

Introduction

In the 1960's, Kato studied *abstract evolution equations* of the form

$$\partial_t u(t) + A(t)u(t) = f(t), \quad u(0) = u_0 \in \mathcal{H} \quad (\text{E})$$

where $t \in [0, T]$ on a Hilbert space \mathcal{H} and $A(t)$ are closed, densely-defined operators with domains $\mathcal{D}(A(t))$. They are also assumed to be *maximally accretive*, by which we mean $\operatorname{Re} \langle A(t)u, u \rangle \geq 0$. Under these conditions, fractional powers $A(t)^\alpha$ exist as closed, densely-defined operators, and if for some $\alpha \in (0, 1]$, $\mathcal{D}(A(t)^\alpha)$ is constant, then under certain smoothness conditions on $A(t)$ and $f(t)$, the abstract evolution equation admits a unique, *strict* (continuously differentiable) solution.

The operators $A(t)$ typically arise naturally, associated to a family of sesquilinear forms (or complex energies) $J_t : \mathcal{W} \times \mathcal{W} \rightarrow \mathbb{C}$ (where $\mathcal{W} \subset \mathcal{H}$). Namely, the operators $A(t)$ are defined as the operators with largest domains $\mathcal{D}(A(t))$ satisfying: $J_t[u, v] = \langle A(t)u, v \rangle$ for all $u \in \mathcal{D}(A(t))$ and $v \in \mathcal{W}$.

For an $\omega \in [0, \pi/2)$, such a form is said to be ω -sectorial if \mathcal{W} is dense in \mathcal{H} , $J_t[u, u] \in \mathbb{S}_{\omega+} = \{\zeta \in \mathbb{C} : |\arg \zeta| \leq \omega\} \cup \{0\}$ (the closed sector of angle ω in the right half complex plane), and \mathcal{W} is complete with respect to the norm $\|u\|_{\mathcal{W}} = \|u\|^2 + \operatorname{Re} J_t[u, u]$. Similarly, we can say that an operator $T : \mathcal{D}(T) \subset \mathcal{H} \rightarrow \mathcal{H}$ is ω -accretive if T is densely-defined and closed, $\langle Tu, u \rangle \in \mathbb{S}_{\omega+}$, and $\sigma(T) \subset \mathbb{S}_{\omega+}$. If $\omega = 0$ then T non-negative self-adjoint.

If $A(t)$ is the associated operator to J_t as defined above, and J_t is ω -sectorial, then the Lax-Milgram Theorem guarantees that $A(t)$ is ω -accretive. If $\omega = 0$, this theorem asserts that $A(t)$ is self-adjoint, $\mathcal{D}(\sqrt{A(t)}) = \mathcal{W}$ (so that in particular, it is constant in t) and for all $u, v \in \mathcal{W}$, $J_t[u, v] = \langle \sqrt{A(t)}u, \sqrt{A(t)}v \rangle$. In the 1961 paper [39],

Kato demonstrates that for every $\alpha < 1/2$,

$$\mathcal{D}(A(t)^\alpha) = \mathcal{D}(A(t)^{* \alpha}) = \mathcal{D}_\alpha \quad \text{and} \quad \|A(t)^\alpha u\| \simeq \|A(t)^{* \alpha} u\|. \quad (\text{K}_\alpha)$$

Counterexamples were known to say (K_α) is in general false when $\alpha > 1/2$. In the same paper, Kato asks two questions (as Remarks 1 and 2 on page 268) about the critical case $\alpha = 1/2$. We paraphrase these questions in our notation:

(K1) Is $\mathcal{D}(\sqrt{A(t)}) = \mathcal{D}(\sqrt{A(t)^*}) = \mathcal{W}$?

(K2) For the case $\omega = 0$, the Lax-Milgram Theorem tells us that (K1) is true, but is $\|\partial_t \sqrt{A(t)} u\| \lesssim \|u\|_{\mathcal{W}}$ for $u \in \mathcal{W}$?

