^2 L e^{-t^2 L}\right)^{M+1} \chi_{T_k^j} t^2 L e^{-t^2 L} f \frac{dt}{t}.
$$

For $K \in \mathbb{N}$, we write

$$
\begin{aligned}
f_N &= \sum_{j+k\le K} \lambda_k^j m_k^j(N) + \sum_{j+k>K} \lambda_k^j m_k^j(N)\\
&= \sigma_K(N) + R_K(N).
\end{aligned}
$$

Then

$$
\sup_N \|R_K(N)\|_{\widetilde{H}_L^1(\mathbb{R}^n)} \le \sum_{j+k>K} |\lambda_k^j| \to 0 \tag{4.28}
$$

as $K \to \infty$. Thus, it suffices to consider

$$
\|\sigma_K(N) - \sigma_K(N')\|_{\widetilde{H}_L^1(\mathbb{R}^n)} = \left\| \sum_{j+k\le K} \lambda_k^j \left(m_k^j(N) - m_k^j(N') \right) \right\|_{\widetilde{H}_L^1(\mathbb{R}^n)}.
$$

Let $\eta > 0$ be given, and choose K so that (4.28) is bounded by η. It is enough to show that for all $p \in (p_L, \widetilde{p}_L)$, for every $\varepsilon > 0$, $M > n/4$, and every $K \in \mathbb{N}$, there exists an integer $N_1 = N_1(\eta, K, p, \varepsilon, M)$ such that

$$
\max_{j+k\le K} \|m_k^j(N) - m_k^j(N')\|_{p,\varepsilon,M,Q_k^j} < \eta, \tag{4.29}
$$

whenever $N' \ge N \ge N_1$, where the "(p, ε, M)-molecular norm adapted to Q" is defined as

$$
\|\mu\|_{p,\varepsilon,M,Q} \equiv \sup_{i\ge 0} 2^{i(n-n/p+\varepsilon)} |Q|^{1-1/p} \sum_{\nu=0}^{M} \|(\ell(Q)^2 L)^{-\nu} \mu\|_{L^p(S_i(Q))}.
$$

To this end, we note that, for N, N' sufficiently large,

$$\mu_k^j(N,N') \equiv m_k^j(N') - m_k^j(N) = \frac{1}{\lambda_k^j}\int_{1/N'}^{1/N} (t^2Le^{-t^2L})^{M+1}\chi_{T_k^j} t^2Le^{-t^2L} f\,\frac{dt}{t},$$

since $t \le C\ell(Q_k^j)$ in T_j^k. Let $h \in L^{p'}(S_i(Q_k^j))$, with $\|h\|_{p'} = 1$. Then, following the argument from (4.11) to (4.19), we obtain that

$$\begin{aligned}|\langle \mu_k^j(N,N'),h\rangle| &= \left|\frac{1}{\lambda_k^j}\int_{1/N'}^{1/N}\left\langle \chi_{T_k^j} t^2Le^{-t^2L}f,(t^2L^*e^{-t^2L^*})^{M+1}h\right\rangle\frac{dt}{t}\right| \\ &\le C\frac{1}{\lambda_k^j}\left(\int_{CQ_k^j\cap {}^cO_{k+1}} (S_h^{1/N}f)^p\,dx\right)^{1/p} 2^{-i(n-n/p+\varepsilon)},\end{aligned}$$

where

$$S_h^{1/N}f \equiv \left(\int\int_{|x-y|<t<1/N} |t^2Le^{-t^2L}f(y)|^2\frac{dydt}{t^{n+1}}\right)^{1/2}.$$

Now, since $f\in L^2$, $S_h^{1/N}f \to 0$ in L^2. We choose N_1 so large that

$$\|S_h^{1/N}f\|_{L^2(\mathbb{R}^n)} \le \frac{1}{C}\,\eta^R \min_{j+k\le K}\lambda_k^j\,|Q_k^j|^{-1/2}, \tag{4.30}$$

whenever $N \ge N_1$, where R will be chosen depending on p. If $p=2$, taking $R=1$, and taking the surpemum over h as above, we obtain immediately that

$$\|\mu_k^j(N,N')\|_{L^2(S_i(Q_k^j))} \le \eta 2^{-i(n/2+\varepsilon)}|Q_k^j|^{-1/2}.$$

The case $p_L < p < 2$ follows by Hölder's inequality. For $2 < p < \widetilde{p}_L$, we choose $r \in (p,\widetilde{p}_L)$, and using that $S_hf \le 2^{k+1}$ on ${}^cO_{k+1}$ by definition, we interpolate between (4.30) and the crude bound

$$\left(\int_{CQ_k^j\cap {}^cO_{k+1}} (S_h^{1/N}f(x))^r\,dx\right)^{1/r} \le C2^k|Q_k^j|^{1/r},$$

to deduce that

$$|\langle \mu_k^j(N,N'),h\rangle| \le \eta 2^{-i(n-n/p+\varepsilon)}|Q_k^j|^{1/p-1},$$

for R chosen large enough depending on p. We now obtain (4.29), by applying $(\ell(Q_k^j)^2 L)^{-\nu}$ to $\mu_k^j(N,N')$, and then repeating the previous argument with minor changes. It follows that $\{f_N\}$ is a Cauchy sequence in $\widetilde{H}^1_L$. This concludes the proof of Lemma 4.2 and therefore also that of Theorem 4.1. □

We conclude this section with

Corollary 4.3 *The spaces $H^1_L(\mathbb{R}^n)$ coincide for different choices of $\varepsilon > 0$, $p_L < p < \widetilde{p}_L$ and $M \in \mathbb{N}$ such that $M > n/4$.*

Indeed, for all permissible values of these parameters, we have established that the corresponding H^1_L space is equivalent to $H^1_{S_h}$.

5 Characterization by the square function associated to the Poisson semigroup

We start with the following auxiliary result.

Lemma 5.1 *Fix $K \in \mathbb{N}$. For all closed sets E, F in $\mathbb{R}^n$ with* $\operatorname{dist}(E,F) > 0$

$$\left\|\left(t\sqrt{L}\right)^{2K} e^{-t\sqrt{L}}\right\|_{L^2(F)} \le C\left(\frac{t}{\operatorname{dist}(E,F)}\right)^{2K+1}\|f\|_{L^2(E)}, \quad \forall t>0, \tag{5.1}$$

if $f \in L^2(\mathbb{R}^n)$ is supported in E.

Proof The subordination formula

$$e^{-t\sqrt{L}}f = C\int_0^\infty \frac{e^{-u}}{\sqrt{u}}\, e^{-\frac{t^2L}{4u}} f\,du \tag{5.2}$$

allows us to write

$$\begin{aligned}\left\|(t\sqrt{L})^{2K}e^{-t\sqrt{L}}\right\|_{L^2(F)} &\le C\int_0^\infty \frac{e^{-u}}{\sqrt{u}}\left\|\left(\frac{t^2L}{4u}\right)^K e^{-\frac{t^2L}{4u}} f\right\|_{L^2(F)} u^K\,du \\ &\le C\|f\|_{L^2(E)}\int_0^\infty e^{-u}\, e^{-\frac{\operatorname{dist}(E,F)^2}{cu^2}}\, u^{K-1/2}\,du. \end{aligned}\tag{5.3}$$

Then we make the change of variables $u \mapsto s := u\frac{\mathrm{dist}\,(E,F)^2}{t^2}$ to bound (5.3) by

$$C\|f\|_{L^2(E)}\int_0^\infty e^{-s\frac{t^2}{\mathrm{dist}(E,F)^2}}e^{-s}\left(s\frac{t^2}{\mathrm{dist}(E,F)^2}\right)^{K-1/2}\frac{t^2}{\mathrm{dist}(E,F)^2}ds$$

$$\leq C\|f\|_{L^2(E)}\left(\frac{t}{\mathrm{dist}(E,F)}\right)^{2K+1}\int_0^\infty e^{-s}s^{K-1/2}ds$$

$$\leq C\left(\frac{t}{\mathrm{dist}(E,F)}\right)^{2K+1}\|f\|_{L^2(E)}, \tag{5.4}$$

as desired. □

Theorem 5.2 *Consider the operator*

$$S_P^K f(x) := \left(\iint_{\Gamma(x)} |\left(t\sqrt{L}\right)^{2K} e^{-t\sqrt{L}} f(y)|^2 \frac{dydt}{t^{n+1}}\right)^{1/2}, \quad x\in\mathbb{R}^n, \quad f\in L^2(\mathbb{R}^n). \tag{5.5}$$

Suppose $K \in \mathbb{N}$, $M \in \mathbb{N}$, $M + K > n/4 - 1/2$, and $\varepsilon = 2M + 2K + 1 - n/2$. If $f \in L^2(\mathbb{R}^n)$, with $\|S_P^K f\|_{L^1(\mathbb{R}^n)} < \infty$, then $f \in H_L^1$. Furthermore, there exists a family of $(2, \varepsilon, M)$-molecules $\{m_i\}_{i=0}^\infty$ and a sequence of numbers $\{\lambda_i\}_{i=0}^\infty$ such that f can be represented in the form $f = \sum_{i=0}^\infty \lambda_i m_i$, with

$$\|f\|_{H_L^1(\mathbb{R}^n)} \leq C\sum_{i=0}^\infty |\lambda_i| \leq C\|S_P^K f\|_{L^1(\mathbb{R}^n)}. \tag{5.6}$$

Proof The lemma can be proved following the argument of Theorem 4.1 with minor modifications. To be more precise, we use the Calderón reproducing formula in the form

$$f = C\int_0^\infty \left((t^2L)^{M+K}e^{-t\sqrt{L}}\right)^2 f\,\frac{dt}{t} = C\int_0^\infty (t^2L)^{2M+K}e^{-t\sqrt{L}}(t^2L)^K e^{-t\sqrt{L}} f\,\frac{dt}{t}, \tag{5.7}$$

for $f \in L^2(\mathbb{R}^n)$. To be completely rigorous, we should truncate and approximate by f_N as in the proof of Theorem 4.1. As the details are similar in the present case, we shall merely sketch a formal proof, and leave the details of the limiting arguments to the reader.

To begin, we define

$$O_k := \{x \in \mathbb{R}^n : S_P^K f(x) > 2^k\}, \tag{5.8}$$

and

$$m_k^j = \frac{1}{\lambda_k^j} \int_0^\infty (t^2 L)^{2M+K} e^{-t\sqrt{L}} \left(\chi_{T_k^j} (t^2 L)^K e^{-t\sqrt{L}} \right) f \, \frac{dt}{t}, \tag{5.9}$$

with T_k^j, $k, j \in \mathbb{Z}$, given analogously to (4.6). The rest of the proof follows the same path, using Lemma 5.1 instead of Gaffney relations, which allows to derive the estimate

$$\|m_k^j\|_{L^2(S_i(Q_k^j))} \leq C\, 2^{-i(4M+2K+1)} |Q_k^j|^{-1/2}, \quad i = 0, 1, 2, \dots, \tag{5.10}$$

for all $k, j \in \mathbb{Z}$.

As for the vanishing moment condition,

$$\left(l(Q_k^j)^{-2} L^{-1} \right)^M m_k^j = \frac{1}{\lambda_k^j} \int_0^\infty \left(\frac{t}{l(Q_k^j)} \right)^{2M} (t^2 L)^{M+K} e^{-t\sqrt{L}} \times \left(\chi_{T_k^j} (t^2 L)^K e^{-t\sqrt{L}} \right) f \, \frac{dt}{t}, \tag{5.11}$$

and hence

$$\left\| (l(Q_k^j)^{-2} L^{-1})^M m_k^j \right\|_{L^2(S_i(Q_k^j))} \leq C 2^{-i(2M+2K+1)} |Q_k^j|^{-1/2}, \quad i = 0, 1, 2, \dots \tag{5.12}$$

Combined with (5.10), this finishes the argument. □

Theorem 5.3 *Let $\varepsilon > 0$ and $M > n/4$. Then for every representation $\sum_{i=0}^\infty \lambda_i m_i$, where $\{m_i\}_{i=0}^\infty$ is a family of $(2, \varepsilon, M)$-molecules and $\sum_{i=0}^\infty |\lambda_i| < \infty$, the series $\sum_{i=0}^\infty \lambda_i m_i$ converges in $H^1_{S_P}(\mathbb{R}^n)$ and*

$$\left\| \sum_{i=0}^\infty \lambda_i m_i \right\|_{H^1_{S_P}(\mathbb{R}^n)} \leq C \sum_{i=0}^\infty |\lambda_i|. \tag{5.13}$$

Proof We will follow the argument of Theorem 4.1, Step II, and mention only necessary changes.

First, by Lemma 3.3, it will be enough to establish a uniform L^1 bound on molecules. To this end, we observe that the operator

$$g_P f := \left(\int_0^\infty |t \nabla e^{-t\sqrt{L}} f|^2 \, \frac{dt}{t} \right)^{1/2}, \tag{5.14}$$

is bounded in $L^2(\mathbb{R}^n)$. This follows from the estimates on the operators having bounded holomorphic functional calculus in L^2 [1] and integration by parts. Then S_P is bounded in $L^2(\mathbb{R}^n)$, since

$$\begin{aligned}\|S_P f\|_{L^2(\mathbb{R}^n)} &\leq C\left(\iint\limits_{\mathbb{R}^n\times(0,\infty)}\left[\int\limits_{|x-y|<t} dx\right]|t\nabla e^{-t\sqrt{L}}f(y)|^2\,\frac{dydt}{t^{n+1}}\right)^{1/2}\\ &\leq C\left(\iint\limits_{\mathbb{R}^n\times(0,\infty)}|t\nabla e^{-t\sqrt{L}}f(y)|^2\,\frac{dydt}{t}\right)^{1/2}\\ &\leq C\|g_P f\|_{L^2(\mathbb{R}^n)}\leq C\|f\|_{L^2(\mathbb{R}^n)}. \end{aligned} \tag{5.15}$$

Therefore, for $j = 0, 1, 2$,

$$\left\|S_P(I-e^{-l(Q)^2L})^M(m\chi_{S_i(Q)})\right\|_{L^2(S_j(Q_i))}\leq C\|m\|_{L^2(S_i(Q))}. \tag{5.16}$$

Turning to the case $j \geq 3$, we write

$$\left\|S_P(I-e^{-l(Q)^2L})^M(m\chi_{S_i(Q)})\right\|^2_{L^2(S_j(Q_i))}\leq I+\sum_{k=0}^{j-2}I_k, \tag{5.17}$$

where

$$I = C\int\limits_{\mathbb{R}^n\setminus Q_{j-2+i}}\int_0^\infty\left|t\nabla e^{-t\sqrt{L}}(I-e^{-l(Q)^2L})^M(m\chi_{S_i(Q)})(x)\right|^2\frac{dtdx}{t} \tag{5.18}$$

and

$$I_k = C\int\limits_{S_k(Q_i)}\int\limits_{(2^{j-1}-2^k)2^il(Q)}^\infty\left|t\nabla e^{-t\sqrt{L}}(I-e^{-l(Q)^2L})^M(m\chi_{S_i(Q)})(x)\right|^2\frac{dtdx}{t} \tag{5.19}$$

for $k = 0, \ldots, j-2$. Then by the subordination formula and Minkowski's inequality we have that $I^{1/2}\leq C\int_0^\infty e^{-u}J^{1/2}du$, where

$$\begin{aligned}J &= \int\limits_{{}^cQ_{j-2+i}}\int_0^\infty\left|\frac{t}{\sqrt{4u}}\nabla e^{-\frac{t^2L}{4u}}(I-e^{-l(Q)^2L})^{2M}(m\chi_{S_i(Q)})(x)\right|^2\frac{dtdx}{t}\\ &= \int\limits_{{}^cQ_{j-2+i}}\int_0^\infty\left|s\nabla e^{-s^2L}(I-e^{-l(Q)^2L})^{4M}(m\chi_{S_i(Q)})(x)\right|^2\frac{dsdx}{s},\end{aligned}$$

and where in the last step we have made the change of variable $t \mapsto s := t/\sqrt{4u}$. However, it can be proved along the lines of Theorem 3.4 that $\tilde{g}_h f := \Big(\int_0^\infty |t\nabla e^{-t^2 L} f|^2 \frac{dt}{t}\Big)^{1/2}$ (similarly to $g_h f$) satisfies the estimates (3.6) with $p = 2$ and therefore

$$I \leq C \left(\frac{l(Q)^2}{\operatorname{dist}(S_i(Q), \mathbb{R}^n \backslash_{j-2+i})^2} \right)^{2M} \|m\|^2_{L^2(S_i(Q))} \leq \left(\frac{1}{2^{i+j}} \right)^{4M} \|m\|^2_{L^2(S_i(Q))}.$$

Concerning I_k, $k = 0, 1, \ldots, j-2$, we use the subordination formula once again to write

$$I_k^{1/2} \leq C \int\limits_0^\infty e^{-u} \left(\int\limits_{S_k(Q_i)} \int\limits_{(2^{j-1}-2^k)2^i l(Q)}^\infty \left| \frac{t}{\sqrt{4u}} \nabla e^{-\frac{t^2 L}{4u}} \right.\right.$$
$$\left.\left. \times (I - e^{-l(Q)^2 L})^M (m\chi_{S_i(Q)})(x) \right|^2 \frac{dt dx}{t} \right)^{1/2} du. \tag{5.20}$$

Then one can make a change of variables $s := \frac{t^2}{4u(m+1)}$, so that following (4.25) and (4.26)

$$I_k^{1/2} \leq C \int\limits_0^\infty e^{-u} \left(\int\limits_{\frac{[(2^{j-1}-2^k)2^i l(Q)]^2}{cu}}^\infty \|\sqrt{s} \nabla e^{-(m+1)sL} \right.$$
$$\left. \times (I - e^{-l(Q)^2 L})^M (m\chi_{S_i(Q)})\|^2_{L^2(S_k(Q_i))} \frac{ds}{s} \right)^{1/2} du$$
$$\leq C \int\limits_0^\infty e^{-u} \left(\int\limits_{\frac{[(2^{j-1}-2^k)2^i l(Q)]^2}{cu}}^\infty e^{-\frac{\operatorname{dist}(S_i(Q), S_k(Q_i))^2}{cs(1+u)}} \left(\frac{l(Q)^2}{s} \right)^{2M} \frac{ds}{s} \right)^{1/2} du$$
$$\times \|m\|_{L^2(S_i(Q))}, \tag{5.21}$$

and hence

$$I_k \leq C \left(\frac{1}{2^{i+j}} \right)^{4M} \|m\|^2_{L^2(S_i(Q))}. \tag{5.22}$$

