

SEMIGROUP GROWTH BOUNDS

version 15

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1 Introduction

The theory of one-parameter semigroups provides a good entry into the study of the properties of non-self-adjoint operators and of the evolution equations associated with them. There are many situations in which such an operator A arises by linearizing some non-linear evolution equation around a stationary point. The stability of the stationary point implies that every eigenvalue of the semigroup $T_t = e^{At}$ has negative real part, but the converse is not true. This was vividly demonstrated in a famous example of Zabczyk, in which the semigroup norm grows exponentially, although every eigenvalue of the operator in question is purely imaginary, [5, Th. 2.17], [34]. One of the main points of this paper is to emphasize that similar phenomena occur for the so-called Schrödinger semigroups, which have extensive applications in quantum theory and stochastic processes. We will see that the long time behaviour of the norms of diffusion semigroups with *self-adjoint generators* may be entirely different for the L^1 and L^2 norms, although the generator has the same spectrum in the two spaces. In other words, growth bounds proved using the spectral theorem for self-adjoint operators may not generalize to the ‘same’ evolution equation acting in other Banach spaces, even when the other norm is physically more relevant than the Hilbert space norm.

We mention in passing that in hydrodynamics Trefethen and others have established that pseudospectral methods may provide stability information unavailable by the use of spectral theory alone; see [27, 28, 10]. On the other hand Renardy has shown that in a number of hydrodynamic problems spectral analysis does indeed suffice to determine stability, [19, 20, 21].

There is an enormous literature studying the asymptotic behaviour of one-parameter semigroups as $t \rightarrow \infty$, [11], but as far as stability is concerned short time bounds on the semigroup norm are often more relevant: if $f_t = T_t f$ grows rapidly for some time, before eventually decaying exponentially, then the linear approximation may become inappropriate before this decay comes into effect (or would do under the

linear approximation). The fact that the short time and long time behaviour of a semigroup may be quite different is physically very clear for the convection-diffusion operator on a bounded interval or region, [18], [30, p.16-19]; see also [7]. In this case the underlying cause is the non-self-adjointness of the operators concerned, which act in a Hilbert space.

Our goal is to obtain information about the short time behaviour of the semigroup from norm bounds on the resolvent operators – closely related to the pseudospectra, for which efficient computations are now available, [26, 27, 31, 30, 32]. We succeed in obtaining lower bounds, not on the semigroup norms themselves, but on certain regularizations, defined in the next section. We also show (Theorem 29) that it is not possible to obtain similar upper bounds from numerical information about the resolvent norms, however accurate this information may be. Both of these facts are completely invisible if one only looks at the spectrum of the relevant operator, which is of limited use for stability analysis.

Some of the results in this paper are already familiar in one form or another, and the paper is written to help communication between experts in the various fields involved. The contents of Sections 2 and 7 and the numerical aspects of Section 5 are, however, entirely new.

2 Lower Bounds

If T_t is a one-parameter semigroup with generator A , we define

$$\begin{aligned}\omega_0 &= \limsup_{t \rightarrow +\infty} t^{-1} \log(\|T_t\|), \\ s &= \sup\{\operatorname{Re}(\lambda) : \lambda \in \operatorname{Spec}(A)\}, \\ s_\varepsilon &= \sup\{\operatorname{Re}(z) : \|R_z\| \geq \varepsilon^{-1}\}, \\ s_0 &= \lim_{\varepsilon \rightarrow 0} s_\varepsilon \\ \rho &= \min\{\omega : \|T_t\| \leq e^{\omega t} \text{ for all } t \geq 0\}\end{aligned}$$

where $R(z)$ is the resolvent operator and $\varepsilon > 0$. s and s_0 are often called the spectral and pseudospectral abscissas respectively. An alternative characterization of ρ , sometimes called the logarithmic norm of A , is given in Lemma 2. One always has $s \leq s_0 \leq \omega_0 \leq \rho$, and each of these may be a strict inequality. In a Hilbert space $\omega_0 = s_0$, [11, Th. 5.1.11], so the value of ω_0 is deducible from knowledge of the pseudospectra (i.e. the resolvent norms). This identity is, however, not always valid in Banach spaces.

The semigroup T_t (or its generator) is sometimes said to satisfy the weak stability principle if $s = \omega_0$, and the strong stability principle if there exists a constant M such that

$$\|T_t\| \leq Me^{st}$$

for all $t \geq 0$. Every diagonalizable matrix satisfies the strong stability principle, as does every operator in a Hilbert space which is similar to a normal operator. In Section 5 we will show that physically important self-adjoint operators need not satisfy the strong stability principle if they are considered with respect to a natural non-Hilbertian norm.

In Example 12 we show that $\|T_t\|$ may oscillate rapidly with time. Because of this possibility we will not study the norm itself, but a regularization of it. Although our main application is to one-parameter semigroups, we work at a more general level to facilitate the discussions in the final section. We assume that \mathcal{B}, \mathcal{D} are two Banach spaces and that $T_t : \mathcal{D} \rightarrow \mathcal{B}$ is a strongly continuous family of operators defined for $t \geq 0$, satisfying $\|T_0\| = 1$ and $\|T_t\| \leq Me^{\omega t}$ for some M, ω and all $t \geq 0$. We define $N(t)$ to be the upper log-concave envelope of $\|T_t\|$. In other words $\nu(t) = \log(N(t))$ is defined to be the smallest concave function satisfying $\nu(t) \geq \log(\|T_t\|)$ for all $t \geq 0$. It is immediate that $N(t)$ is continuous for $t > 0$, and that

$$1 = N(0) \leq \lim_{t \rightarrow 0^+} N(t).$$

In many cases one may have $N(t) = \|T_t\|$, but we do not study this question, asking only for lower bounds on $N(t)$ which are based on pseudospectral information.