A year later, Lions demonstrated in [41] that (K1) is in general invalid for maximal accretive operators. In his 1972 paper [42], McIntosh constructed an ω -accretive operator A (with $\omega < \pi/2$) such that $\mathcal{D}(\sqrt{A}) \neq \mathcal{D}(\sqrt{A^*})$, providing a counterexample to (K1) for *regularly accretive* operators. Ten years later, in [43], McIntosh used similar techniques to construct a counterexample for (K2).

While Kato studied fractional powers of accretive operators motivated by abstract evolution equations of the form (E), the study of such equations were themselves motivated by hyperbolic equations on Euclidean space. Thus, attention became focused on the problem of determining:

$$\mathcal{D}(\sqrt{-a \operatorname{div} A \nabla}) = W^{1,2}(\mathbb{R}^n) \quad \text{and} \quad \|\sqrt{-a \operatorname{div} A \nabla} u\| \simeq \|\nabla u\|, \quad (\text{Kato})$$

where a, A are L^∞ pointwise multiplication operators. The accretivity of the operator follows from assuming an ellipticity condition of the form $\operatorname{Re} \langle A \nabla u, \nabla u \rangle \geq \kappa_1 \|\nabla u\|^2$, for $\kappa_1 > 0$. This was the reincarnation of the abstract problem (K1), which in fact implies (K2) as a consequence of allowing for *complex* coefficients. It is this problem which became popularly known as the *Kato square root problem*.

The Kato square root problem on \mathbb{R}^n was finally settled in 2002 by Auscher, Hofmann, Lacey, McIntosh and Tchamitchian in [5]. Indeed, much development towards the resolution of this problem happened between the years of 1982 and 2002, particularly in terms of $T(b)$ theorems in harmonic analysis. The book [6] by Auscher and Tchamitchian and the paper [35] by Hofmann are a good source of information on the history of the problem. The survey paper [36] by Hofmann and McIntosh illustrates the development and importance of $T(b)$ theorems.

A very significant development for our purposes occurred in 2005 with the paper [8] by Axelsson (Rosén), Keith and McIntosh. There, the authors developed a first-order perspective of the Kato square root problem and rephrased it in terms of the perturbation of *Dirac type* operators. In this paper, they were able to use this *Axelsson-Keith-McIntosh* (AKM) framework to consolidate many of the previous results in harmonic analysis, and in addition, solve similar problems for systems, differential forms on \mathbb{R}^n , and such problems on compact manifolds. This framework is further adapted in [7] to solve inhomogeneous problems on Lipschitz domains $\Omega \subset \mathbb{R}^n$.

We remark that, while [8] proves a Kato square root problem on compact manifolds, the significant advancement in the manifold setting is due to the work of Morris in [46]. There, Morris solves a Kato square root problem on submanifolds of Euclidean space whose second fundamental form is uniformly bounded.

The power of the AKM framework lies in the fact that the operator theory and functional calculi are written out at the level of an abstract Hilbert space, and quadratic estimates, which imply solutions to the Kato square root problem, are obtained under a further set of more concrete hypotheses. More explicitly, the authors consider closed, densely-defined, nilpotent operators Γ on a Hilbert space \mathcal{H} , and bounded operators B_1, B_2 . Defining $\Pi_B = \Gamma + B_1\Gamma^*B_2$, they show that $\mathcal{D}(\sqrt{\Pi_B^2}) = \mathcal{D}(\Pi_B) = \mathcal{D}(\Gamma) \cap \mathcal{D}(\Gamma^*B_2)$ and $\|\sqrt{\Pi_B^2}u\| \simeq \|\Pi_B u\| \simeq \|\Gamma u\| + \|\Gamma^*B_2 u\|$ under a set of hypotheses (H1)-(H8).

