

# Heat Kernels of Second Order Complex Elliptic Operators and Applications

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We study the heat kernels of second order elliptic operators in divergence form with complex bounded measurable coefficients on  $\mathbb{R}^n$ . We obtain Gaussian bounds without further assumption if  $n \leq 2$ , and when the principal part has Hölder continuous coefficients if  $n \geq 3$ . A thorough study of the boundedness properties of the Green operator is made in dimension 1. We construct the fundamental solution of these operators in dimension 2. Boundedness results of the maximal accretive square roots on  $L^p$  Sobolev spaces and Hölder spaces are obtained when  $n \geq 2$  under Hölder continuity assumption on the coefficients. Bounded  $H^\infty$  functional calculi on  $L^p$ ,  $1 < p < +\infty$ , are also discussed. © 1998 Academic Press

## INTRODUCTION

The main objective of this paper is the study of divergence form second order elliptic operators on  $\mathbb{R}^n$  (with lower order terms) having bounded

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complex coefficients with no or little smoothness properties. By no smoothness, we mean measurable. The case of more general domains is also of interest but is not considered here. Some of the results here were announced in [AMcT], though further material has been included.

Our primary goal in this paper is to study the heat kernels of these operators. When the coefficients are real and non-smooth, the well-known estimates of Aronson [Ar] tell that the heat kernel is controlled by a Gaussian bound. This result has been proved since in different ways (see [FS, Da1, R, VSC] and their references) following important ideas developed by Nash in his famous 1958 paper on elliptic and parabolic equations [Na] and by Moser in his paper on Harnack inequalities [Mos]. However, all the methods above use in a crucial way the fact that the coefficients are real. To treat the case of complex coefficients with an ellipticity condition, other arguments are needed.

The method we use relies on the study of the boundedness properties of high powers of the resolvent. In terms of PDE's this means that we start from an elliptic regularity theorem for the operator, which is then iterated by taking successive powers of the resolvent, i.e., the higher the power the better the functional properties. One property we are especially looking for is boundedness from  $L^1$  to  $L^\infty$  as it is equivalent to uniform boundedness of the distribution-kernel. Decay then follows by use of the exponential perturbation method of Davies [Da1] and the Gaussian decay of the heat kernel is obtained via a Cauchy representation of the heat operator in terms of the resolvent.

This type of approach is not new in partial differential equations and functional calculus, and dates back to works of Agmon, R. Beals, Nelson and Stinespring, Nirenberg, Tanabe and many others, e.g., [Ag, B, Na, NS, N, Ta]. It has been used for the spectral analysis of differential operators with smooth coefficients (and even pseudo-differential operators) or operators with little smoothness. However, even with Hölder continuous coefficients, the case of divergence form operators is not covered by those previous works. The main difference lies in the regularity estimates which are at our disposal.

Elliptic regularity results in 1 and 2 dimensions are available without requiring any smoothness on the coefficients. In higher dimensions, we shall use two results, one due to M. Taylor concerning regularity in the  $L^p$ -Sobolev spaces [T], and the other one of Morrey and Stampacchia in the Hölder scale [Mo], both requiring Hölder continuity assumptions on the leading coefficients (and on the other coefficients for more regularity properties of the heat kernel).

In this way we obtain Gaussian bounds for the heat kernels of all second order elliptic operators in divergence form with complex bounded measurable coefficients on  $\mathbb{R}^n$  if  $n \leq 2$ , and when the principal part has

Hölder continuous coefficients if  $n \geq 3$ . We remark that, if  $n \geq 5$ , there exist operators with complex measurable coefficients whose heat kernels do not satisfy Gaussian bounds [AT3].

We also describe the following applications.

In dimension 1, the Green operator is shown to map isomorphically  $W^{-1,p}$  onto  $W^{1,p}$  for all  $p \in [1, +\infty]$  and to map  $L^p$  into  $W^{1,\infty}$  (non-smooth coefficients). This is specific to the monodimensional situation.

In dimension 2, we describe a construction of the fundamental solution of operators of the form  $-\operatorname{div}(AV)$  where  $A$  is a complex matrix of bounded non-smooth coefficients (here, the maximum principle is not available). This fundamental solution has the expected logarithmic singularity. As a corollary we deduce an extension of Wentze's estimate to complex situation [W].

The next two applications make use of the theory of Calderón-Zygmund operators.

First, we present a thorough description of the square root of our operators under Hölder continuity of their coefficients ( $n \geq 2$ ). The  $L^2$  domain of the square root is known to be the Sobolev space  $W^{1,2}$  in this case [Mc1] (in fact, the result there is obtained under a weaker smoothness assumption on the coefficients, i.e., that they are multipliers of Sobolev spaces  $W^{s,2}$  for some  $s > 0$ , allowing step functions as coefficients). However, we obtain a representation in terms of Calderón-Zygmund operators which yields a simpler proof of the result in [Mc1] and also gives new boundedness results on  $L^p$  Sobolev spaces and Hölder spaces.

On the other hand, we prove that the bounded  $H^\infty$  functional calculus defined on  $L^2$  extends to  $L^p$  spaces,  $1 < p < +\infty$  when the dimension is 1 or 2. Results in higher dimensions are also discussed. This is done by showing how functions of  $L$  are related to Calderón-Zygmund operators.

The paper is organized as follows. We set the notations in Section 1. Then Sections 2, 3 and 4 present results specific to one dimension, two dimensions and higher dimensions respectively, and the heat kernel estimates in each case. Sections 5 and 6 are concerned with the square root problem and the  $H^\infty$  functional calculus. We also gather in the Appendix some remarks on the perturbation method of Davies used frequently in the course of the paper.

## 1. NOTATION

The integer  $n$  always denotes dimension. The notation  $L^p$  and  $W^{s,p}$ ,  $1 \leq p \leq \infty$ ,  $s \in \mathbb{R}$ , are used for the Lebesgue and Sobolev spaces on  $\mathbb{R}^n$ . For  $p=2$ , the notation  $H^s$  is also used for  $W^{s,2}$ . The usual norm on  $L^p$  is denoted by  $\|\cdot\|_p$ .

The norm of a bounded linear operator,  $T$ , from  $L^p$  to  $L^q$  is denoted by  $\|T\|_{q;p}$ . The Banach space of these operators is denoted by  $\mathcal{B}(L^p, L^q)$ . We use  $T: E \rightarrow F$  as an alternative way of writing  $T \in \mathcal{B}(E, F)$ .

Define the Hölder spaces as follows. For a function  $f$  defined on  $\mathbb{R}^n$  and  $0 < r < 1$ , we denote by  $|f|_r$  the smallest constant  $C$  for which the inequality  $|f(x) - f(y)| \leq C|x - y|^r$  holds for all  $x, y \in \mathbb{R}^n$ . The space of functions for which  $|f|_r < +\infty$  is denoted by  $\dot{C}^r$ . If  $r > 1$  and is not an integer then  $f \in \dot{C}^r$  if  $\nabla f \in \dot{C}^{r-1}$  etc. For a matrix  $A$ , set  $|A|_r = \sup |a_{ij}|_r$ . Finally  $C^r = \dot{C}^r \cap W^{[r], \infty}$ , where  $[r]$  denotes the integer part of  $r$ .

We turn to some notation on matrices. We denote by  $\mathcal{A}(k)$  the class of all  $k \times k$  matrix valued functions  $B(x)$  defined on  $\mathbb{R}^n$  with complex measurable coefficients for which there exists  $\delta > 0$  such that

$$\forall \zeta \in \mathbb{C}^k \quad \operatorname{Re} b_{ij}(x) \zeta_i \bar{\zeta}_j \geq \delta |\zeta|^2, \quad \text{a.e.} \tag{1.1}$$

and

$$\|B\| = \sup_{x \in \mathbb{R}^n} \sup \{ |b_{ij}(x) \zeta_i \bar{\eta}_j|; \zeta, \eta \in \mathbb{C}^n, |\zeta| = |\eta| = 1 \} < +\infty.$$

We used the summation convention. The supremum in  $x$  is understood as the essential supremum, i.e., the  $L^\infty$  norm. The ellipticity constants of  $B$  are the largest  $\delta$  which occurs in the definition, denoted by  $\delta(B)$ , and  $\|B\|$ . Also let

$$\omega_B = \sup_{x \in \mathbb{R}^n} \{ |\arg\{b_{ij}(x) \zeta_i \bar{\zeta}_j\}|; \zeta \in \mathbb{C}^k \}.$$

Remark that  $\mathcal{A}(k)$  coincides with the class of invertible matrix valued functions  $B(x)$  with bounded measurable coefficients and  $\omega_B < \pi/2$ . Matrix valued functions  $B$  for which this last condition holds are often said to be accretive (uniformly). In this paper, elliptic means the same thing as accretive and bounded and we use both interchangeably.

A second order operator in divergence form on  $\mathbb{R}^n$  is given by

$$\mathcal{L} = -\partial_{x_i} (a_{ij}(x) \partial_{x_j}) + a_{i, n+1}(x) + a_{n+1, j}(x) \partial_{x_j} + a_{n+1, n+1}(x), \tag{1.2}$$

where the  $(n+1) \times (n+1)$  matrix  $(a_{kl}(x))_{1 \leq k, l \leq n+1} = A(x)$  is assumed to have bounded measurable complex valued coefficients. We use the notation  $\mathcal{L} = \mathcal{L}(A)$  or

$$\mathcal{L} = -\operatorname{div}(A_0 \nabla + b) + c \nabla + d$$

to abbreviate (1.2). The leading term of  $\mathcal{L}$  is

$$\mathcal{L}_0 = -\partial_{x_i} (a_{ij}(x) \partial_{x_j}) = -\operatorname{div}(A_0 \nabla) \equiv \mathcal{L}(A_0). \tag{1.3}$$

We say that

$$\mathcal{L}_0 = \mathcal{L}(A_0) \in \mathcal{E}_0 \quad \text{if } A_0 \in \mathcal{A}(n),$$

and that

$$\mathcal{L} = \mathcal{L}(A) \in \mathcal{E} \quad \text{if } A \in \mathcal{A}(n+1).$$

The ellipticity constants for  $\mathcal{L}_0$  (resp.  $\mathcal{L}$ ) are the ellipticity constants for  $A_0$  (resp.  $A$ ). Throughout and unless explicitly mentioned, the subscript 0 is used for the homogeneous second order operators while second order operators with lower order terms are denoted without subscript. The same applies to matrices.

The above operators are defined via their variational form so that an operator  $\mathcal{L}_0$  in  $\mathcal{E}_0$  is maximal-accretive on  $L^2$  and its domain,  $\mathcal{D}(\mathcal{L}_0)$ , is a dense subspace of  $L^2$  and  $W^{1,2}$ . The same thing for  $\mathcal{L} \in \mathcal{E}$ . It is worth noting that these classes of operators are stable under taking adjoints: we have  ${}^t\mathcal{L}(A_0) = \mathcal{L}({}^tA_0)$  and  ${}^t\mathcal{L}(A) = \mathcal{L}({}^tA)$ .

Let us make some remarks of constant use in this paper.

*Remark 1.4.* If  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$  then

$$|\langle \mathcal{L}f, g \rangle| \leq \|A\| \|f\|_{H^1} \|g\|_{H^1},$$

and

$$\operatorname{Re} \langle \mathcal{L}f, f \rangle \geq \delta(A) \|f\|_{H^1}^2.$$

Thus  $\mathcal{L}$  is bounded and invertible from  $H^1$  onto  $H^{-1}$  with norm bounded above by  $\|A\|$ , and bounded below by  $\delta(A)$ . In fact, the uniform ellipticity of  $A$  is a strong assumption and, in most statements, it is enough to suppose that  $A_0$  is uniformly elliptic and that  $\mathcal{L}$  is invertible from  $H^1$  to  $H^{-1}$ .

*Remark 1.5.* For  $\omega < \pi$ , let  $S_\omega^\circ = \{z \in \mathbb{C} \setminus \{0\}; |\arg z| < \omega\}$  and let  $S_\omega$  be its closure. Let  $\mathcal{L}_0 = \mathcal{L}(A_0) \in \mathcal{E}_0$  and  $\lambda \in S_\mu^\circ$  where  $0 \leq \mu < \pi - \omega_{A_0}$ . Then there exists  $z = z(\mu, \omega_{A_0}) \in \mathbb{C}$  with  $|z| = 1$  such that  $z(\mathcal{L}_0 + \lambda) \in \mathcal{E}$ . Moreover, the ellipticity constants of  $z(\mathcal{L}_0 + \lambda)$  are uniform for such  $\lambda \in S_\mu$  with  $|\lambda| = 1$ , and depend only on  $\delta(A_0)$ ,  $\|A_0\|$  and  $\mu$ . For later purpose, observe that  $\mu$  can be chosen larger than  $\pi/2$  since  $\omega_{A_0} < \pi/2$ .

Finally, introduce the Gaussian functions on  $\mathbb{R}^n$ ,

$$G_{\beta,t}(x) = t^{-n/2} \exp \left\{ -\frac{\beta |x|^2}{t} \right\}$$

for  $x \in \mathbb{R}^n$ ,  $\beta > 0$ ,  $t > 0$  and write  $G_{\beta,1} = G_\beta$ .

## 2. THE ONE DIMENSIONAL CASE

### 2.1. The Resolvent and the Green Kernel

We are interested in estimates for the kernels of the resolvent of our differential operators and eventually in heat kernel estimates obtained via a Cauchy contour integral.

The operators of the class  $\mathcal{E}$  defined in Section 1 take the form

$$\mathcal{L} = -d_x(ad_x + b) + cd_x + d, \tag{2.1}$$

where  $d_x = d/dx$  and  $a, b, c, d$  are complex-valued bounded measurable functions. The matrix  $A$  is a two by two matrix with  $a, b, c, d$  for entries and is uniformly elliptic. As mentioned, this implies that  $\mathcal{L}^{-1}$  exists as a bounded operator from  $W^{-1,2}$  onto  $W^{1,2}$ .

**THEOREM 2.2.** *Let  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$ . For any  $p \in [1, +\infty]$ ,  $\mathcal{L}^{-1}$  extends to a bounded operator from  $W^{-1,p}$  onto  $W^{1,p}$ . Moreover,*

$$\|\mathcal{L}^{-1}f\|_{W^{1,p}} \leq C(\delta(A), \|A\|) \|f\|_{W^{-1,p}} \tag{2.3}$$

This theorem is a consequence of the following result.

**THEOREM 2.4.** *Let  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$ . For any  $p \in [1, +\infty]$ ,  $\mathcal{L}^{-1}$ ,  $d_x \mathcal{L}^{-1}$ ,  $\mathcal{L}^{-1}d_x$ ,  $d_x \mathcal{L}^{-1}d_x$ ,  $d_x(ad_x + b)\mathcal{L}^{-1}$  and  $\mathcal{L}^{-1}(d_x a - c)d_x$  extend to bounded operators on  $L^p$  with the following bounds on the Green kernel  $G(x, y)$ :*

$$|G(x, y)| + |\partial_x G(x, y)| + |\partial_y G(x, y)| \leq C e^{-\alpha|x-y|} \quad a.e., \tag{2.5}$$

and

$$\begin{aligned} &|a(x) \partial_x \partial_y G(x, y)| + |\partial_x(a(x)\partial_x + b(x)) G(x, y)| \\ &+ |\partial_y(a(y)\partial_y + c(y)) G(x, y)| \leq C e^{-\alpha|x-y|} \quad a.e. \text{ for } x \neq y. \end{aligned} \tag{2.6}$$

Here  $C$  and  $\alpha > 0$  depend on  $\delta(A)$  and  $\|A\|$  only.

The meaning of  $x \neq y$  is that this inequality holds for the restriction of these kernels away from the diagonal. In fact, on the diagonal the kernels in (2.6) have a Dirac singularity  $\delta(x-y)$  (up to a sign). These estimates were obtained in [AT2] when  $\mathcal{L}$  has no terms of order 1. Those terms complicate the proof of the bounds of the first derivatives of  $G$ .

Theorem 2.2 now follows from this result in the following way. If  $f \in W^{-1,p}$ , write  $f = u + d_x v$  where  $u, v \in L^p$  and  $\|u\|_p + \|v\|_p \leq C_0 \|f\|_{W^{-1,p}}$ . Hence,

$$\mathcal{L}^{-1}f = \mathcal{L}^{-1}u + \mathcal{L}^{-1}d_x v \in L^p$$

and

$$d_x \mathcal{L}^{-1}f = d_x \mathcal{L}^{-1}u + d_x \mathcal{L}^{-1} d_x v \in L^p,$$

which yields that  $\mathcal{L}^{-1}f \in W^{1,p}$  with

$$\|\mathcal{L}^{-1}f\|_{W^{1,p}} \leq C(\|u\|_p + \|v\|_p).$$

This proves (2.3).

Let us mention another corollary of Theorem 2.4.

**COROLLARY 2.7.** *Let  $\mathcal{L} \in \mathcal{E}$  and  $p \in [1, +\infty]$ . Then,  $\mathcal{L}^{-1}: L^p \rightarrow W^{1,\infty}$  is bounded.*

*Proof.* Write  $u = \mathcal{L}^{-1}f$  as  $u(x) = \int G(x, y) f(y) dy$  and apply (2.5) with Young's inequality.

Theorem 2.2 and Corollary 2.7 are specific to dimension one as they are not true in higher dimensions (even when the coefficients are real).

Let us now turn to the proof of Theorem 2.4 with a sequence of lemmata.

**LEMMA 2.8.** *If  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$ , then  $\mathcal{L}^{-1}$  is bounded from  $L^1$  to  $L^\infty$ . Moreover,  $G(x, y)$  satisfies estimate (2.5).*

*Proof.* Using the Sobolev embeddings  $W^{1,2} \subset L^\infty$  and  $L^1 \subset W^{-1,2}$  together with  $\mathcal{L}^{-1}: W^{-1,2} \rightarrow W^{1,2}$ , we obtain the boundedness of  $\mathcal{L}^{-1}$  from  $L^1$  to  $L^\infty$ . Furthermore, (2.5) for  $G(x, y)$  follows directly from the method of perturbation by exponential weights of Davies. Since we use variations of this method several times, we describe it in an Appendix.

The next result is an intermediate step.