If $k \in \mathbf{R}$ and we replace T_t by $T_t e^{kt}$ then $\|T_t\|$ is replaced by $\|T_t\| e^{kt}$ and $N(t)$ is replaced by $N(t) e^{kt}$. We put $k = -\omega_0$ or, equivalently, normalize our problem by assuming that $\omega_0 = 0$. In the semigroup context this implies that $\text{Spec}(A) \subseteq \{z : \text{Re}(z) \leq 0\}$. It also implies that $\|T_t\| \geq 1$ for all $t \geq 0$ by [5, Th. 1.22]. If we define $R_z : \mathcal{D} \rightarrow \mathcal{B}$ by

$$R_z f = \int_0^\infty (T_t f) e^{-zt} dt$$

then $\|R_z\|$ is uniformly bounded on $\{z : \text{Re}(z) \geq \gamma\}$ for any $\gamma > 0$, and the norm converges to 0 as $\text{Re}(z) \rightarrow +\infty$. In the semigroup context R_z is the resolvent of the generator A of the semigroup.

The following lemma compares $N(t)$ with the alternative regularization

$$L(t) = \sup\{\|T_s\| : 0 \leq s \leq t\}$$

of $\|T_t\|$, which was introduced by Trefethen, [29], and implemented in the package Eigtool by Wright, [30, page 82], [31].

Lemma 1 *If $\omega_0 = 0$ then*

$$\|T_t\| \leq L(t) \leq N(t).$$

for all $t > 0$. If T_t is a one-parameter semigroup then we also have

$$N(t) \leq L(t/n)^{n+1}$$

for all positive integers n and $t \geq 0$.

Proof The log-concavity of $N(t)$ and the assumption that $\omega_0 = 0$ imply that $N(t)$ is a non-decreasing function of t . We conclude that $\|T_t\| \leq L(t) \leq N(t)$. If T_t is a one-parameter semigroup we note that $s \rightarrow L(t/n)^{1+ns/t}$ is a log-concave function which dominates $\|T_s\|$ for all $s \geq 0$, and which therefore also dominates $N(s)$.

In the following well-known lemma we put

$$N'(0+) = \lim_{\varepsilon \rightarrow 0+} \varepsilon^{-1} \{N(\varepsilon) - N(0)\} \in [0, +\infty].$$

Lemma 2 *The constant ρ satisfies*

$$\rho = N'(0+) \geq \limsup_{t \rightarrow 0} t^{-1} \{\|T_t\| - 1\}.$$

If T_t is a one-parameter semigroup and \mathcal{B} is a Hilbert space then

$$\rho = \sup\{\operatorname{Re}(z) : z \in \operatorname{Num}(A)\} \tag{1}$$

where $\operatorname{Num}(A)$ is the numerical range of A .

Proof If $N'(0+) \leq \omega$ then, since $N(t)$ is log-concave,

$$\|T_t\| \leq N(t) \leq e^{\omega t}$$

for all $t \geq 0$. The converse is similar. The second statement follows from the fact that, assuming A to be the generator of a one-parameter semigroup, $A - \omega I$ is the generator of a contraction semigroup if and only if $\operatorname{Num}(A - \omega I)$ is contained in $\{z : \operatorname{Re}(z) \leq 0\}$.

We study the function $N(t)$ via a transform, defined for all $\omega > 0$ by

$$M(\omega) = \sup\{\|T_t\|e^{-\omega t} : t \geq 0\}.$$

We see that up to a sign $\mu(\omega) = \log(M(\omega))$ is the Legendre transform of $\nu(t)$ (also called the conjugate function), and must be convex. It is also clear that $M(\omega)$ is a monotonic decreasing function of ω which converges as $\omega \rightarrow +\infty$ to $\limsup_{t \rightarrow 0} \|T_t\|$. Hence $M(\omega) \geq 1$ for all $\omega > 0$. We also have

$$N(t) = \inf\{M(\omega)e^{\omega t} : 0 < \omega < \infty\} \tag{2}$$

for all $t > 0$ by the theory of the Legendre transform, or simple convexity arguments, [25].

In the semigroup context the constant c introduced below measures the deviation of the operator A from any generator of a contraction semigroup.

Lemma 3 *If $a > 0$, $b \in \mathbf{R}$ and $a\|R_{a+ib}\| = c \geq 1$ then*

$$M(\omega) \geq \tilde{M}(\omega) := \begin{cases} (a - \omega)c/a & \text{if } 0 < \omega \leq r = a(1 - 1/c) \\ 1 & \text{otherwise.} \end{cases}$$

Proof The formula

$$R_{a+ib} = \int_0^\infty T_t e^{-(a+ib)t} dt \quad (3)$$

implies that

$$c/a \leq \int_0^\infty N(t) e^{-at} dt \leq \int_0^\infty M(\omega) e^{\omega t - at} dt$$

for all ω such that $0 < \omega < a$. The estimate follows easily.