Then

$$\begin{aligned}
&\left\| S_P(I-e^{-l(Q)^2L})^M(m\chi_{S_i(Q)})\right\|_{L^1(\mathbb{R}^n)}\\
&\quad\le C\sum_{j=3}^{\infty}\left(2^{i+j}l(Q)\right)^{n/2}\sqrt{j}\left(\frac{1}{2^{i+j}}\right)^{2M}\|m\|_{L^2(S_i(Q))}\\
&\qquad+C\left(2^{i}l(Q)\right)^{n/2}\|m\|_{L^2(S_i(Q))}\le C\,2^{-i\varepsilon}.
\end{aligned}$$

A similar argument provides an estimate for $\|S_P[I-(I-e^{-l(Q)^2L})]^M m\|_{L^1(\mathbb{R}^n)}$ and finishes the proof. □

Lemma 5.4 *For all* $f\in L^2(\mathbb{R}^n)$

$$\|S_P^1 f\|_{L^1(\mathbb{R}^n)}\le C\|S_P f\|_{L^1(\mathbb{R}^n)}. \tag{5.23}$$

Proof To start, let us define the family of truncated cones

$$\Gamma^{\varepsilon,R,\alpha}(x):=\{(y,t)\in\mathbb{R}^n\times(\varepsilon,R):|x-y|<t\alpha\},\quad x\in\mathbb{R}^n. \tag{5.24}$$

Then for every function $\eta\in C_0^\infty(\Gamma^{\varepsilon/2,2R,3/2}(x))$ such that $\eta\equiv 1$ on $\Gamma^{\varepsilon,R,1}(x)$ and $0\le\eta\le 1$

$$\begin{aligned}
&\left(\int\!\!\int_{\Gamma^{\varepsilon,R,1}(x)}|t^2Le^{-t\sqrt{L}}f(y)|^2\frac{dydt}{t^{n+1}}\right)^{1/2}\\
&\le\left(\int\!\!\int_{\Gamma^{\varepsilon/2,2R,3/2}(x)}t^2Le^{-t\sqrt{L}}f(y)\,\overline{t^2Le^{-t\sqrt{L}}f(y)}\eta(y,t)\,\frac{dydt}{t^{n+1}}\right)^{1/2}\\
&\le\left(\int\!\!\int_{\Gamma^{\varepsilon/2,2R,3/2}(x)}tA\nabla e^{-t\sqrt{L}}f(y)\cdot t\nabla\left[\,\overline{t^2Le^{-t\sqrt{L}}f(y)}\,\right]\eta(y,t)\frac{dydt}{t^{n+1}}\right)^{1/2}\\
&\quad+\left(\int\!\!\int_{\Gamma^{\varepsilon/2,2R,3/2}(x)}tA\nabla e^{-t\sqrt{L}}f(y)\cdot\overline{t^2Le^{-t\sqrt{L}}f(y)}\,t\nabla\eta(y,t)\frac{dydt}{t^{n+1}}\right)^{1/2}.
\end{aligned} \tag{5.25}$$

We can always assume that $\|\nabla\eta\|_{L^\infty(\Gamma^{\varepsilon/2,2R,2}(x))} \le 1/t$, so that the expression above is bounded by

$$\left(\int\int_{\Gamma^{\varepsilon/2,2R,3/2}(x)} |t\nabla e^{-t\sqrt{L}} f(y)|^2 \frac{dydt}{t^{n+1}}\right)^{1/4} \left(\int\int_{\Gamma^{\varepsilon/2,2R,3/2}(x)} |t\nabla t^2 L e^{-t\sqrt{L}} f(y)|^2 \frac{dydt}{t^{n+1}}\right)^{1/4}$$
$$+\left(\int\int_{\Gamma^{\varepsilon/2,2R,3/2}(x)} |t\nabla e^{-t\sqrt{L}} f(y)|^2 \frac{dydt}{t^{n+1}}\right)^{1/4} \left(\int\int_{\Gamma^{\varepsilon/2,2R,3/2}(x)} |t^2 L e^{-t\sqrt{L}} f(y)|^2 \frac{dydt}{t^{n+1}}\right)^{1/4}.$$

Consider now a covering of the set $\Gamma^{\varepsilon/2,2R,3/2}(x)$ given by collection of balls $\{B(z_k, r_k)\}_{k=0}^\infty$ in $\mathbb{R}^{n+1}$, such that

$$\Gamma^{\varepsilon/2,2R,3/2}(x) \subseteq \bigcup_{k=0}^\infty B(z_k, r_k) \subseteq \bigcup_{k=0}^\infty B(z_k, 2r_k) \subseteq \Gamma^{\varepsilon/4,3R,2}(x),$$
$$\operatorname{dist}\left(z_k, {}^c(\Gamma^{\varepsilon/4,3R,2}(x))\right) \approx r_k \approx \operatorname{dist}\left(B(z_k, r_k), \{t=0\}\right), \tag{5.26}$$

and the collection $\{B(z_k, 2r_k)\}$, has bounded overlaps. Such a collection $\{B(z_k, r_k)\}$ can be constructed using the Whitney decomposition (for the latter see [13,24]). Then we use Caccioppoli's inequality (Lemma 2.7) for the operator

$$\tilde{L} f = -\operatorname{div}_{y,t}(B\,\nabla_{y,t} f),$$

where $\tilde{L}$ is understood in the usual weak sense, B is the $(n+1)\times(n+1)$ block diagonal matrix with components 1 and A and $\operatorname{div}_{y,t}$, $\nabla_{y,t}$ denote, respectively, divergence and gradient taken in space and time variables. Clearly, $\tilde{L} e^{-t\sqrt{L}} f = 0$. We obtain

$$\begin{aligned}
&\int\int_{\Gamma^{\varepsilon/2,2R,3/2}(x)} \left|t\nabla t^2 L e^{-t\sqrt{L}} f(y)\right|^2 \frac{dydt}{t^{n+1}} \\
&\le \sum_{k=0}^\infty \int\int_{B(z_k,r_k)} \left|t\nabla_{y,t} t^2 L e^{-t\sqrt{L}} f(y)\right|^2 \frac{dydt}{t^{n+1}} \\
&\le C\sum_{k=0}^\infty \int\int_{B(z_k,2r_k)} \left|\frac{t}{r_k} t^2 L e^{-t\sqrt{L}} f(y)\right|^2 \frac{dydt}{t^{n+1}} \\
&\le C\int\int_{\Gamma^{\varepsilon/4,3R,2}(x)} \left|t^2 L e^{-t\sqrt{L}} f(y)\right|^2 \frac{dydt}{t^{n+1}}.
\end{aligned} \tag{5.27}$$

Combining this with the formulae above and passing to the limit as $\varepsilon \to 0$ and $R \to \infty$, we arrive at

$$S_P^1 f(x) \le C(S_P f(x))^{1/2}(S_P^1 f(x))^{1/2}, \tag{5.28}$$

and hence (5.23), as desired. □

Corollary 5.5 *$H_L^1(\mathbb{R}^n) = H_{S_P}^1(\mathbb{R}^n)$, in particular, $\|f\|_{H_L^1(\mathbb{R}^n)} \approx \|S_P f\|_{L^1(\mathbb{R}^n)}$.*

Proof The left-to-the-right inclusion follows from Theorem 5.3, the converse from Theorem 5.2 combined with Lemma 5.4; in addition, we use Corollary 4.3 to guarantee that the molecular spaces $H_L^1(\mathbb{R}^n)$ coincide for different choices of $p \in (p_L, \widetilde{p}_L)$ and $\varepsilon > 0$, thus removing the constraints on ε and p in Theorem 5.2. We omit the details. □

Finally, consider two more versions of the square function:

$$\bar{S}_P f(x) := \left(\iint_{\Gamma(x)} \left| t\sqrt{L}e^{-t\sqrt{L}} f(y) \right|^2 \frac{dydt}{t^{n+1}} \right)^{1/2}, \tag{5.29}$$

$$\widehat{S}_P f(x) := \left(\iint_{\Gamma(x)} \left| t\nabla_{x,t} e^{-t\sqrt{L}} f(y) \right|^2 \frac{dydt}{t^{n+1}} \right)^{1/2}, \tag{5.30}$$

where $f \in L^2(\mathbb{R}^n)$, $x \in \mathbb{R}^n$ and $\nabla_{y,t}$ stands for the gradient in space and time variables.

Theorem 5.6 *We have the equivalence*

$$\|f\|_{H_L^1(\mathbb{R}^n)} \approx \|\bar{S}_P f\|_{L^1(\mathbb{R}^n)} \approx \|\widehat{S}_P f\|_{L^1(\mathbb{R}^n)}. \tag{5.31}$$

This result is just a slight modification of the previous ones in this section. In fact, the argument for $\bar{S}_P$ follows the same lines as the proofs of Theorems 5.2 and 5.3 ones we observe that $t\sqrt{L}e^{-t\sqrt{L}} = -t\partial_t e^{-t\sqrt{L}}$, and the result for $\widehat{S}_P$ is a combination of those for S_P and $\bar{S}_P$.

6 Characterization by the non-tangential maximal function associated to the heat semigroup

Theorem 6.1 *For every $f \in L^2(\mathbb{R}^n)$*

$$\|S_h f\|_{L^1(\mathbb{R}^n)} \le C\|\mathcal{N}_h f\|_{L^1(\mathbb{R}^n)}. \tag{6.1}$$

Proof The idea of the proof is based on the analogous argument for the maximal and square functions associated to the Poisson semigroup for the Laplacian that appeared in [17], with some technical modifications owing to the parabolic nature of the heat semigroup. Similar ideas have also been used in [8].

To begin, notice that the argument of Lemma 5.4 also provides the estimate

$$\|S_h f\|_{L^1(\mathbb{R}^n)} \le C\|\tilde{S}_h f\|_{L^1(\mathbb{R}^n)}, \tag{6.2}$$

for $\widetilde{S}_h = \widetilde{S}_h^1$, where

$$\widetilde{S}_h^{\beta} f(x) := \left(\int\!\!\int_{\Gamma^{\beta}(x)} \left| t\nabla e^{-t^2 L} f(y) \right|^2 \frac{dydt}{t^{n+1}} \right)^{1/2}, \quad f \in L^2(\mathbb{R}^n), \quad x \in \mathbb{R}^n. \tag{6.3}$$

Therefore, it is enough to prove (6.1) with $\widetilde{S}_h$ in place of S_h. Also, recall the definition of truncated cone (5.24) and denote

$$\widetilde{S}_h^{\varepsilon,R,\beta} f(x) := \left(\int\!\!\int_{\Gamma^{\varepsilon,R,\beta}(x)} \left| t\nabla e^{-t^2 L} f(y) \right|^2 \frac{dydt}{t^{n+1}} \right)^{1/2}, \quad f \in L^2(\mathbb{R}^n), \quad x \in \mathbb{R}^n. \tag{6.4}$$

In what follows we will work with $\widetilde{S}_h^{\varepsilon,R,\beta}$ rather than $\widetilde{S}_h^{\beta}$ and then pass to the limit as $\varepsilon \to 0$, $R \to \infty$, all constants in estimates will not depend on ε and R unless explicitly stated.

Consider the non-tangential maximal function

$$\mathcal{N}_h^{\beta} f(x) := \sup_{(y,t)\in\Gamma^{\beta}(x)} \left(\frac{1}{(\beta t)^n} \int_{B(y,\beta t)} \left| e^{-t^2 L} f(z) \right|^2 dz \right)^{1/2}, \quad f \in L^2(\mathbb{R}^n), \tag{6.5}$$

where $\Gamma^{\beta}(x)$, $x \in \mathbb{R}^n$, $\beta > 0$, is the cone of aperture β. Let us introduce the following sets:

$$E := \{x \in \mathbb{R}^n : \mathcal{N}_h^{\beta} f(x) \le \sigma\}, \quad \sigma \in \mathbb{R}, \tag{6.6}$$

where β is some fixed constant to be determined later, and

$$E^* := \left\{ x \in \mathbb{R}^n : \text{for every } B(x), \text{ ball in } \mathbb{R}^n \text{ centered at } x, \ \frac{|E \cap B(x)|}{|B(x)|} \ge \frac{1}{2} \right\}, \tag{6.7}$$

the set of points having global $1/2$ density with respect to E. Also,

$$B := {}^{c}E, \quad B^* := {}^{c}E^*. \tag{6.8}$$

Finally, denote

$$\mathcal{R}^{\varepsilon,R,\beta}(E^*) := \bigcup_{x\in E^*} \Gamma^{\varepsilon,R,\beta}(x), \tag{6.9}$$

$$\mathcal{B}^{\varepsilon,R,\beta}(E^*)\text{—the boundary of } \mathcal{R}^{\varepsilon,R,\beta}(E^*), \tag{6.10}$$

and

$$u(y,t) := e^{-t^2L} f(y), \quad t\in(0,\infty), \quad y\in\mathbb{R}^n. \tag{6.11}$$

It is not hard to see that

$$\begin{aligned}\int_{E^*} \left(\widetilde{S}_h^{2\varepsilon,R,1/2} f(x)\right)^2 dx &\le \int_{E^*} \left(\widetilde{S}_h^{\alpha\varepsilon,\alpha R,1/\alpha} f(x)\right)^2 dx \\ &\le C \int\int_{\mathcal{R}^{\alpha\varepsilon,\alpha R,1/\alpha}(E^*)} t|\nabla u(y,t)|^2\, dydt, \quad \forall\alpha\in(1,2),\end{aligned} \tag{6.12}$$

by Lemma 2.1. Going further,

$$\begin{aligned}&\int\int_{\mathcal{R}^{\alpha\varepsilon,\alpha R,1/\alpha}(E^*)} t|\nabla u(y,t)|^2\, dydt = \int\int_{\mathcal{R}^{\alpha\varepsilon,\alpha R,1/\alpha}(E^*)} t\nabla u(y,t)\cdot\overline{\nabla u(y,t)}\, dydt \\ &\le C\Re e\int\int_{\mathcal{R}^{\alpha\varepsilon,\alpha R,1/\alpha}(E^*)} \Big[tA(y)\nabla u(y,t)\cdot\overline{\nabla u(y,t)}+\nabla u(y,t)\cdot t\overline{A(y)\nabla u(y,t)}\Big]\, dydt,\end{aligned} \tag{6.13}$$

using the ellipticity of A. Now we integrate by parts to bound (6.13) by

$$\begin{aligned}&C\Re e\int\int_{\mathcal{R}^{\alpha\varepsilon,\alpha R,1/\alpha}(E^*)} \Big[-t\operatorname{div}A(y)\nabla u(y,t)\overline{u(y,t)} - u(y,t)\overline{t\operatorname{div}A(y)\nabla u(y,t)}\Big]\, dydt \\ &\quad + C\Re e\int_{\mathcal{B}^{\alpha\varepsilon,\alpha R,1/\alpha}(E^*)} \Big[tA(y)\nabla u(y,t)\cdot\nu_y(y,t)\overline{u(y,t)} \\ &\quad + u(y,t)\nu_y(y,t)\cdot t\overline{A(y)\nabla u(y,t)}\Big]\, d\sigma_{y,t},\end{aligned}$$

where $\nu_y(y,t)$, $y\in\mathbb{R}^n$, $t\in\mathbb{R}$, is the projection of normal vector to $\mathcal{B}^{\alpha\varepsilon,\alpha R,1/\alpha}(E^*)$ on $\mathbb{R}^n$ (similarly, ν_t will denote projection on $\mathbb{R}$). However, u given by (6.11) is a solution of system $\partial_t u = -2t\operatorname{div}A\nabla u$, and hence the first integral above can be represented modulo multiplicative constant as

$$\int\int_{\mathcal{R}^{\alpha\varepsilon,\alpha R,1/\alpha}(E^*)} \left[\partial_t u(y,t)\cdot\overline{u(y,t)} + u(y,t)\cdot\overline{\partial_t u(y,t)}\right] dydt$$

$$= \int\int_{\mathcal{R}^{\alpha\varepsilon,\alpha R,1/\alpha}(E^*)} \partial_t |u(y,t)|^2\, dydt = \int_{\mathcal{B}^{\alpha\varepsilon,\alpha R,1/\alpha}(E^*)} |u(y,t)|^2 \nu_t(y,t)\, d\sigma_{y,t}. \tag{6.14}$$

Combining (6.13) and (6.14), one can write

$$\begin{aligned}
&\int_1^2 \int\int_{\mathcal{R}^{\alpha\varepsilon,\alpha R,1/\alpha}(E^*)} t|\nabla u(y,t)|^2\, dydt\, d\alpha \\
&\quad \le C\int_1^2 \int_{\mathcal{B}^{\alpha\varepsilon,\alpha R,1/\alpha}(E^*)} t|\nabla u(y,t)|\,|u(y,t)| d\sigma_{y,t}\, d\alpha \\
&\qquad + C\int_1^2 \int_{\mathcal{B}^{\alpha\varepsilon,\alpha R,1/\alpha}(E^*)} |u(y,t)|^2\, d\sigma_{y,t}\, d\alpha \\
&\quad \le C\int\int_{\widetilde{\mathcal{B}}^{\varepsilon,R}(E^*)} |\nabla u(y,t)|\,|u(y,t)|\, dydt + C\int\int_{\widetilde{\mathcal{B}}^{\varepsilon,R}(E^*)} |u(y,t)|^2 \frac{dydt}{t} \\
&\quad \le C\left(\int\int_{\widetilde{\mathcal{B}}^{\varepsilon,R}(E^*)} t|\nabla u(y,t)|^2\, dydt\right)^{1/2} \left(\int\int_{\widetilde{\mathcal{B}}^{\varepsilon,R}(E^*)} |u(y,t)|^2 \frac{dydt}{t}\right)^{1/2} \\
&\qquad + C\int\int_{\widetilde{\mathcal{B}}^{\varepsilon,R}(E^*)} |u(y,t)|^2 \frac{dydt}{t}
\end{aligned} \tag{6.15}$$

where

$$\widetilde{\mathcal{B}}^{\varepsilon,R}(E^*) := \{(x,t)\in\mathbb{R}^n\times(0,\infty) : (x,t)\in\mathcal{B}^{\alpha\varepsilon,\alpha R,1/\alpha}(E^*) \text{ for some } 1<\alpha<2\}. \tag{6.16}$$

Consider the following three regions:

$$\widetilde{\mathcal{B}}^{\varepsilon}(E^*) := \{(x,t)\in\mathbb{R}^n\times(\varepsilon,2\varepsilon) :\ \operatorname{dist}(x,E^*)<t\}, \tag{6.17}$$

$$\widetilde{\mathcal{B}}^{R}(E^*) := \{(x,t)\in\mathbb{R}^n\times(R,2R) :\ \operatorname{dist}(x,E^*)<t\}, \tag{6.18}$$

$$\widetilde{\mathcal{B}}'(E^*) := \{(x,t)\in B^*\times(\varepsilon,2R) :\ \operatorname{dist}(x,E^*)<t<2\operatorname{dist}(x,E^*)\}, \tag{6.19}$$

and observe that

$$\widetilde{\mathcal{B}}^{\varepsilon,R}(E^*) \subset \widetilde{\mathcal{B}}^{\varepsilon}(E^*) \cup \widetilde{\mathcal{B}}^{R}(E^*) \cup \widetilde{\mathcal{B}}'(E^*). \tag{6.20}$$

Below we will analyze separately the parts of integrals in (6.15) corresponding to the regions (6.17)–(6.19).