**LEMMA 2.9.** *If  $\mathcal{L} \in \mathcal{E}$ , then  $d_x \mathcal{L}^{-1}$  is bounded from  $L^1$  to  $L^p$ , for any  $p \in [2, +\infty)$ .*

*Proof.* Let  $f \in L^1$  and set  $u = \mathcal{L}^{-1}f$ . Let  $p \in [2, +\infty)$  and set  $\varepsilon = 1/p \in (0, 1/2]$ . Observe that  $u \in W^{1,2}$ , hence  $ad_x u + bu \in L^2$  and that

$$-d_x(ad_x u + bu) = f - cd_x u - du - W^{-(1/2)-\varepsilon, 2}$$

since  $L^1 \subset W^{-(1/2)-\varepsilon, 2}$ . Thus,  $ad_x u + bu \in W^{(1/2)-\varepsilon, 2} \subset L^p$  from the Sobolev embedding theorem. By Lemma 2.8,  $bu \in L^p$  so  $ad_x u \in L^p$ . The ellipticity condition implies  $1/a \in L^\infty$ , so we obtain  $d_x u \in L^p$ .

**LEMMA 2.10.** *If  $\mathcal{L} \in \mathcal{E}$ , then  $d_x \mathcal{L}^{-1}$  is bounded from  $L^1$  to  $L^\infty$ , and estimate (2.5) holds for  $\partial_x G(x, y)$ . Moreover, the same is true for  $\mathcal{L}^{-1}d_x$  and  $\partial_y G(x, y)$ .*

*Proof.* We start with the first assertion. Let  $f \in L^1$  and set  $u = D\mathcal{L}^{-1}f$ , where  $D = ad_x + b$ . From Lemma 2.9, we know that  $u \in L^p$  for  $2 \leq p < +\infty$  and we have to show that  $u \in L^\infty$ . Once this is done, we easily obtain from  $1/a \in L^\infty$  and Lemma 2.8 that  $d_x \mathcal{L}^{-1}f \in L^\infty$ .

Let us observe that as unbounded operators on  $L^2$ , the domain of  $D$  is  $W^{1,2}$  and the domain of  $\mathcal{L}$  consists of those  $u \in W^{1,2}$  such that  $Du \in W^{1,2}$ , hence it coincides with the domain of  $D^2$ . Now, completing the square starting from (2.1), we obtain the equality

$$\mathcal{L} = -\frac{1}{a}(D^2 - (b+c)D - (ad-bc)).$$

This implies the following equality between bounded operators on  $L^2$ :

$$D^2\mathcal{L}^{-1} = -a + a(b+c)D\mathcal{L}^{-1} + a(ad-bc)\mathcal{L}^{-1}. \tag{2.11}$$

The right hand side is a bounded operator from  $L^1$  to  $L^1 + L^p$  for all  $p \in [2, +\infty)$ , thus  $Du = D^2\mathcal{L}^{-1}f \in L^1 + L^p$  for  $p$  in the same range. Using again Lemma 2.8 and  $1/a \in L^\infty$ , we see that the same is true for  $d_x u$ .

If  $d_x u$  were in  $L^p$ , we would conclude that  $u \in L^\infty$  from the Sobolev embedding theorem. This is not quite the case but close enough as shown by the following lemma from real analysis.

**LEMMA 2.12.** *Let  $1 < p < q < +\infty$ . Assume that  $u \in L^q$ ,  $v \in L^1$  and  $w \in L^p$  are such that  $d_x u = v + w$  (in the sense of distributions), then  $u \in L^\infty$  and*

$$\|u\|_\infty \leq c(p, q)(\|u\|_q^{q/p} \|v\|_1^{1-q/p} + \|v\|_1 + \|w\|_p).$$

Let us postpone the proof until the end of this argument. This lemma implies that  $u \in L^\infty$  as desired.

The decay estimate for  $\partial_x G(x, y)$  follows from the Appendix.

Finally, the similar results for  $\mathcal{L}^{-1}d_x$  follow by duality since the class of operators under consideration is closed under taking adjoints.

To end the proof of Theorem 2.4, it remains to study operators of the form  $d_x \mathcal{L}^{-1}d_x$ ,  $d_x(ad_x + b)\mathcal{L}^{-1}$  and  $\mathcal{L}^{-1}(d_x a - c)d_x$ .

The preceding argument shows that  $D^2\mathcal{L}^{-1} = -a$  modulo operators that belong to  $\mathcal{B}(L^1, L^\infty)$  (see Section 1 for its definition). Therefore, expanding the first  $D$  in terms of  $d_x$  and using Lemmata 2.8 and 2.10 we have

$$d_x(ad_x + b)\mathcal{L}^{-1} = -I \quad \text{modulo } \mathcal{B}(L^1, L^\infty).$$

Moreover, the operators in  $\mathcal{B}(L^1, L^\infty)$  appearing in this equality all have exponentially decaying kernels. The case of  $\mathcal{L}^{-1}(d_x a - c)d_x$  is now obtained by duality, for its dual is  $d_x(ad_x + c)'\mathcal{L}^{-1}$  where  $'\mathcal{L} = \mathcal{L}('A)$ , and the above argument applies.

We are left with  $d_x \mathcal{L}^{-1}d_x$  and we see from what precedes that we want essentially to exchange  $D$  with  $\mathcal{L}^{-1}$ . There is a quite striking algebraic relation that does this. We need to introduce the following notation.

To any invertible two by two matrix  $B$ , associate an invertible two by two matrix  $\tilde{B}$  by

$$\tilde{B} = \begin{pmatrix} \tilde{a} & \tilde{b} \\ \tilde{c} & \tilde{d} \end{pmatrix} = \frac{1}{\det B} \begin{pmatrix} a & -c \\ -b & d \end{pmatrix} \quad \text{when} \quad B = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

It is clear that  $\tilde{\tilde{B}} = B$ . Observe also that  $B$  is accretive if and only if  $\tilde{B}$  is accretive. Indeed, for  $B$  invertible,  $B$  is accretive if and only if  $B^{-1}$  is accretive and we have that  $\tilde{B}\xi \cdot \tilde{\xi} = B^{-1}\xi \cdot \tilde{\xi}$  whenever  $\xi = (\xi_1, \xi_2)$  and  $\tilde{\xi} = (\xi_2, \xi_1)$ . Hence,  $\operatorname{Re} \tilde{B}\xi \cdot \tilde{\xi} \geq \delta(B^{-1}) |\xi|^2 = \delta(B^{-1}) |\tilde{\xi}|^2$ .

Now, if  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$ , the operator  $\tilde{\mathcal{L}} \equiv \mathcal{L}(\tilde{A})$  also belongs to  $\mathcal{E}$  and the operation  $\mathcal{L} \rightarrow \tilde{\mathcal{L}}$  is an involution of this class of operators. With this notation we have

LEMMA 2.13.

$$(ad_x + b)\mathcal{L}^{-1}f = \tilde{\mathcal{L}}^{-1}(d_x \tilde{a} - \tilde{c})f, \quad f \in L^2. \quad (2.14)$$

Let us recall here that the functions  $a, b \dots$  are identified with the operator of pointwise multiplication they define. Both operators in (2.14) are well-defined and bounded on all  $L^p$  spaces. It suffices to verify formally that

$$\tilde{\mathcal{L}}(ad_x + b)g = (d_x \tilde{a} - \tilde{c})\mathcal{L}g, \quad (2.15)$$

for appropriate functions  $g$ . The justification is an exercise on unbounded operators on  $L^2$  which is left to the reader.

Using (2.11) and (2.14), we see that

$$(ad_x + b)\tilde{\mathcal{L}}^{-1}(d_x \tilde{a} - \tilde{c}) = -a \quad \text{modulo } \mathcal{B}(L^1, L^\infty). \quad (2.16)$$

But, Lemmata 2.8 and 2.10 applied to  $\tilde{\mathcal{L}}$  also yield that

$$(ad_x + b)\tilde{\mathcal{L}}^{-1}(d_x \tilde{a} - \tilde{c}) = ad_x \tilde{\mathcal{L}}^{-1}d_x \tilde{a} \quad \text{modulo } \mathcal{B}(L^1, L^\infty). \quad (2.17)$$

Hence, we deduce from (2.16–17) and  $1/a, 1/\tilde{a} \in L^\infty$  that

$$d_x \tilde{\mathcal{L}}^{-1} d_x = -\frac{1}{\tilde{a}} \text{ modulo } \mathcal{B}(L^1, L^\infty).$$

By symmetry, this means that we have shown

$$d_x \mathcal{L}^{-1} d_x = -\frac{1}{a} \text{ modulo } \mathcal{B}(L^1, L^\infty).$$

The exponential decay away from the diagonal of the kernel of  $d_x \mathcal{L}^{-1} d_x$  now follows by inspection of the above argument, tracing back all operators in  $\mathcal{B}(L^1, L^\infty)$  whose kernels have exponential decay by the previous lemmata (variations on the methods in the Appendix could also be used).

*Proof of Lemma 2.12.* First, by separating imaginary and real parts, we may and do assume that  $u, v, w$  are real-valued. Since  $u, d_x u \in L^1_{loc}$ , standard arguments show that the derivative of  $u$  exists almost everywhere in the classical sense with  $u' = v + w$  a.e. and that  $u$  can be redefined pointwise to be continuous with

$$u(x) = f(x) + g(x), \quad x \in \mathbb{R},$$

where  $f'(x) = v(x)$  and  $g'(x) = w(x)$  a.e.. Since  $v \in L^1, f \in L^\infty$  and call  $M = \|v\|_1 \geq \|f\|_\infty$ . We show that  $g = g_1 + g_2$  where  $g_1 \in L^\infty$  and  $g_2 \in W^{1,p}$ . From the Sobolev embedding theorem  $W^{1,p} \subset L^\infty$ , we conclude that  $g \in L^\infty$ , hence  $u \in L^\infty$ .

For  $s > 0$  let  $O_s = \{|g| > s\}$ . If  $s \geq 2M$ , Tchebychev's inequality yields

$$\begin{aligned} |O_s| &\leq |\{|f| > s/2\}| + |\{|u| > s/2\}| = |\{|u| > s/2\}| \\ &\leq \left\{ \frac{2 \|u\|_q}{s} \right\}^q < \infty \end{aligned} \tag{2.18}$$

since  $u \in L^q$ . Let  $\varphi \in \mathcal{C}^1(\mathbb{R})$  be an odd non-decreasing real-valued function with  $\varphi(y) = 0$  if  $0 \leq y \leq 2M$  and  $\varphi(y) = y$  if  $y \geq 4M$ . If  $\psi(y) = y - \varphi(y)$ , it is clear that  $\|\psi\|_\infty \leq 2M$ . For each  $x \in \mathbb{R}$ , we have  $g(x) = \psi(g(x)) + \varphi(g(x)) \equiv g_1(x) + g_2(x)$ , where  $\|g_1\|_\infty \leq \|\psi\|_\infty$ . We show that  $g_2 \in W^{1,p}$ .

Let  $t > 0$ , since  $|\varphi(y)| > 0$  implies  $|y| > 2M$ , we have  $\{|g_2| > t\} \subset O_{2M}$ . Furthermore, if  $t \geq 4M$  then  $\{|g_2| > t\} = \{|g| > t\} = O_t$  since  $|\varphi(y)| > t \geq 4M$  is equivalent to  $|y| > t \geq 4M$ . Hence,

$$\begin{aligned}
\int |g_2|^p &= p \int_0^\infty t^{p-1} |\{|g_2| > t\}| dt \\
&\leq p \int_0^{4M} t^{p-1} |O_{2M}| dt + p \int_{4M}^\infty t^{p-1} |O_t| dt \\
&\leq (4M)^p |O_{2M}| + p2^q \|u\|_q^q \int_{4M}^\infty t^{p-q-1} dt \\
&\leq C(p, q) \|u\|_q^q M^{p-q}
\end{aligned}$$

since  $p < q$ . We have used (2.18) to obtain the second inequality. Thus,  $g_2 \in L^p$ . Furthermore,  $g_2'(x) = \varphi'(g(x)) g'(x) = \varphi'(g(x)) w(x)$  a.e. and since  $\varphi' \in L^\infty$  and  $w \in L^p$ , we have  $g_2' \in L^p$ . This completes the proof.

The uniform ellipticity used in this section can be slightly relaxed and this is the object of the next result.

**THEOREM 2.19.** *Let  $\mathcal{L} = \mathcal{L}(A)$  be as in (2.1) where the entries  $a, b, c, d$  of  $A$  are bounded measurable complex-valued functions. Assume that  $|\arg a(x)| \leq \omega$  a.e. for some  $\omega < \pi/2$  and that  $\mathcal{L}$  is invertible from  $H^1$  onto  $H^{-1}$ . Then  $\mathcal{L}^{-1}$  extends to a bounded operator from  $W^{-1,p}$  onto  $W^{1,p}$  for any  $p \in [1, +\infty]$  and the conclusion of Theorem 2.4 holds.*

Let us start with the following classical lemma, the proof of which can be done via rescaling considerations and is skipped.

**LEMMA 2.20.** *If  $\mathcal{L} = \mathcal{L}(A)$  is an isomorphism between  $H^1$  and  $H^{-1}$  then  $a$  has a bounded inverse and  $\|a^{-1}\|_\infty \leq \|\mathcal{L}^{-1}\|_{H^{-1} \rightarrow H^1}$ .*

The proof of Theorem 2.19 is the same as that of Theorem 2.4. A careful examination of the argument shows that without the assumption on  $\arg a(x)$ , the conclusion of Theorem 2.4 holds with the exception of the control on  $|\partial_x \partial_y G(x, y)|$ . As a consequence, Corollary 2.7 holds under the hypothesis that  $\mathcal{L}$  is invertible from  $H^1$  onto  $H^{-1}$ .

Now, to obtain control on the cross and second derivative of  $G(x, y)$  one could try to find an analog to (2.14), but this seems harder to do. Instead, observe that for a large positive number  $\lambda$ ,  $\begin{pmatrix} a & c \\ b & d+\lambda \end{pmatrix}$  is uniformly accretive. This is where we use the hypothesis on  $\arg a$ . Thus, Theorem 2.4 applies to  $\mathcal{L} + \lambda$ . Next, the resolvent formula

$$d_x \mathcal{L}^{-1} d_x = d_x (\mathcal{L} + \lambda)^{-1} d_x + d_x (\mathcal{L} + \lambda)^{-1} \lambda \mathcal{L}^{-1} d_x$$

yields a representation of  $\partial_x \partial_y G(x, y)$  that gives estimate (2.6).

2.2. *The Heat Kernel*

Let  $\mathcal{L}_0 = -d_x a d_x \in \mathcal{E}_0$  and call  $S_t = e^{-t\mathcal{L}_0}$ ,  $t > 0$ , the contraction semi-group on  $L^2$  generated by  $-\mathcal{L}_0$ . Recall that the function  $a(x)$  takes complex values. We prove Gaussian estimates on the heat kernel of  $\mathcal{L}_0$ , i.e., on the kernel  $K_t^0(x, y)$  of  $S_t$ .

**THEOREM 2.21.** *For each  $t > 0$ ,  $K_t^0(x, y)$  is a Lipschitz continuous function which satisfies the following bounds,*

$$|K_t^0(x, y)| \leq c G_{\beta, t}(x - y), \tag{2.22}$$

$$|\partial_x K_t^0(x, y)| + |\partial_y K_t^0(x, y)| \leq ct^{-1/2} G_{\beta, t}(x - y) \quad a.e. \tag{2.23}$$

and

$$\begin{aligned} & |\partial_x \partial_y K_t^0(x, y)| + |\partial_x a(x) \partial_x K_t^0(x, y)| + |\partial_y a(y) \partial_y K_t^0(x, y)| \\ & \leq ct^{-1} G_{\beta, t}(x - y) \quad a.e.. \end{aligned} \tag{2.24}$$

The constants  $c$  and  $\beta > 0$  depend only on the ellipticity constants of  $\mathcal{L}_0$ . (See Section 1 for the definition of  $G_{\beta, t}$ .)

*Proof.* The argument relies on a contour integral, the estimates of Theorem 2.4, and rescaling.

The contour integral is the following

$$e^{-t\mathcal{L}_0} = \frac{1}{2\pi i} \int_{\gamma} e^{t\lambda} (\lambda + \mathcal{L}_0)^{-1} d\lambda. \tag{2.25}$$

The path  $\gamma$  consists of two half-rays  $\gamma_{\pm 1} = \{\lambda = re^{\pm i\mu}, r \geq R\}$  and of the arc  $\gamma_0 = \{\lambda = Re^{i\theta}, |\theta| \leq \mu\}$ , where  $\mu \in (\pi/2, \pi)$ . Because of the exponential factor, we have to choose  $\mu \in (\pi/2, \pi)$  to obtain convergence. This we can do by Remark 1.5 in Section 1. The integral does not depend on the choice of  $R$  and  $\mu$ . In terms of kernels this equality becomes

$$K_t^0(x, y) = \frac{1}{2\pi i} \int_{\gamma} e^{t\lambda} R_{\lambda}(x, y) d\lambda, \tag{2.26}$$

where  $R_{\lambda}(x, y)$  is the kernel of  $(\lambda + \mathcal{L}_0)^{-1}$ .

Now, we use a rescaling argument to deduce estimates on  $R_{\lambda}(x, y)$  from Theorem 2.4 with the correct dependence on  $\lambda$ . Set  $\lambda = re^{i\theta}$ , then it is easy to see that

$$R_{\lambda}(x, y) = r^{-1/2} G_{r, \theta}(r^{1/2}x, r^{1/2}y),$$

where  $G_{r,\theta}(x,y)$  is the Green kernel of  $\mathcal{L}_{r,\theta} = -d_x a(r^{-1/2} \cdot) d_x + e^{i\theta}$ . As explained in Remark 1.5, this operator is, up to a rotation factor, in  $\mathcal{E}$ , and the estimates of Theorem 2.4 hold uniformly for  $e^{i\theta} \in \mathcal{S}_\mu$  and  $r > 0$ . Thus,

$$|R_\lambda(x,y)| \leq c |\lambda|^{-1/2} \exp\{-\alpha |\lambda|^{1/2} |x-y|\} \quad (2.27)$$

where  $c$  and  $\alpha$  depend only on  $\delta(a)$ ,  $\|a\|_\infty$  and  $\mu$ . We also obtain the estimates on the derivatives of  $R_\lambda(x,y)$  in the same way.