This lemma is most useful when c is much larger than 1. If $c = 1$ then $r = 0$ and the lemma reduces to $M(\omega) \geq 1$ for all $\omega > 0$.

Theorem 4 *If $a\|R_{a+ib}\| = c \geq 1$ and $r = a(1 - 1/c)$ then*

$$N(t) \geq \min\{e^{rt}, c\}$$

for all $t \geq 0$.

Proof This uses

$$N(t) \geq \inf\{\tilde{M}(\omega) e^{\omega t} : \omega > 0\},$$

which follows from (2).

Trefethen and Wright give a related lower bound in [29, 30], namely

$$L(t) \geq \frac{e^{at}}{1 + (e^{at} - 1)/c}.$$

Although these are lower bounds for different quantities and under slightly different conditions, the bound of Theorem 4 is better in the following sense. The two sides of (4) are asymptotically equal as $t \rightarrow 0+$ and $t \rightarrow \infty$, but for intermediate t we have:

Lemma 5 *Let $a > 0$, $t \geq 0$ and $c \geq 1$ then*

$$\frac{e^{at}}{1 + (e^{at} - 1)/c} \leq \min\{e^{a(1-1/c)t}, c\}. \quad (4)$$

Proof Put $s = at$. There are two inequalities to prove for all $s \geq 0$.

$$\begin{aligned} \frac{e^s}{1 + (e^s - 1)/c} &\leq c, \\ \frac{e^s}{1 + (e^s - 1)/c} &\leq e^{(1-1/c)s}. \end{aligned}$$

After some algebraic manipulations, both are seen to be elementary.

The above theorem provides a lower bound on $N(t)$ from a single value of the resolvent norm. The well-known constants $c(a)$, defined for $a > 0$ by

$$c(a) = a \sup\{\|R_{a+ib}\| : b \in \mathbf{R}\},$$

are immediately calculable from the pseudospectra. it follows from (3) and $\omega_0 = 0$ that $c(a)$ remains bounded as $a \rightarrow +\infty$. The transform $\tilde{c}(\cdot)$ defined below is easily calculated from $c(\cdot)$.

Corollary 6 *Under the above assumptions one has*

$$N(t) \geq \tilde{c}(t) := \sup_{\{a:c(a) \geq 1\}} \left\{ \min\{e^{r(a)t}, c(a)\} \right\}. \quad (5)$$

where

$$r(a) = a(1 - 1/c(a)).$$

Theorem 7 *If T_t is a one-parameter semigroup and $s_0 = \omega_0 = 0$ then $c(a) \geq 1$ for all $a > 0$.*

Proof If $c(a) < 1$ then by using the resolvent expansion one obtains

$$\|R_{a+ib+z}\| \leq \frac{c(a)}{a} (1 - |z|c(a)/a)^{-1}$$

for all $|z| < a/c(a)$. This implies that $s_0 < 0$.

Examples show that $c(a)$ is often a decreasing function of a , but this is not true in Example 15 below. The supremum in (5) need only be taken over those a at which $c(a)$ is decreasing. The following transform of $c(\cdot)$ may sometimes be easier to compute than $\tilde{c}(\cdot)$.

Lemma 8 *If $c(\cdot) \geq 1$ is a monotonic decreasing function then $N(t) \geq \hat{c}(t)$ for all $t \geq 0$, where $\hat{c}(\cdot)$ is the function inverse to*

$$t(c) := \frac{\log(c)}{a(c)(1 - 1/c)}$$

and $c \rightarrow a(c)$ is the function inverse to $a \rightarrow c(a)$. The function $\hat{c}(t)$ is defined for all $0 < t < \infty$.

Proof We only consider the case in which $c(\cdot)$ is differentiable with a negative derivative at each point. The graph of $t \rightarrow N(t)$ lies above each of the points $(t(c), c)$ by Theorem 4. Putting $g(c) = \log(c)/(1 - 1/c)$ a direct calculation shows that $g'(c) \geq 0$ for all $c \geq 1$. Its definition implies that $a'(c) < 0$ for all c . Hence

$$t'(c) = \frac{a(c)g'(c) - a'(c)g(c)}{a(c)^2} > 0$$

The domain of $\hat{c}(\cdot)$ is the same as the range of $t(\cdot)$, and one may show that $t(c(a)) \rightarrow 0$ as $a \rightarrow \infty$, while $t(c(a)) \rightarrow \infty$ as $a \rightarrow 0$.

Although much recent progress has been made, the numerical computation of the pseudospectra is still relatively expensive. All of the examples of one-parameter

semigroups in the next section are positivity-preserving, in the sense that $f \geq 0$ implies $T_t f \geq 0$ for all $t \geq 0$. In this situation the evaluation of $c(a)$ is particularly simple. The following is only one of many special properties of positivity-preserving semigroups to be found in [17].

Lemma 9 *Let T_t be a positivity-preserving one-parameter semigroup acting in $L^p(X, dx)$ for some $1 \leq p < \infty$. If $\omega_0 = 0$ then*

$$\|R_{a+ib}\| \leq \|R_a\|$$

for all $a > 0$ and $b \in \mathbf{R}$. Hence $c(a) = a\|R_a\|$.