Let us start with

$$I_1^\varepsilon := \iint\limits_{\widetilde{\mathcal{B}}^{\varepsilon}(E^*)} |u(y,t)|^2 \,\frac{dydt}{t}. \tag{6.21}$$

For every $(y,t) \in \widetilde{\mathcal{B}}^{\varepsilon}(E^*)$ there exists $y^* \in E^*$ such that $y^* \in B(y,t)$. By definition of E^* this implies that $|E \cap B(y^*,t)| \geq C|B(y^*,t)|$ and therefore $|E \cap B(y,2t)| \geq Ct^n$. Then

$$\begin{aligned} I_1^\varepsilon &\leq C \iint\limits_{\widetilde{\mathcal{B}}^{\varepsilon}(E^*)} \int\limits_{E\cap B(y,2t)} |u(y,t)|^2 \,dz\, \frac{dydt}{t^{n+1}} \\ &\leq C \int_\varepsilon^{2\varepsilon}\int_E \left(\frac{1}{t^n} \int\limits_{B(z,2t)} |u(y,t)|^2\,dy \right) dz \frac{dt}{t} \\ &\leq C \int_\varepsilon^{2\varepsilon}\int_E \left|\mathcal{N}_h^\beta f(z)\right|^2 dz \frac{dt}{t} \leq C \int_E \left|\mathcal{N}_h^\beta f(z)\right|^2 dz, \end{aligned} \tag{6.22}$$

for every $\beta \geq 2$.

Using similar ideas,

$$I_2^\varepsilon := \iint\limits_{\widetilde{\mathcal{B}}^{\varepsilon}(E^*)} t|\nabla u(y,t)|^2\,dydt \leq C \int_\varepsilon^{2\varepsilon}\int_E \left(\frac{1}{t^{n-2}} \int\limits_{B(z,2t)} |\nabla u(y,t)|^2\,dy \right) dz \frac{dt}{t}. \tag{6.23}$$

Recall now parabolic Caccioppoli inequality (2.15). By definition $u(y,t) = e^{-t^2L} f(y)$, therefore, making the change of variables in (2.15), one can see that

$$\int_{t_0-cr}^{t_0} \int\limits_{B(x_0,r)} t|\nabla u(x,t)|^2\,dxdt \leq \frac{C}{r^2} \int_{t_0-2cr}^{t_0} \int\limits_{B(x_0,2r)} t|u(x,t)|^2\,dxdt, \tag{6.24}$$

for every $x_0 \in \mathbb{R}^n$, $r > 0$, $t_0 > 2cr$. Here $c > 0$ and the constant C depends on c. Next, we divide the integral in $t \in (\varepsilon, 2\varepsilon)$ from (6.21) into integrals over $(\varepsilon, 3\varepsilon/2)$ and

$(3\varepsilon/2, 2\varepsilon)$, and apply (6.24) with $t_0 = 2\varepsilon$ and $t_0 = 3\varepsilon/2$, $r = 2\varepsilon$, $c = 1/4$ to obtain the bound

$$I_2^\varepsilon \le C \int_{\varepsilon/2}^{2\varepsilon} \int_E \left(\frac{1}{t^n} \int_{B(z,8\varepsilon)} |u(y,t)|^2 \, dy \right) dz \frac{dt}{t}$$

$$\le C \int_{\varepsilon/2}^{2\varepsilon} \int_E \left(\frac{1}{t^n} \int_{B(z,16t)} |u(y,t)|^2 \, dy \right) dz \frac{dt}{t} \le C \int_E |\mathcal{N}_h^\beta f(z)|^2 \, dz, \tag{6.25}$$

where $\beta \ge 16$.

Observe that the same argument applies to estimates

$$\iint_{\widetilde{\mathcal{B}}^R(E^*)} |u(y,t)|^2 \frac{dydt}{t} \le C \int_E |\mathcal{N}_h^\beta f(z)|^2 \, dz, \tag{6.26}$$

$$\iint_{\widetilde{\mathcal{B}}^R(E^*)} t |\nabla u(y,t)|^2 \, dydt \le C \int_E |\mathcal{N}_h^\beta f(z)|^2 \, dz, \tag{6.27}$$

with $\beta \ge 16$.

To control the integral over $\widetilde{\mathcal{B}}'(E^*)$, we first decompose B^* into a family of Whitney balls, $\{B(x_k, r_k)\}_{k=0}^\infty$, such that $\cup_{k=0}^\infty B(x_k, r_k) = B^*$, $c_1 \operatorname{dist}(x_k, E^*) \le r_k \le c_2 \operatorname{dist}(x_k, E^*)$, and every point $x \in B^*$ belongs at most to c_3 balls, $0 < c_1 < c_2 < 1$ and $c_3 \in \mathbb{N}$ are some fixed constants, independent of B^* [13,24]. Then

$$I_1' := \iint_{\widetilde{\mathcal{B}}'(E^*)} |u(y,t)|^2 \frac{dydt}{t} \le \sum_{k=0}^\infty \int_{r_k(1/c_2-1)}^{2r_k(1/c_1+1)} \int_{B(x_k,r_k)} |u(y,t)|^2 \frac{dydt}{t}$$

$$\le C \sum_{k=0}^\infty r_k^n \int_{r_k(1/c_2-1)}^{2r_k(1/c_1+1)} \left[\frac{1}{t^n} \int_{B(x_k, \frac{c_2}{1-c_2} t)} |u(y,t)|^2 dy \right] \frac{dt}{t}. \tag{6.28}$$

On the other side, $E^* \subset E$, hence, $\operatorname{dist}(x_k, E) \le \operatorname{dist}(x_k, E^*) \le \frac{c_2}{(1-c_2)c_1} t$ and the expression in brackets above can be majorized by the square of non-tangential maximal function $\mathcal{N}^\beta f(z)$ for some $z \in E$ and $\beta \ge \frac{c_2}{(1-c_2)c_1}$. Hence,

$$I_1' \le C \sum_{k=0}^\infty r_k^n \left(\sup_{z \in E} \mathcal{N}_h^\beta f(z) \right)^2 \le C |B^*| \left(\sup_{z \in E} \mathcal{N}_h^\beta f(z) \right)^2. \tag{6.29}$$

Similarly to (6.28) and (6.29) we can prove that there exists $C_0 = C_0(c_1, c_2) > 0$ such that

$$I_2' := \int\int_{\widetilde{\mathcal{B}}'(E^*)} t|\nabla u(y,t)|^2\, dydt \le C|B^*| \left(\sup_{z\in E} \mathcal{N}_h^\beta f(z)\right)^2, \tag{6.30}$$

for $\beta \ge C_0$, using (6.24) to control the gradient of u.

Let us choose now

$$\beta := \max\left\{16, \frac{c_2}{(1-c_2)c_1}, C_0\right\} \tag{6.31}$$

in (6.6). Then

$$I_1' \le C\sigma^2|B^*| \quad \text{and} \quad I_2' \le C\sigma^2|B^*|. \tag{6.32}$$

Combining all the estimates above allows us to write

$$\int_{E^*} \left(\widetilde{S}_h^{2\varepsilon,R,1/2} f(x)\right)^2 dx \le C\sigma^2|B^*| + C\int_E |\mathcal{N}_h^\beta f(z)|^2 dz, \tag{6.33}$$

and therefore, passing to the limit as $\varepsilon \to 0$ and $R \to \infty$,

$$\int_{E^*} \left(\widetilde{S}_h^{1/2} f(x)\right)^2 dx \le C\sigma^2|B^*| + C\int_E |\mathcal{N}_h^\beta f(z)|^2 dz. \tag{6.34}$$

Denote by $\lambda_{\mathcal{N}_h^\beta f}$ the distribution function of $\mathcal{N}_h^\beta f$ and recall that $\mathcal{N}_h^\beta \le \sigma$ on E. Then

$$\int_{E^*} \left(\widetilde{S}_h^{1/2} f(x)\right)^2 dx \le C\sigma^2 \lambda_{\mathcal{N}_h^\beta f}(\sigma) + C\int_0^\sigma t\lambda_{\mathcal{N}_h^\beta f}(t)dt, \tag{6.35}$$

since $|B^*| \le C|B| \le C\lambda_{\mathcal{N}_h^\beta f}(\sigma)$. Next,

$$\begin{aligned}
\lambda_{\widetilde{S}_h^{1/2} f}(\sigma) &\le \left|\left\{x \in E^* : \widetilde{S}_h^{1/2} f(x) > \sigma\right\}\right| + |{}^c E^*| \\
&\le C\frac{1}{\sigma^2} \int_{E^*} \left(\widetilde{S}_h^{1/2} f(x)\right)^2 dx + C\lambda_{\mathcal{N}_h^\beta f}(\sigma) \\
&\le C\frac{1}{\sigma^2} \int_0^\sigma t\lambda_{\mathcal{N}_h^\beta f}(t)\, dt + C\lambda_{\mathcal{N}_h^\beta f}(\sigma),
\end{aligned} \tag{6.36}$$

and therefore,

$$\|\widetilde{S}_h^{1/2} f\|_{L^1(\mathbb{R}^n)} = \int_0^\infty \lambda_{\widetilde{S}_h^{1/2} f}(\sigma)\, d\sigma \leq C\|\mathcal{N}_h^\beta f\|_{L^1(\mathbb{R}^n)}, \tag{6.37}$$

for β as in (6.31). In view of Lemma 2.2 and (6.2) the theorem is proved modulo the result we present below. □

Lemma 6.2 *For all $f \in L^2(\mathbb{R}^n)$ and $\beta \geq 1$*

$$\|\mathcal{N}_h^\beta f\|_{L^1(\mathbb{R}^n)} \leq C\beta^n \|\mathcal{N}_h^1 f\|_{L^1(\mathbb{R}^n)}. \tag{6.38}$$

Proof Fix $\sigma \in (0, \infty)$ and consider the following sets:

$$E_\sigma := \{x \in \mathbb{R}^n : \mathcal{N}_h^1 f(x) > \sigma\} \quad \text{and} \quad E_\sigma^* := \{x \in \mathbb{R}^n : \mathcal{M}(\chi_{E_\sigma})(x) > C/\beta^n\}. \tag{6.39}$$

It is not hard to see that $|E_\sigma^*| \leq C\beta^n |E_\sigma|$.

Assume now that $x \not\in E_\sigma^*$. Then $B(y, t) \not\subset E_\sigma$ for every $(y, t) \in \Gamma^{2\beta}(x)$. Indeed, if $B(y, t) \subset E_\sigma$, then

$$\mathcal{M}(\chi_{E_\sigma})(x) > C\frac{|B(y, t)|}{|B(x, 2\beta t)|} \geq C/\beta^n, \tag{6.40}$$

which implies $x \in E_\sigma^*$.

Therefore, there exists $z \in B(y, t)$ such that $\mathcal{N}_h^1 f(z) \leq \sigma$, in particular,

$$\left(\frac{1}{t^n}\int_{B(y,t)} |e^{-t^2 L} f(z)|^2\, dz\right)^{1/2} \leq \sigma. \tag{6.41}$$

Recall that the above inequality holds for all $(y, t) \in \Gamma^{2\beta}(x)$. Now for every $w \in B(x, \beta t)$ one can cover $B(w, \beta t)$ by $C\beta^n$ balls $B(y_i, t)$, where $y_i \in \Gamma^{2\beta}(x)$, to prove that

$$\frac{1}{(\beta t)^n}\int_{B(w,\beta t)} |e^{-t^2 L} f(z)|^2\, dz \leq \frac{C}{\beta^n}\sum_i \frac{1}{t^n}\int_{B(y_i,t)} |e^{-t^2 L} f(z)|^2\, dz \leq C\sigma^2, \tag{6.42}$$

hence,

$$\mathcal{N}_h^\beta f(x) \leq C\sigma \quad \text{for every } x \notin E_\sigma^*. \tag{6.43}$$

Having this at hand, we simply write

$$\|\mathcal{N}_h^\beta f\|_{L^1(\mathbb{R}^n)} \leq C \int_0^\infty \Big|\{x \in \mathbb{R}^n : \mathcal{N}_h^\beta f > C\sigma\}\Big| d\sigma$$
$$\leq C \int_0^\infty |E_\sigma^*| d\sigma \leq C \int_0^\infty \beta^n |E_\sigma| d\sigma \leq C\beta^n \|\mathcal{N}_h^1 f\|_{L^1(\mathbb{R}^n)}, \quad (6.44)$$

and finish the argument. □

Theorem 6.3 *Let $\varepsilon > 0$ and $M > n/4$. Then for every representation $\sum_{i=0}^\infty \lambda_i m_i$, where $\{m_i\}_{i=0}^\infty$ is a family of $(2, \varepsilon, M)$-molecules and $\sum_{i=0}^\infty |\lambda_i| < \infty$, the series $\sum_{i=0}^\infty \lambda_i m_i$ converges in $H^1_{\mathcal{N}_h}(\mathbb{R}^n)$ and*

$$\left\|\sum_{i=0}^\infty \lambda_i m_i\right\|_{H^1_{\mathcal{N}_h}(\mathbb{R}^n)} \leq C \sum_{i=0}^\infty |\lambda_i|. \quad (6.45)$$

Proof As usual, by Lemma 3.3 we need only establish a uniform L^1 bound on molecules. Consider the following modifications of the non-tangential maximal function

$$\mathcal{N}_h^* f(y) = \sup_{t>0} \left(\frac{1}{t^n} \int_{|x-y|<t} |e^{-t^2 L} f(x)|^2 dx\right)^{1/2}, \quad (6.46)$$

$$\mathcal{N}_h^{*,M} f(y) = \sup_{t>0} \left(\frac{1}{t^n} \int_{|x-y|<t} |t^{2M} L^M e^{-t^2 L} f(x)|^2 dx\right)^{1/2}, \quad (6.47)$$

where $y \in \mathbb{R}^n$, $M \in \mathbb{N}$ and $f \in L^2(\mathbb{R}^n)$. Both of the operators above are bounded on $L^2(\mathbb{R}^n)$.

Indeed

$$\|\mathcal{N}_h^* f\|^2_{L^2(\mathbb{R}^n)}$$
$$\leq C \int_{\mathbb{R}^n} \left[\sup_{t>0} \sum_{j=0}^\infty \left(\frac{1}{t^n} \int_{B(y,t)} |e^{-t^2 L}(f\chi_{S_j(B(y,t))})(x)|^2 dx\right)^{1/2}\right]^2 dy$$
$$\leq C \int_{\mathbb{R}^n} \left[\sup_{t>0} \sum_{j=0}^\infty \frac{1}{t^{n/p}} e^{-\frac{\operatorname{dist}(B(y,t), S_j(B(y,t)))^2}{ct^2}} \|f\|_{L^p(S_j(B(y,t)))}\right]^2 dy, \quad (6.48)$$

for every $p_L < p \le 2$ by $L^p - L^2$ off-diagonal estimates. Therefore, for every $\varepsilon > 0$ and $p < 2$ as above

$$\|\mathcal{N}_h^* f\|_{L^2(\mathbb{R}^n)}^2 \le C \int_{\mathbb{R}^n} \left[\sup_{t>0} \sum_{j=0}^{\infty} \frac{1}{t^{n/p}} 2^{-j(n/p+\varepsilon)} \|f\|_{L^p(S_j(B(y,t)))} \right]^2 dy$$
$$\le C \int_{\mathbb{R}^n} \left[\mathcal{M}(|f|^p)(y) \right]^{2/p} dy \le C \int_{\mathbb{R}^n} |f(y)|^2 \, dy, \tag{6.49}$$

using $L^{2/p}(\mathbb{R}^n)$ boundedness of the Hardy–Littlewood maximal function.

Along the same lines we can prove L^2 boundedness of the function $\mathcal{N}_h^{*,M}$.

On the other side, by Lemma 6.2

$$\|\mathcal{N}_h f\|_{L^1(\mathbb{R}^n)} \le C \|\mathcal{N}_h^{1/2} f\|_{L^1(\mathbb{R}^n)} \le C \|\mathcal{N}_h^* f\|_{L^1(\mathbb{R}^n)}, \tag{6.50}$$

and therefore, by Lemma 3.3, it is enough to show that

$$\|\mathcal{N}_h^* m\|_{L^1(\mathbb{R}^n)} \le C \tag{6.51}$$

for every m a $(2, \varepsilon, M)$-molecule associated to some cube Q.