Inserting (2.27) in (2.26) we obtain

$$\begin{aligned} |K_t^0(x,y)| &\leq c_0 \int_\gamma e^{t \operatorname{Re} \lambda} |\lambda|^{-1/2} e^{-\alpha |\lambda|^{1/2} |x-y|} |d\lambda| \\ &\leq I_1 + I_0 + I_{-1}, \end{aligned} \quad (2.28)$$

where  $I_k$  is the contribution from the path  $\gamma_k$ . First

$$\begin{aligned} I_1 &\leq c_1 \int_R^{+\infty} e^{tr \cos \mu} r^{-1/2} dr e^{\alpha R^{1/2} |x-y|} \\ &\leq c_2 t^{-1/2} e^{-\alpha R^{1/2} |x-y|}. \end{aligned} \quad (2.29)$$

The contribution from  $\gamma_{-1}$  is the same. For the last term, we make use of

$$\int_0^{2\pi} e^{s \cos \theta} d\theta \leq \frac{c_3 e^s}{s^{1/2}}, \quad s > 0 \quad (2.30)$$

(which is a bad estimate if  $s$  is small). Hence,

$$\begin{aligned} I_0 &\leq c_4 \int_{|\theta| \leq \mu} e^{tR \cos \theta} R d\theta R^{-1/2} e^{-\alpha R^{1/2} |x-y|} \\ &\leq c_5 t^{-1/2} e^{tR - \alpha R^{1/2} |x-y|} \end{aligned} \quad (2.31)$$

Now, we choose  $R = (\alpha^2 |x-y|^2)/4t^2$ . Hence,  $\alpha R^{1/2} |x-y| = \alpha^2 |x-y|^2/2t$  and  $tR = (\alpha^2 |x-y|^2)/4t$ . Combining all the inequalities (2.29–2.31), we obtain

$$|K_t(x,y)| \leq c_6 t^{-1/2} e^{-(\alpha^2 |x-y|^2)/4t}.$$

The estimates for the derivatives can be done in the same way except for a minor technical change in the choice of  $R$ . Let us quickly look at  $\partial^v K_t(x,y)$ , where  $\partial$  is  $a(x)\partial_x$  or  $a(y)\partial_y$ , and  $v = 1$  or  $2$  (with this definition, all second derivatives make sense). First, the same rescaling argument yields

$$|\partial^v R_\lambda(x,y)| \leq C |\lambda|^{-1/2-v} e^{-\alpha |\lambda|^{1/2} |x-y|}. \quad (2.32)$$

Following the same decomposition of the path  $\gamma$ , the first and third contributions for  $\partial^v K_t(x, y)$  are of the order of

$$c_7 \int_{Rt}^{+\infty} e^{s \cos \mu} s^{-1/2-v} ds t^{-1/2-v} e^{-\alpha R^{1/2} |x-y|},$$

while the second contribution is

$$c_8 \frac{(tR)^v}{t^{1/2+v}} e^{tR - \alpha R^{1/2} |x-y|}.$$

Choosing  $R = \sup((\alpha^2 |x-y|^2/4t^2), t^{-1})$  we obtain that

$$|\partial^v K_t(x, y)| \leq c_9(\varepsilon) t^{-1/2-v} \exp \left\{ \frac{-\alpha^2 |x-y|^2}{4(1+\varepsilon)t} \right\} \quad \text{a.e.}, \quad (2.33)$$

for all  $\varepsilon > 0$ . (It is not necessary to use (2.30) as an estimate in  $2\pi e^s$  suffices in these computations.)

*Remark 2.34.* The constant  $\beta$  in (2.22) is  $\alpha^2/4$  where  $\alpha$  is the best constant in (2.5) for the kernels  $G_{r, \theta}(x, y)$ . This number depends on the ellipticity constants and on  $\mu$ . Optimizing over  $\mu$  would not give Davies sharp bound when  $a(x)$  is real-valued [Da2].

*Remark 2.35.* The kernels  $\partial^2 K_t^0(x, y)$  have no singularity on the diagonal. For example, recall from (2.16–17) that

$$ad_x(\mathcal{L}_0 + \lambda)^{-1} d_x a = -a + T_\lambda$$

where  $T_\lambda$  has a bounded kernel satisfying (2.32) with  $\nu = 2$ . Now, inserting this identity in (2.25) we see that

$$ad_x S_t d_x a = - \left( \frac{1}{2\pi i} \int_\gamma e^{t\lambda} d\lambda \right) a + \frac{1}{2\pi i} \int_\gamma e^{t\lambda} T_\lambda d\lambda.$$

Because of Cauchy’s theorem, the first term of the right hand side in the above equality vanishes and the part with  $T_\lambda$  does not bring any singularity. The other second derivatives can be dealt with in the same way.

The same technique applies for any operator  $\mathcal{L} \in \mathcal{E}$  of type (2.1) and a similar result holds for the heat kernel of this operator. First, the rescaling goes only for  $|\lambda|$  large and since 0 is not in the spectrum of such operators we can use estimates of Theorem 2.4 directly for  $|\lambda|$  small. This yields a decreasing exponential function of  $t$  in all estimates. Also, the “second derivatives” for the heat kernel have to be taken as for the Green function in Theorem 2.4. The precise statement is the following.

**THEOREM 2.36.** *Let  $\mathcal{L} = -d_x(ad_x + b) + cd_x + d \in \mathcal{E}$ . For each  $t > 0$ , the heat kernel  $K_t(x, y)$  of  $e^{-t\mathcal{L}}$  is a Lipschitz continuous function which satisfies the following bounds,*

$$|K_t(x, y)| \leq ce^{-\omega t} G_{\beta, t}(x, y), \quad (2.37)$$

$$|\partial_x K_t(x, y)| + |\partial_y K_t(x, y)| \leq ct^{-1/2} e^{-\omega t} G_{\beta, t}(x - y) \quad a.e. \quad (2.38)$$

and

$$\begin{aligned} & |a(x) \partial_x \partial_y K_t(x, y)| \\ & \quad + |\partial_x(a(x) \partial_x + b(x)) K_t(x, y)| + |\partial_y(a(y) \partial_y + c(y)) K_t(x, y)| \\ & \leq ct^{-1} e^{-\omega t} G_{\beta, t}(x - y) \quad a.e.. \end{aligned} \quad (2.39)$$

The constants  $c, \beta > 0$  and  $\omega > 0$  depend only on the ellipticity constants of  $\mathcal{L}$ .

### 3. THE TWO DIMENSIONAL CASE

In dimension two, the Green function of  $\mathcal{L} \in \mathcal{E}$  is expected to have a logarithmic singularity on the diagonal. On the other hand, we prove that the kernel of  $\mathcal{L}^{-2}$  is bounded and Hölder continuous. Then, we transfer these estimates to heat kernels, and finally show that the Green kernel has indeed the expected behavior. If  $\mathcal{L}_0 \in \mathcal{E}_0$ , its fundamental solution does not exist as a distribution, but we give it a sense modulo constants and describe its properties. As a consequence, a generalization of Wentz's estimate is obtained.

#### 3.1. Taking High Powers

We begin with a perturbation result, valid in all dimensions.

**PROPOSITION 3.1.** *Let  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$ . Then there exists  $v \in (0, 1/2)$  depending on  $\delta(A)$ ,  $\|A\|$  and dimension only such that  $\mathcal{L}^{-1}$  extends as a bounded and invertible operator from  $W^{-1, p}$  onto  $W^{1, p}$  for all  $p$  with  $|1/p - 1/2| < v$ .*

This result is well-known when  $A$  is symmetric, see [BLP]. One needs the following observation to extend the argument to the accretive case. There exists a large constant  $M$  such that  $\|A - MI\| < M$ . Thus,  $A = M(I - B)$  where  $\|B\| < 1$ . This means that

$$\mathcal{L}(A) = M(I - \Delta - \mathcal{L}(B)) = MA(I - A^{-1}\mathcal{L}(B)A^{-1})A,$$

where  $\Delta$  denotes the ordinary Laplacian and  $A = (I - \Delta)^{1/2}$ . Expressing precisely  $A^{-1}\mathcal{L}(B)A^{-1}$  in terms of Riesz transforms, one sees that this operator is bounded on  $L^p$ ,  $1 < p < +\infty$  with norm in  $\mathcal{B}(L^2, L^2)$  not exceeding  $\|B\| < 1$ . Proceeding by convexity as in [BLP], its norm in  $\mathcal{B}(L^p, L^p)$  remains strictly less than 1 if  $p$  is close to 2. Therefore, one inverts  $I - A^{-1}\mathcal{L}(B)A^{-1}$  by a converging Neumann series in  $\mathcal{B}(L^p, L^p)$  for  $p$  close to 2. This proves the Proposition.

We return to dimension  $n = 2$  for the rest of this section.

LEMMA 3.2. *Let  $\mathcal{L} \in \mathcal{E}$ . If  $\nu$  is as in Proposition 3.1, then  $\mathcal{L}^{-2}$  extends to a bounded operator from  $L^1$  to  $L^\infty \cap C^\eta$  for all  $\eta \in (0, 2\nu)$ . Moreover, the kernel  $G^{(2)}(x, y)$  of  $\mathcal{L}^{-2}$  satisfies the following bounds*

$$|G^{(2)}(x, y)| \leq c \exp\{-\alpha |x - y|\} \tag{3.3}$$

$$\begin{aligned} & |G^{(2)}(x, y) - G^{(2)}(x + h, y)| + |G^{(2)}(x, y) - G^{(2)}(x, y + h)| \\ & \leq c |h|^\eta \exp\{-\alpha |x - y|\} \end{aligned} \tag{3.4}$$

when  $2|h| \leq |x - y|$ , the constants  $c$  and  $\alpha > 0$  depending only the ellipticity constants.

*Proof.* We start by showing that  $\mathcal{L}^{-2}$  is bounded from  $L^1$  to  $L^\infty \cap C^\eta$ . Pick  $p > 2$  with  $1/p - 1/2 < \nu$ . Since  $L^1 \subset W^{-1,p}$ , Proposition 3.1 yields

$$\mathcal{L}^{-1} : L^1 \rightarrow W^{1,p}.$$

Now, the Sobolev embedding theorem yields  $W^{1,p} \subset W^{-1,q}$  for any  $q > 2$  with  $1/2 - 1/q < \nu$  (recall that dimension is 2). Applying Proposition 3.1 again we obtain

$$\mathcal{L}^{-2} : L^1 \rightarrow W^{1,q}$$

and we conclude with the Sobolev embedding  $W^{1,q} \subset L^\infty \cap \dot{C}^\eta$  with  $\eta = 1 - 2/q$ .

This implies that  $G^{(2)}(x, y)$  is bounded a.e. in  $\mathbb{R}^2 \times \mathbb{R}^2$ , and that it is a Hölder continuous function of  $y$  uniformly in  $x$ . Applying the method in the Appendix, we obtain the exponential decay in (3.3) and half of (3.4), the other half being obtained by duality since  ${}^t\mathcal{L} \in \mathcal{E}$ .

### 3.2. The Heat Kernel

We first restrict our attention to the heat kernels of operators in  $\mathcal{E}_0$ .

THEOREM 3.5. *Let  $\mathcal{L}_0 \in \mathcal{E}_0$  and let  $K_t^0(x, y)$  be the distribution-kernel of the  $L^2$  contraction semi-group  $e^{-t\mathcal{L}_0}$ ,  $t > 0$ . Then, for all  $t > 0$ ,  $K_t^0(x, y)$*

is a bounded Hölder continuous function which satisfies the following bounds:

$$|K_t^0(x, y)| \leq c G_{\beta, t}(x - y), \quad (3.6)$$

$$\begin{aligned} & |K_t^0(x, y) - K_t^0(x + h, y)| + |K_t^0(x, y) - K_t^0(x, y + h)| \\ & \leq c \left( \frac{|h|}{t^{1/2} + |x - y|} \right)^\eta G_{\beta, t}(x - y), \end{aligned} \quad (3.7)$$

when  $2|h| \leq t^{1/2} + |x - y|$  and  $\eta \in (0, 2\nu)$  where  $c, \beta > 0$  and  $\nu > 0$  depend on the ellipticity constants only.

The proof goes along the same lines as the argument in one dimension with one modification. From formula (2.25), one can integrate by parts successively and obtain

$$e^{-t\mathcal{L}_0} = \frac{(m-1)!}{2\pi i t^{m-1}} \int_\gamma e^{t\lambda} (\lambda + \mathcal{L}_0)^{-m} d\lambda \quad (3.8)$$

for any integer  $m$ . Here, we take  $m = 2$ . Thus,

$$K_t^0(x, y) = \frac{1}{2\pi i t} \int_\gamma e^{t\lambda} R_\lambda^2(x, y) d\lambda \quad (3.9)$$

where  $R_\lambda^2(x, y)$  is the kernel of  $(\lambda + \mathcal{L})^{-2}$ . As before, the path  $\gamma$  consists of two half-rays  $\gamma_{\pm 1} = \{\lambda = r e^{\pm i\mu}, r \geq R\}$  and of the arc  $\gamma_0 = \{\lambda = R e^{i\theta}, |\theta| \leq \mu\}$  with  $\mu \in (\pi/2, \pi)$  (Remark 1.5 in Section 1) and  $R = \sup((\alpha^2 |x - y|^2)/4t^2, t^{-1})$ , where  $\alpha > 0$  as the constant in (3.3) for a uniform family of operators in  $\mathcal{E}$  (same explanation as in dimension one). Using rescaling, one has

$$|R_\lambda^2(x, y)| \leq c |\lambda|^{-1} \exp\{-\alpha |\lambda|^{1/2} |x - y|\}, \quad (3.10)$$

Breaking up the integral (3.9) as in Section 2 leads to the desired estimate (3.6). We skip the details for (3.7), which are similar. The proof is complete.

Let us make a remark. Even though this theorem says, in particular, that the semi-group extends to a bounded semi-group on  $L^p$  (with usual care if  $p = +\infty$ ), this does not say what is the domain of the  $L^p$ -infinitesimal generator of this semi-group (except if  $p = 2$ ). It is in fact a difficult question which is open even when  $\mathcal{L} = \mathcal{L}(A_0)$ , with  $A_0$  real symmetric and positive definite.

**THEOREM 3.11.** *Let  $\mathcal{L} \in \mathcal{E}$  and let  $K_t(x, y)$  be the distribution-kernel of the  $L^2$  contraction semi-group  $e^{-t\mathcal{L}}$ ,  $t > 0$ . Then, for all  $t > 0$ ,  $K_t(x, y)$*

is a bounded Hölder continuous function which satisfies the following bounds:

$$|K_t(x, y)| \leq c e^{-\omega t} G_{\beta, t}(x - y), \tag{3.12}$$

$$\begin{aligned} & |K_t(x, y) - K_t(x + h, y)| + |K_t(x, y) - K_t(x, y + h)| \\ & \leq c e^{-\omega t} \left( \frac{|h|}{t^{1/2} + |x - y|} \right)^\eta G_{\beta, t}(x - y), \end{aligned} \tag{3.13}$$

when  $2|h| \leq t^{1/2} + |x - y|$  and  $\eta \in (0, 2v)$  where  $c, \beta > 0, \omega$  and  $v > 0$  depend on the ellipticity constants only.

The proof is similar to the proof of Theorem 3.5, though a little more technical especially when writing the appropriate substitute for (3.10). We skip the proof.

**COROLLARY 3.14.** *Let  $\mathcal{L} \in \mathcal{E}$ . Then its Green kernel,  $G(x, y)$ , satisfies*

$$\begin{aligned} |G(x, y)| & \leq c \ln \left( \frac{1}{|x - y|} + e \right) \exp\{-\alpha |x - y|\}, \quad a.e., \\ |G(x, y) - G(x + h, y)| + |G(x, y) - G(x, y + h)| \\ & \leq c \left( \frac{|h|}{|x - y|} \right)^\eta \exp\{-\alpha |x - y|\} \end{aligned}$$

when  $2|h| \leq |x - y|$  and  $\eta \in (0, 2v)$  where  $c, \alpha$  and  $v > 0$  depend on the ellipticity constants only.

Denoting by  $K_t(x, y)$  the kernel of  $e^{-t\mathcal{L}}$ , we have

$$G(x, y) = \int_0^{+\infty} K_t(x, y) dt \tag{*}$$

and breaking up the integral at  $\tau \equiv \sup(|x - y|, 1)$ , we obtain

$$\begin{aligned} |G(x, y)| & \leq c \int_0^\tau G_{\beta, t}(x - y) dt + c \int_\tau^{+\infty} e^{-t\omega} \frac{dt}{t} \\ & \leq c \ln \left( \frac{1}{|x - y|} + e \right) \exp\{-\beta |x - y|\} + c \exp\{-\beta |x - y|\}, \end{aligned}$$

where  $c$  and  $\beta > 0$  change at each occurrence.

It remains to establish the Hölder estimate in the  $x$  variable. The Hölder estimate in the  $y$  variable follows by duality. If  $2|h| \leq |x-y|$ , the estimate

$$|K_t(x+h, y) - K_t(x, y)| \leq ce^{-\omega t} \left( \frac{|h|}{t^{1/2}} \right)^n G_{\beta, t}(x-y),$$

is valid for all  $t > 0$ . Hence, integration from 0 to  $\infty$ , gives

$$|G(x, y) - G(x+h, y)| \leq c \left( \frac{|h|}{|x-y|} \right)^n.$$

This is sufficient as long as  $|x-y| \leq 1$ . If  $|x-y| \geq 1$  break the integral (\*) at  $t = |x-y|$ , and use the regularity estimate (3.13) for small  $t$  and the size estimate (3.12) for large  $t$ . Further details are skipped.

### 3.3. Fundamental Solution of $-\operatorname{div}(A\nabla)$

Let  $\mathcal{L} = -\operatorname{div}(A\nabla) \in \mathcal{E}_0$  (in this section, we drop the subscript 0). Although there is no distribution  $\Gamma(x, y) \in \mathcal{S}'(\mathbb{R}^2 \times \mathbb{R}^2)$  such that  $L_x \Gamma(x, y) = \delta_y$ , there is a possible definition of a fundamental solution as a distribution modulo constants. We come to this now.

We first observe that  $\mathcal{L}$  is an isomorphism from the homogeneous Sobolev space  $\dot{W}^{1,2}$  onto its dual  $\dot{W}^{-1,2}$ . The notation  $\mathcal{L}^{-1}$  stands for its inverse. For  $f \in \dot{W}^{-1,2}$ ,  $\mathcal{L}^{-1}f$  is the unique solution  $u \in \dot{W}^{1,2}$  of the problem

$$\langle A \nabla u, \nabla \varphi \rangle = (\bar{\varphi}, f), \quad \forall \varphi \in \dot{W}^{1,2}.$$

The first bracket is the usual sesquilinear form acting on scalar- or vector-valued  $L^2$  functions. The second bracket is the bilinear duality form between  $\dot{W}^{1,2}$  and  $\dot{W}^{-1,2}$ . We recall that this bracket coincides with the duality brackets between distribution modulo constants and test functions with vanishing mean or between BMO and  $\mathcal{H}^1$  when  $f$  and  $\varphi$  are appropriately chosen. We refer to [St] for definitions and properties of BMO and  $\mathcal{H}^1$ .