In this thesis, we are primarily concerned with formulating and solving Kato square root problems on manifolds. Similar to the case of boundary value problems, we expect the formulation of such problems to be inhomogeneous (due to geometry). Let \mathcal{M} be a manifold with metric g , $S = (I, \nabla) : W^{1,2}(\mathcal{M}) \rightarrow L^2(\mathcal{M}) \oplus L^2(T^*\mathcal{M})$ and write $L_A = aS^*AS$, where $A = (A_{ij})$ is a matrix of L^∞ pointwise multiplication operators and $a \in L^\infty(\mathcal{M})$. Explicitly, the operator $L_A u = -a \operatorname{div}(A_{11} \nabla u) - a \operatorname{div}(A_{10} u) + a A_{01} \nabla u + a A_{00} u$, which can be seen as an L^∞ perturbation of the Bochner Laplacian $\Delta_B = -\operatorname{div} \nabla$ with lower-order terms. We require L_A to be uniformly elliptic in order to talk about its square roots. The *Kato square root problem on manifolds* is then to determine conditions on the geometry for which we can obtain:

$$\mathcal{D}(\sqrt{L_A}) = W^{1,2}(\mathcal{M}) \quad \text{and} \quad \|\sqrt{L_A}u\| \simeq \|u\|_{W^{1,2}} = \|u\| + \|\nabla u\|. \quad (\text{Kato}_{\mathcal{M}})$$

In the setting of a Lie group, which has more structure than an abstract manifold, we can ask questions about perturbations of *subelliptic* operators. These questions are the natural sort to generalise the homogeneous problem (Kato). Let \mathcal{G} be a Lie group and \mathfrak{a} an *algebraic basis* for the Lie algebra \mathfrak{g} . We can consider the right translation and span of these vectors to yield global vector fields. Associated with these vector fields is a natural sub-Riemannian distance as well as a sub-connection ∇ (which lands in the span of the co-vector fields obtained from \mathfrak{a} rather than the whole co-tangent space). Letting $W^{1,2}(\mathcal{G})'$ denote the domain of ∇ , the homogeneous Kato square root problem for subelliptic operators on Lie groups is then to determine when:

$$\mathcal{D}(\sqrt{-a \operatorname{div} A \nabla}) = W^{1,2'}(\mathcal{G}) \quad \text{and} \quad \|\sqrt{-a \operatorname{div} A \nabla} u\| \simeq \|\nabla u\|, \quad (\text{Kato}_{\mathcal{G}})$$

where $a, A \in L^\infty$ are multiplication operators and the operator $-\operatorname{div} A \nabla$ is uniformly subelliptic. In fact, this particular problem has been asked by ter Elst since the resolution of the Kato square root problem on \mathbb{R}^n in 2002.

For the purposes of the research we present in this thesis, the profound resolution of the Kato square problem in 2002 is where we begin. We propose the term *geometric Kato square root problem* to describe the geometric problems of the form (Kato $_{\mathcal{M}}$) and (Kato $_{\mathcal{G}}$). The material we present in this thesis advances the understanding of the problem by providing some natural geometric conditions under which (Kato $_{\mathcal{M}}$) and (Kato $_{\mathcal{G}}$) can be solved in the affirmative.

The way in which we attack these problems is to make modifications to the AKM framework and list a set of mild, operator theoretic hypotheses (H1)-(H6) in §1.8. Quadratic estimates, the fundamental objects which allow us to prove Kato square root type estimates, are obtained under two additional hypotheses. We label these hypotheses geometric and outline them in Chapter 3.

A first advancement to the theory we provide is to show that the quadratic estimates can be obtained on measure metric spaces. There are a few difficulties in generalising the proofs in [8] to the metric space setting, but the primary one is the lack of a differentiable structure. We compensate for this by rephrasing the argument in terms of Lipschitz functions and controlling such functions using the *pointwise Lipschitz constant*. Our first theorem is then the following, which allows us to obtain *homogeneous* Kato square root estimates (Kato $_{\mathcal{G}}$), directly generalising (Kato).