To this end, we use the annular decomposition of $\mathbb{R}^n$ along with Hölder's inequality to write

$$\|\mathcal{N}_h^* m\|_{L^1(\mathbb{R}^n)} \le C \sum_{j=0}^{\infty} (2^j l(Q))^{n/2} \|\mathcal{N}_h^* m\|_{L^2(S_j(Q))}$$
$$\le C \sum_{j=0}^{10} (2^j l(Q))^{n/2} \|\mathcal{N}_h^* m\|_{L^2(S_j(Q))}$$
$$+ C \sum_{j=10}^{\infty} (2^j l(Q))^{n/2} \|\mathcal{N}_h^* m\|_{L^2(S_j(Q))}. \tag{6.52}$$

The finite sum above is bounded by some constant in view of $L^2(\mathbb{R}^n)$ boundedness of $\mathcal{N}_h^*$ and (1.9) condition on molecules.

To handle the second sum in (6.52), we fix some number $0 < a < 1$ such that $n/2 - 2aM < 0$ and split $\mathcal{N}_h^* m$ according to whether $t \le c\, 2^{aj} l(Q)$ or $t \ge c\, 2^{aj} l(Q)$. Consider the former case first. Set

$$U_j(Q) := 2^{j+3} Q \backslash 2^{j-3} Q, \quad R_j(Q) := 2^{j+5} Q \backslash 2^{j-5} Q, \quad \text{and} \quad E_j(Q) =^c R_j(Q), \tag{6.53}$$

for every $j \ge 10$ and split $m = m\chi_{R_j(Q)} + m\chi_{E_j(Q)}$.

For $x \in S_j(Q)$, $|x-y|<t$ and $t \le c\,2^{aj}l(Q)$ we have $y \in U_j(Q)$. Moreover, $\mathrm{dist}(U_j(Q), E_j(Q)) \approx C2^j l(Q)$. Then the Gaffney estimates (Lemma 2.4) guarantee that for every such t, $y \in \mathbb{R}^n$, $a<1$ and $N \in \mathbb{N}$

$$\left(\frac{1}{t^n}\int_{|x-y|<t}\left|e^{-t^2L}(m\chi_{E_j(Q)})(x)\right|^2 dx\right)^{1/2}$$

$$\le \frac{C}{t^{n/2}}e^{-\frac{(2^j l(Q))^2}{ct^2}}\|m\|_{L^2(E_j(Q))} \le \frac{C}{t^{n/2}}\left(\frac{t}{2^j l(Q)}\right)^N \|m\|_{L^2(\mathbb{R}^n)}, \quad (6.54)$$

so that

$$\sum_{j=10}^{\infty}(2^j l(Q))^{n/2}\left\|\sup_{t\le c\,2^{aj}l(Q)}\left(\frac{1}{t^n}\int_{|x-\cdot|<t}\left|e^{-t^2L}(m\chi_{E_j(Q)})(x)\right|^2 dx\right)^{1/2}\right\|_{L^2(S_j(Q))}$$

$$\le \sum_{j=10}^{\infty}2^{j(1-a)(n/2-N)} \le C, \quad (6.55)$$

when $N>n/2$.

As for the contribution of $m\chi_{R_j(Q)}$, by L^2 boundedness of $\mathcal{N}_h^*$ we have

$$\sum_{j=10}^{\infty}(2^j l(Q))^{n/2}\|\mathcal{N}_h^*(m\chi_{R_j(Q)})\|_{L^2(S_j(Q))}$$

$$\le C\sum_{j=10}^{\infty}(2^j l(Q))^{n/2}\|m\chi_{R_j(Q)}\|_{L^2(R_j(Q))} \le C\sum_{j=10}^{\infty}2^{-j\varepsilon} \le C. \quad (6.56)$$

Now we consider the case $t \ge c\,2^{aj}l(Q)$. For every $y \in \mathbb{R}^n$

$$\sup_{t\ge c2^{aj}l(Q)}\left(\frac{1}{t^n}\int_{|x-y|<t}|e^{-t^2L}m(x)|^2 dx\right)^{1/2}$$

$$= \sup_{t\ge c\,2^{aj}l(Q)}\left(\frac{1}{t^n}\int_{|x-y|<t}\left|(t^{2M}L^M e^{-t^2L})(t^{-2M}L^{-M}m)(x)\right|^2 dx\right)^{1/2}$$

$$\le C2^{-2aMj}\mathcal{N}_h^{*,M}(l(Q)^{-2M}L^{-M}m)(y), \quad (6.57)$$

so we use the boundedness of $\mathcal{N}_h^{*,M}$ on $L^2(\mathbb{R}^n)$ to finish the argument. □

Corollary 6.4 *$H^1_L(\mathbb{R}^n) = H^1_{\mathcal{N}_h}(\mathbb{R}^n)$, in particular, $\|f\|_{H^1_L(\mathbb{R}^n)} \approx \|\mathcal{N}_h f\|_{L^1(\mathbb{R}^n)}$.*

Proof The right-to-the-left inclusion is a direct consequence of Theorems 4.1 and 6.1, the converse follows from Theorem 6.3 and Corollary 4.3. □

7 Characterization by the non-tangential maximal function associated to the Poisson semigroup

Theorem 7.1 *For every $f \in L^2(\mathbb{R}^n)$*

$$\|\widehat{S}_P f\|_{L^1(\mathbb{R}^n)} \leq C\|\mathcal{N}_P f\|_{L^1(\mathbb{R}^n)}, \tag{7.1}$$

where $\widehat{S}_P$ is the operator defined in (5.30).

Proof We follow the proof in [17] for the case of the Laplacian, and also the proof of our Theorem 6.1. More precisely, at the step corresponding to (6.11) we assign

$$u(y,t) := e^{-t\sqrt{L}} f(y), \quad t \in (0,\infty), \quad y \in \mathbb{R}^n. \tag{7.2}$$

The analogue of (6.13) and (6.14) can be obtained observing that $-\mathrm{div}_{y,t} B\nabla_{y,t} u = 0$, where as before B is the $(n+1)\times(n+1)$ block diagonal matrix with entries 1 and A and $\mathrm{div}_{y,t}$ is divergence in space and time variables. Concretely, we can write

$$\begin{aligned}
&\int\int_{\mathcal{R}^{\alpha\varepsilon,\alpha R,\frac{1}{\alpha}}(E^*)} t|\nabla_{y,t} u(y,t)|^2\,dydt \\
&\leq C\Re e \int\int_{\mathcal{R}^{\alpha\varepsilon,\alpha R,\frac{1}{\alpha}}(E^*)} \Big[-\mathrm{div}_{y,t}[tB(y)\nabla_{y,t} u(y,t)]\overline{u(y,t)} \\
&\quad - u(y,t)\overline{\mathrm{div}_{y,t}[tB(y)\nabla_{y,t} u(y,t)]}\Big]\,dydt \\
&\quad + C\Re e \int_{\mathcal{B}^{\alpha\varepsilon,\alpha R,\frac{1}{\alpha}}(E^*)} \Big[tB(y)\nabla_{y,t} u(y,t)\cdot \nu(y,t)\overline{u(y,t)} \\
&\quad + u(y,t)\nu(y,t)\cdot \overline{tB(y)\nabla_{y,t} u(y,t)}\Big]\,d\sigma_{y,t} \\
&\leq C\Re e \int\int_{\mathcal{R}^{\alpha\varepsilon,\alpha R,\frac{1}{\alpha}}(E^*)} \Big[-\partial_t u(y,t)\cdot\overline{u(y,t)} - u(y,t)\cdot\overline{\partial_t u(y,t)}\Big]\,dydt \\
&\quad + C\Re e \int_{\mathcal{B}^{\alpha\varepsilon,\alpha R,\frac{1}{\alpha}}(E^*)} \Big[tB(y)\nabla_{y,t} u(y,t)\cdot \nu(y,t)\overline{u(y,t)} \\
&\quad + u(y,t)\nu(y,t)\cdot \overline{tB(y)\nabla_{y,t} u(y,t)}\Big]\,d\sigma_{y,t},
\end{aligned}$$

so that (6.14) and (6.15) with $\nabla_{y,t}$ in place of space gradient holds.

The rest of the argument is essentially the same as the proof of Theorem 6.1, just employing elliptic instead of parabolic Caccioppoli inequality. □

To handle the converse to (7.1), we start with two auxiliary Lemmas.

Lemma 7.2 *Define*

$$\bar{g}_P f(x) := \left(\int_0^\infty \left| t\sqrt{L} e^{-t\sqrt{L}} f(x) \right|^2 \frac{dt}{t} \right)^{1/2}. \tag{7.3}$$

Then

$$\bar{g}_P f(x) \leq C g_h f(x), \quad x \in \mathbb{R}^n, \tag{7.4}$$

for every $f \in L^2(\mathbb{R}^n)$.

Proof By subordination formula (5.2) and Minkowski inequality

$$\begin{aligned} \bar{g}_P f(x) &= \left(\int_0^\infty \left| t\partial_t e^{-t\sqrt{L}} f(x) \right|^2 \frac{dt}{t} \right)^{1/2} \\ &\leq C \int_0^\infty \frac{e^{-u}}{\sqrt{u}} \left(\int_0^\infty \left| t\partial_t e^{-\frac{t^2 L}{4u}} f(x) \right|^2 \frac{dt}{t} \right)^{1/2} du. \end{aligned} \tag{7.5}$$

After the change of variables $t \mapsto s = \frac{t^2}{4u}$, $s \in (0, \infty)$, $\frac{dt}{t} = \frac{ds}{2s}$, the expression above can be written as

$$C \int_0^\infty \frac{e^{-u}}{\sqrt{u}} \left(\int_0^\infty |sLe^{-sL} f(x)|^2 \frac{ds}{s} \right)^{1/2} du \leq C g_h(x), \tag{7.6}$$

as desired. □

Lemma 7.3 *Define*

$$g_P^{\mathrm{aux}} f(x) := \left(\int_0^\infty \left| (e^{-t\sqrt{L}} - e^{-t^2 L}) f(x) \right|^2 \frac{dt}{t} \right)^{1/2}. \tag{7.7}$$

Then

$$g_P^{\mathrm{aux}} f(x) \leq C g_h f(x), \quad x \in \mathbb{R}^n, \tag{7.8}$$

for every $f \in L^2(\mathbb{R}^n)$.

Proof By the subordination formula (5.2)

$$g_P^{\text{aux}} f(x) = C \left(\int_0^\infty \left| \int_0^\infty \frac{e^{-u}}{\sqrt{u}} (e^{-\frac{t^2 L}{4u}} - e^{-t^2 L}) f(x)\, du \right|^2 \frac{dt}{t} \right)^{1/2}$$

$$= C \left(\int_0^\infty \left| \int_0^\infty \frac{e^{-u}}{\sqrt{u}} \int_t^{t/\sqrt{4u}} 2rLe^{-r^2 L} f(x)\, dr du \right|^2 \frac{dt}{t} \right)^{1/2}. \tag{7.9}$$

We now split the integral in u according to whether $u < 1/4$ or $u > 1/4$. In the first case,

$$\left| \int_0^{1/4} \frac{e^{-u}}{\sqrt{u}} \int_t^{t/\sqrt{4u}} 2rLe^{-r^2 L} f(x)\, dr du \right| \le \int_t^\infty \left| \int_0^{t^2/(4r^2)} \frac{e^{-u}}{\sqrt{u}}\, du \right| |2rLe^{-r^2 L} f(x)|\, dr$$

$$\le \int_t^\infty \left| tLe^{-r^2 L} f(x) \right| dr. \tag{7.10}$$

As for the second part,

$$\left| \int_{1/4}^\infty \frac{e^{-u}}{\sqrt{u}} \int_{t/\sqrt{4u}}^t 2rLe^{-r^2 L} f(x)\, dr du \right| = \int_0^t \left| \int_{t^2/(4r^2)}^\infty \frac{e^{-u}}{\sqrt{u}}\, du \right| |2rLe^{-r^2 L} f(x)|\, dr$$

$$\le C \int_0^t \left| (r^2/t)\, Le^{-r^2 L} f(x) \right| dr. \tag{7.11}$$

Inserting the results into (7.9), we get

$$g_P^{\text{aux}} f(x) \le C \left(\int_0^\infty t^2 \left(\int_t^\infty |rLe^{-r^2 L} f(x)| \frac{dr}{r} \right)^2 \frac{dt}{t} \right)^{1/2}$$

$$+ C \left(\int_0^\infty \frac{1}{t^2} \left(\int_0^t |r^2 Le^{-r^2 L} f(x)|\, dr \right)^2 \frac{dt}{t} \right)^{1/2}$$

$$\leq C\left(\int_0^\infty\int_t^\infty |rLe^{-r^2L}f(x)|^2\,dr\,dt\right)^{1/2}$$

$$+ C\left(\int_0^\infty\int_0^t |r^2Le^{-r^2L}f(x)|^2\,dr\frac{dt}{t^2}\right)^{1/2}$$

$$\leq C\left(\int_0^\infty |r^2Le^{-r^2L}f(x)|^2\,\frac{dr}{r}\right)^{1/2} = Cg_h f(x).$$

This finishes the argument. □

Theorem 7.4 *Let $\varepsilon > 0$ and $M > n/4$. Then for every representation $\sum_{i=0}^\infty \lambda_i m_i$, where $\{m_i\}_{i=0}^\infty$ is a family of $(2, \varepsilon, M)$-molecules and $\sum_{i=0}^\infty |\lambda_i| < \infty$, the series $\sum_{i=0}^\infty \lambda_i m_i$ converges in $H^1_{\mathcal{N}_P}(\mathbb{R}^n)$ and*

$$\left\|\sum_{i=0}^\infty \lambda_i m_i\right\|_{H^1_{\mathcal{N}_P}(\mathbb{R}^n)} \leq C\sum_{i=0}^\infty |\lambda_i|. \tag{7.12}$$

Proof Let $2 < p < \widetilde{p}_L$, $\epsilon > 0$, $M > \frac{n}{4}$. Similarly to Theorem 6.3, it is enough to prove that

$$\|\mathcal{N}_P^* m\|_{L^1(\mathbb{R}^n)} \leq C, \tag{7.13}$$

for every (p, ϵ, M)-molecule m, where

$$\mathcal{N}_P^* f(x) := \sup_{t>0}\left(\frac{1}{t^n}\int_{|x-y|<t}\left|e^{-t\sqrt{L}}f(y)\right|^2 dy\right)^{1/2}, \quad x\in\mathbb{R}^n, \quad f\in L^2(\mathbb{R}^n). \tag{7.14}$$

To this end, by the standard dyadic annular decomposition and Hölder's inequality, it will suffice to establish the estimate

$$\|\mathcal{N}_P^* m\|_{L^p(S_j(Q))} \leq C(2^j l(Q))^{n\left(\frac{1}{p}-1\right)}2^{-j\gamma}, \quad j\in\mathbb{N}\cup\{0\}, \tag{7.15}$$

where Q is a cube associated to the molecule m and γ is some fixed positive number.

Fix some a such that $n\left(\frac{n}{2}+2M\right)^{-1} < a < 1$. Then

$$\left\| \sup_{t \geq 2^{aj} l(Q)} \left(\frac{1}{t^n} \int_{|\cdot - y| < t} |e^{-t\sqrt{L}} m(y)|^2 dy \right)^{1/2} \right\|_{L^p(S_j(Q))}$$

$$= \left\| \sup_{t \geq 2^{aj} l(Q)} \left(\frac{l(Q)}{t} \right)^{2M} \left(\frac{1}{t^n} \int_{|\cdot - y| < t} \left| (t^2 L)^M e^{-t\sqrt{L}} (l(Q)^2 L)^{-M} m(y) \right|^2 dy \right)^{\frac{1}{2}} \right\|_{L^p(S_j(Q))}$$

$$\leq C \left(\frac{1}{2^{aj}} \right)^{2M} \left(\frac{1}{2^{aj} l(Q)} \right)^{n/2}$$

$$\times \left\| \sup_{t>0} \left(\int_{\mathbb{R}^n} |(t^2 L)^M e^{-t\sqrt{L}} (l(Q)^2 L)^{-M} m(y)|^2 dy \right)^{1/2} \right\|_{L^p(S_j(Q))} .$$

Resting on Lemma 5.1, one can prove that for $M > n/4$ the family of operators $(t^2 L)^M e^{-t\sqrt{L}}$ is uniformly bounded in $L^2(\mathbb{R}^n)$. Also,

$$\|(l(Q)^2 L)^{-M} m\|_{L^2(\mathbb{R}^n)} \leq C|Q|^{-1/2}, \quad j \in \mathbb{N}, \tag{7.16}$$

by the definition of molecule and Hölder's inequality. Then

$$\left\| \sup_{t \geq 2^{aj} l(Q)} \left(\frac{1}{t^n} \int_{|\cdot - y| < t} |e^{-t\sqrt{L}} m(y)|^2 dy \right)^{1/2} \right\|_{L^p(S_j(Q))}$$

$$\leq C 2^{aj(-2M-n/2)} 2^{jn/p} l(Q)^{n/p-n} = C(2^j l(Q))^{n\left(\frac{1}{p}-1\right)} 2^{-j\varepsilon_1}, \tag{7.17}$$

for $\varepsilon_1 = a(2M + n/2) - n > 0$ by the assumptions on a.