Now, the Sobolev embeddings in  $\mathbb{R}^2$  imply that  $\mathcal{L}^{-1}$  maps the Hardy space  $\mathcal{H}^1$  continuously into its dual, BMO. In fact, we prove that the range of this map is contained in  $C_0$ , the space of continuous functions on  $\mathbb{R}^2$  vanishing at infinity. In the case where the matrix has real coefficients, the existence of the fundamental solution is known (see, e.g., [CL]) and can be achieved by use of the maximum principle. In the complex case, this tool is not available and we use instead the functional calculus and especially the heat kernel. The issue here is to give a meaning to the formula  $\mathcal{L}^{-1}f = \left( \int_0^\infty e^{-t\mathcal{L}} dt \right) f$  when  $f \in \mathcal{H}^1$ . The problem is the logarithmic divergence of the integral  $\int_1^{+\infty} K_t(x, y) dt$  and we are led to the following definition.

For  $x, y \in \mathbb{R}^2$ ,  $x \neq y$ , define

$$\Gamma(x, y) = \int_0^1 K_t(x, y) dt + \int_1^{+\infty} K_t(x, y) - K_t(x, x) dt. \quad (3.15)$$

**THEOREM 3.16.** *Suppose that  $\mathcal{L} \in \mathcal{E}_0$ . Then for all  $x \in \mathbb{R}^2$ ,  $\Gamma(x, \cdot) \in BMO$  and the function defined by  $Tf(x) = (\Gamma(x, \cdot), f)$  for  $f \in \mathcal{H}^1$  belongs to  $C_0$ . The linear map  $T$  thus defined is continuous from  $\mathcal{H}^1$  into  $C_0$  and coincides with the restriction to  $\mathcal{H}^1$  of  $\mathcal{L}^{-1}$ . Finally, there are constants  $c$  and  $\eta \in (0, 1)$ , depending only the ellipticity constants, such that for all  $x, y, h$  with  $0 < |h| \leq \frac{1}{2}|x - y|$ ,*

$$|\Gamma(x, y)| \leq c |\ln |x - y||, \quad (3.17)$$

$$|\Gamma(x, y + h) - \Gamma(x, y)| \leq c \left( \frac{|h|}{|x - y|} \right)^\eta, \quad (3.18)$$

$$|\Gamma(x + h, y) - \Gamma(x, y) - g(x, h)| \leq c \left( \frac{|h|}{|x - y|} \right)^\eta, \quad (3.19)$$

where  $|g(x, h)| \leq c \min\{|h|^\eta, \ln(e + |h|)\}$  for all  $x$ .

The function  $\Gamma(x, y)$  can be considered as the fundamental solution of  $\mathcal{L}$ , with the expected properties. An example of application of this result is an extension of a result of Wentz to complex elliptic operators (see [CL] and [BG] for the extension to the case of general real elliptic operators).

**COROLLARY 3.20.** *Suppose  $A$  is a uniformly accretive matrix with bounded complex measurable coefficients on  $\mathbb{R}^2$ . Let  $u, v$  belong to  $W^{1,2}$ . Then the equation*

$$\operatorname{div}(A \nabla w) = \partial_{x_1} u \partial_{x_2} v - \partial_{x_2} u \partial_{x_1} v$$

has a unique solution in  $W^{1,2}$ . Moreover, this solution belongs to  $C_0$  and

$$\|w\|_\infty + \|\nabla w\|_2 \leq c \|\nabla u\|_2 \|\nabla v\|_2,$$

where  $c$  depends on  $\delta(A)$  and  $\|A\|$  only.

As shown in [CLMS], the function  $f = \partial_{x_1} u \partial_{x_2} v - \partial_{x_2} u \partial_{x_1} v$  belongs to  $\mathcal{H}^1$ , with norm controlled by  $c_0 \|\nabla u\|_2 \|\nabla v\|_2$  where  $c_0$  is a universal constant. Hence,  $w = Tf$  is the desired solution.

We now turn to the proof of the Theorem 3.16, which is done in three steps.

*Step 1. Definition of an approximation of  $T$ .* For  $R > 1$ , define  $T_R = \int_0^R e^{-t\mathcal{L}} dt$ . Note that it follows from Theorem 3.5 that  $T_R$  is defined on all  $L^p$  spaces,  $p \geq 1$ , with norm not exceeding  $cR$ , for some numerical constant  $c$ . Hence, the action of  $T_R$  on atoms makes sense. Let  $a$  be an atom supported in a ball  $B$ , i.e., we assume  $\int a = 0$  and  $\|a\|_\infty \leq |B|^{-1}$ , where  $|B|$  denotes the Lebesgue measure of  $B$  (see, e.g., [St]). For each  $x \in \mathbb{R}^2$ , Theorem 3.5, Fubini's theorem and the mean value property of  $a$  yields

$$\begin{aligned} T_R a(x) &= \int_0^R \int K_t(x, y) a(y) dy dt \\ &= \int_0^1 \int K_t(x, y) a(y) dy dt + \int_1^R \int (K_t(x, y) - K_t(x, x)) a(y) dy dt \\ &= \int \Gamma_R(x, y) a(y) dy, \end{aligned} \tag{3.21}$$

where

$$\Gamma_R(x, y) = \int_0^1 K_t(x, y) dt + \int_1^R K_t(x, y) - K_t(x, x) dt. \tag{3.22}$$

Both integrals are absolutely convergent if  $x \neq y$  and we have

$$|\Gamma_R(x, y)| \leq C |\ln |x - y||, \tag{3.23}$$

uniformly for all  $R$ . We postpone the proof of this.

LEMMA 3.24. (i)  $\Gamma_R(x, \cdot) \in BMO$  and its norm satisfies

$$\sup_{R > 1} \sup_{x \in \mathbb{R}^2} \|\Gamma_R(x, \cdot)\|_* = c_0 < +\infty.$$

(ii) There exists  $c_1$  such that for all atoms  $a$

$$\sup_{R > 1} \|T_R a\|_\infty \leq c_1.$$

(iii) For all atoms,  $T_R a$  is a Hölder continuous function vanishing at infinity.

Admitting this lemma, we can define  $T_R$  on  $\mathcal{H}^1$  as follows. Let  $f \in \mathcal{H}^1$  and choose an atomic decomposition of  $f(x) = \sum_1^\infty \lambda_i a_i(x)$  a.e. where  $a_i$

are atoms and  $(\lambda_i)$  is an  $l^1$  sequence whose norm is comparable to  $\|f\|_{\mathcal{H}^1}$ . We set

$$T_R f(x) = \sum_1^\infty \lambda_i T_R a_i(x). \tag{3.25}$$

First, the sum converges uniformly to a  $C_0$  function by (ii) and (iii) above. To show that this definition does not depend on the choice of the decomposition of  $f$ , we establish that

$$\sum_1^\infty \lambda_i T_R a_i(x) = (\Gamma_R(x, \cdot), f), \quad \forall x \in \mathbb{R}^2. \tag{3.26}$$

Both sides of (3.26) are well-defined at every point and call  $g(x)$  the difference. Set  $f_n = \sum_1^n \lambda_i a_i$ . Since  $T_R a_i(x) = \int \Gamma_R(x, y) a_i(y) dy = (\Gamma_R(x, \cdot), a_i)$ , we have

$$g(x) = \sum_{n+1}^\infty \lambda_i T_R a_i(x) - (\Gamma_R(x, \cdot), f - f_n).$$

Fix  $\varepsilon > 0$  and choose  $n$  such that  $\sum_{n+1}^\infty |\lambda_i| \leq \varepsilon$ . Then from (ii)

$$\left| \sum_{n+1}^\infty \lambda_i T_R a_i(x) \right| \leq c_1 \varepsilon.$$

Also, since  $f - f_n \in L^1$  with  $\|f - f_n\|_1 \leq \varepsilon$ ,

$$\int_{\mathbb{R}^2} |(\Gamma_R(x, \cdot), f - f_n)| dx = \int_{\mathbb{R}^2} |T_R(f - f_n)(x)| dx \leq cR\varepsilon.$$

As this holds for all  $\varepsilon > 0$ , it follows that  $g$  is identically 0.

*Step 2: Definition of  $T$ .*

LEMMA 3.27. *For each  $x \in \mathbb{R}^2$ ,  $\Gamma_R(x, \cdot)$  converges to  $\Gamma(x, \cdot)$  in BMO for the weak star topology as  $R \rightarrow +\infty$ . For each atom  $a$ ,  $T_R a$  converges as  $R$  tends to  $+\infty$  uniformly to a function  $Ta$  and we have the pointwise equalities*

$$Ta(x) = \int \Gamma(x, y) a(y) dy = (\Gamma(x, \cdot), a).$$

To prove this lemma, we start by observing for each  $x$ ,  $\Gamma_R(x, \cdot)$  converges to  $\Gamma_R(x, \cdot)$  in  $L^1_{\text{loc}}$  by dominated convergence, which applies by (3.23). Thus,  $T_R a(x) = \int \Gamma_R(x, y) a(y) dy$  converges to  $\int \Gamma(x, y) a(y) dy$  pointwise and the fact that this convergence is uniform will be proved later.

On the other hand, we also have  $Ta_R(x) = (\Gamma_R(x, \cdot), a)$ . By Lemma 3.24,  $\Gamma_R(x, \cdot)$  is a bounded sequence in BMO, hence, there is a subsequence converging weak star in BMO to a function  $\beta$ . By testing against all atoms, we see that  $\beta = \Gamma(x, \cdot)$  (equality in BMO). Hence,  $\Gamma_R(x, \cdot)$  converges weak star to  $\Gamma(x, \cdot)$  in BMO and the second equality in the lemma follows.

For an arbitrary  $f \in \mathcal{H}^1$ , we set

$$Tf(x) = \sum_1^\infty \lambda_i Ta_i(x), \quad (3.28)$$

where  $f(x) = \sum_1^\infty \lambda_i a_i(x)$  a.e. with  $a_i$  atoms and  $(\lambda_i) \in l^1$  of norm comparable to  $\|f\|_{\mathcal{H}^1}$ . Using the previous lemmata, the sum converges uniformly to a  $C_0$  function and letting  $R \rightarrow +\infty$  in (3.26) yields

$$\sum_1^\infty \lambda_i Ta_i(x) = (\Gamma(x, \cdot), f), \quad \forall x \in \mathbb{R}^2. \quad (3.29)$$

This shows that the definition of  $Tf$  is independent of the choice of the atomic decomposition for  $f$ . The equation (3.28) shows that  $Tf \in C_0$  and equation (3.29) gives

$$\|Tf\|_\infty \leq \sup_{x \in \mathbb{R}^2} \|\Gamma(x, \cdot)\|_* \|f\|_{\mathcal{H}^1}.$$

From weak star convergence, we have

$$\sup_{x \in \mathbb{R}^2} \|\Gamma(x, \cdot)\|_* \leq \sup_{x \in \mathbb{R}^2} \sup_{R \geq 1} \|\Gamma_R(x, \cdot)\|_* \leq c_0$$

by Lemma 3.24(i). Thus, boundedness of  $T$  from  $\mathcal{H}^1$  to  $C_0$  is proved.

*Step 3: Coincidence of  $T$  and  $\mathcal{L}^{-1}$ .* By linearity, it suffices to show that for any atom  $a$ ,

$$\mathcal{L}Ta = a,$$

i.e.,

$$\langle A \nabla Ta, \nabla \varphi \rangle = \langle \bar{\varphi}, a \rangle \quad \forall \varphi \in W^{1,2}.$$

We use the approximation  $T_R$  once again. Since  $a \in L^2$ ,  $T_R a = \int_0^R e^{-t\mathcal{L}} a dt$  belongs to the  $L^2$ -domain of  $\mathcal{L}$  by usual arguments from semi-group theory. Moreover,

$$\mathcal{L}T_R a = \int_0^R \mathcal{L} e^{-t\mathcal{L}} a dt = - \int_0^R \frac{d}{dt} e^{-t\mathcal{L}} a dt = a - e^{-R\mathcal{L}} a. \quad (3.30)$$

This can be written as

$$\langle A \nabla T_R a, \nabla \varphi \rangle = (\bar{\varphi}, a) - (\bar{\varphi}, e^{-R\mathcal{L}} a) \quad \forall \varphi \in W^{1,2}. \quad (3.31)$$

Also  $a \in \mathcal{H}^1 \subset \dot{W}^{-1,2}$ , hence  $a = \operatorname{div} f$  with  $f \in L^2$ . This implies

$$\langle A \nabla T_R a, \nabla \varphi \rangle = -(\nabla \bar{\varphi}, f) - (\bar{\varphi}, e^{-R\mathcal{L}} a) \quad \forall \varphi \in W^{1,2}.$$

Taking in particular  $\bar{\varphi} = T_R a$  and using ellipticity, the Cauchy Schwarz inequality gives

$$\delta \|\nabla T_R a\|_2^2 \leq \|f\|_2 \|\nabla T_R a\|_2 + \|T_R a\|_2 \|e^{-R\mathcal{L}} a\|_2.$$

Now, easy rescaling considerations give us

$$\|e^{-t\mathcal{L}} a\|_2 = \|e^{-t\mathcal{L}} \operatorname{div} f\|_2 \leq C t^{-1/2} \|f\|_2,$$

so

$$\|T_R a\|_2 \leq c \int_0^R t^{-1/2} dt \|f\|_2 = c R^{1/2} \|f\|_2,$$

Hence,

$$\|\nabla T_R a\|_2 \leq c \|f\|_2.$$

Since this estimate is uniform in  $R$ , this implies the existence of a subsequence  $\nabla T_{R_j} a$  converging weakly in  $L^2$  as  $R_j \rightarrow +\infty$ . Together with the uniform convergence of  $T_R a$  to  $Ta$ , this means that this limit must be  $\nabla Ta$  (taken in the sense of distributions). Therefore,  $\nabla Ta \in L^2$  and letting  $R \rightarrow +\infty$  in (3.31) yields the desired equality.

To complete the proof of Theorem 3.16, it remains to establish (3.23), Lemma 3.24, the uniform convergence in Lemma 3.27, as well as (3.18) and (3.19), to the proofs of which we now turn. They all rely on the estimates of Theorem 3.5. The constants in the following will only depend on the constants there, i.e.,  $c$ ,  $\beta$  and  $\eta < 2\nu$  in (3.6–3.7).

Let us start with (3.23). If  $|x - y| \leq 1$ , we have

$$\begin{aligned} \int_0^1 |K_t(x, y)| dt &\leq c \int_0^1 G_{\beta,t}(x, y) dt \\ &= c \int_0^1 \exp \left\{ -\frac{\beta |x - y|^2}{t} \right\} \frac{dt}{t} \leq c |\ln |x - y||, \end{aligned}$$

and

$$\begin{aligned} \int_1^R |K_t(x, y) - K_t(x, x)| dt &\leq c \int_1^R \left( \frac{|x-y|}{t^{1/2}} \right)^\eta G_{\beta, t}(x-y) dt \\ &\leq c \int_1^R \left( \frac{|x-y|}{t^{1/2}} \right)^\eta \frac{dt}{t} \leq c |x-y|^\eta. \end{aligned}$$

Next, if  $|x-y| \geq 1$ , we break up the integrals in a different way:

$$\begin{aligned} \int_0^{|x-y|^2} |K_t(x, y)| dt &\leq c \int_0^{|x-y|^2} \exp \left\{ \frac{\beta |x-y|^2}{t} \right\} \frac{dt}{t} \leq c, \\ \int_1^{|x-y|^2} |K_t(x, x)| dt &\leq c \int_1^{|x-y|^2} \frac{dt}{t} \leq c |\ln |x-y||, \end{aligned}$$

and

$$\int_{|x-y|^2}^R |K_t(x, y) - K_t(x, x)| dt \leq c \int_{|x-y|^2}^R \left( \frac{|x-y|}{t^{1/2}} \right)^\eta \frac{dt}{t} \leq c.$$

(This last integral occurs only when  $|x-y|^2 \leq R$ .) This proves (3.23).

Let us now prove (3.18) and (3.19). By a limiting argument, it suffices to prove them with  $\Gamma_R$  in place of  $\Gamma$  with uniform constants in  $R$ . Let  $x, y, h$  with  $0 < |h| \leq \frac{1}{2} |x-y|$ . From the definition of  $\Gamma_R$  we have

$$\Gamma_R(x, y+h) - \Gamma_R(x, y) = \int_0^R K_t(x, y+h) - K_t(x, y) dt$$

Since  $|h| \leq \frac{1}{2} |x-y|$  we have

$$\begin{aligned} \int_0^R |K_t(x, y+h) - K_t(x, y)| dt &\leq c \int_0^R \left( \frac{|h|}{t^{1/2}} \right)^\eta G_{\beta, t}(x-y) dt \\ &\leq c \left( \frac{|h|}{|x-y|} \right)^\eta. \end{aligned}$$

On the other hand we have

$$\begin{aligned} &\Gamma_R(x+h, y) - \Gamma_R(x, y) \\ &= \int_0^R K_t(x+h, y) - K_t(x, y) dt + \int_1^R K_t(x+h, x+h) - K_t(x, x) dt \end{aligned}$$

The last integral depends on  $R$ ,  $x$  and  $h$  only, and a direct estimate is  $c \min\{|h|^n, \ln(e + |h|)\}$  uniformly in  $R$  and  $x$ . The first integral is estimated as above and gives  $c(|h|/(|x - y|))^n$ .

We now turn to the proof Lemma 3.24, part (i). Fix  $x \in \mathbb{R}^2$  and a ball  $B = B(z, r)$  of center  $z$  and radius  $r$ . We want to show that

$$\int_B |\Gamma_R(x, y) - c_{R, B, x}| dy \leq c |B|$$

for some constant  $c_{R, B, x}$  with  $c$  uniform in  $B$ ,  $R$  and  $x$ . If  $(2r)^2 \leq R$ , write

$$\Gamma_R(x, y) = \int_0^{(2r)^2} K_t(x, y) dt + \int_{(2r)^2}^R K_t(x, y) - K_t(x, z) dt + c_{R, B, x},$$

while if  $(2r)^2 > R$ , write

$$\Gamma_R(x, y) = \int_0^R K_t(x, y) dt + \tilde{c}_{R, B, x},$$

where the numbers  $c_{R, B, x}$ ,  $\tilde{c}_{R, B, x}$  do not depend on  $y$ . Proceeding as above we see that in the first case

$$|\Gamma_R(x, y) - c_{R, B, x}| \leq c + c \ln_+ \left( \frac{2r}{|x - y|} \right) + c \left( \frac{|y - z|}{r} \right)^n,$$

where  $\ln_+ u = \sup(0, \ln u)$ . Hence,

$$\int_B |\Gamma_R(x, y) - c_{R, B, x}| dy \leq c |B| + c \int_B \ln_+ \left( \frac{2r}{|x - y|} \right) dy.$$

Observe that the last integral is 0 if  $|x - z| > 4r$ . If  $|x - z| \leq 4r$ , then  $B \subset B(x, 5r)$  and, therefore, this integral does not exceed  $25 \int_{B(0, 1)} \ln_+ (2/(5|u|)) du |B|$ . The same considerations apply in the second case and we have shown that  $\|\Gamma_R(x, \cdot)\|_*$  is bounded uniformly in  $x$  and  $R$ .

