An Abstract Kato's Inequality for Generators of Positivity Preserving Semigroups

BARRY SIMON

§ 1. Introduction. Several years ago, Kato [11] proved a simple but extremely useful inequality:

$$\Delta|u| \geq (\operatorname{sgn} u)\Delta u \tag{1}$$

for u real valued with $u \in L^1_{\text{loc}}$ and $\Delta u \in L^1_{\text{loc}}$ (distribution inequality). (1) is to be interpreted as a distributional inequality although it is proven by a limiting argument starting with nice u's. The use Kato made of (1) was to prove:

Theorem 1.1. *(Kato* [11]*). Let $V \in L^2_{\text{loc}}(\mathbb{R}^n)$, $V \geq 0$. Then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.*

Kato was motivated in part by a result of Simon [15] who used hypercontractive semigroup methods (see §X.9 and its notes in [12]) to prove the weaker result where $V \in L^2_{\text{loc}}(\mathbb{R}^n)$ is replaced by $L^2(\mathbb{R}^n, \exp(-ax^2)dx)$ for some a. By using the simpler contractive semigroup methods, Semenov [14] (see also Davies [4] and Faris [5]) noted that one can prove the result with $V \in L^2(\mathbb{R}^n, dx)$. There is clearly a relation between the hypercontractive and contractive semigroup methods, but there seems to be little connection between those proofs and Kato's proof. Our main purpose in this note is to show that the methods are related since both depend on the fact that $e^{t\Delta}$ has a positive kernel: this positivity and $\Delta 1 = 0$ lead to the fact that $e^{t\Delta}$ is a contractive semigroup: our point in this note is that (1) is "essentially" equivalent to this positivity.

The link between (1) and positivity preserving semigroups is via the following theorem of Beurling-Deny [2]:

Theorem 1.2. *(Beurling-Deny* [2]*). Let H be a positive self-adjoint operator on $L^2(M, d\mu)$. Then $\exp(-tH)$ is positivity preserving for all $t > 0$, if and only if $u \in Q(H)$, the form domain of H implies $|u| \in Q(H)$ with $(|u|, H|u|) \leq (u, Hu)$.*

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(We note that the statement in [2] is very different looking involving "pure potentials being positive"; moreover, the result is only stated for finite-dimensional L^2 spaces! but the method extends, and the more general result is announced in [1]. For additional discussion, see [7, 13].)

If we proceed formally from (1), we see that multiplying (1) by $|u|$ and integrating $(|u|, \Delta|u|) \geq (u, \Delta u)$ so that (1) is related to positivity of $e^{t\Delta}$ via Theorem 1.2. We make a precise statement of this in §2 and discuss the resulting self-adjointness theorems in §3, 4. In §5, we consider relations between two different operators, the prototype being Kato's inequality with magnetic fields [11, 16]. Finally in §6, we mention a connection between two apparently different proofs of nodelessness of ground states.

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§ 2. The Basic Inequality.

Definition. Let H be an operator on $L^2(M, d\mu)$. We say that *H obeys Kato's inequality* if and only if

(i) $u \in Q(H)$ implies $|u| \in Q(H)$

(ii) For $u \in D(H)$ and $f \in Q(H)$ with $f \geq 0$

$$\mathrm{Re}(f, H|u|) \leq \mathrm{Re}((\mathrm{sgn}\, u)^* f, Hu). \tag{2}$$

The left side of (2) is to be interpreted in the sense of a quadratic form expression which makes sense since $f, |u| \in Q(H)$. We note that *a posteriori*, it will turn out that $(f, H|u|)$ is real so that (2) really says

$$H|u| \leq (\mathrm{sgn}\, u) Hu. \tag{2'}$$

The right side of (2) is interpreted in the sense of the inner product of Hu and $(\mathrm{sgn}\, u)^* f$. We note that

$$\begin{aligned} (\mathrm{sgn}\, u)\,(x) &= 0 \qquad \text{if} \quad u(x) = 0 \\ &= u^*(x)/|u(x)| \quad \text{otherwise.} \end{aligned}$$

Finally, we remark, that by (i) $Q(H)$ has many positive elements so that (ii) is a severe restriction on H.