Turning to the case $t \leq 2^{aj} l(Q)$, we follow a suggestion of P. Auscher, and split

$$\sup_{t \leq 2^{aj} l(Q)} \left(\frac{1}{t^n} \int_{|x-y|<t} |e^{-t\sqrt{L}} m(y)|^2 dy \right)^{1/2}$$

$$\leq \sup_{t \leq 2^{aj} l(Q)} \left(\frac{1}{t^n} \int_{|x-y|<t} |(e^{-t\sqrt{L}} - e^{-t^2 L}) m(y)|^2 dy \right)^{1/2} + \mathcal{N}_h m(x). \tag{7.18}$$

We remark that Auscher has observed [2] that this splitting yields L^2 boundedness of $\mathcal{N}_P$; a similar idea has appeared previously in the work of Stein [26]. An argument similar to the proof of Theorem 6.3 shows that $\mathcal{N}_h m$ satisfies the desired estimate, so we will concentrate on the first term on the right hand side of (7.18). Observe that

$$
\begin{aligned}
&t\left|(e^{-t\sqrt{L}}-e^{-t^2L})m(y)\right|^2\\
&\quad=\left|\int_0^t \partial_s\left(s^{1/2}(e^{-s\sqrt{L}}-e^{-s^2L})m(y)\right)\,ds\right|^2\\
&\quad\leq\left|\int_0^t s^{1/2}\partial_s(e^{-s\sqrt{L}}-e^{-s^2L})m(y)\,ds+\frac{1}{2}\int_0^t s^{-1/2}(e^{-s\sqrt{L}}-e^{-s^2L})m(y)\,ds\right|^2\\
&\quad\leq Ct\left(\int_0^t \left|(e^{-s\sqrt{L}}-e^{-s^2L})m(y)\right|^2\,\frac{ds}{s}\right.\\
&\qquad\left.+\int_0^t\left|s\sqrt{L}e^{-s\sqrt{L}}m(y)\right|^2\frac{ds}{s}+\int_0^t\left|s^2Le^{-s^2L}m(y)\right|^2\frac{ds}{s}\right). \qquad (7.19)
\end{aligned}
$$

Given Lemmas 7.2 and 7.3, this allows to control the first term in (7.18) by

$$
\sup_{t\leq 2^{aj}l(Q)}\left(\frac{1}{t^n}\int_{|x-y|<t}\int_0^\infty |s^2Le^{-s^2L}m(y)|^2\,\frac{ds}{s}\,dy\right)^{1/2}, \quad x\in\mathbb{R}^n. \qquad (7.20)
$$

Much as for $t\geq 2^{aj}l(Q)$, we have

$$
\begin{aligned}
&\sup_{t\leq 2^{aj}l(Q)}\left(\frac{1}{t^n}\int_{|x-y|<t}\int_{2^{aj}l(Q)}^\infty \left|s^2Le^{-s^2L}m(y)\right|^2\,\frac{ds}{s}\,dy\right)^{1/2}\\
&\quad\leq\left(\mathcal{M}\left(\int_{2^{aj}l(Q)}^\infty\left(\frac{l(Q)}{s}\right)^{4M}\left|(s^2L)^Me^{-s^2L}(l(Q)^2L)^{-M}m(y)\right|^2\,\frac{ds}{s}\right)(x)\right)^{1/2},
\end{aligned} \qquad (7.21)
$$

where $\mathcal{M}$ denotes the Hardy–Littlewood maximal operator. Thus,

$$
\begin{aligned}
&\left\|\sup_{t\leq 2^{aj}l(Q)}\left(\frac{1}{t^n}\int_{|\cdot-y|<t}\int_{2^{aj}l(Q)}^\infty\left|s^2Le^{-s^2L}m(y)\right|^2\,\frac{ds}{s}\,dy\right)^{1/2}\right\|_{L^p(S_j(Q))}\\
&\quad\leq C\left(\int_{2^{aj}l(Q)}^\infty\left(\frac{l(Q)}{s}\right)^{4M}\left(\int_{\mathbb{R}^n}\left|(s^2L)^Me^{-s^2L}(l(Q)^2L)^{-M}m(x)\right|^p\,dx\right)^{2/p}\frac{ds}{s}\right)^{1/2}
\end{aligned}
$$

$$\leq C\left(\int_{2^{aj}l(Q)}^{\infty}\left(\frac{l(Q)}{s}\right)^{4M} s^{-2\left(\frac{n}{2}-\frac{n}{p}\right)}\frac{ds}{s}\right)^{1/2}\|(l(Q)^2L)^{-M}m\|_{L^2(\mathbb{R}^n)}$$

$$\leq C2^{aj(-2M-n/2+n/p)}l(Q)^{n\left(\frac{1}{p}-1\right)} = C(2^j l(Q))^{n\left(\frac{1}{p}-1\right)}2^{-j\varepsilon_2}, \tag{7.22}$$

where $\varepsilon_2 = a(2M+n/2)-n+(1-a)n/p > \varepsilon_1 > 0$ by our assumptions on a.

It remains to estimate

$$\left\|\sup_{t\leq 2^{aj}l(Q)}\left(\frac{1}{t^n}\int_{|\cdot-y|<t}\int_0^{2^{aj}l(Q)}\left|s^2Le^{-s^2L}m(y)\right|^2\frac{ds}{s}\,dy\right)^{1/2}\right\|_{L^p(S_j(Q))}. \tag{7.23}$$

Consider first the case $j\geq 10$. Observe that for $x\in S_j(Q)$, $j\geq 10$, and $|x-y|<t$ we have $y\in U_j(Q)$, a slightly fattened version of $S_j(Q)$ (see (6.53)). Then, in the notation of (6.53),

$$\left\|\sup_{t\leq 2^{aj}l(Q)}\left(\frac{1}{t^n}\int_{|\cdot-y|<t}\int_0^{2^{aj}l(Q)}|s^2Le^{-s^2L}(m\chi_{R_j(Q)})(y)|^2\frac{ds}{s}\,dy\right)^{1/2}\right\|_{L^p(S_j(Q))}$$

$$\leq C\left\|\left(\mathcal{M}\left(\int_0^{2^{aj}l(Q)}|s^2Le^{-s^2L}(m\chi_{R_j(Q)})|^2\frac{ds}{s}\right)\right)^{1/2}\right\|_{L^p(S_j(Q))}$$

$$\leq C\left\|g_h(m\chi_{R_j(Q)})\right\|_{L^p(\mathbb{R}^n)} \leq C\|m\|_{L^p(R_j(Q))} \leq C(2^jl(Q))^{n\left(\frac{1}{p}-1\right)}2^{-j\epsilon}, \tag{7.24}$$

where the next-to-the-last inequality follows from L^p-boundedness of g_h for $p_L < p < \widetilde{p}_L$ [3] and the last inequality follows from the definition of molecule. On the other hand,

$$\left\|\sup_{t\leq 2^{aj}l(Q)}\left(\frac{1}{t^n}\int_{|\cdot-y|<t}\int_0^{2^{aj}l(Q)}\left|s^2Le^{-s^2L}(m\chi_{E_j(Q)})(y)\right|^2\frac{ds}{s}\,dy\right)^{1/2}\right\|_{L^p(S_j(Q))}$$

$$\leq C\left\|\left(\mathcal{M}\left(\chi_{U_j(Q)}\int_0^{2^{aj}l(Q)}\left|s^2Le^{-s^2L}(m\chi_{E_j(Q)})\right|^2\frac{ds}{s}\right)\right)^{1/2}\right\|_{L^p(S_j(Q))}$$

$$\leq C\left(\int_0^{2^{aj}l(Q)}\left\|s^2Le^{-s^2L}(m\chi_{E_j(Q)})\right\|^2_{L^p(U_j(Q))}\frac{ds}{s}\right)^{1/2}\leq C2^{(a-1)jN}\|m\|_{L^p(\mathbb{R}^n)},$$

where N is any natural number and the last inequality follows from the Gaffney estimates. Clearly, we can take N large enough to bound the expression above by $C(2^jl(Q))^{n\left(\frac{1}{p}-1\right)}2^{-j\epsilon}$.

Finally, in the case $j\leq 10$ following (7.24) we show

$$\left\|\sup_{t\leq 2^{aj}l(Q)}\left(\frac{1}{t^n}\int_{|\cdot-y|<t}\int_0^{2^{aj}l(Q)}|s^2Le^{-s^2L}m(y)|^2\frac{ds}{s}\,dy\right)^{1/2}\right\|_{L^p(S_j(Q))}$$

$$\leq C\,\|g_hm\|_{L^p(\mathbb{R}^n)}\leq C\,\|m\|_{L^p(\mathbb{R}^n)}\leq Cl(Q)^{n\left(\frac{1}{p}-1\right)},\tag{7.25}$$

as desired.

Collecting all the terms, we arrive at (7.15) with $\gamma=\min\{\varepsilon_1,\epsilon\}$. □

Corollary 7.5 *$H^1_L(\mathbb{R}^n)=H^1_{\mathcal{N}_P}(\mathbb{R}^n)$, in particular, $\|f\|_{H^1_L(\mathbb{R}^n)}\approx\|\mathcal{N}_Pf\|_{L^1(\mathbb{R}^n)}$.*

Proof The Corollary follows from Theorems 7.1, 7.4 and 5.6. □

8 $BMO_L(\mathbb{R}^n)$: duality with Hardy spaces

We start with an auxiliary lemma that gives an equivalent characterization of $BMO_L(\mathbb{R}^n)$ using the resolvent in place of the heat semigroup. In the sequel we shall frequently use the characterization below as the definition of $BMO_L(\mathbb{R}^n)$ without additional comments. In addition, by the results of Sect. 4, we are at liberty to choose the molecular parameters $\varepsilon>0$ and $M>n/4$ at our convenience. In the sequel, we shall use this fact without further comment.

Lemma 8.1 *An element $f\in\cap_{\varepsilon>0}(\mathbf{M}_0^{2,\varepsilon,M}(L^*))^*\equiv(\mathbf{M}_0^{2,M}(L^*))^*$ belongs to $BMO_L(\mathbb{R}^n)$ if and only if*

$$\sup_{Q\subset\mathbb{R}^n}\left(\frac{1}{|Q|}\int_Q\left|(I-(1+l(Q)^2L)^{-1})^Mf(x)\right|^2dx\right)^{1/2}<\infty,\tag{8.1}$$

where $M>n/4$ and Q stands for a cube in $\mathbb{R}^n$.

Proof For brevity in this proof we shall distinguish (8.1) as $\|f\|_{BMO_L^{res}(\mathbb{R}^n)}$. In the rest of the paper both the norm based on the heat semigroup and the one based on the resolvent will be denoted by $\|f\|_{BMO_L(\mathbb{R}^n)}$.

Step I. Let us start with the "$\leq$" inequality. To this end, we split

$$f = \Big(I - (1 + l(Q)^2 L)^{-1}\Big)^M f + \Big[I - \Big(I - (1 + l(Q)^2 L)^{-1}\Big)^M\Big] f. \quad (8.2)$$

For every $Q \subset \mathbb{R}^n$

$$\begin{aligned}
&\left(\frac{1}{|Q|} \int_Q \Big| (I - e^{-l(Q)^2 L})^M (I - (1 + l(Q)^2 L)^{-1})^M f(x) \Big|^2 \, dx \right)^{1/2} \\
&\leq C \sum_{k=0}^{M} \sum_{j=0}^{\infty} \left(\frac{1}{|Q|} \int_Q \Big| e^{-kl(Q)^2 L} \Big[\chi_{S_j(Q)} (I - (1 + l(Q)^2 L)^{-1})^M f \Big](x) \Big|^2 \, dx \right)^{1/2} \\
&\leq C \|f\|_{BMO_L^{res}(\mathbb{R}^n)} \\
&\quad + C \sum_{j=2}^{\infty} e^{-\frac{(2^j l(Q))^2}{cl(Q)^2}} \left(\frac{1}{|Q|} \int_{S_j(Q)} \Big| (I - (1 + l(Q)^2 L)^{-1})^M f(x) \Big|^2 \, dx \right)^{1/2}, \quad (8.3)
\end{aligned}$$

where we used Lemmas 2.3, 2.4 for the second inequality. Now one can cover $S_j(Q)$ by approximately 2^{jn} cubes of the sidelength $l(Q)$, this allows to bound the second term in the expression above by

$$C \sum_{j=2}^{\infty} e^{-c\, 2^{2j}} 2^{jn/2} \, \|f\|_{BMO_L^{\mathrm{res}}(\mathbb{R}^n)} \leq C \|f\|_{BMO_L^{\mathrm{res}}(\mathbb{R}^n)}, \quad (8.4)$$

as desired.

As for the remaining term, observe that

$$\begin{aligned}
\frac{I - (I - (1 + l(Q)^2 L)^{-1})^M}{(I - (1 + l(Q)^2 L)^{-1})^M} &= \Big(I - (1 + l(Q)^2 L)^{-1}\Big)^{-M} - I \\
&= \left(\frac{1 + l(Q)^2 L}{l(Q)^2 L} \right)^M - I \\
&= \Big(1 + (l(Q)^2 L)^{-1}\Big)^M - I \\
&= \sum_{k=1}^{M} \frac{M!}{(M-k)!\, k!} \, (l(Q)^2 L)^{-k}, \quad (8.5)
\end{aligned}$$

and therefore,

$$\left(\frac{1}{|Q|}\int_Q \left|(I-e^{-l(Q)^2L})^M[I-(I-(1+l(Q)^2L)^{-1})^M]f(x)\right|^2 dx\right)^{1/2}$$

$$\leq C\sum_{k=1}^M \left(\frac{1}{|Q|}\int_Q \left|(I-e^{-l(Q)^2L})^{M-k}\left(-\int_0^{l(Q)}\partial_\tau e^{-\tau^2L}\,d\tau\right)^k (l(Q)^2L)^{-k}\right.\right.$$

$$\left.\left.\times(I-(1+l(Q)^2L)^{-1})^M f(x)\right|^2 dx\right)^{1/2}$$

$$\leq C\sum_{k=1}^M \left(\frac{1}{|Q|}\int_Q \left|(I-e^{-l(Q)^2L})^{M-k}\left(\int_0^{l(Q)}\frac{\tau}{l(Q)^2}e^{-\tau^2L}\,d\tau\right)^k\right.\right.$$

$$\left.\left.\times(I-(1+l(Q)^2L)^{-1})^M f(x)\right|^2 dx\right)^{1/2}. \tag{8.6}$$

Having this at hand, we obtain the required estimate changing the order of integration above and using the annular decomposition and Gaffney estimates, much as in (8.3) and (8.4).

Step II. Let us now consider the "$\geq$" part of (8.1). For every $x\in\mathbb{R}^n$

$$f(x)=2^M\left(l(Q)^{-2}\int_{l(Q)}^{\sqrt{2}l(Q)}s\,ds\right)^M f(x)$$

$$=2^M\,l(Q)^{-2}\int_{l(Q)}^{\sqrt{2}l(Q)}s_1(I-e^{-s_1^2L})^M\,ds_1\left(l(Q)^{-2}\int_{l(Q)}^{\sqrt{2}l(Q)}s\,ds\right)^{M-1}f(x)$$

$$+\sum_{k=1}^M C_{k,M}l(Q)^{-2}\int_{l(Q)}^{\sqrt{2}l(Q)}s_1e^{-ks_1^2L}\,ds_1\left(l(Q)^{-2}\int_{l(Q)}^{\sqrt{2}l(Q)}s\,ds\right)^{M-1}f(x), \tag{8.7}$$

where $C_{k,M}\in\mathbb{R}$ are some constants depending on k and M only. However, $\partial_s e^{-ks^2L}=-2kLse^{-ks^2L}$ and therefore,

$$2kL \int_{l(Q)}^{\sqrt{2}l(Q)} se^{-ks^2L}\,ds = e^{-kl(Q)^2L} - e^{-2kl(Q)^2L}$$
$$= e^{-kl(Q)^2L}(I - e^{-kl(Q)^2L})$$
$$= e^{-kl(Q)^2L}(I - e^{-l(Q)^2L})\sum_{i=0}^{k-1} e^{-il(Q)^2L}. \tag{8.8}$$

Applying the procedure outlined in (8.7) and (8.8) M times, we arrive at the following formula

$$f(x) = \sum_{i=1}^{(M+1)^M} l(Q)^{-2M}L^{-N_i}\prod_{k=1}^{M} C(i,k,M)\,p_{i,k}f(x), \tag{8.9}$$

where $0 \le N_i \le M$ and for all i, k as above either

$$p_{i,k} = \int_{l(Q)}^{\sqrt{2}l(Q)} s(I - e^{-s^2L})^M\,ds \tag{8.10}$$

or $p_{i,k}$ is of the form (8.8).

Fix some $Q \subset \mathbb{R}^n$ and $x \in Q$ and consider $(I - (1 + l(Q)^2L)^{-1})^M f(x)$ with f represented in the form (8.9). The negative powers of L can be handled writing

$$\Big(I - (1 + l(Q)^2L)^{-1}\Big)^{N_i} l(Q)^{-2N_i}L^{-N_i} = \Big(1 + l(Q)^2L\Big)^{-N_i}. \tag{8.11}$$

Then the new expression for $(I - (1 + l(Q)^2L)^{-1})^M f(x)$ is a linear combination of terms, with the property that each term contains

$$\text{either}\quad l(Q)^{-2}\int_{l(Q)}^{\sqrt{2}l(Q)} s(I - e^{-s^2L})^M\,ds \quad\text{or}\quad (I - e^{-l(Q)^2L})^M, \tag{8.12}$$

and a finite number of factors (almost) in the form of resolvent or heat semigroup corresponding to $t \approx l(Q)$. One can now build an argument similar to Step I, (8.3) and (8.4), using dyadic annular decomposition and Gaffney estimates, to single out $(I - e^{-l(Q)^2L})^M$ or $(I - e^{-s^2L})^M$, $s \approx l(Q)$, and obtain the desired estimate. We leave the details to the interested reader. □

Theorem 8.2 *Let $f \in BMO_{L^*}(\mathbb{R}^n)$ for some $M \in \mathbb{N}$. Then the linear functional given by*

$$l(g) = \langle f, g\rangle, \tag{8.13}$$

initially defined on the dense subspace of finite linear combinations of $(2, \varepsilon, M)$*-molecules,* $\varepsilon > 0$*, via the pairing of* $\mathbf{M}_0^{2,\varepsilon,M}$ *with its dual, has a unique bounded extention to* $H_L^1(\mathbb{R}^n)$ *with*

$$\|l\| \leq C\|f\|_{BMO_{L^*}(\mathbb{R}^n)}. \tag{8.14}$$

Proof Let us prove first that for every $(2, \varepsilon, M)$-molecule m

$$|\langle f, m\rangle| \leq C\|f\|_{BMO_{L^*}(\mathbb{R}^n)}. \tag{8.15}$$

By definition, $f \in (\mathbf{M}_0^{2,M}(L))^*$, so in particular $(I - (1 + l(Q)^2L^*)^{-1})^M f \in L^2_{\text{loc}}$ (see the discussion preceding (1.21)). Thus, we may write

$$\begin{aligned}\langle f, m\rangle &= \int_{\mathbb{R}^n} \left(I - (1 + l(Q)^2L^*)^{-1}\right)^M f(x)\overline{m(x)}\,dx \\ &\quad + \left\langle \left[I - (I - (1 + l(Q)^2L^*)^{-1})^M\right] f, m\right\rangle \\ &=: I_1 + I_2,\end{aligned} \tag{8.16}$$

where Q is the cube associated to m. Then

$$\begin{aligned}|I_1| &\leq \sum_{j=0}^{\infty} \left(\int_{S_j(Q)} \left|(I - (1 + l(Q)^2L^*)^{-1})^M f(x)\right|^2 dx\right)^{1/2} \\ &\quad \times \left(\int_{S_j(Q)} |m(x)|^2\,dx\right)^{1/2} \\ &\leq \sum_{j=0}^{\infty} 2^{-j\varepsilon}\left(\frac{1}{(2^j l(Q))^n}\int_{S_j(Q)} \left|(I - (1 + l(Q)^2L^*)^{-1})^M f(x)\right|^2 dx\right)^{1/2} \\ &\leq C\|f\|_{BMO_{L^*}(\mathbb{R}^n)},\end{aligned} \tag{8.17}$$

where we used (1.9) for the second inequality, and the third one follows by covering $S_j(Q)$ by $C2^{jn}$ cubes of the sidelength $l(Q)$. □

To analyze I_2 recall (8.5) (with L^* in place of L), and write

$$|I_2| \le C \sum_{k=1}^{M} \left| \int_{\mathbb{R}^n} (I - (1 + l(Q)^2 L^*)^{-1})^M f(x) \, \overline{(l(Q)^2 L)^{-k} m(x)} \, dx \right|$$

$$\le C \sum_{k=1}^{M} \sum_{j=0}^{\infty} \left(\int_{S_j(Q)} \left| (I - (1 + l(Q)^2 L^*)^{-1})^M f(x) \right|^2 dx \right)^{1/2}$$

$$\times \left(\int_{S_j(Q)} |(l(Q)^2 L)^{-k} m(x)|^2 \, dx \right)^{1/2}. \tag{8.18}$$

We finish as in (8.17) using (1.10). Thus, (8.15) is now established.