Proof Let $f \in L^p$ and $g \in L^q = (L^p)^*$, where $1/p + 1/q = 1$. Then

$$\begin{aligned} |\langle R_{a+ib}f, g \rangle| &= \left| \int_0^\infty \langle T_t f, g \rangle e^{-(a+ib)t} dt \right| \\ &\leq \int_0^\infty |\langle T_t f, g \rangle| e^{-at} dt \\ &\leq \int_0^\infty \langle T_t |f|, |g| \rangle e^{-at} dt \\ &= \langle R_a |f|, |g| \rangle \\ &\leq \|R_a\| \|f\|_p \|g\|_q. \end{aligned}$$

By letting f and g vary we obtain the statement of the lemma. (The inequality $|\langle Xf, g \rangle| \leq \langle X|f|, |g| \rangle$ for all positivity-preserving operators X may be proved by considering first the case in which f, g take only a finite number of values.)

3 A Direct Method

The direct calculation of $\|T_t\|$ for $t \geq 0$ is not straightforward for very large matrices, i.e in dimensions of order 10^6 , particularly when using the l^1 norm: even if A is sparse, e^{At} is usually a full matrix. If the generator A of the semigroup has enough eigenvalues the following method may be useful. Let $\{f_r\}_{r=1}^n$ be a linearly independent set of vectors in \mathcal{B} , and suppose that $Af_r = \lambda_r f_r$ for $1 \leq r \leq n$. Let \mathcal{L} denote the linear span of $\{f_1, \dots, f_n\}$ and let $T_{\mathcal{L},t}$ denote the restriction of T_t to \mathcal{L} . It is clear that

$$\|T_t\| \geq \|T_{\mathcal{L},t}\|$$

for all $t \geq 0$. If \mathcal{L} is large enough one might hope that this is a reasonably good lower bound. If A has a large number of eigenvalues, then one might choose some of them to carry out the above computation after inspecting the pseudospectra of A .

The operator $T_{\mathcal{L},t}$ must be distinguished from $P_n T_t P_n$, where P_n is the spectral projection of A associated with the set of eigenvalues $\{\lambda_1, \dots, \lambda_n\}$. If $n = 1$ the norm of the first operator is $|e^{-\lambda_1 t}|$ while the norm of the second is $\|P_1\| |e^{-\lambda_1 t}|$.

We will see in Table 4 that the norm of P_1 may be very large. Unfortunately the norm of $P_n T_t P_n$ is much easier to compute than that of $T_{\mathcal{L},t}$ in the l^1 context, using Matlab's **eigs** and **norm**($\cdot, \mathbf{1}$) routines, and it is easy to confuse the two.

The following standard result is included for completeness.

Lemma 10 *Under the above assumptions, suppose also that the linear span of $\{f_r\}_{r=1}^\infty$ is dense in \mathcal{B} . Let $T_{n,t}$ denote the restriction of T_t to $\mathcal{L}_n = \text{lin}\{f_1, \dots, f_n\}$. Then*

$$\lim_{n \rightarrow \infty} \|T_{n,t}\| = \|T_t\|$$

for all $t \geq 0$. If $t \rightarrow \|T_t\|$ is continuous on $[a, b]$ then the limit is locally uniform with respect to t on that interval.

Proof Given $\varepsilon > 0$ and $t \geq 0$ there exists $f \in \mathcal{B}$ such that $\|f\| = 1$ and $\|T_t f\| > \|T_t\| - \varepsilon$. By the assumed density property, we may assume that $f \in \mathcal{L}_n$ for some n . This immediately yields $\|T_t\| \geq \|T_{n,t}\| > \|T_t\| - \varepsilon$.

The final statement is a general property of any pointwise, monotonically convergent sequence of continuous functions to a continuous limit.

Clearly this lemma is of limited use in the absence of any information about the rate of convergence. If \mathcal{B} is a Hilbert space, the norms of the approximating semigroups may be evaluated by the following standard result. We know of no analogue of this lemma for subspaces of Banach spaces. The problem is that the unit balls of subspaces of L^1 may have very complicated shapes, which makes operator norms difficult to compute. For example the unit ball of a generic, real, two-dimensional subspace of $l^1\{1, \dots, n\}$ is a polygon with $2n$ sides, and higher dimensional subspaces are even more complicated.

Lemma 11 *If $B_{r,s} = \langle f_s, f_r \rangle$ and $D_{r,s,t} = e^{\lambda r t} \delta_{r,s}$ for $1 \leq r, s \leq n$, then*

$$\|T_{n,t}\| = \|B^{1/2} D_t B^{-1/2}\|$$

where the norm on the RHS is the operator norm, \mathbf{C}^n being provided with its standard inner product.

Proof The $n \times n$ matrix B is readily seen to be self-adjoint and positive. If $S : \mathbf{C}^n \rightarrow \mathcal{L}_n$ is defined by

$$S\alpha = \sum_{r=1}^n \beta_r f_r$$

where $\beta = B^{-1/2}\alpha$, then S is unitary and

$$S^{-1} T_t S = B^{1/2} D_t B^{-1/2}.$$

This yields the statement of the lemma.

4 Exactly Soluble Examples

Example 12 Let T_t be the positivity-preserving, one-parameter semigroup acting on $L^2(\mathbf{R}^+)$ with generator

$$Af(x) = f'(x) + v(x)f(x)$$

where v is any real-valued, bounded measurable function on \mathbf{R}^+ . Explicitly

$$T_t f(x) = \frac{a(x+t)}{a(x)} f(x+t) \quad (6)$$

for all $f \in L^2$ and all $t \geq 0$, where

$$a(x) = \exp \left\{ \int_0^x v(s) \, ds \right\}.$$

The function a is continuous and satisfies

$$e^{-\|v\|_\infty t} a(x) \leq a(x+t) \leq e^{\|v\|_\infty t} a(x)$$

for all x, t . hence $\|T_t\| \leq e^{\|v\|_\infty t}$ for all $t \geq 0$.