The proof of Lemma 3.24, part (ii), readily follows from part (i) and is skipped.

Finally, we prove Lemma 3.24, part (iii), starting with the Hölder continuity. Let  $a$  be an atom supported in  $B = B(z, r)$ . We have

$$T_R a(x + h) - T_R a(x) = \int_B (\Gamma_R(x + h, y) - \Gamma_R(x, y)) a(y) dy$$

which by (3.19) and the mean value property of  $a$  is controlled by

$$c \int_B \left( \frac{|h|}{|x-y|} \right)^\eta |a(y)| dy \leq c \left( \frac{|h|}{\sup(|x-z|, 2r)} \right)^\eta.$$

We continue with the behavior at infinity of  $T_R a$ . If  $|x-z| \geq 4r$ , using another representation for  $T_R$ ,

$$\begin{aligned} |T_R a(x)| &= \left| \int_B \int_0^R K_t(x, y) - K_t(x, z) dt a(y) dy \right| \\ &\leq c \int_B \int_0^R \left( \frac{|y-z|}{t^{1/2}} \right)^\eta \exp \left\{ -\frac{\beta |x-y|^2}{t} \right\} \frac{dt}{t} |a(y)| dy \\ &\leq c \int_B \left( \frac{|y-z|}{|x-z|} \right)^\eta |a(y)| dy \\ &\leq c \left( \frac{|r|}{|x-z|} \right)^\eta. \end{aligned}$$

Finally, we show that the convergence of  $T_R a$  to  $Ta$  is uniform. Let  $R \leq R'$ , then as before,

$$T_R a(x) - T_{R'} a(x) = \int_B \int_R^{R'} K_t(x, y) - K_t(x, z) dt a(y) dy,$$

which gives an estimate of the form  $cr^\eta R^{-\eta/2}$  uniformly in  $x$ . The conclusion is immediate.

The proof of Theorem 3.16 is complete.

*Remark 3.32.* The following can also be shown.  $T$  maps  $L^p$  to  $C^\mu$  with  $\mu = 2(1 - 1/p)$  as long as  $0 < \mu < 2\nu$ , where  $\nu$  is given by Theorem 3.5. For  $(1 + \eta)^{-1} < p < 1$ ,  $T$  maps the Hardy space  $\mathcal{H}^p$  to  $L^q$  provided  $-1 + 1/p = 2/q$ ; it is immediately seen on  $\mathcal{H}^p$  atoms. The limit case  $p = 1$  is the object of Theorem 3.16. However, completely analogous arguments to those of the proof of this theorem show that  $T$  maps  $L^1$  to VMO. We refer to, e.g., [St] for a definition of  $\mathcal{H}^p$  and VMO.

#### 4. HIGHER DIMENSIONS

In this section, we consider operators in  $\mathcal{E}$  with  $n \geq 3$  and we assume a Hölder condition on the coefficients of the principal part. We recall that such operators have the form

$$\mathcal{L} = \mathcal{L}(A) = -\operatorname{div}(A_0 \nabla + b) + c \nabla + d,$$

and, here,  $A_0$  has Hölder continuous coefficients. We also mention results where, in addition, the coefficients  $b, c$  are Hölder continuous.

#### 4.1. Taking High Powers

Let us start by recalling two elliptic regularity results, the first one in the Sobolev scale and the second one in the Hölder scale. Notice that we are stating these results globally over  $\mathbb{R}^n$ .

LEMMA 4.1. *Let  $A_0(x)$  be uniformly bounded and accretive (i.e.,  $A_0 \in \mathcal{A}(n)$ ). Then the conditions*

$$\begin{aligned} \operatorname{div}(A_0 \nabla u) &= f, \\ u &\in W^{1,p}, \quad 1 < p, \\ f &\in W^{-1,q}, \quad p < q < \infty, \\ A_0 &\in C^r, \quad r > 0, \end{aligned}$$

imply

$$u \in W^{1,q}.$$

Moreover,

$$\|u\|_{W^{1,q}} \leq c(\delta(A_0), \|A_0\|)(1 + |A_0|_r)^k (\|u\|_{W^{1,p}} + \|f\|_{W^{-1,q}}),$$

where  $k$  is the smallest integer satisfying  $q \leq p(1 + (rp/2n))^k$ .

This is due to M. Taylor by use of the pseudo-differential calculus [T], Theorem 2.2.H. The bound on  $k$  is not the sharpest one derived from Taylor's argument but is sufficient here.

LEMMA 4.2. *Let  $A_0(x)$  be uniformly bounded and accretive. Then the conditions*

$$\begin{aligned} \operatorname{div}(A_0 \nabla u) &= f + \operatorname{div} g, \\ A_0 &\in C^r, \quad 0 < r < 1, \\ f &\in L^p, \quad -1 - n/p \geq r, \\ g &\in C^r, \\ u &\in W^{1,q}, \quad q > n/r, \end{aligned}$$

imply

$$u \in C^{r+1}.$$

Moreover,

$$\|u\|_{C^{r+1}} \leq c(1 + |A_0|_r)^2 (\|\nabla u\|_q + \|f\|_p + |g|_r),$$

where  $c$  depends on ellipticity, dimension and  $r$ ,  $p$  and  $q$ .

This is a variation of a result due to Morrey, which can be derived following the proof of [G], Theorem 3.2. The unusual hypothesis  $u \in W^{1,q}$  for  $q > 2$  makes the growth in the constant polynomial in  $|A_0|_r$ . It can also be obtained via the pseudo-differential calculus as in [T], Chapter 2.

The idea of the method is the same as in dimension 2, though it is more involved here. The use of these results with an iteration improves on the regularity so as to reach Hölder regularity in the end. Let us recall the convention that  $T: E \rightarrow F$  means that  $T$  is bounded from  $E$  into  $F$ .

**PROPOSITION 4.3.** *There exists an integer  $m(n)$  with the following properties. Let  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$  and assume that  $A_0 \in C^r$  for some  $0 < r < 1$ .*

- (i) *For all  $m \geq m(n)$  and  $p \in [2, +\infty)$*

$$\mathcal{L}^{-m}: L^1 \rightarrow W^{1,p}$$

*with a norm not exceeding  $C(\delta(A), \|A\|, n, p)^m (1 + |A_0|_r^{1/r})^{M(n,p)}$ .*

- (ii) *In addition, assume  $b \in C^r$ . Then, for all  $m \geq m(n)$ ,*

$$\mathcal{L}^{-m}: L^1 \rightarrow C^{1+r}$$

*with a norm not exceeding  $C(\delta(A), \|A\|, n, r)^m (1 + |b|_r)(1 + |A_0|_r^{1/r})^{M(n,r)}$ .*

The exact control of the norm is not of great importance as long as its growth remains polynomial in  $|A_0|_r^{1/r}$ . The reason becomes apparent when we come to heat kernel estimates. We do not write details, however we provide the necessary ingredients for the reader to check this polynomial growth. The proof goes in several steps.

*Step 1:  $A$  boundedness result.*

**LEMMA 4.4.** *Let  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$  and assume that  $A_0 \in C^r$  for some  $0 < r < 1$ . Then, for all  $p \geq 2$ ,*

$$\mathcal{L}^{-1}: W^{1,2} \cap W^{1,p} \rightarrow W^{1,2} \cap W^{1,q},$$

*where  $n/q = n/p - 2$  if  $n/p - 2 > 0$  and  $q \in [p, +\infty)$  if  $n/p - 2 \leq 0$ .*

*Proof.* Define a sequence of numbers by  $p_0 = 2$  and  $n/(p_{k+1}) = n/p_k - 2$  as long as this quantity remains non-negative. In dimensions 3 and 4, the

sequence stops at  $p_0$ , and in higher dimensions, we see that  $p_k$  is strictly increasing and stops at  $k = k(n)$ . Indeed,

$$\frac{n}{p_k} = \frac{n}{p_{k-1}} - 2 \leq \frac{n}{p_{k-1}} \left(1 - \frac{4}{n}\right) \leq \frac{n}{2} \left(1 - \frac{4}{n}\right)^k.$$

The last term goes to 0 as  $k$  increases while we want  $(n/p_k) > 2$ . Finally notice that this sequence of numbers coincides with the one given by the sharp Sobolev embeddings  $W^{1,p_k} \subset W^{-1,p_{k+1}}$ .

By complex interpolation, it suffices to show by induction on  $k$  that the conclusion of the lemma holds for the numbers  $p_k$ .

Suppose that  $f \in W^{1,2}$ . Let us assume for simplicity that  $q = p_1$  exists, otherwise the following applies to any  $q \in [2, +\infty)$ . Since  $f \in W^{-1,2}$ ,  $u = \mathcal{L}^{-1}f \in W^{1,2}$ . We want to show that  $u \in W^{1,q}$ .

This function satisfies the equation

$$\operatorname{div}(A_0 \nabla u) = -f + du + c \nabla u - \operatorname{div}(bu). \tag{4.5}$$

Since the coefficients are bounded, the Sobolev embedding theorems imply that

$$du \in L^{q_1} \subset W^{-1,q}, \quad c \nabla u \in L^2 \subset W^{-1,q_1} \quad \text{and} \quad bu \in L^{q_1},$$

where  $(n/q_1) = (n/2) - 1$ . Hence the right hand side of (4.5) belongs to  $W^{-1,q_1}$  and an application of Lemma 4.1 yields  $u \in W^{1,q_1}$ . Using this information back again in (4.5), we see that the right hand side belongs to  $W^{-1,q}$ . Again by Lemma 4.1,  $u \in W^{1,q}$  as desired.

Now assume that the induction hypothesis holds for  $k - 1$ . Let  $f \in W^{1,2} \cap W^{1,p_k}$ , we wish to show that  $u = \mathcal{L}^{-1}f \in W^{1,2} \cap W^{1,p_{k+1}}$  (or  $f \in W^{1,p}$ ,  $p < +\infty$ , if  $p_{k+1}$  does not exist). Certainly  $u \in W^{1,2}$ . Since  $f \in W^{1,p_{k-1}}$  by complex interpolation, the induction hypothesis yields  $u \in W^{1,p_k}$ . Now, it suffices to write down (4.5) again and to adapt the exponents in the previous arguments to obtain  $u \in W^{1,p_{k+1}}$ . The lemma is proved.

*Step 2: Iteration and conclusion of part (i).*

It follows from the previous lemma that  $\mathcal{L}^{-k}: L^2 \rightarrow W^{1,p}$  for all  $k \geq k(n) + 1$  and  $p \in [2, +\infty)$ . Indeed, write

$$\mathcal{L}^{-k} = \mathcal{L}^{-k(n)} \mathcal{L}^{-1} \mathcal{L}^{-k+k(n)-1}. \tag{4.6}$$

Starting from the right, the first operator maps  $L^2$  into  $L^2$ , then  $\mathcal{L}^{-1}$  maps  $L^2$  into  $W^{1,2}$  and for the last term, we can apply the previous lemma iteratively.

In particular, we have obtained

$$\mathcal{L}^{-k}: L^2 \rightarrow L^\infty, \quad k \geq k(n) \quad (4.7)$$

by Sobolev embeddings. Since the class of operators under the assumption for (i) is self-adjoint, the same is true for the dual of  $\mathcal{L}$ , or in other words,

$$\mathcal{L}^{-k}: L^1 \rightarrow L^2. \quad (4.8)$$

Combining these completes the proof of (i).

*Step 3: Part (ii) (under smoothness assumption for b).*

By the Sobolev embeddings of the type  $W^{1,p} \subset C^\mu$  for appropriate  $p$  and  $\mu$  we have obtained that  $\mathcal{L}^{-k}$  maps  $L^2$  into  $C^\mu$  for any  $\mu \in (0, 1)$  and the same range of  $k$  as above. We now use the smoothness of  $b$ .

Fix  $s > \sup(1-r, r)$  and  $q = (n/(1-s))$ , i.e.,  $1 - n/q = s$  and observe that  $q > n/r$ . Pick  $k$  for which

$$\mathcal{L}^{-k}: L^2 \rightarrow W^{1,2} \cap W^{1,q} \subset W^{1,2} \cap C^s.$$

Let  $g \in L^2$ , define  $f = \mathcal{L}^{-k}g$  and  $u = \mathcal{L}^{-1}f$ . First since  $\mathcal{L}^{-1}g \in L^2$ ,

$$u = \mathcal{L}^{-k} \mathcal{L}^{-1}g \in W^{1,q} \in C^s.$$

Next, we write the equation

$$\operatorname{div}(A_0 \nabla u) = -f + du + c \nabla u - \operatorname{div}(bu) \equiv f_1 + \operatorname{div} g.$$

By the regularity assumption on  $b$  and the choice of  $s$ ,  $g \in C^r$ . Also,  $f_1 \in L^q$  and  $1 - n/q = s > r$ . Thus, Lemma 4.2 applies and yields  $u \in C^{r+1}$ .

Hence,

$$\mathcal{L}^{-k-1}: L^2 \rightarrow C^{r+1}, \quad k \geq k(n). \quad (4.9)$$

Combining this with (4.8), the conclusion of (ii) follows.

The norm of all these linear maps can be estimated using formulæ of the type (4.6), the estimates in Lemmata 4.1–2 and the norm of  $\mathcal{L}^{-1}$  from  $L^2$  to  $L^2$  or  $W^{1,2}$  that depends only on the ellipticity constant (see Remark 1.4 in Section 1). The proposition is proved.

*Remark 4.10.* If, in addition to the hypothesis in (ii), we impose that  $c \in C^r$ , the proof also gives  $\mathcal{L}^{-m}\partial: L^1 \rightarrow C^{r+1}$  for  $m \geq 2k(n) + 2$ , where  $\partial$  denotes any of the first partial derivatives. Let us prove it for  $m = 2k(n) + 2$ . Let  $k = k(n) + 1$ . From (4.9), we have

$$\partial \mathcal{L}^{-k}: L^2 \rightarrow C^r \subset L^\infty.$$

Since  $\mathcal{L}$  satisfies the same hypotheses, this implies by duality  $\mathcal{L}^{-k}\partial: L^1 \rightarrow L^2$ . Using (4.8) the remark follows.

In the sequel, we take  $m(n) = 2k(n) + 2$  so that both the proposition and the remark apply.

**COROLLARY 4.11.** *Let  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$ , assume that  $A_0 \in C^r$  for some  $0 < r < 1$  and denote by  $G^{(m)}(x, y)$  the kernel of  $\mathcal{L}^{-m}$ .*

(i) *For  $m \geq m(n)$ ,  $G^{(m)}(x, y)$  is  $C^\mu$  in both variables for any  $\mu \in (0, 1)$  and we have the following bounds:*

$$|G^{(m)}(x, y)| \leq c \exp\{-\alpha |x - y|\}, \tag{4.12}$$

and

$$\begin{aligned} &|G^{(m)}(x, y) - G^{(m)}(x + h, y)| + |G^{(m)}(x, y) - G^{(m)}(x, y + h)| \\ &\leq c |h|^\mu \exp\{-\alpha |x - y|\}, \end{aligned} \tag{4.13}$$

when  $2|h| \leq |x - y|$ . The constant  $\alpha > 0$  depends only the ellipticity bounds and dimension. The constant  $c$  is of the order of  $c_0^m(1 + |A|_r^{1/r})^{M(n, \mu)}$ , where  $c_0$  depends on the ellipticity constant, dimension and  $\mu$ .

(ii) *If, in addition, the coefficients  $b, c \in C^r$ , then  $G^{(m)}(x, y)$  is  $C^{r+1}$  in both variables,  $\nabla_x G^{(m)}(x, y)$  and  $\nabla_y G^{(m)}(x, y)$  both satisfy (4.12) and (4.13) with  $\mu = r$ ,  $\alpha > 0$  depending on the ellipticity constant and dimension only. The constant  $c$  is controlled by  $c_1^m(1 + |A|_r^{1/r})^{M(n, r)}(1 + |b|_r)(1 + |c|_r)$ , where  $c_1$  depends on the ellipticity constant, dimension and  $r$ .*

*Remark 4.14.* In fact, a little more holds under the assumption in (ii): we also have that  $\nabla_x \nabla_y G^{(m)}(x, y)$  exists pointwise and satisfies both estimates (4.12–13) with  $\mu = r$  with an analogous description for the constant.

In view of the perturbation method of the Appendix, it suffices to establish the bounds without the exponential decay since the class of operators under condition (i) (resp. (ii)) is stable under exponential perturbation. By duality considerations we are reduced to establishing boundedness

- (a) from  $L^1$  to  $L^\infty \cap \dot{C}^\mu$  of  $\mathcal{L}^{-m}$  in part (i),
- (b) from  $L^1$  to  $L^\infty \cap \dot{C}^r$  of  $\partial \mathcal{L}^{-m}$  in part (ii) and
- (c) from  $L^1$  to  $L^\infty \cap \dot{C}^r$  of  $\partial \mathcal{L}^{-m} \partial$  in the remark.

Parts (i) and (ii) of Proposition 4.3 give us (a) and (b). Only (c) requires an explanation. If  $k = k(n) + 1$  then we have seen that  $\partial \mathcal{L}^{-k}: L^2 \rightarrow C^r$

which implies  $\partial \mathcal{L}^{-k}: L^2 \rightarrow L^\infty$ . The same holds for  ${}^t \mathcal{L}$ , hence  $\mathcal{L}^{-k} \partial: L^1 \rightarrow L^2$ . Now let  $m \geq 2k$  and write

$$\partial \mathcal{L}^{-m} \partial = (\partial \mathcal{L}^{-k}) \mathcal{L}^{-m+2k} (\mathcal{L}^{-k} \partial): L^1 \rightarrow L^\infty \cap \dot{C}^r$$

by composition. The corollary is proved.