The main result of this note is:

Theorem 2.1. *$H \geq 0$ obeys Kato's inequality if and only if e^{-tH} is positivity preserving for all t.*

Proof. If Kato's inequality holds, given $u \in D(H)$ take $f = |u|$ and obtain $(|u|, H|u|) \leq (u, Hu)$. By a limiting argument this extends to all $u \in Q(H)$ whence e^{-tH} is positivity preserving by the Beurling-Deny Theorem (Theorem 1.2). Conversely, if e^{-tH} is positivity preserving for any u and any $f \geq 0$

$$\operatorname{Re}((\operatorname{sgn} u)^* f,\ e^{tH} u) \leq (f,\ e^{-tH}|u|)$$

with equality at $t = 0$. Thus, if $u \in D(H), f, |u| \in Q(H)$ we can differentiate at $t = 0$ and obtain (2).

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§ 3. **The Self-Adjointness Theorem.** To use Kato's inequality as a self-adjointness tool, we need a regularity assumption.

Hypothesis R. We say that $e^{-tH} : L^2(M, d\mu) \to L^2(M, d\mu)$ obeys Hypothesis R if and only if

$$\sup_{t \geq 0} \left\{ \|e^{-tH} f\|_1 \,\middle|\, f \in L^1 \cap L^2,\ \|f\|_1 \leq 1 \right\} < \infty$$

and

$$\lim_{t \to 0} \quad \|e^{-tH} f - f\|_1 = 0 \quad \text{for all} \quad f \in L^1.$$

Remarks. 1. By replacing H by $H + c$, it suffices to take the sup over $t \leq 1$.
2. Since $e^{-tH} f \to f$ in L^1 and for any $\delta > 0$:

$$(1 + \delta H)^{-1} f = \int_0^\infty e^{-t}\, e^{-t\delta H} f\, dt$$

we have

(3) $$\lim_{\delta \downarrow 0} (1 + \delta H)^{-1} f = f; \text{ all } f \in L^1.$$

Moreover, if e^{-tH} is positivity preserving, so is $(1 + \delta H)^{-1}$.
3. Notice we do not suppose that $\lim_{t \downarrow 0} \|e^{-tH}\|_{1,1} = 1$.

Definition. A subset $\mathscr{D}$ of L^2 is called a *fundamental domain* for H if and only if:

(i) $\mathscr{D} \subset L^\infty \cap D(H)$ where $D(H)$ is the (L^2)-domain of H.

(ii) $\mathscr{D}$ is left invariant by $(1 + \delta H)^{-1}$ for all $\delta > 0$.

(iii) For any $g \in L^2 \cap L^\infty$, there exists a sequence $g_n \in \mathscr{D}$ with $\|g_n - g\|_2 \to 0$ and $\sup_n \|g_n\|_\infty < \infty$. If $g \geq 0$, g_n can be chosen ≥ 0.

Remarks. 1. By (iii) $\int g_n f \to \int g f$ for any $f \in L^1 \cap L^2$ and so any $f \in L^1$.

2. Under hypothesis R and e^{-tH} positivity preserving $\mathscr{D} = L^\infty \cap D(H)$ is a fundamental domain, as is easy to see ($C^\infty(H) \cap L^\infty$ will also do!).

We can now give an abstract version of Kato's basic self-adjointness result [11]. Our proof is closely related to his.

Theorem 3.1. *Let e^{-tH} be a positivity preserving semigroup on $L^2(M, d\mu)$ obeying Hypothesis R. Let V be a multiplication operator so that* (i) $V_+ = \max(V, 0) \in L^2(M, d\mu)$, (ii) $V_- = \max(-V, 0)$ *is a multiplication operator which is H bounded with relative bound $\alpha < 1$. Then $H + V$ is essentially self-adjoint on any fundamental domain, $\mathscr{D}$, for H.*