The precise behaviour of $\|T_t\|$ depends on the choice of v , or of a , and there is a wide variety of possibilities. For example if $c > 1$ and $b > 0$ then the choice

$$a(x) = 1 + (c-1) \sin^2(\pi x/2b) \quad (7)$$

leads to $\|T_{2nb}\| = 1$ and $\|T_{(2n+1)b}\| = c$ for all positive integers n . In the case (7), the regularizations $N(t)$ and $L(t)$ are not equal, but both are equal to c for $t \geq b$.

If $c > 0$ and $0 < \gamma < 1$ then the unbounded potential $v(x) = c(1-\gamma)x^{-\gamma}$ corresponds to the choice

$$a(x) = \exp\{cx^{1-\gamma}\}.$$

Instead of deciding the precise domain of the generator A , we define the one-parameter semigroup T_t directly by (6), and observe that

$$N(t) = \|T_t\| = \exp\{ct^{1-\gamma}\}$$

for all $t \geq 0$. If c is large and γ is close to 1, the semigroup norm grows rapidly for small t , before becoming almost stationary. The behaviour of $\|T_t f\|$ as $t \rightarrow \infty$ depends upon the choice of f , but for any f with compact support $T_t f = 0$ for all large enough t . On the other hand $\|T_t f\|$ cannot be a bounded function of t for all $f \in L^2(\mathbf{R}^+)$, because of the uniform boundedness theorem.

For this unbounded potential v , every z with $\operatorname{Re}(z) < 0$ is an eigenvalue, the corresponding eigenvector being

$$f(x) = \exp\{zx - c(1-\gamma)x^{1-\gamma}\}.$$

Hence

$$\text{Spec}(A) = \{z : \text{Re}(z) \leq 0\}.$$

On the other hand $\rho = +\infty$, and $\text{Num}(A)$, which is always a convex set, must equal the entire complex plane by Lemma 2.

Example 13 If we put

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

acting in \mathbf{C}^2 with the Euclidean norm, and $|\lambda| = r > 0$ then

$$\|R_\lambda\| = \frac{1}{2r^2} + \frac{\sqrt{1 + 1/4r^2}}{r}$$

so

$$c(a) = \frac{1}{2a} + \sqrt{1 + 1/4a^2}$$

for all $a > 0$. We also have

$$\|T_t\| = t/2 + \sqrt{1 + t^2/4}$$

which is log-concave, so $\|T_t\| = N(t)$ for all $t \geq 0$. The choice $a = 2$ provides a fairly good lower bound on $N(t)$ for $0 \leq t \leq 0.5$. As a gets smaller we get a better lower bound on $N(t)$ for large $t > 0$, while as a gets bigger we get a better lower bound for small $t > 0$.

Example 14 Let A be the $n \times n$ Jordan matrix

$$A_{i,j} = \begin{cases} 1 & \text{if } j = i + 1 \\ 0 & \text{otherwise} \end{cases}$$

acting in \mathbf{C}^n with the l^1 norm. Then

$$T_t = I + At + A^2 t^2 / 2! + \dots + A^{n-1} t^{n-1} / (n-1)!$$

and

$$\|T_t\| = 1 + t + t^2 / 2! + \dots + t^{n-1} / (n-1)!$$

for all $t \geq 0$. A direct calculation shows that

$$\|T_t\| = N(t) = L(t)$$

for all $t \geq 0$, and that $\rho = 1$.

Direct calculations are not so easy for this example if one uses the l^2 norm. However, in this case it follows from (1) that ρ equals the largest eigenvalue of $B = (A + A^*)/2$. Since the set of eigenvalues is $\{\cos(r\pi/(n+1))\}_{r=1}^n$, it follows that

$$\rho = \cos(\pi/(n+1)) < 1.$$

Example 15 Given $\gamma > 0$, let

$$A = \begin{bmatrix} -\gamma & 1 & 0 \\ 0 & -\gamma & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

act in \mathbf{C}^3 with the Euclidean norm. We have

$$\|T_t\| = \max \left\{ 1, e^{-\gamma t} \left\{ t/2 + \sqrt{1 + t^2/4} \right\} \right\}.$$

If $0 < \gamma < 1$ then this is not log-concave, and for γ close to 0, it increases linearly in t for a long time, before eventually dropping to 1. The functions $L(t)$ and $N(t)$ are equal, and they are constant for large enough $t > 0$. In this example

$$c(a) = \max \left\{ 1, \frac{a}{2(a + \gamma)^2} + \frac{a}{a + \gamma} \sqrt{1 + \frac{1}{4(a + \gamma)^2}} \right\}.$$

This equals 1 for small $a > 0$, and converges to 1 as $a \rightarrow \infty$, but it is not a monotonic decreasing function of a .

5 Schrödinger Semigroups

Semigroups with generators of the form $A = -H = \Delta - V$ have been extensively studied, and provide a fascinating insight into the importance of the Banach space on which they are chosen to act.