#### 4.2. The Heat Kernel

Following the now familiar procedure, we derive bounds for the heat kernel.

**THEOREM 4.15.** *Let  $\mathcal{L}_0 = \mathcal{L}(A_0) \in \mathcal{L}(A_0) \in \mathcal{E}_0$  and let  $K_t^0(x, y)$  be the distribution-kernel of  $e^{-t\mathcal{L}_0}$ ,  $t > 0$ . Assume that  $A_0 \in C^r$ . Then, for all  $t > 0$ ,  $K_t^0(x, y)$  is a bounded  $C^{r+1}$  function, and there are constants  $\beta = \beta(n, \delta) > 0$ ,  $\omega = \omega(n, \delta)$ ,  $c = c(n, \delta, r, |A_0|_r)$  and  $M = M(n, r)$  for which the following bounds hold. For all  $t > 0$ , and  $x, y \in \mathbb{R}^n$ :*

$$|K_t^0(x, y)| + |t^{1/2} \nabla_x K_t^0(x, y)| \leq c(1 + |A_0|_r^{1/r} t^{1/2})^M G_{\beta, t}(x - y), \quad (4.16)$$

and

$$\begin{aligned} & |t^{1/2} \nabla_x K_t^0(x, y) - t^{1/2} \nabla_x K_t^0(x + h, y)| \\ & \quad + |t^{1/2} \nabla_x K_t^0(x, y) - t^{1/2} \nabla_x K_t^0(x, y + h)| \\ & \leq c(1 + |A_0|_r^{1/r} t^{1/2})^M \left( \frac{|h|}{t^{1/2} + |x - y|} \right)^r G_{\beta, t}(x - y) \end{aligned} \quad (4.17)$$

when  $2|h| \leq t^{1/2} + |x - y|$ , and the similar bounds for  $t^{1/2} \nabla_y K_t^0(x, y)$ .

The proof follows the same pattern as before. We use

$$e^{-t\mathcal{L}_0} = \frac{(m-1)!}{2\pi i t^{m-1}} \int_{\gamma} e^{t\lambda} (\lambda + \mathcal{L}_0)^{-m} d\lambda$$

for a large integer  $m$  for which Corollary 4.11 applies. Thus,

$$K_t^0(x, y) = \frac{(m-1)!}{2\pi i t^{m-1}} \int_{\gamma} e^{t\lambda} R_{\lambda}^m(x, y) d\lambda, \quad (4.18)$$

where  $R_{\lambda}^m(x, y)$  is the kernel of  $(\lambda + \mathcal{L}_0)^{-m}$ . The path of integration is chosen as in Section 2. If  $\lambda = \rho e^{i\theta}$ , a rescaling gives

$$R_{\lambda}^m(x, y) = \rho^{(n/2)-m} G_{\rho, \theta}^{(m)}(\rho^{1/2} x, \rho^{1/2} y),$$

where  $G_{\rho, \theta}^{(m)}(x, y)$  is the kernel of  $\mathcal{L}_{\rho, \theta}^{-m} = (-\operatorname{div}(A_0(\rho^{-1/2} \cdot) \nabla) + e^{i\theta})^{-m}$ . In the sector of integration the ellipticity constants of the family  $\mathcal{L}_{\rho, \theta} \in \mathcal{E}$  are

uniform in  $\rho, \theta$  (modulo a rotation explained in Remark 1.5, Section 1) but  $|A_0(\rho^{-1/2} \cdot)|_r = |A_0|_r \rho^{-r/2}$ . Because of the control of the constants in Corollary 4.11, we finally have

$$|R_\lambda^{(m)}(x, y)| \leq c(1 + |A_0|_r^{1/r} |\lambda|^{-1/2})^{M(n, r)} |\lambda|^{n/2 - m} \exp\{-\alpha |\lambda|^{1/2} |x - y|\}.$$

Next, we perform the same estimates as in Section 1. Similar considerations apply to the first derivatives of  $K_t^0(x, y)$  and their Hölder estimates, using Corollary 4.11 applied to operators of the form  $\mathcal{L}_0 + \lambda$ . Further details skipped.

**THEOREM 4.19.** *Let  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$  with ellipticity constant  $\delta$  and let  $K_t(x, y)$  be the distribution-kernel of  $e^{-t\mathcal{L}}$ ,  $t > 0$ . Assume that  $A_0 \in C^r$ . Then, for all  $t > 0$ , and  $\mu \in (0, 1)$ ,  $K_t(x, y)$  is a bounded  $C^\mu$  function, and there are constants  $\beta = \beta(n, \delta) > 0$ ,  $\omega = \omega(n, \delta)$ ,  $c = c(n, \delta, \mu, r, |A_0|_r)$  for which the following bounds hold. For all  $t > 0$ , and  $x, y \in \mathbb{R}^n$ :*

$$|K_t(x, y)| \leq ce^{-\omega t} G_{\beta, t}(x - y), \tag{4.20}$$

and

$$\begin{aligned} &|K_t(x, y) - K_t(x + h, y)| + |K_t(x, y) - K_t(x, y + h)| \\ &\leq ce^{-\omega t} \left( \frac{|h|}{t^{1/2} + |x - y|} \right)^\mu G_{\beta, t}(x - y) \end{aligned} \tag{4.21}$$

when  $2|h| \leq t^{1/2} + |x - y|$ . Moreover, if, in addition,  $b \in C^r$  and  $c \in C^r$  then  $K_t(x, y)$  is a  $C^{r+1}$  function and bounds similar to (4.20) and (4.21) with  $\mu < r$  hold for both  $t^{1/2} \nabla_x K_t(x, y)$  and  $t^{1/2} \nabla_y K_t(x, y)$ .

Note that the factor  $e^{-\omega t}$  comes from the strong ellipticity of  $\mathcal{L}$  and kills the polynomial factor in  $t$  coming from the method of proof. We skip the proof.

*Remark 4.22.* In dimension 2, both of the above theorems apply. This gives information which we did not derive in Section 3. See Section 5 for a use of this.

**COROLLARY 4.23.** *Let  $\mathcal{L}(A_0) \in \mathcal{E}_0$  with  $A_0 \in C^r$ . Then for all  $\lambda$  with  $|\arg \lambda| < \pi - \omega_{A_0}$  (see Remark 1.5 for the definition of  $\omega_{A_0}$ ) we have  $(\lambda + \mathcal{L}_0)^{-1} \in \mathcal{B}(L^p, L^p)$  for  $1 \leq p \leq \infty$ .*

This follows from Theorem 4.19 applied to  $\lambda + \mathcal{L}_0$  and the Laplace formula. The resolvent kernel is in fact integrable on the diagonal and at infinity.

*Remark 4.24.* We do not know the sharp value of the exponent  $M$  in (4.16) and whether polynomial growth in time is best possible. A question posed by E. B. Davies (personal communication) is whether it is necessary to have a growth under smoothness assumption on the coefficients. The answer is yes in general. We sketch a *reductio ad absurdum* argument.

Indeed, fix  $r \in (0, 1)$  and assume that for all  $\mathcal{L}(A_0) \in \mathcal{E}_0$  with ellipticity constants  $\delta$  and  $\|A_0\|_\infty$ , and with  $A_0 \in C^r$ , one obtains with the above notations,

$$|K_t^0(x, y)| \leq cG_{\beta, t}(x - y), \quad t > 0, \quad x, y \in \mathbb{R}^n, \quad (4.25)$$

with  $c = c(n, \delta, \|A_0\|_\infty, r, |A|_r)$  and  $\beta = \beta(n, \delta) > 0$ . (In general the Gaussian rate of decay does not depend on smoothness, so we assume  $\beta$  does not as well.)

First, by rescaling considerations, we see that we can choose  $c = c(n, \delta, \|A_0\|_\infty, r)$  in (4.25).

Next, for any  $\mathcal{L}(B_0) \in \mathcal{E}_0$ , one can approximate in the pointwise sense  $B_0$  by a family  $(B_k)_{k \geq 1}$  of smooth matrices (say Hölder with  $r = 1/2$ ) with uniform ellipticity constants. By a result of Kato,  $\lim_{k \rightarrow \infty} e^{-t\mathcal{L}(B_k)} = e^{-t\mathcal{L}(B_0)}$  in the strong topology of  $L^2$  for any  $t > 0$ . Hence, the heat kernel for  $\mathcal{L}(B_k)$  converges to the corresponding heat kernel for  $\mathcal{L}(B_0)$  in the sense of distributions. From this and the first step it easily follows that the heat kernel for  $\mathcal{L}(B_0)$  satisfies

$$|K_t^0(x, y)| \leq cG_{\beta, t}(x - y), \quad t > 0, \quad x, y \in \mathbb{R}^n, \quad (4.26)$$

with  $c = c(n, \delta, \|A_0\|_\infty, 1/2)$  and  $\beta = \beta(n, \delta) > 0$ .

Hence, (4.25) implies Gaussian bounds for heat kernels of any operator in  $\mathcal{E}_0$ . The existence of a counterexamples [AT3] to such an estimate for dimensions large than 5, shows that (4.25) cannot hold for smooth coefficients if  $n \geq 5$ . Nothing is known when  $n = 3$  or 4 and Section 3 treats the case  $n = 2$ .

## 5. THE KATO SQUARE ROOT PROBLEM

In this section, we study the square roots of operators in the classes  $\mathcal{E}_0$  and  $\mathcal{E}$  under mild smoothness assumptions on the leading coefficients.

Any operator in  $\mathcal{E}_0$  or  $\mathcal{E}$  is maximal accretive in  $L^2$  and has a uniquely defined maximal accretive square root on  $L^2$  [K], whose domain is a dense subspace of  $L^2$ . The Kato square root problem consists in determining whether this domain is  $W^{1,2}$ . Under our smoothness assumptions, this question has been answered affirmatively in [Mc1]. See also [Mc3] for a survey of what was known about this problem by 1989.

Our aim, here, is to obtain a better description of the square root in terms of Calderón–Zygmund operators as a consequence of our estimates in the previous sections. This provides a simple proof of the above mentioned result and gives  $L^p$  results,  $p \neq 2$ , and regularity results, which are new.

We restrict to dimension  $n \geq 2$  since for  $n = 1$ , the solution of this problem is known in all generality for operators in  $\mathcal{E}_0$  [CMcM], and indeed in  $\mathcal{E}$  [AT2]. An optimal description in terms of Calderón–Zygmund operators is given in [AT1]. Our method also relies on Calderón–Zygmund operators and on the T(1) theorem. We refer the reader to [M] for an account on this topic.

### 5.1. Operators without Lower Order Terms

**THEOREM 5.1.** *Let  $\mathcal{L}_0 = \mathcal{L}(A_0) \in \mathcal{E}_0$ , where  $n \geq 2$  and  $A_0 = (a_{jk})$ ,  $a_{jk} \in C^r$  for some  $0 < r < 1$ . Then the domain of  $\mathcal{L}_0^{1/2}$  coincides with  $W^{1,2}$ . Furthermore,*

$$\mathcal{L}_0^{1/2} = T_i a_{ij} \partial_{x_j} + R, \tag{5.2}$$

where the operators  $T_i$  are Calderón–Zygmund operators, and  $R$  is bounded on  $L^p$  with  $p_0 < p < q_0$ , where  $p_0 < 2 < q_0$  depend only  $n, r$ . Moreover, if  $n = 2$ , or if  $n \geq 3$  and  $A_0$  is real, then  $R$  extends boundedly on all  $L^p$ ,  $1 \leq p \leq \infty$ , hence  $\mathcal{L}_0^{1/2}$  extends continuously from  $W^{1,p}$  into  $L^p$  for  $1 < p < \infty$ .

Let us mention that a similar result was obtained by Alexopoulos under the extra assumptions that the coefficients are real and periodic [Al], which implies a better control of the heat kernel for large time. In this case, the operator  $R$  can be taken as 0 in the statement.

The proof of Theorem 5.1 was briefly sketched in the announcement [AMcT]. Here we give some more details.

Let  $\mathcal{L}_0 \in \mathcal{E}_0$  with the assumption in the statement. First, by a result of Lions, the domain of  $\mathcal{L}_0^{1/2}$  is  $W^{1,2}$  if we can show that  $\mathcal{L}_0^{1/2}$  and its adjoint are bounded from  $W^{1,2}$  into  $L^2$ . Since the class of operators under consideration is self-adjoint, it suffices to show that  $\mathcal{L}_0^{1/2}$  has this boundedness property. We do this by establishing (5.2).

A possible definition of  $\mathcal{L}_0^{1/2}$  is by means of the heat semi-group. This yields the following representation.

$$\begin{aligned} \mathcal{L}_0^{1/2} &= \frac{1}{\sqrt{\pi}} \int_0^{+\infty} e^{-t\mathcal{L}_0} \mathcal{L}_0 \frac{dt}{t^{1/2}} \\ &= -\frac{1}{\sqrt{\pi}} \int_0^1 e^{-t\mathcal{L}_0} t^{1/2} \partial_{x_i} \frac{dt}{t} a_{ij} \partial_{x_j} + \frac{1}{\sqrt{\pi}} \int_1^{+\infty} e^{-t\mathcal{L}_0} t \mathcal{L}_0 \frac{dt}{t^{3/2}} \\ &\equiv T_i a_{ij} \partial_{x_j} + R. \end{aligned} \tag{5.3}$$

Let us treat the case of  $T_i$  first. Its kernel is given by

$$T_i(x, y) = \frac{1}{\sqrt{\pi}} \int_0^1 t^{1/2} \partial_{y_i} K_t^0(x, y) \frac{dt}{t}.$$

Estimates (4.16–4.17) apply to  $t^{1/2} \partial_{y_i} K_t(x, y)$ ,  $t \leq 1$ , and give Calderón–Zygmund estimates for the kernel,  $T_i(x, y)$ , of  $T_i$ . For example,

$$\begin{aligned} |T_i(x, y)| &\leq \frac{C}{\sqrt{\pi}} \int_0^1 G_{\beta, t}(x-y) \frac{dt}{t} \\ &= C |x-y|^{-n} \int_{|x-y|^2}^{+\infty} u^{n/2} \exp\{-\beta u\} \frac{du}{u} \\ &\leq C |x-y|^{-n} \exp\{-\gamma |x-y|^2\} \end{aligned}$$

for any  $\gamma < \beta$ . The estimates for the Hölder regularity in  $x$  and  $y$  with exponent  $r$  of  $T_i(x, y)$  can be dealt with similarly.

Next, we have for all  $t > 0$ ,  $e^{-t\mathcal{L}_0} t^{1/2} \partial_{x_i}(1) = 0 = \{e^{-t\mathcal{L}_0} t^{1/2} \partial_{x_i}\}^* (1)$  pointwise, where 1 denotes the constant function with value 1. The first identity is obvious and the second follows from the pointwise equality

$$e^{-t\mathcal{L}_0^*}(1) = 1. \quad (5.4)$$

Admitting this equality, the T(1) theorem applies and shows that  $T_i$  is bounded on  $L^2$  and  $T_i(1) = T_i^*(1) = 0$  in BMO. Hence  $T_i$  is bounded on  $L^p$ ,  $1 < p < +\infty$ , by Calderón–Zygmund theory (see [DJ] or [M]).

Now, let us look at  $R$ . It is well-known that  $t\mathcal{L}_0 e^{-t\mathcal{L}_0} = -t(d/dt) e^{-t\mathcal{L}_0} \in \mathcal{B}(L^2, L^2)$  and

$$\|t\mathcal{L}_0 e^{-t\mathcal{L}_0}\|_{2,2} \leq c < +\infty.$$

See, e.g., Chapter IX of [K]. Moreover, the kernel of  $t\mathcal{L}_0 e^{-t\mathcal{L}_0}$  is  $-t(\partial/\partial t) K_t^0(x, y)$ . By differentiating (4.18) and adapting the proof of Theorem 4.15, we find that  $t(\partial/\partial t) K_t^0(x, y)$  satisfies an estimate of the type (4.16).

Thus  $\|t\mathcal{L}_0 e^{-t\mathcal{L}_0}\|_{p,p} \leq C(1+t)^{M/2}$  for  $p=1$  and  $p=+\infty$  with the same  $M$  as in (4.16). Using the uniform estimate for  $p=2$  and interpolation we obtain that

$$\|t\mathcal{L}_0 e^{-t\mathcal{L}_0}\|_{p,p} \leq C(1+t)^{M|1/2-1/p|} \text{ for all } p.$$

As long as  $M|\frac{1}{2}-1/p| < \frac{1}{2}$  the integral that defines  $R$  converges uniformly in  $\mathcal{B}(L^p, L^p)$ .

In dimension 2,  $M=0$  hence  $\sup_{t>0} \|t\mathcal{L}_0 e^{-t\mathcal{L}_0}\|_{p,p} < +\infty$  for all  $p$ . Thus,  $R$  is bounded on all  $L^p$ . In fact, more is true: the kernel of  $t\mathcal{L}_0 e^{-t\mathcal{L}_0}$

satisfies the Gaussian estimate (3.6), which implies that the kernel of  $R$  satisfies

$$|R(x, y)| \leq C(1 + |x - y|)^{-3}. \tag{5.5}$$

In dimension larger than 3, for real coefficients, Aronson's theorem [Ar] gives the Gaussian bounds (with no growth for large time). By standard techniques, we also have that  $\sup_{t>0} \|t\mathcal{L}_0 e^{-t\mathcal{L}_0}\|_{p,p} < +\infty$  for all  $p$  and that

$$|R(x, y)| \leq C(1 + |x - y|)^{-n-1}. \tag{5.6}$$

We have obtained (subject to proving (5.4)) that

$$\|\mathcal{L}_0^{1/2}f\|_p \leq C(\|f\|_p + \|\nabla f\|_p), \tag{5.7}$$

for  $1 < p < +\infty$  if  $n=2$  or if  $n \geq 3$  and the coefficients are real, and for  $1 \leq p_0 < p < q_0 \leq +\infty$  if  $n \geq 3$  in general. In particular, in the case of  $p=2$ , we deduce that  $\mathcal{L}_0^{1/2}$  is bounded from  $W^{1,2}$  into  $L^2$ . By the remark at the beginning of the proof, this implies that its domain is  $W^{1,2}$ .