Proof. Suppose first that $V_- = 0$. Suppose that u obeys $[(H + V + 1) \mid \mathscr{D}]^* u = 0$, *i.e.*

$$(4) \qquad (Hf, u) = -((V + 1)f, u) \text{ all } f \in \mathscr{D}.$$

Let $u_\delta = (1 + \delta H)^{-1} u \in D(H)$. Let $f \in \mathscr{D}$ with $f \geq 0$. Then by Theorem 2.1,

$$(5) \qquad (f, H|u_\delta|) \leq ((\text{sgn } u_\delta)^* f, Hu_\delta).$$

As $\delta \downarrow 0$, the left side of (5) converges to $(Hf, |u|)$ since $f \in D(H)$ $u_\delta \to u$ in L^2 so that $|u_\delta| \to |u|$ in L^2.

Now let $g \in \mathscr{D}$, arbitrary. Then, by (4):

$$\begin{aligned}(g, Hu_\delta) &= (H(1 + \delta H)^{-1} g, u) \\ &= -((1 + \delta H)^{-1} g, (V + 1)u) \\ &= -(g, (1 + \delta H)^{-1} (V + 1)u)\end{aligned}$$

where $(1 + \delta H)^{-1} (V + 1) u$ = sum of L^1 term + L^2 term. By Remark 1 above, this extends to all $g \in L^2 \cap L^\infty$ so that

$$(6) \qquad ((\text{sgn } u_\delta)^* f, Hu_\delta) = -((\text{sgn } u_\delta)^* f, (1 + \delta H)^{-1} (V + 1)u).$$

Now, let $w = (V + 1)u$, $w_\delta = (1 + \delta H)^{-1} w$, $s_\delta = (\text{sgn } u_\delta)^*$, $s = (\text{sgn } u)^*$. Then

$$(7) \qquad (s_\delta f, w_\delta) - (sf, w) = (s_\delta f, w_\delta - w) + ((s_\delta - s)f, w).$$

The first term in (7) goes to zero since $\|w_\delta - w\|_1 \to 0$ (see Remark 2 following Hypothesis R). The second goes to zero, if we pass to a subsequence, since $s_\delta - s \to 0$ on $\{x \mid u \neq 0\} = \{x \mid w \neq 0\}$ and $|(s_\delta - s) fw| \leq 2f|w|$. Thus by (5), (6), (7):

$$(Hf, |u_\delta|) \leq -(f, (V + 1)|u|)$$

so that

$$((H + 1)f, |u_\delta|) \leq 0.$$

Letting $f = (H + 1)^{-1} g$ with $g \geq 0$, $g \in \mathscr{D}$:

$$(g, |u_\delta|) \leq 0$$

so that $|u_\delta| = 0$ by (iii) of the properties of $\mathscr{D}$. This completes the proof when $V_- = 0$.

The V_- part can be added by using the Davies-Faris Theorem (see Theorem X.31 of [12]).

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There is a close connection between Theorem 3.1 and the contractive semigroup theorem of [10]. An important difference is that the latter theorem depends critically on $\lim_{t \downarrow 0} \|e^{-tH}\|_{1,1} = 1$, while Theorem 3.1 does not (on the other hand Theorem 3.7 needs positivity of e^{-tH}).

Remark. Using the idea of Faris, [5, 6], Theorem 3.1 can be made applicable to $P(\varnothing)_2$ spatially cutoff Hamiltonian [8, 17]. Several years ago, Faris (private communication) remarked to the author that he had a "Kato's inequality" proof for $P(\phi)_2$.

§4. **Localization.** The advantage of Kato's method of proving Theorem 1.1 is that his method allows localization. Here we give an abstraction of this idea.

Theorem 4.1. *Let e^{-tH} be a positivity preserving semigroup on $L^2(M, d\mu)$. Let $M = \bigcup X_n$, $X_1 \subset X_2 \subset \cdots \subset X_n \subset \cdots$. Suppose that there are bounded functions f_n so that*

(a) supp $g \subset X_k$ *implies* supp$[f_n(H)g] \subset X_{k+1}$.