If one assumes that the potential (multiplication operator) $V : \mathbf{R}^N \rightarrow \mathbf{R}$ lies in the so-called Kato class, then the self-adjoint operator $H = -\Delta + V$ may be interpreted as a quadratic form sum in $L^2(\mathbf{R}^N)$, and the one-parameter ‘Schrödinger semigroup’ $\{e^{-Ht}\}_{t \geq 0}$ on L^2 may be extended consistently to all of the L^p spaces, $1 \leq p \leq \infty$, [24].

If H is interpreted as a quantum-mechanical Hamiltonian, then there are good reasons for being interested primarily in the choice $p = 2$. We show in the next section that the time-dependent Schrödinger equation $f'(t) = -iHf(t)$ is only soluble in L^p for $p = 2$, but in addition the use of the L^2 norm is fundamental to the probabilistic interpretation of quantum mechanics. In this context Schrödinger semigroups are only of technical interest; they enable one to investigate a variety of spectral questions very efficiently.

When studied in L^2 the spectral theorem yields the strong stability condition

$$\|e^{-Ht}\| = e^{-\lambda t}$$

where

$$\lambda = \min\{\text{Spec}(H)\}.$$

If the potential V depends upon a parameter c , then one often has $\lambda(c) = 0$ for some range of values of c , with transitions to $\lambda(c) < 0$ at certain critical values of c . These critical values describe the sharp emergence of instability.

Schrödinger semigroups also have direct physical significance in problems involving diffusion, but in this context the equation should be studied in $L^1(\mathbf{R}^N)$. The point here is that the semigroup e^{-Ht} is positivity-preserving, and $f_t = e^{-Ht} f$ describes the distribution of some continuous quantity in \mathbf{R}^N at time $t \geq 0$ given its initial distribution f . Assuming $f \geq 0$, the total amount of the quantity at time t is given by

$$\int_{\mathbf{R}^N} f(t, x) \, d^N x = \|f_t\|_1.$$

It is known that, in the technical context described above, the spectrum of H_p (the operator H considered as acting in L^p) is independent of p , [13]. The operators e^{-Ht} are known to have positive ‘heat’ kernels $K(t, x, y)$, [23], and

$$\|e^{-H_1 t}\| = \sup_{y \in \mathbf{R}^N} \int_{\mathbf{R}^N} K(t, x, y) \, d^N x.$$

We will see that these integrals of the heat kernel are not determined by the spectral properties of H_1 . We start by showing that the value of the constant ρ may be entirely different in the L^1 and L^2 contexts. The conditions on the potential V in the following theorem can clearly be weakened, and we refer to [1] for a comprehensive treatment of the problem.

Theorem 16 *Let $H_1 = -\Delta + V$, where V is continuous and bounded below, with*

$$c = \inf\{V(x) : x \in \mathbf{R}^N\}.$$

Then $c = -\rho$.

Proof The inequality $\rho \leq -c$, or equivalently

$$\|e^{-H_1 t}\| \leq e^{-ct} \text{ for all } t \geq 0$$

may be proved by the use of functional integration or the Trotter product formula, [23].

Conversely, let $\varepsilon > 0$ and let $|x - a| < \delta$ imply $c \leq V(x) < c + \varepsilon$. Let $f \in C_c^\infty(\{x : |x - a| < \delta\})$ be non-negative with $\|f\|_1 = 1$. Then

$$\begin{aligned} \rho &\geq \left\{ \frac{d}{dt} \|T_t f\| \right\}_{t=0} \\ &= \lim_{t \rightarrow 0} t^{-1} \{ \langle T_t f, 1 \rangle - \langle f, 1 \rangle \} \\ &= -\langle H_1 f, 1 \rangle \\ &= \langle \Delta f - V f, 1 \rangle \\ &= -\langle V f, 1 \rangle \\ &\geq -(c + \varepsilon) \langle f, 1 \rangle \\ &= -c - \varepsilon. \end{aligned}$$

This implies that $\rho \geq -c$.

Corollary 17 *If $H_1 = -\Delta + V$ where V is not bounded below, then $\rho = \infty$, whatever the spectral properties of H_1 .*

The above results show that the short time L^1 semigroup growth properties do not depend only upon whether the spectrum is non-negative. We cannot give a complete analysis of the long time behaviour, since the requisite theorems do not exist, but discuss a typical case below. Our main purpose is to emphasize that one may have a failure of the strong stability principle for such semigroups. Generalizations of this example have been studied in considerable detail by Murata, [15, 16], and by Davies and Simon, [8]. The most general results which we know about are by Zhang, [35].

Example 18 Let $N \geq 3$ and let

$$\alpha_{\pm} = \frac{N-2}{2} \pm \sqrt{\frac{(N-2)^2}{4} - c}, \quad 0 < c < \frac{(N-2)^2}{4}, \quad (8)$$

so that

$$0 < \alpha_- < \frac{N-2}{2} < \alpha_+ < N-2.$$

Now consider the operator $H_p = -\Delta + V$ acting in $L^p(\mathbf{R}^N)$, where the bounded, strongly subcritical potential V is defined by

$$V(x) = \begin{cases} -c|x|^{-2} & \text{if } |x| \geq 1 \\ 0 & \text{otherwise.} \end{cases}$$

It is known that the operator H_p has spectrum $[0, \infty)$ for all $1 \leq p \leq \infty$, and that $c = (N-2)^2/4$ is a critical value for the emergence of a negative eigenvalue, [13, 8]