Theorem 1 (Theorem 3.1.1). *Let (\mathcal{X}, d, μ) be a complete measure metric space which is at most polynomial in growth and (Γ, B_1, B_2) satisfy (H1)-(H6) (§1.8),*

(H7-H) and (H8-H) (§3.1). Then, Π_B satisfies the quadratic estimate

$$\int_0^\infty \|\Pi_B(\mathbf{I} + t^2\Pi_B^2)^{-1}u\|^2 \frac{dt}{t} \simeq \|u\|^2$$

for all $u \in \overline{\mathcal{R}(\Pi_B)} \subset L^2(\mathcal{X}, \mathbb{C}^N)$

We are predominantly interested in obtaining solutions to $(\text{Kato}_{\mathcal{M}})$ for manifolds under *intrinsic* geometric conditions. It is worth mentioning here that, at least from our perspective, the quadratic estimates see the geometry because we need to analyse a first-order formulation of the problem on the space $L^2(\mathcal{M}) \oplus L^2(T^*\mathcal{M})$. In [46], Morris obtains quadratic estimates on $L^2(\mathbb{C}^N)$ and uses bounds on extrinsic curvature (second fundamental form) to move from analysis on $L^2(T^*\mathcal{M})$ to $L^2(\mathbb{C}^N)$.

Motivated by the existence of *harmonic coordinates* which provides us with the right kind of uniform intrinsic control on the geometry, we formulate a notion called *generalised bounded geometry* for a vector bundle \mathcal{V} on a measure metric space \mathcal{X} (§1.4). This notion captures a uniform locally Euclidean structure on the bundle. We allow for this very general situation of vector bundles because from our perspective, they capture the notion of *systems* in the presence of geometry. The quadratic estimates used to solve inhomogeneous problems of the form $(\text{Kato}_{\mathcal{M}})$ is then guaranteed by the following theorem.

Theorem 2 (Theorem 3.2.4). *Suppose that (\mathcal{X}, d, μ) is a complete measure metric space that is at most exponential in growth, \mathcal{V} satisfies the generalised bounded geometry criterion (§1.4), and that (Γ, B_1, B_2) satisfy (H1)-(H6) (§1.8), (H7-I) and (H8-I) (§3.2). Then, Π_B satisfies the quadratic estimate*

$$\int_0^\infty \|t\Pi_B(\mathbf{I} + t^2\Pi_B^2)^{-1}u\|^2 \frac{dt}{t} \simeq \|u\|^2$$

for all $u \in \overline{\mathcal{R}(\Pi_B)} \subset L^2(\mathcal{V})$.

We acknowledge that the harmonic analytic technology which Morris develops in [46] assists a great deal in proving this theorem. However, this theorem is by no means an immediate consequence. A crucial difficulty is that, in the harmonic analysis, we use techniques such as integral averaging in our proofs. This is not, in general, well defined on a vector bundle. Hence, we are forced to define notions of integration and averaging after fixing a set of coordinates seen through an abstract dyadic decomposition that is valid up to a certain scale. These coordinates may

indeed jump at the boundaries of the cubes, but our techniques allow us to absorb such jumps. This construction permits us to import the Euclidean tools to this vector bundle setting.

As aforementioned, the point of these quadratic estimates is that they allow us to solve Kato square root problems. The following theorem is obtained through analysis on Lie groups and due to our first-order perspective of the problem. We also mention that obtaining the quadratic estimates on measure metric spaces is of paramount importance in proving the following theorem as we need to depart from any Riemannian structure of the Lie group to a sub-Riemannian setting.

Theorem 3 (Theorem 4.3.1). *Let (\mathcal{G}, d, μ) be a connected, nilpotent Lie group with \mathfrak{a} an algebraic basis, d the associated subelliptic distance, and μ the left Haar measure. Suppose that $a, A \in L^\infty$ and that there exist $\kappa_1, \kappa_2 > 0$ satisfying*

$$\operatorname{Re} \langle au, u \rangle \geq \kappa_1 \|u\|^2 \quad \text{and} \quad \operatorname{Re} \langle A\nabla v, \nabla v \rangle \geq \kappa_2 \|\nabla v\|^2,$$

for every $u \in L^2(\mathcal{G})$ and $v \in W^{1,2}(\mathcal{G})'$. Then, **(Kato \mathcal{G})** holds.