(b) *For some C independent of n and all p*

$$\|f_n(H)g\|_p \leq C\|g\|_p.$$

(c) *$f_n(H)g \to g$ in L^2 for all $g \in L^2$.*

(d) *Given $f \geq 0$, there are $g_n \geq 0$ so that each g_n is in $C^\infty(H)$ and has support in some X_k so that*

$$g_n \to (H + 1)^{-1} f$$

in L^2.

Let $\mathscr{D} = \bigcup_n \{ f \in C^\infty(H) \mid \text{supp } f \subset X_n\}$. Then for any V with $\int_{X_n} |V(x)|^2 dx < \infty$ all n, $V \geq 0$, $H + V$ is essentially self-adjoint on $\mathscr{D}$.

Proof. The same as Theorem 3.1 with u_δ replaced by $f_n(H)u$. This leads to

$$((H + 1)f, |u|) = 0$$

for $f \in \mathscr{D}$ so $|u| = 0$ by (d).

■

§5. **Comparing Different Operators.**

Theorem 5.1. *Let A, B be positive self-adjoint operators. Suppose that*

$$|e^{-tA}g| \leq e^{-tB}|g| \tag{8}$$

for all g. Then, $u \in D(A)$ implies that $|u| \in D(B)$ and for all $f \geq 0$ in $Q(B)$:

$$(f, B|u|) \leq Re((sgn\ u)^* f, A\ u). \tag{9}$$

Proof. First

$$(u, e^{-tA}u) \leq (|u|, e^{-tB}|u|)$$

so $u \in Q(A)$ implies $(u, (1 - e^{-tA})u)t^{-1}$ has a finite limit so $(|u|, (1 - e^{-tB}|u|)t^{-1}$ has a finite limit so $|u| \in Q(B)$. Now

$$Re((sgn\ u)^* f, (1 - e^{-tA})u) \geq (|f|, (1 - e^{-tB})|u|)$$

so that (9) results.

■

Conjecture. *Theorem 5.1 has a converse, i.e. (9) implies (8).*

Example. Let $B = -\Delta$ on $\mathbb{R}^n$. Let $A = -(\partial - ia)^2$. Then one can show that (8) holds following an argument of Nelson (private communication). There is a formula for e^{-tA} in terms of stochastic and Weiner path integrals. For example if div $a = 0$ (Colomb gauge),

$$(e^{-tA})(x, y) = \int \exp\left(\int i\, a(\omega(t))d\omega\right) d\mu_{x,y,t}(\omega)$$

so that

$$|e^{-tA}(x, y)| \leq \int d\mu_{x,y,t}(\omega) = e^{-tB}(x, y).$$

This yields a proof of Kato's inequality with magnetic fields [11, 16].

§6. Ground State Energies. There are two general proofs of the nodelessness property of ground states in quantum systems. One in Courant-Hilbert [3] uses

$$\int (\nabla |u|)^2 dx \leq \int |\nabla u|^2 dx$$

The other ([9, 19]) uses Perron-Frobenius arguments. The Beurling-Deny Theorems shows these proofs are really the same and suggests Kato's inequality might be connected with ground states. In fact, we proved in [18]:

Theorem 6.1. *Let $H = -\Delta + V$, $\tilde{H} = -(\partial\text{-}ia)^2 + V$. Then for any a,* inf spec$(\tilde{H}) \geq$ inf spec(H).

Proof. This follows from

$$(|u|, H|u|) \leq (u, \tilde{H}\, u)$$

which in turn follows from Kato's inequality (see §5)

$$H|u| \leq \mathrm{Re}((\mathrm{sgn}\, u)\tilde{H}\, u).$$

■

Remark. By the remarks in the example of §5, this result extends to free energies, *i.e.*

$$Tr((\exp(-\beta\tilde{H})) \leq Tr(\exp(-\beta H)).$$

Added note. E. B. Davies has kindly pointed out that a result similar to what we have called the Beurling Deny Theorem appears earlier in Aronszajn and Smith. The conjecture in §5 has been proven independently by the author (University of Geneva preprint) and by Hess, Schrader and Uhlenbrock (University of Berlin preprint).

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Princeton University, Princeton, NJ 08540