Having at hand (8.15), our goal is to show that for every $N \in \mathbb{N}$ and for every $g = \sum_{j=0}^{N} \lambda_j m_j$, where $\{m_j\}_{j=0}^{N}$ are $(2, \varepsilon, M')$-molecules, and $M' > n/4$ is chosen large enough relative to M, we have

$$|\langle f, g \rangle| \le C \|g\|_{H^1_L(\mathbb{R}^n)} \|f\|_{BMO_{L^*}(\mathbb{R}^n)}. \tag{8.19}$$

Since the space of finite linear combinations of $(2, \varepsilon, M')$-molecules is dense in $H^1_L(\mathbb{R}^n)$, the linear functional l will then have a unique bounded extension to $H^1_L(\mathbb{R}^n)$ defined in a standard fashion by continuity. We point out that this extension by continuity depends on having a bound in terms of $\|g\|_{H^1_L(\mathbb{R}^n)}$ in (8.19), as opposed to $\sum_{j=0}^{N} |\lambda_j|$. The latter bound is immediately obtainable from (8.15) (since in particular, a $(2, \varepsilon, M')$-molecule is a $(2, \varepsilon, M)$-molecule whenever $M' \ge M$), but may be much larger than the H^1_L norm. To obtain the sharper bound (8.19) will be somewhat delicate. In the classical setting, the same issue arises, but may be handled in a fairly routine fashion by truncating the BMO function so that it may be approximated in $(H^1)^*$ by bounded functions (see, e.g. [25, pp. 142–143]). This avenue is not available to us, as we cannot expect that any L^∞ truncation will interact well with our operator L. Instead, we should seek a "truncation" in L^p, $p \in (p_L, \widetilde{p}_L)$. In fact, approximating by L^2 functions will be most convenient, and this is what we shall do. We note that it is to deal with this difficulty that we have been forced to introduce the equivalent norm $\| \cdot \|_{\widetilde{H}^1_L}$. The reason for our doing so will become apparent in the sequel.

We shall require some rather extensive preliminaries. In particular, we shall use the "tent space" approach of Coifman–Meyer–Stein [12]. Let us now recall the basic theory.

For some $F : \mathbb{R}^{n+1}_+ \to \mathbb{C}$, $\mathbb{R}^{n+1}_+ = \mathbb{R}^n \times (0,\infty)$, consider the square function $SF := S^1 F$, where $S^\alpha F$, $\alpha > 0$, was defined in (2.6) and

$$CF(x) := \sup_{B:\, x\in B} \left(\frac{1}{|B|} \iint_{\widehat{B}} |F(y,t)|^2 \, \frac{dydt}{t} \right)^{1/2}, \quad x \in \mathbb{R}^n, \tag{8.20}$$

where B stands for a ball in $\mathbb{R}^n$ and

$$\widehat{B} := \{(x,t) \in \mathbb{R}^n \times (0,\infty) :\ \mathrm{dist}(x, {}^cB) \geq t\}, \tag{8.21}$$

is the tent region above ball B. Define the tent spaces

$$\begin{aligned} T^1(\mathbb{R}^{n+1}_+) &:= \{F : \mathbb{R}^{n+1}_+ \longrightarrow \mathbb{C}; \\ &\quad \|F\|_{T^1(\mathbb{R}^{n+1}_+)} := \|SF\|_{L^1(\mathbb{R}^n)} < \infty\}, \end{aligned} \tag{8.22}$$

and

$$\begin{aligned} T^\infty(\mathbb{R}^{n+1}_+) &:= \{F : \mathbb{R}^{n+1}_+ \longrightarrow \mathbb{C}; \\ &\quad \|F\|_{T^\infty(\mathbb{R}^{n+1}_+)} := \|CF\|_{L^\infty(\mathbb{R}^n)} < \infty\}, \end{aligned} \tag{8.23}$$

and recall from [12] that $(T^1(\mathbb{R}^{n+1}_+))^* = T^\infty(\mathbb{R}^{n+1}_+)$.

We now prove the following analogue of a classical estimate of [17].

Lemma 8.3 *The operator*

$$f \mapsto C\left((t^2L)^M e^{-t^2L} f\right)$$

maps $BMO_L(\mathbb{R}^n) \to T^\infty(\mathbb{R}^{n+1}_+)$; i.e.,

$$\begin{aligned} &\sup_B \left(\frac{1}{|B|} \iint_{\widehat{B}} \left|(t^2L)^M e^{-t^2L} f(x)\right|^2 \, \frac{dxdt}{t} \right)^{1/2} \\ &\quad \leq C\|f\|_{BMO_L(\mathbb{R}^n)}. \end{aligned}$$

Proof For every cube $Q \subset \mathbb{R}^n$

$$\left(\frac{1}{|Q|}\int_0^{l(Q)}\int_Q \left|(t^2L)^M e^{-t^2L} f(y)\right|^2 \frac{dydt}{t}\right)^{1/2}$$

$$= \left(\frac{1}{|Q|}\int_0^{l(Q)}\int_Q \left|(t^2L)^M e^{-t^2L}(I-(1+l(Q)^2L)^{-1})^M f(y)\right|^2 \frac{dydt}{t}\right)^{1/2}$$

$$+ \left(\frac{1}{|Q|}\int_0^{l(Q)}\int_Q \left|(t^2L)^M e^{-t^2L}\left[I-(I-(1+l(Q)^2L)^{-1})^M\right] f(y)\right|^2 \frac{dydt}{t}\right)^{1/2}$$

$$=: I_1 + I_2. \tag{8.24}$$

Then

$$I_1 \le \sum_{j=0}^{\infty}\left(\frac{1}{|Q|}\int_0^{l(Q)}\int_Q \left|(t^2L)^M e^{-t^2L}\left[\chi_{S_j(Q)}(I-(1+l(Q)^2L)^{-1})^M f\right](y)\right|^2 \frac{dydt}{t}\right)^{1/2}$$

$$\le \frac{1}{|Q|^{1/2}}\left\|g_h^M\left(\chi_{2Q}(I-(1+l(Q)^2L)^{-1})^M f\right)\right\|_{L^2(\mathbb{R}^n)}$$

$$+ \sum_{j=2}^{\infty}\frac{C}{|Q|^{1/2}}\left(\int_0^{l(Q)} e^{-\frac{(2^j l(Q))^2}{ct^2}}\frac{dt}{t}\right)^{1/2}\left\|(I-(1+l(Q)^2L)^{-1})^M f\right\|_{L^2(S_j(Q))}, \tag{8.25}$$

where

$$g_h^M f(x) := \left(\int_0^{\infty}|(t^2L)^M e^{-t^2L} f(x)|^2 \frac{dt}{t}\right)^{1/2}, \quad M \in \mathbb{N}, \quad x \in \mathbb{R}^n, \tag{8.26}$$

is bounded in $L^2(\mathbb{R}^n)$ according to [1]. Therefore, for every $N \in \mathbb{N}$

$$I_1 \le \frac{C}{|Q|^{1/2}}\left\|(I-(1+l(Q)^2L)^{-1})^M f\right\|_{L^2(2Q)}$$

$$+ \sum_{j=2}^{\infty} 2^{-jN}\frac{C}{(2^j l(Q))^{n/2}}\left\|(I-(1+l(Q)^2L)^{-1})^M f\right\|_{L^2(S_j(Q))}$$

$$\le C\|f\|_{BMO_L(\mathbb{R}^n)}. \tag{8.27}$$

To estimate I_2 we use (8.5) and write

$$I_2 \leq C \sup_{1\leq k\leq M} \left(\frac{1}{|Q|} \int_0^{l(Q)} \int_Q \left| (t^2L)^M e^{-t^2L} (l(Q)^2L)^{-k} (I-(1+l(Q)^2L)^{-1})^M f(y) \right|^2 \frac{dydt}{t} \right)^{1/2}$$

$$\leq C \sup_{1\leq k\leq M} \left(\frac{1}{|Q|} \int_0^{l(Q)} \left(\frac{t}{l(Q)} \right)^{2k} \int_Q \left| (t^2L)^{M-k} e^{-t^2L} (I-(1+l(Q)^2L)^{-1})^M f(y) \right|^2 \frac{dydt}{t} \right)^{1/2},$$

the rest of the argument is similar to (8.25)–(8.27). This finishes the proof of Lemma 8.3. □

We shall also require an extension of the "Calderón reproducing formula":

Lemma 8.4 *Suppose that $f \in (\mathbf{M}_0^{2,M}(L))^*$ satisfies the "controlled growth estimate"*

$$\int_{\mathbb{R}^n} \frac{|(I-(1+L^*)^{-1})^M f(x)|^2}{1+|x|^{n+\varepsilon_1}}\, dx < \infty, \tag{8.28}$$

for some $\varepsilon_1 > 0$ (in particular, this holds trivially for every $\varepsilon_1 > 0$ if $f \in BMO_{L^*}$). Then for every $g \in H^1_L$ that can be represented as a finite linear combination of $(2, \varepsilon, M')$ molecules, with ε, M' sufficiently large compared to ε_1, M, we have

$$\langle f, g\rangle = C_M \iint_{\mathbb{R}^{n+1}_+} (t^2L^*)^M e^{-t^2L^*} f(x)\, \overline{t^2Le^{-t^2L}g(x)}\, \frac{dtdx}{t}. \tag{8.29}$$

Proof For $\delta, R > 0$ consider

$$\begin{aligned} &\int_{\mathbb{R}^n} \int_\delta^R (t^2L^*)^M e^{-t^2L^*} f(x)\, \overline{t^2Le^{-t^2L}g(x)}\, \frac{dtdx}{t} \\ &= \left\langle f, \left(\int_\delta^R \left(t^2L\right)^{M+1} e^{-2t^2L} g\, \frac{dt}{t} \right) \right\rangle \\ &= C_M^{-1} \langle f, g\rangle - \left\langle f, \left(C_M^{-1} g - \int_\delta^R \left(t^2L\right)^{M+1} e^{-2t^2L} g\, \frac{dt}{t} \right) \right\rangle. \end{aligned} \tag{8.30}$$

We will now write f in the following way

$$\begin{aligned} f &= \left(I-(1+L^*)^{-1}+(1+L^*)^{-1}\right)^M f \\ &= \sum_{k=0}^{M} \frac{M!}{(M-k)!\,k!}\left(I-(1+L^*)^{-1}\right)^{M-k}(1+L^*)^{-k} f \\ &= \sum_{k=0}^{M} \frac{M!}{(M-k)!\,k!}(L^*)^{-k}\left(I-(1+L^*)^{-1}\right)^{M} f \end{aligned} \tag{8.31}$$

Thus, the last expression in (8.30) equals $\sum_{k=0}^{M} C_{k,M}$ times

$$\begin{aligned} &\left\langle (I-(1+L^*)^{-1})^M f, \left(C_M^{-1}L^{-k}g-\int_\delta^R \left(t^2L\right)^{M+1} e^{-2t^2L}L^{-k}g\,\frac{dt}{t}\right)\right\rangle \\ &= \left\langle (I-(1+L^*)^{-1})^M f, \int_0^\delta \left(t^2L\right)^{M+1} e^{-2t^2L}L^{-k}g\,\frac{dt}{t}\right\rangle \\ &\quad+\left\langle (I-(1+L^*)^{-1})^M f, \int_R^\infty \left(t^2L\right)^{M+1} e^{-2t^2L}L^{-k}g\,\frac{dt}{t}\right\rangle, \end{aligned} \tag{8.32}$$

since for $L^{-k}g \in L^2(\mathbb{R}^n)$ the Calderón reproducing formula is valid. The last term in (8.32) is bounded by a constant times

$$\begin{aligned} &\left(\int_{\mathbb{R}^n} \frac{|(I-(1+L^*)^{-1})^M f(x)|^2}{1+|x|^{n+\varepsilon_1}}\,dx\right)^{1/2} \\ &\times \sup_{0\le k\le M}\left(\int_{\mathbb{R}^n}\left|\int_R^\infty \left(t^2L\right)^{M+1} e^{-2t^2L}L^{-k}g(x)\,\frac{dt}{t}\right|^2 (1+|x|^{n+\varepsilon_1})\,dx\right)^{1/2} \\ &\le C\Upsilon \sup_{0\le k\le M}\sum_{j=0}^{\infty} 2^{j(n+\varepsilon_1)/2}\left(\int_{S_j(Q_0)}\left|\int_R^\infty \left(t^2L\right)^{M+1} e^{-2t^2L}L^{-k}g(x)\,\frac{dt}{t}\right|^2 dx\right)^{1/2} \\ &\le C\Upsilon \sup_{0\le k\le M}\sum_{j=0}^{\infty} 2^{j(n+\varepsilon_1)/2} \\ &\quad\times\int_R^\infty \left\|\left(t^2L\right)^{M+M'-k+1} e^{-2t^2L}L^{-M'}g\right\|_{L^2(S_j(Q_0))}\frac{dt}{t^{2(M'-k)+1}}, \end{aligned} \tag{8.33}$$

where Υ is the finite quantity defined in (8.28), and Q_0 is the cube centered at 0 with the sidelength 1. Then the expression under the sup sign above is bounded modulo multiplicative constant by

$$\int_R^\infty \left\| \left(t^2 L\right)^{M+M'-k+1} e^{-2t^2 L} L^{-M'} g \right\|_{L^2(4Q_0)} \frac{dt}{t^{2(M'-k)+1}}$$
$$+ \sum_{j=3}^\infty 2^{j(n+\varepsilon_1)/2} \int_R^\infty \left\| \left(t^2 L\right)^{M+M'-k+1} e^{-2t^2 L} \left[\chi_{\mathbb{R}^n \setminus 2^{j-2} Q_0} L^{-M'} g \right] \right\|_{L^2(S_j(Q_0))} \frac{dt}{t^{2(M'-k)+1}}$$
$$+ \sum_{j=3}^\infty 2^{j(n+\varepsilon_1)/2} \int_R^\infty \left\| \left(t^2 L\right)^{M+M'-k+1} e^{-2t^2 L} \left[\chi_{2^{j-2} Q_0} L^{-M'} g \right] \right\|_{L^2(S_j(Q_0))} \frac{dt}{t^{2(M'-k)+1}}$$
$$\leq \frac{C}{R^{2(M'-k)}} \left\| L^{-M'} g \right\|_{L^2(\mathbb{R}^n)} + \frac{C}{R^{2(M'-k)}} \sum_{j=3}^\infty 2^{j(n+\varepsilon_1)/2} \left\| L^{-M'} g \right\|_{L^2(\mathbb{R}^n \setminus 2^{j-2} Q_0)}$$
$$+ \sum_{j=3}^\infty 2^{j(n+\varepsilon_1)/2} \left(\int_R^\infty e^{-\frac{2^{2j}}{ct^2}} \frac{dt}{t^{2(M'-k)+1}} \right) \left\| L^{-M'} g \right\|_{L^2(\mathbb{R}^n)}. \tag{8.34}$$

However,

$$\int_R^\infty e^{-\frac{2^{2j}}{ct^2}} \frac{dt}{t^{2(M'-k)+1}} \leq C \frac{1}{2^{2(M'-k)j}} \int_{R/2^j}^\infty e^{-\frac{1}{s^2}} \frac{ds}{s^{2(M'-k)+1}} \leq C \frac{1}{2^{2(M'-k)j}} (2^j/R)^{\epsilon'} \tag{8.35}$$

for every $\epsilon' > 0$. Also, g is a finite linear combination of $(2, \varepsilon, M')$- molecules, therefore for large j

$$\left\| L^{-k'} g \right\|_{L^2(S^j(Q_0))} \leq C 2^{-j(n/2+\varepsilon)}, \quad 0 \leq k' \leq M', \tag{8.36}$$

which allows to estimate the second term in (8.34). Without loss of generality we can assume that $\varepsilon > \varepsilon_1/2$ and $M' > \frac{n+\varepsilon_1}{4} + M$. Then there exists $\epsilon_0 > 0$ such that the quantity in (8.34), and hence the one in (8.33), does not exceed C/R^{ϵ_0}.