It remains to prove (5.4) for arbitrary  $\mathcal{L}_0 \in \mathcal{E}_0$  with the  $C^r$  assumption. This equality is classical when the matrix  $A_0$  has real measurable coefficients, as it follows from the positivity of the heat kernel together with the maximum principle (see [Da1]), both of which are not available in our situation. An argument is as follows. First we use again the contour formula

$$e^{-t\mathcal{L}_0^*} = \frac{1}{2\pi i} \int_{\gamma} e^{t\lambda} (\lambda + \mathcal{L}_0^*)^{-1} d\lambda$$

with the same contour as in Section 2 and  $R=1/t$ . By our estimates in Section 3 and 4 (Proposition 3.14, Remark 4.22 and Proposition 4.23) the resolvent of  $\mathcal{L}_0^*$  is bounded on all  $L^p$ . It suffices to show

LEMMA 5.8. *For all  $\mathcal{L}(A_0) \in \mathcal{E}_0$  with  $A_0 \in C^r$*

$$(\lambda + \mathcal{L}_0^*)^{-1}(1) = \lambda^{-1}, \quad \text{for all } \lambda \text{ with } |\arg \lambda| < \pi - \omega_{A_0}.$$

(See Remark 1.5 for the definition of  $\omega_{A_0}$ .)

By duality, this is equivalent to (changing  $\lambda$  to  $\bar{\lambda}$ )

$$\int (\lambda + \mathcal{L}_0)^{-1}(\varphi)(x) dx = \lambda^{-1} \int \varphi(x) dx \quad \text{for all } \varphi \in L^1.$$

By a density argument, we only have to check this equality for  $\varphi \in L^1 \cap L^2$ . Let  $h = (\lambda + \mathcal{L}_0)^{-1}(\varphi) \in W^{1,2}$  defined by the variational formulation. We also have that  $h \in L^1$  by Corollary 4.23. Since  $\lambda h - \operatorname{div}(A_0 \nabla h) = \varphi$  (in the sense of distributions) it follows that  $\operatorname{div}(A_0 \nabla h) \in L^1$  and by an easy argument  $\int \operatorname{div}(A_0 \nabla h)(x) dx = 0$ . Thus,  $\int \lambda h(x) dx = \int \varphi(x) dx$ , which is the desired equality. This completes the proof of (5.4) and hence of Theorem 5.1.

**COROLLARY 5.9.** *Let  $\mathcal{L}_0 = \mathcal{L}(A_0) \in \mathcal{E}_0$  with  $A_0 \in C^r$  for some  $0 < r < 1$ . Assume that  $A_0$  has real coefficients if  $n \geq 3$  and complex coefficients if  $n = 2$ . Then  $\mathcal{L}_0^{1/2}$  extends as a bounded operator from  $W^{s+1,p}$  into  $W^{s,p}$  for  $1 < p < \infty$  and  $-1 - r < s < r$ . In particular we have that*

$$\|\mathcal{L}_0^{1/2} f\|_{W^{s,p}} \leq c \|f\|_{W^{1+s,p}},$$

where  $c$  depends on  $n, r, p, s$ , the ellipticity bounds of  $A_0$  and  $|A_0|_r$ .

First note that by an easy duality  $\|\mathcal{L}_0^{1/2} f\|_{W^{s,p}} \leq c \|f\|_{W^{1+s,p}}$  implies  $\|\mathcal{L}_0^{*1/2} f\|_{W^{-s-1,p'}} \leq c \|f\|_{W^{-s,p'}}$  where  $p'$  is the conjugate exponent of  $p$ . Since the class of operators under consideration is self-adjoint, complex interpolation shows that it suffices to restrict our attention to proving the corollary for  $0 < s < r$  and  $1 < p < \infty$ .

Using the decomposition (5.3), and since multiplication by a  $C^r$  function preserves the space  $W^{s,p}$  for  $s, p$  as above, we see that it suffices to show that

$$T_i, R: W^{s,p} \rightarrow W^{s,p}.$$

As we saw,  $T_i$  is a Calderón–Zygmund operator with  $T_i(1) = T_i^*(1) = 0$ . Moreover, it can be seen that its kernel has rapid decay at  $\infty$  and is Hölder continuous away from the diagonal with exponent  $r$ . Thus it extends to a bounded operator on  $W^{s,p}$  (see Chapter 10 of [M], or [FJW]).

It remains to prove the boundedness of  $R$  on  $W^{s,p}$ . In fact, we claim that  $R$  is smoothing of order 1 on any  $L^p$ ,  $1 \leq p \leq +\infty$ , which implies the result. More precisely, we claim that for any  $i$ ,  $\partial_{x_i} R$  is an operator with kernel bounded by  $(1 + |x - y|)^{-n-1}$ .

Setting  $Q_t = e^{-t\mathcal{L}_0} t \mathcal{L}_0$ , we have  $\partial_{x_i} R = c \int_1^{+\infty} \partial_{x_i} Q_t(dt/t^{3/2})$  and we need estimates on  $\nabla_x Q_t(x, y)$ .

Let us start with the two dimensional situation. We have already seen that for arbitrary  $\mathcal{L}_0 \in \mathcal{E}_0$ ,

$$|Q_t(x, y)| \leq CG_{\beta,t}(x - y), \tag{5.10}$$

which follows from the same estimate for the heat kernel of  $\mathcal{L}_0$ . If, in addition,  $A_0 \in C^r$ , then  $Q_t(x, y)$  has bounded first order derivative by Theorem 4.15, and for  $t \geq 1$

$$|\nabla_x Q_t(x, y)| \leq Ct^{M-1/2} G_{\beta, t}(x-y) \tag{5.11}$$

for some  $M \geq 1/2$ . In fact, one can take  $M = 1/2$ . To see this, we make use of the semi-group property of the heat operator: for  $f \in \mathcal{D}(\mathcal{L}_0)$

$$\nabla Q_t f = -t \nabla \frac{d}{dt} e^{-t\mathcal{L}_0} f = -t \nabla e^{-t\mathcal{L}_0} \frac{d}{dt} e^{-(t-1)\mathcal{L}_0} f = \frac{t}{t-1} \nabla e^{-\mathcal{L}_0} Q_{t-1} f.$$

Hence, using (4.16) for  $\nabla e^{-\mathcal{L}_0}$  and (5.10), we obtain for all  $t \geq 2$

$$|\nabla_x Q_t(x, y)| \leq CG_{\beta, 1} * G_{\beta, t-1}(x-y),$$

and we conclude using the convolution inequality for  $G_{\beta, r} * G_{\beta, s}(x) \leq c(\beta, n) G_{\beta, r+s}(x)$  for all  $x \in \mathbb{R}^n$  and  $r, s > 0$ . Using (5.11) in  $\int_1^{+\infty} \partial_{x_i} Q_t(x, y) (dt/t^{3/2})$  finishes the proof.

In dimension  $n \geq 3$ , the argument is the same, but we need to start with the analog of (5.10) for  $Q_t$ . Assuming that  $A$  has real coefficients, then this follows from Aronson’s Gaussian estimate [Ar] and holomorphic functional calculus adapting the calculations in, e.g., chapter 3 of [Da1]). We skip further details.

*Remark 5.12.* Under the assumptions of Corollary 5.9, we also have that  $\mathcal{L}_0^{1/2}$  is bounded from  $C^{s+1}$  to  $C^s$  for  $0 < s < r$ . The proof relies on Calderón–Zygmund theory for the  $T_i$ , the above estimates for  $R(x, y)$  and  $\nabla_x R(x, y)$  and interpolation.

### 5.2. Operators with lower order terms.

**THEOREM 5.13.** *Let  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$ , where  $n \geq 2$  and  $A_0 = (a_{ij})$ ,  $b, c \in C^r$  for some  $0 < r < 1$ . Then the domain of  $\mathcal{L}^{1/2}$  coincides with  $W^{1,2}$ . Furthermore,*

$$\mathcal{L}^{1/2} = U_i(a_{ij} \partial_{x_j} + b_i) + V(c_j \partial_{x_j} + d), \tag{5.14}$$

where

- (1)  $U_i$  are Calderón–Zygmund operators satisfying:

$$U_i(1) = 0 \quad \text{and} \quad U_i^*(1) \in L^\infty, \tag{5.15}$$

$$|U_i(x, y)| \leq C |x - y|^{-n} \exp\{-\alpha |x - y|\}, \tag{5.16}$$

and

$$|U_i(x+h, y) - U_i(x, y)| \leq C \frac{|h|^r}{|x-y|^{n+r}} \exp\{-\alpha|x-y|\} \\ \text{for } |h| \leq |x-y|/2, \quad (5.17)$$

and symmetrically exchanging the roles of  $x, y$ ;

(2)  $V$  is bounded on all  $L^p$  with kernel estimate

$$|V(x, y)| \leq C|x-y|^{-n+1} \exp\{-\alpha|x-y|\} \quad (5.18)$$

and for all  $i$ ,  $V\partial_{x_i} = -U_i$  and  $\partial_{x_i}V = \tilde{U}_i^*$  where  $\tilde{U}_i$  satisfy the same properties as  $U_i$  in point (1).

Here  $\alpha > 0$  depends on  $n$  and the ellipticity bounds of  $\mathcal{L}$  only, and  $C$  depends on  $n, r$ , the ellipticity bounds of  $\mathcal{L}$  and  $|A_0|_r, |b|_r, |c|_r$ .

**COROLLARY 5.19.** *Under the above assumptions, we have*

$$\mathcal{L}^{1/2}: W^{1,p} \rightarrow L^p, \quad \text{for } 1 < p < +\infty \quad (5.20)$$

If, in addition,  $d \in C^r$ , then

$$\mathcal{L}^{1/2}: W^{s+1,p} \rightarrow W^{s,p}, \quad \text{for } 1 < p < +\infty \quad \text{and} \quad -1-r < s < r, \quad (5.21)$$

and

$$\mathcal{L}^{1/2}: C^{s+1} \rightarrow C^s, \quad \text{for } 0 < s < r. \quad (5.22)$$

Furthermore,  $\mathcal{L}^{1/2}$  is an isomorphism in the three cases.

This corollary applies for example to the operators  $(\lambda + \mathcal{L}_0)$  where  $\mathcal{L}_0 \in \mathcal{E}_0$  and  $\lambda$  in the sector defined by Remark 1.5.

Let us prove this corollary first. The first assertion follows from (5.14) and Calderón–Zygmund theory. That  $\mathcal{L}^{1/2}: W^{1,p} \rightarrow L^p$  is an isomorphism can be seen as follows. By standard arguments, it suffices to show that its inverse extends as a bounded operator from  $L^p$  into  $W^{1,p}$ . In fact,  $\mathcal{L}^{-1/2} = V$  and by the properties of  $V$  in Theorem 5.13,  $\mathcal{L}^{-1/2}$  is smoothing of order 1 on  $L^p$  for  $1 < p < +\infty$ , which is the desired result.

By the same remark as in the beginning of the proof of Corollary 5.9, it suffices to prove (5.21) for  $0 < s < r$ . Since the multiplication by a  $C^r$  function preserves  $W^{s,p}$  and  $C^s$ , (5.21) and (5.22) follow from

$$U_i: W^{s,p} \text{ (resp. } C^s) \rightarrow W^{s,p} \text{ (resp. } C^s)$$

for  $p$  as above and  $0 < s < r$ , and the same thing for  $V$ . For  $U_i$ , this comes from well-known results for singular integral operators under condition

(5.15–5.17), which we already used in the proof of Corollary 5.9. The reader is referred again to Chapter 10 of [M].

As for  $V$ , it is smoothing of order 1 on  $L^p$  for  $1 < p < +\infty$ , hence  $V$  is clearly bounded on  $W^{s,p}$  for  $0 \leq s \leq 1$  and  $1 < p < +\infty$ . Furthermore, interpolating between (5.18) for  $V(x, y)$  and the Calderón–Zygmund estimate for  $\partial_{x_i} V(x, y)$  for all  $i$ , one finds that if  $0 < s < 1$

$$|V(x+h, y) - V(x, y)| \leq C \frac{|h|^s}{|x-y|^{n+s-1}} \exp\{-\alpha|x-y|\} \text{ for } |h| \leq |x-y|/2.$$

This easily implies that  $V: L^\infty \rightarrow C^s$  for  $0 < s < 1$ , which is stronger than what we need.

The argument for the invertibility is left to the reader.

*Proof of Theorem 5.13.* Let  $\mathcal{L} \in \mathcal{E}$  be as in the statement. Define

$$U_i = -\frac{1}{\sqrt{\pi}} \int_0^{+\infty} e^{-t\mathcal{L}} t^{1/2} \partial_{x_i} \frac{dt}{t}$$

and

$$V = \frac{1}{\sqrt{\pi}} \int_0^{+\infty} e^{-t\mathcal{L}} \frac{dt}{t^{1/2}} = \mathcal{L}^{-1/2}.$$

From the equality  $\mathcal{L}^{1/2} = 1/\sqrt{\pi} \int_0^{+\infty} e^{-t\mathcal{L}} \mathcal{L}(dt/t^{1/2})$ , we obtain (5.14) easily. We have to describe  $U_i$  and  $V$ .

Let us start by studying  $V$ . First, it is clear on a formal level that  $V\partial_{x_i} = -U_i$  and  $\partial_{x_i} V = \tilde{U}_i^*$ , where  $\tilde{U}_i$  is similar to  $U_i$  (in fact, change  $\mathcal{L}$  to  $\mathcal{L}^*$  in the definition of  $U_i$ ). We only need to look at the kernel of  $V$ . By (4.20),

$$|V(x, y)| \leq C \int_0^{+\infty} \exp\{-\omega t\} G_{\beta, t}(x-y) \frac{dt}{t^{1/2}}$$

and we break the integral at  $\tau = |x-y|$ . The contribution for  $t \leq \tau$  is dominated by

$$\begin{aligned} & C \int_0^\tau G_{\beta, t}(x-y) \frac{dt}{t^{1/2}} \\ & \leq C\tau^{-n+1} \int_\tau^{+\infty} \exp\{-\beta v\} v^{(n-3)/2} dv \leq C\tau^{-n+1} \exp\{-\beta\tau\}, \end{aligned}$$

since  $(n-3)/2 > -1$ . After a change of variable, the other term is dominated by

$$C\tau^{-n+1} \exp\{-\omega\tau\} \int_0^\tau \exp\{-\beta s\} s^{(n-3)/2} ds \leq C\tau^{-n+1} \exp\{-\omega\tau\}.$$

We now turn to  $U_i$ . We skip the proof of the Calderón–Zygmund estimates on the kernel, which requires only the estimates (4.20–21) on  $K_t(x, y)$  and the same breakings of the integrals. Also, it is clear that  $U_i(1) = 0$ . Thus, the only thing to check is  $U_i^*(1) \in L^\infty$ , which implies  $L^2$  boundedness from the T(1) theorem.

**LEMMA 5.23.** *For all  $\mathcal{L}(A) \in \mathcal{E}$  with  $A_0, b, c \in C^r$ . for all  $\mu < \pi - \omega_A$  and for all  $\lambda$  with  $|\arg \lambda| \leq \mu$ ,*

$$(\lambda + \mathcal{L})^{-1}(1)(x) = \lambda^{-1} + \lambda^{-3/2} f_\lambda(x) + \lambda^{-2} g_\lambda(x) \quad (5.24)$$

where

$$\|f_\lambda\|_\infty + \|g_\lambda\|_\infty \leq C, \quad (5.25)$$

$$\|\nabla f_\lambda\|_\infty + \|\nabla g_\lambda\|_\infty \leq C |\lambda|^{1/2}, \quad (5.26)$$

the constant  $C$  being independent of  $\lambda$ . Furthermore,  $f_\lambda = 0$  if  $b = 0$  and  $g_\lambda = 0$  if  $d = 0$ .

**COROLLARY 5.27.** *Under the hypotheses above, for all  $t > 0$ ,*

$$e^{-t\mathcal{L}}(1)(x) = 1 + t^{1/2} f^t(x) + t g^t(x)$$

where

$$\|f^t\|_\infty + \|g^t\|_\infty \leq C,$$

$$\|\nabla f^t\|_\infty + \|\nabla g^t\|_\infty \leq C t^{-1/2}$$

Furthermore,  $f^t = 0$  if  $b = 0$  and  $g^t = 0$  if  $d = 0$ .

To compute  $U_i^*(1)$ , write  $\mathcal{L} = \mathcal{L} - \omega + \omega$ , for  $\omega$  small enough depending on ellipticity so that the corollary applies to  $\mathcal{L}^* - \omega$ . Thus,

$$\begin{aligned} U_i^*(1) &= \frac{1}{\sqrt{\pi}} \int_0^{+\infty} t^{1/2} \partial_{x_i} e^{-t(\mathcal{L}^* - \omega)}(1) \exp\{-\omega t\} \frac{dt}{t} \\ &= \frac{1}{\sqrt{\pi}} \int_0^{+\infty} (\partial_{x_i} f^t + t^{1/2} \partial_{x_i} g^t) \exp\{-\omega t\} dt \end{aligned}$$

and this integral belongs to  $L^\infty$  (with convergence for the weak \* topology).

It remains to prove the lemma and its corollary. The proof of the latter readily follows from the Cauchy representation for the exponential

$$e^{-t\mathcal{L}} = \frac{1}{2\pi i} \int_{\gamma} e^{t\lambda} (\lambda + \mathcal{L})^{-1} d\lambda$$

with the same contour as in Section 2 and  $R = 1/t$ . It suffices to insert (5.24) in this equality. Let us turn to the proof of (5.24).

Define

$$f_\lambda = \lambda^{1/2} (\lambda + {}^t\mathcal{L})^{-1} \operatorname{div} b$$

and

$$g_\lambda = -\lambda (\lambda + {}^t\mathcal{L})^{-1} d.$$

It follows easily from the estimates of Theorem 4.19 and the Laplace transform that  $f_\lambda$  and  $g_\lambda$  satisfy the estimates (5.25–5.26). The right behavior in  $\lambda$  is obtained by rescaling. It remains to check (5.24).

We know that  $u_\lambda = (\lambda + \mathcal{L})^{-1} (1) \in L^\infty$ . For all  $\varphi \in L^1 \cap L^2$  we have, therefore,

$$\int u_\lambda \varphi = \int (\lambda + {}^t\mathcal{L})^{-1} (\varphi).$$

Let  $h = (\lambda + {}^t\mathcal{L})^{-1} (\varphi) \in W^{1,2}$ , then  $h \in W^{1,1}$  by Corollary 4.11. By definition,

$$\operatorname{div}({}^tA_0 \nabla h + ch) = (\lambda + d)h + b \nabla h - \varphi \in L^1.$$

Also  ${}^tA_0 \nabla h + ch \in L^1$ , therefore  $\int \operatorname{div}({}^tA_0 \nabla h + ch) = 0$ . Consequently

$$\begin{aligned} \int u_\lambda \varphi &= \int h \\ &= \int \lambda^{-1} \varphi - \int \lambda^{-1} dh - \int \lambda^{-1} b \nabla h \\ &= \int \lambda^{-1} \varphi - \int \lambda^{-1} b \nabla (\lambda + {}^t\mathcal{L})^{-1} (\varphi) - \int \lambda^{-1} d (\lambda + {}^t\mathcal{L})^{-1} (\varphi) \\ &= \int (\lambda^{-1} + \lambda^{-3/2} f_\lambda + \lambda^{-2} g_\lambda) \varphi. \end{aligned}$$

This proves (5.24) and finishes the proof of Lemma 5.23 (it can be observed that for  $|\lambda|$  small (5.24) and the accompanying estimates (5.25–5.26) can be improved since 0 does not belong to the spectrum of  $\mathcal{L}$ ).