Through the use of the quadratic estimates in Theorem 2, we are able to solve the following inhomogeneous problem on general Lie groups. In the following theorem, the operator $S = (I, \nabla)$ where ∇ is the sub-connection associated to the algebraic basis \mathfrak{a} .

Theorem 4 (Theorem 4.4.1). *Let (\mathcal{G}, d, μ) be a connected Lie group, \mathfrak{a} an algebraic basis, d the associated subelliptic distance, and μ the left Haar measure. Let $a, A \in L^\infty$ such that*

$$\operatorname{Re} \langle au, u \rangle \geq \kappa_1 \|u\|^2 \quad \text{and} \quad \operatorname{Re} \langle ASv, Sv \rangle \geq \kappa_2 \|v\|_{W^{1,2'}}^2,$$

for all $u \in L^2(\mathcal{G})$ and $v \in W^{1,2}(\mathcal{G})'$. Then, $\mathcal{D}(\sqrt{aS^*AS}) = W^{1,2}(\mathcal{G})'$ with $\|\sqrt{aS^*AS}u\| \simeq \|u\|_{W^{1,2'}} = \|u\| + \|\nabla u\|$. That is, we solve **(Kato \mathcal{M})** with ∇ being a sub-connection, which is the inhomogeneous version of **(Kato \mathcal{G})**.

Since Lie groups have trivial tangent bundles, Theorem 2 is actually a much stronger result than necessary to prove Theorem 4. A relatively easy adaptation of the proof in [46] can be used instead.

As we have previously mentioned, the real strength of our quadratic estimates in Theorem 2 is that they allow us to tackle problems on manifolds with non-trivial

tangent bundles. We present the following highlight theorem solving the Kato problem on manifolds for functions. The notation Ric stands for the Ricci curvature of \mathcal{M} and inj its injectivity radius.

Theorem 5 (Theorem 5.3.3). *Let (\mathcal{M}, g) be a smooth, complete Riemannian manifold with $|\text{Ric}| \leq C$ and $\text{inj}(\mathcal{M}) \geq \kappa > 0$. Let $a, A \in L^\infty$ and suppose that the following ellipticity condition holds: there exist $\kappa_1, \kappa_2 > 0$ such that*

$$\text{Re} \langle au, u \rangle \geq \kappa_1 \|u\|^2 \quad \text{and} \quad \text{Re} \langle ASv, Sv \rangle \geq \kappa_2 \|v\|_{W^{1,2}}^2$$

for all $u \in L^2(\mathcal{M})$ and $v \in W^{1,2}(\mathcal{M})$. Then the problem $(\text{Kato}_{\mathcal{M}})$ is solved in the positive.

This theorem is obtained as a consequence of a more general theorem on tensors, which is obtained through an even more general theorem on vector bundles satisfying generalised bounded geometry. We refrain from listing these more general results here because they require additional technical assumptions which are arduous to define. These results are presented in detail in Chapter 5.

Let us remark that Theorems 3, 4, 5 provide solutions to Kato's question (K1). However, these theorems also have an accompanying stability theorem of the type (K2). More explicitly, these theorems assert that the (non-linear) operator $(a, A) \mapsto L_A = \sqrt{aS^*AS}$ (or in the case of nilpotent Lie groups the operator $(a, A) \mapsto \sqrt{-a \text{div} A \nabla}$), satisfies Lipschitz bounds. Since we allow the coefficients a and A to be complex, we are able to obtain solutions to (K2) immediately from (K1). These results are listed in detail in §4.5 and §5.4.

The fundamental objects of the AKM setup are Dirac type operators, and indeed, the authors of [8] obtain a version of the Kato square root problem for differential forms. We are able to consider a similar, inhomogeneous problem in our case. We emphasise again that the following theorem is possible because we obtain quadratic estimates on non-trivial bundles. In this theorem, $\Omega(\mathcal{M})$ denotes the space of differential forms on \mathcal{M} , R the curvature endomorphism (§6.3) (which can be seen to generalise Ricci curvature to forms), and $D_A = d + A^{-1}d^*A$ for an invertible $A \in L^\infty(\mathcal{L}(\Omega(\mathcal{M})))$.