We now turn to the integral over $(0, \delta)$. For convenience of notation, we set

$$\tilde{f} \equiv \left(I - (1 + L^*)^{-1}\right)^M f.$$

Since $-2tLe^{-t^2L} = \partial_t e^{-t^2L}$, we may write

$$\left|\left\langle \tilde{f}, \int_0^\delta \left(t^2L\right)^{M+1} e^{-2t^2L} L^{-k} g(x)\,\frac{dt}{t}\right\rangle\right| = C\left|\left\langle \tilde{f}, \int_0^\delta \left(t^2L\right)^{M} \partial_t e^{-2t^2L} L^{-k} g(x) dt\right\rangle\right|$$
$$\leq C\left|\left\langle \tilde{f}, \int_0^\delta \left(t^2L\right)^{M} e^{-2t^2L} L^{-k} g(x)\,\frac{dt}{t}\right\rangle\right| + C\left|\left\langle \tilde{f}, \left(\delta^2L\right)^{M} e^{-2\delta^2L} L^{-k} g(x)\right\rangle\right|$$
$$\leq C\sum_{k=1}^{M}\left|\left\langle \tilde{f}, \left(\delta^2L\right)^{k} e^{-2\delta^2L} L^{-k} g(x)\right\rangle\right| + C\left|\left\langle \tilde{f}, \left(e^{-2\delta^2L} - I\right) L^{-k} g(x)\right\rangle\right|,$$

repeatedly integrating by parts in t. Therefore, as in (8.33),

$$\left|\left\langle \tilde{f}, \int_0^\delta \left(t^2L\right)^{M+1} e^{-2t^2L} L^{-k} g(x)\,\frac{dt}{t}\right\rangle\right|$$
$$\leq C\Upsilon \sup_{0\leq k'\leq M}\sum_{k=1}^{M}\sum_{j=0}^{\infty} 2^{j(n+\varepsilon_1)/2}\left\|\left(\delta^2L\right)^{k} e^{-2\delta^2L} L^{-k'} g\right\|_{L^2(S_j(Q_0))}$$
$$+ C\Upsilon \sup_{0\leq k'\leq M}\sum_{j=0}^{\infty} 2^{j(n+\varepsilon_1)/2}\left\|\left(e^{-2\delta^2L} - I\right) L^{-k'} g\right\|_{L^2(S_j(Q_0))}. \tag{8.37}$$

Now let us split $L^{-k'}g = \chi_{R_j} L^{-k'} g + \chi_{{}^cR_j} L^{-k'} g$ where

$$R_j = 2^{j+2}Q_0, \quad \text{if } j = 0, 1, 2,$$
$$R_j = 2^{j+2}Q_0 \backslash 2^{j-2}Q_0, \quad \text{if } j = 3, 4, \ldots,$$

and start with the part of (8.37) corresponding to $\chi_{R_j} L^{-k'} g$. Fix some $\eta > 0$. Then for $N \in \mathbb{N}$ and for all $0 \leq k' \leq M$

$$C\sum_{k=1}^{M}\sum_{j=N}^{\infty} 2^{j(n+\varepsilon_1)/2}\Bigg(\left\|\left(\delta^2L\right)^{k} e^{-2\delta^2L}(\chi_{R_j} L^{-k'} g)\right\|_{L^2(S_j(Q_0))}$$
$$+ \left\|\left(e^{-2\delta^2L} - I\right)(\chi_{R_j} L^{-k'} g)\right\|_{L^2(S_j(Q_0))}\Bigg) \tag{8.38}$$
$$\leq C\sum_{j=N}^{\infty} 2^{j(n+\varepsilon_1)/2}\|L^{-k'}g\|_{L^2(R_j)} \leq C\sum_{j=N}^{\infty} 2^{j(n+\varepsilon_1)/2} 2^{-j(n/2+\varepsilon)}, \tag{8.39}$$

where the last inequality uses (8.36). Recall that $\varepsilon > \varepsilon_1/2$. Then choosing $N \approx -\ln\eta$, we can control the expression above by η. As for the remaining part, for δ small enough

$$C\sum_{k=1}^{M}\sum_{j=0}^{N} 2^{j(n+\varepsilon_1)/2}\left(\left\|\left(\delta^2 L\right)^k e^{-2\delta^2 L}(\chi_{R_j}L^{-k'}g)\right\|_{L^2(S_j(Q_0))}\right.$$
$$\left.+\left\|\left(e^{-2\delta^2 L}-I\right)(\chi_{R_j}L^{-k'}g)\right\|_{L^2(S_j(Q_0))}\right)\leq C\eta \tag{8.40}$$

using that $\left(\delta^2 L\right)^k e^{-2\delta^2 L}\to 0$ and $e^{-2\delta^2 L}-I\to 0$ in the strong operator topology as $\delta\to 0$.

The integral corresponding to $\chi_{{}^cR_j}L^{-k'}g$ is analyzed similarly, with the only difference that the Gaffney estimates instead of L^2-decay of $L^{-k'}g$ are used to control an analogue of (8.39).

We have proved that the second term in (8.30) vanishes as $\delta\to 0$ and $R\to\infty$. Therefore, the formula (8.29) is justified for every g belonging to the space of finite linear combinations of molecules. $\square$

We return now to the proof of (8.19). We shall approximate f by

$$f_K \equiv \int_{1/K}^{K} t^2L^*e^{-t^2L^*}\left(\chi_{B_K}(t^2L^*)^M e^{-t^2L^*}f\right)\frac{dt}{t},$$

where $B_K\equiv\{x\in\mathbb{R}^n : |x|<K\}$. We claim that $f_K\in L^2$, and that

$$\sup_K \|f_K\|_{BMO_{L^*}(\mathbb{R}^n)}\leq C\left\|(t^2L^*)^M e^{-t^2L^*}f\right\|_{T^\infty(\mathbb{R}^{n+1}_+)}\leq C\|f\|_{BMO_{L^*}(\mathbb{R}^n)}. \tag{8.41}$$

We note that the second inequality in (8.41) is just Lemma 8.3, so the key issue is the first inequality. Let us take the claim for granted momentarily. Since g is a finite linear combination of $(2,\varepsilon,M')$-molecules, in particular we have that$g\in\widehat{H}^1_L$. Consequently, there is a $\delta>0$ and a δ-representation $g=\sum\lambda_i m_i$, converging in L^2, with $\sum|\lambda_i|\approx\|g\|_{\widehat{H}^1_L}\approx\|g\|_{H^1_L}$ (by (3.3)). Thus, for $f_K\in L^2$, we have that

$$|\langle f_K,g\rangle| = \left|\sum\lambda_i\langle f_K,m_i\rangle\right|$$
$$\leq C\sum|\lambda_i|\,\|f_K\|_{BMO_{L^*}}\leq C\|f\|_{BMO_{L^*}}\|g\|_{H^1_L}, \tag{8.42}$$

where we have used the claim (8.41). Now, we also have that

$$\langle f_K,g\rangle\to\iint_{\mathbb{R}^{n+1}_+}(t^2L^*)^M e^{-t^2L^*}f(x)\,\overline{t^2Le^{-t^2L}g(x)}\,\frac{dxdt}{t},$$

by a dominated convergence argument which uses Lemma 4.2 (ii), Lemma 8.3, and the duality of T^1 and T^∞ [12]. But by Lemma 8.4, the last expression equals $\langle f, g\rangle$; i.e.,

$$\langle f_K, g\rangle \to \langle f, g\rangle,$$

so that (8.19) follows from (8.42).

To complete the proof of Theorem 8.2, it remains only to establish the claims concerning f_K. To see that $f_K \in L^2(\mathbb{R}^n)$, it suffices by Lemma 8.3 to observe that for all $F_t \in T^\infty(\mathbb{R}^{n+1}_+)$, we have

$$\begin{aligned}\left\| \int_{1/K}^{K} t^2 L^* e^{-t^2 L^*} \left(\chi_{B_K} F_t\right) \frac{dt}{t} \right\|_{L^2(\mathbb{R}^n)} &\leq C \int_{1/K}^{K} \|F_t\|_{L^2(B_K)} \frac{dt}{t} \\ &\leq C_K \left(\int_0^K \int_{B_K} |F_t(x)|^2 dx \frac{dt}{t} \right)^{1/2} \\ &\leq C_K \|F_t\|_{T^\infty(\mathbb{R}^{n+1}_+)} |B_K|^{1/2}. \end{aligned} \tag{8.43}$$

To prove the claim (8.41), again by Lemma 8.3 it suffices to prove the following

Lemma 8.5 *Suppose that* $F_t \in T^\infty(\mathbb{R}^{n+1}_+)$, *and set*

$$f_K \equiv \int_{1/K}^{K} t^2 L^* e^{-t^2 L^*} \left(\chi_{B_K} F_t\right) \frac{dt}{t}.$$

Then

$$\sup_K \|f_K\|_{BMO_{L^*}(\mathbb{R}^n)} \leq C \|F_t\|_{T^\infty(\mathbb{R}^{n+1}_+)}.$$

Proof We need to prove that for every cube $Q \subset \mathbb{R}^n$

$$\begin{aligned}&\left(\frac{1}{|Q|} \int_Q \left| (I - (1 + l(Q)^2 L^*)^{-1})^M \int_{1/K}^{K} t L^* e^{-t^2 L^*} \left(\chi_{B_K} F_t\right) dt \right|^2 dx \right)^{\frac{1}{2}} \\ &\quad \leq C \|F_t\|_{T^\infty(\mathbb{R}^{n+1}_+)}, \end{aligned} \tag{8.44}$$

uniformly in K. To this end, we split the integral in t in (8.44) into two integrals over $(1/K, l(Q)]$ and $(l(Q), K)$ (these are of course vacuous if $\ell(Q) < 1/K$, or if $\ell(Q) > K$, respectively), and consider first the case $t \leq l(Q)$. Let $h \in L^2(\mathbb{R}^n)$ such that $\operatorname{supp} h \subset Q$ and $\|h\|_{L^2(\mathbb{R}^n)} = 1$. The left hand side of (8.44), restricted to $t \leq l(Q)$, is bounded by the supremum over all such h of the following:

$$\frac{1}{|Q|^{1/2}}\left|\int_Q \left(I-(1+l(Q)^2L^*)^{-1}\right)^M \int_{1/K}^{l(Q)} tL^*e^{-t^2L^*}\left(\chi_{B_K}F_t\right)(x)\,dt\,\overline{h(x)}\,dx\right|$$

$$\leq \frac{C}{|Q|^{1/2}}\left|\int_{1/K}^{l(Q)}\int_{\mathbb{R}^n}\left(\chi_{B_K}F_t(x)\right)\overline{t^2Le^{-t^2L}(I-(1+l(Q)^2L)^{-1})^M h(x)}\,\frac{dxdt}{t}\right|$$

$$\leq C\sum_{j=0}^{\infty}\left(\frac{1}{|Q|}\int_0^{l(Q)}\int_{S_j(Q)}|F_t(x)|^2\,\frac{dxdt}{t}\right)^{1/2}$$

$$\times\left(\int_0^{l(Q)}\int_{S_j(Q)}\left|t^2Le^{-t^2L}(I-(1+l(Q)^2L)^{-1})^M h(x)\right|^2\,\frac{dxdt}{t}\right)^{1/2}$$

$$\leq C\sum_{j=0}^{\infty}2^{jn/2}\|F_t\|_{T^\infty(\mathbb{R}^{n+1}_+)}$$

$$\times\left(\int_0^{l(Q)}\int_{S_j(Q)}\left|t^2Le^{-t^2L}(I-(1+l(Q)^2L)^{-1})^M h(x)\right|^2\,\frac{dxdt}{t}\right)^{1/2}, \quad (8.45)$$

where we majorized the integral over $S_j(Q)\times(0,l(Q))$ by the integral over $\widehat{B}$ for some ball B with size comparable to $(2^j l(Q))^n$ in the last inequality.

If $j=0,1$

$$\left(\int_0^{l(Q)}\int_{S_j(Q)}\left|t^2Le^{-t^2L}(I-(1+l(Q)^2L)^{-1})^M h(x)\right|^2\,\frac{dxdt}{t}\right)^{1/2}$$

$$\leq C\sup_{0\leq k\leq M}\|g_h(1+l(Q)^2L)^{-k}h\|_{L^2(\mathbb{R}^n)}\leq C, \quad (8.46)$$

since g_h is bounded on $L^2(\mathbb{R}^n)$ (see [1]) and $(1+l(Q)^2L)^{-1}$ is uniformly bounded on $L^2(\mathbb{R}^n)$ (see Lemma 2.4).

Assume now that $j\geq 2$. Then

$$\left(\int_0^{l(Q)}\int_{S_j(Q)}\left|t^2Le^{-t^2L}(I-(1+l(Q)^2L)^{-1})^M h(x)\right|^2\,\frac{dxdt}{t}\right)^{1/2}$$

$$\leq C \sup_{0\leq k\leq M} \left(\int_0^{l(Q)} \int_{S_j(Q)} \left| t^2 L e^{-t^2 L} (1 + l(Q)^2 L)^{-k} h(x) \right|^2 \frac{dxdt}{t} \right)^{1/2}. \tag{8.47}$$

When $k = 0$,

$$\left(\int_0^{l(Q)} \int_{S_j(Q)} \left| t^2 L e^{-t^2 L} h(x) \right|^2 \frac{dxdt}{t} \right)^{1/2} \leq C \left(\int_0^{l(Q)} e^{-\frac{(2^j l(Q))^2}{ct^2}} \frac{dt}{t} \right)^{1/2} \leq C 2^{-jN}, \tag{8.48}$$

for every $N \in \mathbb{N}$. Here we used Gaffney estimates and the fact that $\operatorname{supp} h \subset Q$, $\|h\|_{L^2(\mathbb{R}^n)} = 1$.

When $1 \leq k \leq M$, the quantity under the sup sign in (8.47) can be rewritten as

$$\left(\int_0^{l(Q)} \int_{S_j(Q)} \frac{t^4}{l(Q)^4} \left| e^{-t^2 L} \left[(l(Q)^2 L)(1+l(Q)^2 L)^{-1} \right] (1+l(Q)^2 L)^{-k+1} h(x) \right|^2 \frac{dxdt}{t} \right)^{1/2}$$

$$\leq C \left(\int_0^{l(Q)} \int_{S_j(Q)} \frac{t^4}{l(Q)^4} \left| e^{-t^2 L} (I - (1 + l(Q)^2 L)^{-1})(1+l(Q)^2 L)^{-k+1} h(x) \right|^2 \frac{dxdt}{t} \right)^{1/2}$$

$$\leq C \left(\int_0^{l(Q)} \frac{t^4}{l(Q)^4} e^{-\frac{(2^j l(Q))^2}{ct^2}} \frac{dt}{t} \right)^{1/2} + C \left(\int_0^{l(Q)} \frac{t^4}{l(Q)^4} e^{-\frac{(2^j l(Q))^2}{cl(Q)^2}} \frac{dt}{t} \right)^{1/2},$$

where the first term above comes from the case $k = 1$ and we use Lemmas 2.4 and 2.3. The last sum in (8.49) is bounded by $C2^{-jN}$ for every $N \in \mathbb{N}$, and combining (8.45)–(8.49) we deduce the desired estimate for (8.45) when $t \leq l(Q)$.

As for the case $t \in (l(Q), K)$,

$$\frac{1}{|Q|^{1/2}} \int_Q \left(I - (1 + l(Q)^2 L^*)^{-1} \right)^M \int_{l(Q)}^K t L^* e^{-t^2 L^*} \left(\chi_{B_K} F_t \right)(x)\, dt\, \overline{h(x)}\, dx$$

$$\leq C \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \left(\frac{1}{|Q|} \int_{2^k l(Q)}^{2^{k+1} l(Q)} \int_{S_j(2^k Q)} |F_t(x)|^2 \frac{dxdt}{t} \right)^{1/2}$$

$$\times\left(\int_{2^k l(Q)}^{2^{k+1}l(Q)}\int_{S_j(2^kQ)}\left|t^2Le^{-t^2L}(I-(1+l(Q)^2L)^{-1})^M h(x)\right|^2\,\frac{dxdt}{t}\right)^{1/2}$$

$$\leq C\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}2^{(j+k)n/2}\|F_t\|_{T^\infty(\mathbb{R}^{n+1}_+)}$$

$$\times\left(\int_{2^k l(Q)}^{2^{k+1}l(Q)}\int_{S_j(2^kQ)}\left(\frac{l(Q)}{t}\right)^{4M}\left|(t^2L)^{M+1}e^{-t^2L}(1+l(Q)^2L)^{-M}h(x)\right|^2\,\frac{dxdt}{t}\right)^{1/2}$$

$$\leq C\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}2^{jn/2}2^{k(n/2-2M)}\|F_t\|_{T^\infty(\mathbb{R}^{n+1}_+)}$$

$$\times\left(\int_{2^k l(Q)}^{2^{k+1}l(Q)}\int_{S_j(2^kQ)}\left|(t^2L)^{M+1}e^{-t^2L}(1+l(Q)^2L)^{-M}h(x)\right|^2\,\frac{dxdt}{t}\right)^{1/2}. \tag{8.49}$$

From this point the argument is essentially the same as the one for small t. For $j=0,1$ the expression in the parentheses above is bounded by $C\|h\|^2_{L^2(\mathbb{R}^n)}\leq C$, and the sum in k converges for $M>n/4$. For $j\geq 2$ we use Gaffney estimates to bound the quantity in (8.49) by

$$\sum_{k=0}^{\infty}\sum_{j=2}^{\infty}2^{jn/2}2^{k(n/2-2M)}\|F_t\|_{T^\infty(\mathbb{R}^{n+1}_+)}\left(\int_{2^k l(Q)}^{2^{k+1}l(Q)}e^{-\frac{(2^{j+k})^2}{ct^2}}\,\frac{dt}{t}\right)^{1/2}\leq C\|F_t\|_{T^\infty(\mathbb{R}^{n+1}_+)}. \tag{8.50}$$

Therefore, (8.44) is valid for all $M>n/4$. This concludes the proof of Lemma 8.5, and thus also that of Theorem 8.2. □

Next, we prove the converse:

Theorem 8.6 *Suppose $M>n/4$, $\varepsilon>0$, and that l is a bounded linear functional on $H^1_L(\mathbb{R}^n)$. Then in fact, $l\in BMO_{L^*}(\mathbb{R}^n)$ and for all $g\in H^1_L(\mathbb{R}^n)$ which can be represented as finite linear combinations of $(2,\varepsilon,M)$-molecules, we have*

$$l(g)=\langle l,g\rangle, \tag{8.51}$$

where the latter pairing is in the sense of $\mathbf{M}_0^{2,\varepsilon,M}(L)$ and its dual. Moreover,

$$\|l\|_{BMO_{L^*}(\mathbb{R}^n)}\leq C\|l\|. \tag{8.52}$$

We observe that the combination of Theorems 8.2 and 8.6 gives Theorem 1.3.