## 6. BOUNDED $H^\infty$ FUNCTIONAL CALCULUS ON $L^p$ SPACES

### 6.1. Holomorphic Extension of Heat Kernels

We give here a short account on the holomorphic extension of heat kernels. See [Dal] for more details.

Let  $n \geq 1$  and let  $\mathcal{L}_0 = \mathcal{L}(A_0) \in \mathcal{E}_0$ . From Remark 1.5, we see that  $\zeta \mathcal{L}_0 = \mathcal{L}(\zeta A_0) \in \mathcal{E}_0$  for  $|\arg \zeta| < (\pi/2) - \omega_{A_0}$ , i.e.,  $\zeta \in S_{(\pi/2) - \omega_{A_0}}^o$ . Moreover, the ellipticity constants are uniform provided  $|\zeta| = 1$  and  $\zeta \in S_{(\pi/2) - \theta}^o$ , where  $\pi/2 > \theta > \omega_{A_0}$ . Hence,  $\zeta \mathcal{L}_0$  generates an  $L^2$  contraction semi-group to which can be applied the results of Sections 2, 3 and 4.

For  $z = t\zeta$  with  $\zeta$  as above, define  $K_z^0(x, y)$  as the heat kernel of  $e^{-t(\zeta \mathcal{L}_0)}$ . It can be shown that as a function of  $z$  it is a holomorphic distribution-valued function on the open sector  $S_{(\pi/2) - \theta}^o$ .

The estimates of Theorems 2.21, 3.5 and 4.15 apply in full to  $K_z^0(x, y)$  provided  $t$  is replaced by  $|z|$  on the right hand side. In particular, we have for all  $(x, y) \in \mathbb{R}^{2n}$  and  $z \in S_{(\pi/2) - \theta}^o$ ,

$$|K_z^0(x, y)| \leq c(1 + |z|^{1/2})^M G_{\beta, |z|}(x - y), \quad (6.1)$$

and

$$\begin{aligned} & |K_z^0(x, y) - K_z^0(x + h, y)| + |K_z^0(x, y) - K_z^0(x, y + h)| \\ & \leq c(1 + |z|^{1/2})^M \left( \frac{|h|}{|z|^{1/2} + |x - y|} \right)^r G_{\beta, |z|}(x - y) \end{aligned} \quad (6.2)$$

when  $2|h| \leq |z|^{1/2} + |x - y|$  and where  $M = M(n)$  with  $M(1) = M(2) = 0$ .

Note that when (6.1) applies,  $K_z^0(x, y)$  is a holomorphic function of  $z \in S_{(\pi/2) - \theta}^o$  for each  $(x, y)$ .

A consequence of the holomorphy which we already used in Section 5 is that the same estimates holds for  $z$ -derivatives of  $K_z^0(x, y)$  correctly renormalized.

### 6.2. Bounded $H^\infty$ Functional Calculus

Let  $n \geq 1$  and  $\mathcal{L}_0$  be as above. The maximal accretive operator  $\mathcal{L}_0$  is one-one and has a bounded  $H^\infty$  functional calculus in  $L^2$ , meaning that  $b(\mathcal{L}_0) \in \mathcal{B}(L^2, L^2)$  and

$$\|b(\mathcal{L}_0)\|_{2,2} \leq c_\mu \|b\|_\infty$$

for all functions  $b \in H^\infty(S_\mu^o)$ , where  $S_\mu^o$  is the open sector  $\{z \in \mathbb{C} : |\arg z| < \mu\}$ , and  $\mu > \omega_{A_0} = \sup\{|\arg a_{ij}(x) \zeta_i \bar{\zeta}_j| : \zeta \in \mathbb{C}^n, x \in \mathbb{R}^n\}$ . See, e.g., [Mc2].

It is natural to ask whether  $b(\mathcal{L}_0)$  is a Calderón–Zygmund operator, and hence is bounded in  $L^p$ ,  $1 < p < \infty$ .

**THEOREM 6.3.** *Let  $\mathcal{L}_0$  satisfy the inequalities (6.1–6.2). Let  $b \in H^\infty(S_\mu^o)$  such that*

$$|b(\zeta)| \leq c_0(1 + |\zeta|^{-1/2})^{-M}, \quad \zeta \in S_\mu^o, \tag{6.4}$$

where  $M$  is the smallest positive constant in (6.1–6.2). Then  $b(\mathcal{L}_0)$  is a Calderón–Zygmund operator. Furthermore, we have

$$\|b(\mathcal{L}_0)\|_{p,p} \leq c(\mu, n, p)c_0$$

for  $1 < p < \infty$ .

**COROLLARY 6.5.** *Let  $n \leq 2$  and  $\mathcal{L}_0 = \mathcal{L}(A_0) \in \mathcal{E}_0$ . Then  $\mathcal{L}_0$  has a bounded  $H^\infty$  functional calculus on  $L^p$ ,  $1 < p < \infty$ .*

In dimensions 1 and 2, we obtain the optimal result for this class of complex elliptic operators.

The decay of  $b$  at the origin in (6.4) compensates the polynomial growth at the origin in (6.1–6.2) when  $n \geq 3$ . It would, therefore, be interesting to estimate the smallest value for  $M$  under the Hölder continuity of  $A_0$  (see the discussion in Section 4). Also, note that an exponential growth for large  $|z|$  in (6.1–6.2) in lieu of a polynomial growth would forbid us to state Theorem 6.3 when  $n \geq 3$  since there is no non trivial holomorphic function with exponential decay at the origin.

Theorem 6.3 can be proved by the method of [Du]. See also [DuMc], where operators with real measurable symmetric coefficients are considered in dimension  $\geq 3$  (with  $\mu > \omega_{A_0} = 0$ ) (in which case the estimates with  $M = 0$  were previously known [Ar]).

To derive Theorem 6.3 directly from heat kernel estimates, proceed as follows. Let  $b \in H^\infty(S_\mu^o)$  satisfy (6.4) and choose  $\theta$  with  $\omega_{A_0} < \theta < \mu$ . Let  $\gamma$  consist of the two half-rays  $re^{i(\pi + \theta)}$  and  $re^{-i\theta}$  where  $r > 0$ , and note that for  $z \in \gamma$ , we have  $|\arg iz| = \pi/2 - \theta < \pi/2 - \omega_{A_0}$ , i.e.,  $iz \in S_{\pi/2 - \omega_{A_0}}^o$ . We define  $b(\mathcal{L}_0)$  by the equality

$$b(\mathcal{L}_0) = \frac{1}{2\pi} \lim_{\delta \rightarrow 0} \int_\gamma e^{-iz\mathcal{L}_0} \check{b}(z + i\delta) dz, \tag{6.6}$$

with strong convergence in  $L^2$ . This definition coincides with the usual ones as can be seen by applying the convergence lemma of [Mc2]. The function  $\check{b}$  denotes the inverse Fourier transform of  $b$  (where we have set  $b(\zeta) = 0$  for  $\operatorname{Re} \zeta < 0$ ) extended holomorphically to the sector  $iS_{(\pi/2)+\mu}^o$ . By standard Fourier transform estimates, one obtains

$$|\check{b}(z)| \leq c_\nu |z|^{-1} (1 + |z|^{1/2})^{-M} \quad (6.7)$$

on every smaller sector  $iS_{(\pi/2)+\nu}^o$ ,  $\nu < \mu$  (see [McQ]).

Therefore the kernel  $K_b(x, y)$  of  $b(\mathcal{L}_0)$  satisfies

$$K_b(x, y) = \frac{1}{2\pi} \lim_{\delta \rightarrow 0} \int_\gamma K_{iz}^0(x, y) \check{b}(z + i\delta) dz,$$

so that using (6.1) and (6.7)

$$\begin{aligned} |K_b(x, y)| &\leq c \int_\gamma \frac{(1 + |z|^{1/2})^M}{|z|^{n/2}} \exp \left\{ -\frac{\beta |x - y|^2}{|z|} \right\} |z|^{-1} (1 + |z|^{1/2})^{-M} |dz| \\ &= c |x - y|^{-n}. \end{aligned}$$

Similar reasoning gives Hölder bounds for  $K_b(x, y)$ . Since we already have the  $L^2$  boundedness of  $b(\mathcal{L}_0)$ , we conclude that  $b(\mathcal{L}_0)$  is a Calderón–Zygmund operator, and thus obtain  $L^p$  boundedness.

We conclude with the case of operators with lower order terms.

**THEOREM 6.8.** *Let  $n \geq 1$  and  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$ , where, in addition,  $A_0(x)$  is Hölder continuous when  $n \geq 3$ . Then,  $\mathcal{L}$  has a bounded  $H^\infty$  functional calculus on  $L^p$ ,  $1 < p < \infty$ . More precisely, if  $b \in H^\infty(S_\mu^o)$ , where  $\omega_A < \pi < \pi/2$ , then  $b(\mathcal{L})$  is a Calderón–Zygmund operator and*

$$\|b(\mathcal{L})\|_{p,p} \leq c(\mu, n, p) \|b\|_\infty,$$

for  $1 < p < \infty$ .

The methods are similar and include the fact that (6.1–6.2) are valid for the heat kernel of  $\mathcal{L}$  with an exponentially decaying factor  $e^{-\alpha|z|}$ ,  $\alpha > 0$ , instead of  $(1 + |z|)^M$ . No further assumption on the lower order coefficients is necessary (see Sections 2, 3 and 4). We skip further details.

We remark that the  $L^p$  bounds for  $b(\mathcal{L}_0)$  and  $b(\mathcal{L})$  can be proved without using the Hölder estimates on the heat kernel, by adapting the results of Duong and Robinson [DuR].

APPENDIX:

REMARKS ON THE PERTURBATION TECHNIQUE OF DAVIES

E. B. Davies developed a useful technique to derive pointwise bounds on heat kernels. We wish to make a few simple comments and remarks on this method that we have used throughout this paper.

A class,  $\mathcal{C}$ , of unbounded operators on  $L^2$  is said to be stable under exponential perturbation if whenever  $\mathcal{L} \in \mathcal{C}$ , there is a  $\rho = \rho(\mathcal{L}) > 0$  such that  $\mathcal{L}^\phi \equiv e^{-\phi} \mathcal{L} e^\phi \in \mathcal{C}$  for all real-valued  $\phi \in \mathcal{C}^\infty$  (with compact support) and  $\|\nabla\phi\|_\infty < \rho$ . Here,  $e^{-\phi}$  denotes the operator of pointwise multiplication by the function  $e^{-\phi(x)}$ .

An example of such a class is  $\mathcal{E}$ . This follows from the following calculation. Suppose  $\mathcal{L} = -\text{div}(A_0 \nabla + b) + c \nabla + d = \mathcal{L}(A) \in \mathcal{E}$ . Then,

$$e^{-\phi} \mathcal{L} e^\phi = -\text{div}(A_0 \nabla + b + {}^t(\nabla\phi)A_0) + (c - A_0 \nabla\phi) \cdot \nabla + d + c \cdot \nabla\phi - b \cdot \nabla\phi - A_0 \nabla\phi \cdot \nabla\phi. \tag{A.1}$$

Thus,  $e^{-\phi} \mathcal{L}(A) e^\phi = \mathcal{L}(A_\phi)$  for some matrix  $A_\phi(x)$  and it is easy to show that  $A \in \mathcal{A}$  and  $\|\nabla\phi\|_\infty < \rho = \rho(\delta(A), \|A\|)$  imply  $A_\phi \in \mathcal{A}$ . Moreover, any smoothness assumptions made on the leading coefficients is preserved under exponential perturbation. Additional smoothness on lower order coefficients is also preserved. We denote by  $|A|$  a semi-norm which measures the smoothness of the coefficients if assumed.

We note that here and hereafter, the constants  $\rho$  (which change from line to line) depend only on the ellipticity bounds and dimension.

Suppose that  $\mathcal{C}$  is the above class  $\mathcal{E}$  (what follows could be easily generalized). Let  $F(z) = z^{-m}$  for some  $m \geq 1$ . (More general holomorphic functions in a neighborhood of the spectrum can be considered, such as  $\exp\{-z\}$ .)

Assume:

(1) For all  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$ ,  $F(\mathcal{L})$  is defined on  $L^2$  and has a kernel satisfying

$$|K_{F(\mathcal{L})}(x, y)| \leq c_1 g(|x - y|) \quad \text{for a.e. } (x, y) \in \Omega, \tag{A.2}$$

for some constant  $c_1 = C(\delta(A), \|A\|, |A|, n)$ , where  $g: \mathbb{R}^+ \rightarrow \mathbb{R}^+$  is a measurable function and  $\Omega$  is some measurable subset of  $\mathbb{R}^n \times \mathbb{R}^n$ , independent of the choice of  $\mathcal{L}$ .

The conclusion is that for all  $\mathcal{L} \in \mathcal{E}$ , there are constants  $c_2 = C(\delta(A), \|A\|, |A|, n)$  and  $\rho > 0$ , such that

$$|K_{F(\mathcal{L})}(x, y)| \leq c_2 g(|x - y|) e^{-\rho|x-y|} \quad \text{for a.e. } (x, y) \in \Omega. \tag{A.3}$$

The proof is classical. Applying the hypothesis to  $\mathcal{L}^\phi$ , we have

$$|K_{F(\mathcal{L}^\phi)}(x, y)| \leq c_1 g(|x - y|) \quad \text{for a.e. } (x, y) \in \Omega,$$

and  $c_1$  is uniform in  $\phi$  as long as  $\|\nabla\phi\|_\infty$  is small enough. But  $K_{F(\mathcal{L}^\phi)}(x, y) = K_{F(\mathcal{L})}(x, y)e^{\phi(y) - \phi(x)}$ . Thus, fixing  $x$  and  $y$  and selecting  $\phi$  with  $\|\nabla\phi\|_\infty = \rho$ ,  $\rho$  small enough and  $\phi(y) - \phi(x) = \rho|x - y|$  give us (A.3).

The most common choice for  $g$  is  $g = 1$  identically which means, if  $\Omega = \mathbb{R}^{2n}$ , that  $F(\mathcal{L})$  extends boundedly from  $L^1$  to  $L^\infty$ . However,  $g(t) = |\ln t|$  or  $t^{-q}$ ,  $q > 0$ , can also be expected if  $F$  does not decay enough at infinity.

Let us take  $g = 1$  for simplicity in the next discussion. In addition to (1) above assume that

(2)  $F(\mathcal{L})$  extends boundedly from  $L^1(\mathbb{R}^n)$  to  $\dot{C}^s(\mathbb{R}^n)$  for some  $s \in (0, 1)$ , its norm depending on dimension, the ellipticity bounds of  $A$ , and the seminorm  $|A|$ .

Then the conclusion is that for  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$ , there are constants  $c_3 = C(\delta(A), \|A\|, |A|, n)$  and  $\rho > 0$ , such that for all  $x, y, h$  with  $|h| \leq |x - y|/2$ ,

$$|K_{F(\mathcal{L})}(x + h, y) - K_{F(\mathcal{L})}(x, y)| \leq c_3 |h|^s e^{-\rho|x - y|}. \quad (\text{A.4})$$

To see this, we remark that the extra hypothesis gives us by an easy duality argument

$$|K_{F(\mathcal{L})}(x + h, y) - K_{F(\mathcal{L})}(x, y)| \leq c_4 |h|^s$$

for all  $x, y, h$  and all  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$  where  $c_4 = C(\delta(A), \|A\|, |A|, n)$ . Now, applying this to  $\mathcal{L}^\phi$  for an appropriate  $\phi$  gives us

$$|K_{F(\mathcal{L})}(x + h, y)e^{\phi(y) - \phi(x + h)} - K_{F(\mathcal{L})}(x, y)e^{\phi(y) - \phi(x)}| \leq c_5 |h|^s$$

where  $c_5 = C(\delta(A), \|A\|, |A|, n)$ . Next, we fix  $x, y, h$  with  $|h| \leq |x - y|/2$  and select  $\phi$  with support in a ball centered at  $y$  of radius not exceeding  $|x - y|/2$  and  $\|\nabla\phi\|_\infty = \rho$ ,  $\rho$  small enough and  $\phi(y) = \rho|x - y|/4$ . Then if  $z = x$  or  $x + h$ ,  $\phi(y) - \phi(z) = \phi(y) = \rho|x - y|/4$  and (A.4) follows easily.

Finally, we can replace (2) by

(3) A partial derivative  $\partial_i F(\mathcal{L})$  extends boundedly from  $L^1(\mathbb{R}^n)$  to  $L^\infty(\mathbb{R}^n)$ , its norm depending on the ellipticity bounds of  $\mathcal{L}$  and on any seminorm  $|A|$  as above.

Then the conclusion is that for all  $\mathcal{L} = \mathcal{L}(A) \in \mathcal{E}$ , there are constants  $c_6 = C(\delta(A), \|A\|, |A|, n)$  and  $\rho > 0$ , such that for all  $x, y, h$  with  $|h| \leq |x - y|/2$ ,

$$|\partial_{x_i} K_{F(\mathcal{L})}(x, y)| \leq c_6 e^{-\rho|x - y|}.$$

The proof is similar using (A.3) and the formula

$$\partial_{x_i} K_{F(\mathcal{L}\phi)}(x, y) = \partial_{x_i} K_{F(\mathcal{L})}(x, y) e^{\phi(y) - \phi(x)} - K_{F(\mathcal{L})}(x, y) e^{\phi(y) - \phi(x)} \partial_{x_i} \phi(x).$$

Details are skipped.

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*Note added in proof.* After this work was completed, the first author derived a new proof for Aronson's estimates by using the method of this paper together with appropriate elliptic regularity results [Au]. He also weakened the Hölder continuity assumption to that of uniform continuity. Nevertheless, the specific treatment of dimensions 1 and 2 and the applications of our results remain of independent interest.

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