The operator H_p possesses a zero energy resonance η given by

$$0 < \eta(x) = \begin{cases} |x|^{-\alpha_-} - \beta|x|^{-\alpha_+} & \text{if } |x| \geq 1 \\ 1 - \beta & \text{otherwise.} \end{cases}$$

where

$$0 < \beta = \frac{\alpha_-}{\alpha_+} < 1.$$

The operator $-H_p$ generates a positivity-preserving one-parameter semigroup acting in $L^p(\mathbf{R}^N)$ for all $1 \leq p \leq \infty$, and for $p = 2$ it is a self-adjoint contraction semigroup. On the other hand it is proved in [8, Th. 14] that for any σ_1, σ_2 satisfying $0 < \sigma_1 < \alpha_-/2 < \sigma_2 < \infty$ there exist positive constants c_1, c_2 such that

$$c_1(1+t)^{\sigma_1} \leq \|e^{-H_1 t}\| \leq c_2(1+t)^{\sigma_2} \quad (9)$$

for all $t \geq 0$, the norm being the operator norm in $L^1(\mathbf{R}^N)$. We conclude that $s = s_0 = \omega_0 = 0$ for this example, whether the operator is considered to act in $L^1(\mathbf{R}^N)$ or $L^2(\mathbf{R}^N)$.

The above example exhibits polynomial growth of the L^1 operator norm as $t \rightarrow \infty$. It exhibits the weak, but not the strong, stability property.

Theorem 19 *For every $\gamma > 0$ there exists a Schrödinger semigroup $e^{-K_p t}$ acting in $L^p(\mathbf{R}^N)$ for all $1 \leq p \leq \infty$ such that*

$$c_1(1 + \gamma^2 t)^{\sigma_1} \leq \|e^{-K_1 t}\| \leq c_2(1 + \gamma^2 t)^{\sigma_2}$$

for all $t \geq 0$, even though $K_2 = K_2^* \geq 0$ in $L^2(\mathbf{R}^N)$.

Proof The operator is given by $K_p = -\Delta + V_\gamma$, where

$$V_\gamma(x) = \begin{cases} -c|x|^{-2} & \text{if } |x| \geq 1/\gamma \\ 0 & \text{otherwise.} \end{cases}$$

The bounds are proved by reducing to the case $\gamma = 1$ by using the scaling transformation $(U_\gamma f)(x) = \gamma^{N/2} f(\gamma x)$.

By exploiting the rotational invariance, it is easily seen that the above example is associated with a similar example on the half-line. However, the transference procedure is different for the L^1 and L^2 norms.

Lemma 20 *Let the potential V be rotationally invariant and bounded below on \mathbf{R}^N . Then the self-adjoint operator $H = -\Delta + V$, defined as a quadratic form sum, is bounded below, and the one-parameter semigroup T_t defined for $t \geq 0$ by $T_t = e^{-Ht}$ acts consistently on $L^p(\mathbf{R}^N)$ for all $1 \leq p < \infty$ and commutes with rotations. If we identify the rotationally invariant subspace of $L^2(\mathbf{R}^N)$ with $L^2((0, \infty), dr)$ in the usual way, then the restriction of H_2 to this subspace is given by*

$$L_2 f(r) = -\frac{d^2 f}{dr^2} + \frac{(N-1)(N-3)}{4r^2} f(r) + V(r)f(r)$$

subject to Dirichlet boundary conditions at $r = 0$. On the other hand if we identify the rotationally invariant subspace of $L^1(\mathbf{R}^N)$ with $L^1((0, \infty), dr)$ in the usual way, then the restriction of H_1 to this subspace is given by

$$L_1 f(r) = -\frac{d^2 f}{dr^2} + (N-1)(f(r)/r)' + V(r)f(r)$$

subject to Dirichlet boundary conditions at $r = 0$.

Proof The operator H acts on the space $L^2((0, \infty), r^{N-1} dr)$ of rotationally invariant functions according to the formula

$$H_2 f(r) = -\frac{1}{r^{N-1}} \frac{d}{dr} \left\{ r^{N-1} \frac{df}{dr} \right\} + V(r)f(r).$$

We transfer H_2 to $L^2((0, \infty), dr)$ by means of the unitary map $Uf(r) = r^{(N-1)/2} f(r)$, obtaining the stated formula for $L_2 = UH_2U^{-1}$.

The operator H_1 acts on the space $L^1((0, \infty), r^{N-1} dr)$ of rotationally invariant functions according to the same formula as for H_2 . We transfer H_1 to $L^1((0, \infty), dr)$ by means of the isometric map $Vf(r) = r^{N-1}f(r)$, obtaining the stated formula for $L_1 = VH_1V^{-1}$.

There are two ways of seeing that one should impose Dirichlet boundary conditions at $r = 0$. If one calculates the heat kernels using functional integration, the relevant fact is that the probability of Brownian motion passing through the origin in \mathbf{R}^N for $N \geq 2$ is zero, [23]. Alternatively, subject to minimal regularity conditions on f at the origin, we see from their definitions that $Uf(0) = Vf(0) = 0$, at least if $N \geq 3$.

There are several ways of discretizing the operator L_1 . One obtains a discretization which has real eigenvalues and generates a positivity-preserving semigroup by starting from the formula

$$L_1f(r) = r^{(N-1)/2}L_2\{r^{-(N-1)/2}f(r)\}.$$

The last part of the following lemma will be used when carrying out numerical calculations below.