Theorem 6 (Theorem 6.4.3). *Let (\mathcal{M}, g) be a smooth, complete Riemannian manifold and let $\beta \in \mathbb{C} \setminus \{0\}$. Suppose there exist $\eta, \kappa > 0$ such that $|\text{Ric}| \leq \eta$ and $\text{inj}(\mathcal{M}) \geq \kappa$. Furthermore, suppose there exists $\zeta \in \mathbb{R}$ satisfying $g(R\omega, \omega) \geq \zeta |\omega|^2$ for $\omega \in \Omega_x(\mathcal{M})$ and all $x \in \mathcal{M}$, and that $A \in L^\infty(\mathcal{L}(\Omega(\mathcal{M})))$ such that there exists*

$\kappa_1 > 0$ satisfying

$$\operatorname{Re} \langle Au, u \rangle \geq \kappa_1 \|u\|^2$$

for all $u \in L^2(\Omega(\mathcal{M}))$. Then, $\mathcal{D}(\sqrt{D_A^2 + |\beta|^2}) = \mathcal{D}(D_A) = \mathcal{D}(d) \cap \mathcal{D}(d^*A)$ and $\|\sqrt{D_A^2 + |\beta|^2}u\| \simeq \|D_A u\| + \|u\|$.

The proofs of the Kato square root theorems we have presented here rely upon the analysis of canonical differential operators such as ∇ and $\operatorname{div} = -\nabla^*$ to obtain estimates such as cancellations with respect to these operators or the control of the Hessian via the Laplacian. To obtain such results, and more generally in PDE, it is useful to know that smooth compactly supported functions are dense in the domains of such operators. While a slight departure from geometric Kato square problems, but very much motivated by it, we study these *density problems*. The first theorem we present is the following very general result on vector bundles, and it is made possible by taking a first-order perspective, very much motivated by the AKM framework. We note that to say ∇ and a metric h on a vector bundle are compatible means that ∇ satisfies a product rule with respect to h .

Theorem 7 (Theorem 2.2.6). *Let \mathcal{M} be a smooth, complete Riemannian manifold with smooth metric g and let \mathcal{V} be a smooth vector bundle over \mathcal{M} with smooth metric h and connection ∇ . Suppose that h and ∇ are compatible. Then, $C_c^\infty(\mathcal{V})$ is dense in $\mathcal{D}(\nabla) = W^{1,2}(\mathcal{V})$ and $C_c^\infty(T^*\mathcal{M} \otimes \mathcal{V})$ is dense in $\mathcal{D}(\operatorname{div})$. Furthermore, $C_c^\infty(\mathcal{V})$ is dense in $\mathcal{D}(-\operatorname{div} \nabla)$ (Bochner Laplacian) and $C_c^\infty(T^*\mathcal{M} \otimes \mathcal{V})$ is dense in $\mathcal{D}(-\nabla \operatorname{div})$ (co-Laplacian).*

In the book [33], Hebey states that the best known conditions for determining that compactly supported functions are dense in the second-order Sobolev space $W^{2,2}(\mathcal{M})$ (associated to the Hessian) is under both Ricci curvature bounds and injectivity radius bounds. To the best of our knowledge, no improvement has been made to this result since the writing of this book in 2001. We make the following improvement by dispensing the injectivity radius bounds.

Theorem 8 (Theorem 2.4.1). *Let \mathcal{M} be a smooth, complete Riemannian manifold with metric g and Levi-Cevita connection ∇ . If there exists $\eta \in \mathbb{R}$ such that $\operatorname{Ric} \geq \eta g$, then $C_c^\infty(\mathcal{M})$ is dense in $W^{2,2}(\mathcal{M})$.*

We conclude this thesis by listing a set of open problems in Chapter 7, whose solutions we expect would advance our understanding of geometric Kato square root problems.