Proof By Theorem 4.1 and its proof, we have in particular that for any $(2, \varepsilon, M)$-molecule m, $\|m\|_{H^1_L} \leq C$. Thus,

$$l(m) \leq C\|l\|$$

for every $(2, \varepsilon, M)$-molecule m. In particular, l defines a linear functional on $\mathbf{M}_0^{2,\varepsilon,M}(L)$ for every $\varepsilon > 0$, $M > n/4$. Thus, $(I - (I + t^2L^*)^{-1})^M l$ is well defined and belongs to L^2_{loc} for every $t > 0$ (recall (1.20) and the related discussion). Fix a cube Q, and let $\varphi \in L^2(Q)$, with $\|\varphi\|_{L^2(Q)} \leq |Q|^{-1/2}$. As we have observed above (1.13),

$$\tilde{m} \equiv (I - (I + \ell(Q)^2 L)^{-1})^M \varphi$$

is (up to a harmless multiplicative constant) a $(2, \varepsilon, M)$-molecule for every $\varepsilon > 0$. Thus,

$$\begin{aligned}\left|\left\langle (I - (I + t^2L^*)^{-1})^M l, \varphi\right\rangle\right| &\equiv \left|\left\langle l, (I - (I + t^2L)^{-1})^M \varphi\right\rangle\right| \\ &= |\langle l, \tilde{m}\rangle| \leq C\|l\|.\end{aligned}$$

Taking a supremum over all such φ supported in Q, we obtain that

$$\frac{1}{|Q|}\int\limits_Q \left|(I - (I + t^2L^*)^{-1})^M l(x)\right|^2 dx \leq C\|l\|^2.$$

Since Q was arbitrary, the conclusion of the theorem follows. □

Corollary 8.7 *The operator $(L^*)^{-1/2}\operatorname{div} = \left(\nabla L^{-1/2}\right)^*$ is bounded from $L^\infty(\mathbb{R}^n)$ to $BMO_{L^*}(\mathbb{R}^n)$.*

Proof The corollary follows from Theorems 3.4 and 1.3 or can be proved directly. The argument is standard, we leave the details to the interested reader. □

We conclude this section with the following consequence of Theorems 8.2 and 8.6, and Corollary 4.3.

Corollary 8.8 *For every $M > n/4$, the spaces $BMO_L(\mathbb{R}^n)$ defined by the norms (1.22) are equivalent.*

9 $BMO_L(\mathbb{R}^n)$: connection with Carleson measures

A Carleson measure is a positive measure μ on $\mathbb{R}^{n+1}_+$ such that

$$\|\mu\|_{\mathcal{C}} := \sup_B \frac{1}{|B|}\mu\left(\widehat{B}\right) < \infty, \tag{9.1}$$

where B denotes a ball in $\mathbb{R}^n$ and $\widehat{B}$ is a tent over B (see (8.21)). Recall the definition of the operator C in (8.20) and observe that

$$\|CF\|^2_{L^\infty(\mathbb{R}^n)} = \left\| |F(y,t)|^2 \frac{dydt}{t} \right\|_{\mathcal{C}}. \tag{9.2}$$

Theorem 9.1 *Assume that $M \in \mathbb{N}$, $M > n/4$. Then for every $f \in BMO_L(\mathbb{R}^n)$*

$$\mu_f := \left|(t^2L)^M e^{-t^2L} f(y)\right|^2 \frac{dydt}{t} \tag{9.3}$$

is a Carleson measure and

$$\|\mu_f\|_{\mathcal{C}} \le C\|f\|^2_{BMO_L(\mathbb{R}^n)}. \tag{9.4}$$

Conversely, if $f \in (\mathbf{M}_0^{2,M}(L^*))^*$ satisfies the controlled growth bound (8.28) (with L in place of L^*) for some $\varepsilon_1 > 0$, and if μ_f defined in (9.3) is a Carleson measure, then $f \in BMO_L(\mathbb{R}^n)$ and

$$\|f\|^2_{BMO_L(\mathbb{R}^n)} \le C\,\|\mu_f\|_{\mathcal{C}}. \tag{9.5}$$

Proof The direction BMO_L implies (9.4) is just a restatement of Lemma 8.3.

For the converse we follow [12], using the duality of the tent spaces. More precisely, for f satisfying (8.28) and every $g \in H^1_{L^*}(\mathbb{R}^n)$ that can be represented as a finite linear combination of $(2, \varepsilon, M')$-molecules, $\varepsilon > \varepsilon_1/2$ and $M' > n/4$ large enough compared to M, we have by Lemma 8.4 that

$$\langle f, g\rangle = C_M \iint_{\mathbb{R}^{n+1}_+} (t^2L)^M e^{-t^2L} f(x)\, \overline{t^2L^*e^{-t^2L^*} g(x)}\, \frac{dtdx}{t}. \tag{9.6}$$

Now according to Theorem 1 in [12]

$$\begin{aligned}
&\iint_{\mathbb{R}^{n+1}_+} \left|(t^2L)^M e^{-t^2L} f(x)\, \overline{t^2L^*e^{-t^2L^*} g(x)}\right| dx \\
&\quad \le C \int_{\mathbb{R}^n} C((t^2L)^M e^{-t^2L} f)(x)\, S(t^2L^*e^{-t^2L^*} g)(x)\, dx \\
&\quad \le C \left\| C\left((t^2L)^M e^{-t^2L} f\right)\right\|_{L^\infty(\mathbb{R}^n)} \left\| S(t^2L^*e^{-t^2L^*} g)\right\|_{L^1(\mathbb{R}^n)}.
\end{aligned} \tag{9.7}$$

Then using (9.2) and Theorem 4.1, we have

$$|\langle f, g\rangle| \le C \left\| \left|(t^2L)^M e^{-t^2L} f(y)\right|^2 \frac{dydt}{t} \right\|^{1/2}_{\mathcal{C}} \|g\|_{H^1_{L^*}(\mathbb{R}^n)}, \tag{9.8}$$

for every $g \in H^1_{L^*}(\mathbb{R}^n)$. By Theorem 8.6 this gives the desired conclusion (9.5). $\square$

Remark Fix some $p \in (p_L, 2)$. Using the finite linear combinations of (p', ε, M')-molecules in the proof of Lemma 8.4, $\frac{1}{p} + \frac{1}{p'} = 1$, we can prove that the condition (8.28) can be replaced by

$$\int\limits_{\mathbb{R}^n} \frac{|(I-(1+L)^{-1})^M f(x)|^p}{1+|x|^{n+\varepsilon_1}}\, dx < \infty \tag{9.9}$$

for some $\varepsilon_1 > 0$. We will use this fact later in conjunction with the fact that every $f \in BMO^p_L(\mathbb{R}^n)$ satisfies (9.9).

10 John–Nirenberg inequality

We start with the following auxiliary result, which is a modification of Lemma 2.14 in [6].

Lemma 10.1 *Suppose there exist numbers $0 < \alpha < 1$ and $0 < N < \infty$ such that for some function $F \in L^2_{loc}((0,\infty) \times \mathbb{R}^n)$, some $a \in \mathbb{R}$ and every cube $Q \subset \mathbb{R}^n$*

$$\left|\left\{x \in Q : \left(\int\limits_{|x-y|<3at<3al(Q)} \int |F(t,y)|^2 \frac{dydt}{t^{n+1}}\right)^{1/2} > N\right\}\right| \le \alpha|Q|. \tag{10.1}$$

Then there exists $C > 0$ such that

$$\sup_{Q \subset \mathbb{R}^n} \frac{1}{|Q|} \int\limits_Q \left(\int\limits_{|x-y|<at<al(Q)} \int |F(t,y)|^2 \frac{dydt}{t^{n+1}}\right)^{p/2} dx \le C, \tag{10.2}$$

for all $p \in (1,\infty)$.

Proof Denote the set on the left-hand side of (10.1) by Ω, so that $|\Omega| \le \alpha|Q|$, and let $\cup Q_j$ be a Whitney decomposition of Ω. Also,

$$M(\delta) := \sup_{Q' \subseteq Q} \frac{1}{|Q'|} \int\limits_{Q'} \left(\int\limits_{\substack{|x-y|<a(t-\delta)\\ \delta<t<l(Q')}} \int |F(t,y)|^2 \frac{dydt}{t^{n+1}}\right)^{p/2} dx,$$

where the integral is set to be zero whenever $l(Q') \leq \delta$. Then

$$\begin{aligned}
&\int_Q \left(\iint_{\substack{|x-y|<a(t-\delta)\\ \delta<t<l(Q)}} |F(t,y)|^2 \frac{dydt}{t^{n+1}} \right)^{p/2} dx \\
&\leq \int_{Q\setminus\Omega} \left(\iint_{\substack{|x-y|<3at\\ t<l(Q)}} |F(t,y)|^2 \frac{dydt}{t^{n+1}} \right)^{p/2} dx \\
&\quad + \sum_{j:l(Q_j)>\delta} \int_{Q_j} \left(\iint_{\substack{|x-y|<a(t-\delta)\\ \delta<t<l(Q_j)}} |F(t,y)|^2 \frac{dydt}{t^{n+1}} \right)^{p/2} dx \\
&\quad + \sum_j \int_{Q_j} \left(\iint_{\substack{|x-y|<a(t-\delta)\\ \max\{l(Q_j),\delta\}<t<l(Q)}} |F(t,y)|^2 \frac{dydt}{t^{n+1}} \right)^{p/2} dx \\
&\leq N^p|Q| + M(\delta)\alpha|Q| + \sum_j \int_{Q_j} \left(\iint_{\substack{|x-y|<a(t-\delta)\\ \max\{l(Q_j),\delta\}<t<l(Q)}} |F(t,y)|^2 \frac{dydt}{t^{n+1}} \right)^{p/2} dx.
\end{aligned} \tag{10.3}$$

By the properties of the Whitney decomposition $\operatorname{dist}(x', Q_j) \approx l(Q_j)$ for some $x' \in Q\setminus\Omega$. Therefore, without loss of generality we can assume that for every $x \in Q_j$ there exists $x' \in Q\setminus\Omega$ such that

$$\begin{aligned}
&\left\{y : |x-y| < a(t-\delta),\ \max\{l(Q_j),\delta\} < t < l(Q)\right\} \\
&\quad \subset \left\{y : |x'-y| < 3at,\ t < l(Q)\right\}.
\end{aligned} \tag{10.4}$$

Then the last term in (10.3) can be bounded by

$$|Q| \sup_{x'\in Q\setminus\Omega} \left(\iint_{\substack{|x'-y|<3at\\ t<l(Q)}} |F(t,y)|^2 \frac{dydt}{t^{n+1}} \right)^{p/2} \leq N^p|Q|. \tag{10.5}$$

Repeating the procedure in (10.3)–(10.5) for every cube $Q' \subset Q$, we arrive at

$$(1-\alpha)M(\delta) \leq CN^p, \tag{10.6}$$

and the argument can be finished taking limit as $\delta \to 0$. □

Proof of Theorem 1.2 *Step I.* It is an easy consequence of Hölder's inequality that

$$\|f\|_{BMO_L^p(\mathbb{R}^n)} \leq C\|f\|_{BMO_L(\mathbb{R}^n)} \leq C\|f\|_{BMO_L^q(\mathbb{R}^n)} \quad \text{for } p_L < p < 2 < q < \widetilde{p}_L, \tag{10.7}$$

so we will concentrate on the reverse estimates.

Step II. In this part we will show that $f \in BMO_L^{p_0}(\mathbb{R}^n)$ implies $f \in BMO_L(\mathbb{R}^n)$ with $p_L < p_0 < 2$. Let us first prove that whenever $f \in BMO_L^{p_0}$ the inequality (10.1) holds with $p = p_0$, $a = 1$. We split f as in (8.2). Then the contribution of the first part is handled as follows. Making the dyadic annular decomposition,

$$\begin{aligned}
&\left(\frac{1}{|Q|}\int_Q \left(\int\int_{|x-y|<t<l(Q)} |(t^2L)^M e^{-t^2L}\right.\right. \\
&\qquad \left.\left. \times\ (I-(1+l(Q)^2L)^{-1})^M f(y)|^2 \frac{dydt}{t^{n+1}}\right)^{\frac{p_0}{2}} dx\right)^{\frac{1}{p_0}} \\
&\leq C\sum_{j=0}^{\infty}\left(\frac{1}{|Q|}\int_Q \left(\int\int_{|x-y|<t<l(Q)} |(t^2L)^M e^{-t^2L}\right.\right. \\
&\qquad \left.\left. \times\ \left[\chi_{S_j(Q)}(I-(1+l(Q)^2L)^{-1})^M f\right](y)|^2 \frac{dydt}{t^{n+1}}\right)^{\frac{p_0}{2}} dx\right)^{\frac{1}{p_0}} \\
&\leq C\frac{1}{|Q|^{1/p_0}}\left(\int_{4Q} |(I-(1+l(Q)^2L)^{-1})^M f(x)|^{p_0}\,dx\right)^{\frac{1}{p_0}} \\
&\quad + C\sum_{j=3}^{\infty}\frac{1}{|Q|^{1/2}}\left(\int\int_{2Q\times(0,l(Q))} |(t^2L)^M e^{-t^2L}\right. \\
&\qquad \left. \times\ \left[\chi_{S_j(Q)}(I-(1+l(Q)^2L)^{-1})^M f\right](x)|^2 \frac{dxdt}{t}\right)^{\frac{1}{2}}.
\end{aligned} \tag{10.8}$$

Here we have used $L^{p_0}(\mathbb{R}^n)$ boundedness of the conical square function (see Lemma 2.6) for the first term above. To handle the second one we have applied Hölder's inequality to pass from the L^{p_0} to the L^2 norm and then Lemma 2.1. Using $L^{p_0} - L^2$ off-diagonal estimates (Lemma 2.5) the second term can be further bounded by

$$C\sum_{j=3}^{\infty}\frac{1}{|Q|^{1/2}}\left(\int_0^{l(Q)} e^{-\frac{(2^j l(Q))^2}{ct^2}}\left(\int_{S_j(Q)} |(I-(1+l(Q)^2L)^{-1})^M \;\; f(x)|^{p_0}dx\right)^{\frac{2}{p_0}}\frac{dt}{t^{1-\frac{n}{2}+\frac{n}{p_0}}}\right)^{\frac{1}{2}}. \tag{10.9}$$

Covering $S_j(Q)$ by approximately 2^{jn} cubes of the sidelength $l(Q)$ and integrating in t, we control (10.9) and hence (10.8) by $\|f\|_{BMO_L^{p_0}(\mathbb{R}^n)}$.

The contribution of

$$\left[I-(I-(1+l(Q)^2L)^{-1})^M\right]f=\sum_{k=1}^{M} C_{k,M}\,(l(Q)^2L)^{-k}(I-(1+l(Q)^2L)^{-1})^M f \tag{10.10}$$

(cf. (8.5)) can be estimated in the same way as (10.8)–(10.9), first combining L^{-k}, $1\le k\le M$, with L^M.

We have thus proved that $F := F(t,y) = t^2Le^{-t^2L}f(y)$ satisfies (10.2) for some $p = p_0$ and $a = 1$. Then by Chebyshev's inequality F satisfies (10.1) with $a = 1/3$. Hence (10.2) holds for $p = 2, a = 1/3$ and F as above by Lemma 10.1. The latter fact implies that $f \in BMO_L(\mathbb{R}^n)$ using Theorem 9.1 and the Remark after Theorem 9.1.

Step III. Let us consider the estimate

$$\|f\|_{BMO_L^q(\mathbb{R}^n)} \le C\|f\|_{BMO_L(\mathbb{R}^n)} \quad \text{for } 2<q<\widetilde{p}_L. \tag{10.11}$$

Fix a cube Q, and let $\varphi \in L^2(Q) \supseteq L^p(Q)$, where $p = q'$, i.e.,

$$(\widetilde{p}_L)' \equiv \widetilde{p}_L/(\widetilde{p}_L-1) < p \equiv q/(q-1) < 2,$$

and suppose that

$$\|\varphi\|_p \le |Q|^{1/p-1}.$$

We claim that for some harmless constant C_0,

$$m \equiv \frac{1}{C_0}\left(I-(I+\ell(Q)^2L^*)^{-1}\right)^M\varphi$$

is a (p, ε, M)-molecule, for the operator L^*, adapted to Q, for every $\varepsilon > 0$. Indeed, by a simple duality argument, we have that

$$(\widetilde{p}_L)' = p_{L^*}, \quad p_L' = \widetilde{p}_{L^*}.$$

Thus, for $(\widetilde{p}_L)' = p_{L^*} < p < 2$, the resolvent kernel $(I + t^2L^*)^{-1}$ satisfies the $L^p - L^p$ off-diagonal estimates by Lemma 2.5. Taking $E = Q$, and $F = S_i(Q)$, the reader may then readily verify that m is a molecule as claimed. We omit the details.

Now, suppose that $f \in BMO_L$. Then by Theorem 8.2, $f \in (H^1_{L^*})^*$. Thus, since $\|m\|_{H^1_{L^*}} \le C$, we have that

$$\frac{1}{C_0}\left|\left\langle\left(I - (I + \ell(Q)^2L)^{-1}\right)^M f, \varphi\right\rangle\right| \equiv |\langle f, m\rangle| \le C\|f\|_{BMO_L(\mathbb{R}^n)}.$$

Thus, taking a supremum over all φ as above, we obtain (10.11). □

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