Lemma 21 *Let M_2 be a self-adjoint $n \times n$ matrix with non-positive off-diagonal entries, and let D be a diagonal $n \times n$ matrix with positive entries. Then the matrix*

$$M_1 = DM_2D^{-1}$$

*has the same, real, spectrum as M_2 , and e^{-M_1t} is positivity-preserving for all $t \geq 0$. If also $M_1^*1 \geq 0$ then e^{-M_1t} is a contraction semigroup on \mathbf{C}^n provided with the l^1 norm. If λ is an eigenvalue of M_2 with multiplicity 1 and $f \neq 0$ is a corresponding eigenvector, then the spectral projection P_λ of M_1 corresponding to the eigenvalue λ has norm*

$$\|P_\lambda\| = \frac{\|Df\|_1 \|(D^{-1})^*f\|_\infty}{\langle f, f \rangle} \quad (10)$$

calculated with respect to the l^1 norm of \mathbf{C}^n .

Proof See [5, Th. 7.14] or the proof of Lemma 24 for the positivity-preservation. The second statement is also classical, but we include a proof for completeness. Since the coefficients of the matrix e^{-M_1t} are non-negative, we have

$$\begin{aligned} \|e^{-M_1t}f\|_1 - \|f\|_1 &= \sum_{r=1}^n \left\{ |(e^{-M_1t}f)_r| - |f_r| \right\} \\ &\leq \sum_{r=1}^n \left\{ (e^{-M_1t}|f|)_r - |f_r| \right\} \\ &= \langle e^{-M_1t}|f| - |f|, 1 \rangle \\ &= - \int_0^t \langle M_1 e^{-M_1s}|f|, 1 \rangle ds \\ &= - \int_0^t \langle e^{-M_1s}|f|, M_1^*1 \rangle ds \\ &\leq 0. \end{aligned}$$

The expression for $\|P_\lambda\|$ is obtained from the formula

$$P_\lambda \phi = \frac{\langle \phi, (D^{-1})^* f \rangle}{\langle f, f \rangle} Df.$$

Example 22 We describe a discretization of the operator L_1 , with the critical value of the parameter c in (8), namely $c = (N - 2)^2/4$, and with $N = 3$, acting in the space C^n of finite sequences. We put

$$(M_2 f)_r = \begin{cases} (2 - v_1)f_1 - f_2 & \text{if } r = 1 \\ (2 - v_r)f_r - f_{r-1} - f_{r+1} & \text{if } 2 \leq r \leq n - 1 \\ (2 - v_n)f_n - f_{n-1} & \text{if } r = n \end{cases}$$

We choose

$$v_r = \begin{cases} 2 - s_1 & \text{if } r = 1 \\ 2 - s_{r-1}^{-1} - s_r & \text{if } 2 \leq r \leq n \end{cases}$$

where $s_r = (1 + 1/r)^{1/2}$. We note that

$$\frac{1}{4r^2} \leq v_r \leq \frac{1}{4r^2} + O(r^{-4})$$

as $r \rightarrow \infty$. We finally put $M_1 = DM_2D^{-1}$ where $D_{r,s} = r\delta_{r,s}$ for all r, s .

Theorem 23 *The matrix M_2 is non-negative and self-adjoint. The operators $e^{-M_1 t}$ on C^n are positivity-preserving for all $t \geq 0$, and their eigenvalues $\lambda_{r,t}$ all satisfy $0 < \lambda_{r,t} \leq 1$. If we replace v_r by 0 in the above definitions, then $e^{-M_1 t}$ is a one-parameter contraction semigroup on C^n provided with the l^1 norm.*

Proof The self-adjointness of M_2 is evident. The fact that M_2 is non-negative depends upon a discrete analogue of the Hardy inequality. There is a substantial literature on discrete analogues of differential inequalities, but we can prove the result which we need very quickly. The relevant quadratic form is

$$\begin{aligned} Q(a) &= |a_1|^2 + |a_{n+1}|^2 + \sum_{r=1}^n \left\{ |a_r - a_{r-1}|^2 - v_r |a_r|^2 \right\} \\ &= \sum_{r=1}^n (2 - v_r) |a_r|^2 - \sum_{r=2}^n \{ a_r \bar{a}_{r-1} + a_{r-1} \bar{a}_r \} \\ &= \sum_{r=2}^n |s_{r-1}^{1/2} a_{r-1} - s_{r-1}^{-1/2} a_r|^2 + |s_n^{1/2} a_n|^2 \\ &\geq 0. \end{aligned}$$

Since M_1 and M_2 are similar, the comments about the eigenvalues of $e^{-M_1 t}$ follow immediately. The fact that $e^{-M_1 t}$ is positivity preserving for $t \geq 0$ follows using Lemma 21, as does the final statement of the theorem.

In spite of the above, Theorem 19 suggests that the norm of $e^{-M_1 t}$, considered as an operator on C^n provided with the l^1 norm, should grow with t . Table 1 shows

the results of testing this numerically using Matlab. Our computations used the formula

$$e^{-M_1 t} = D e^{-M_2 t} D^{-1}$$

and exploited the self-adjointness of M_2 when calculating the exponential. One can use this formula directly to obtain the bound

$$\|e^{-M_1 t}\| \leq n^{1/2} \|D\| \|e^{-M_2 t}\| \|D^{-1}\| \leq n^{3/2}$$

for all $t \geq 0$, using the fact that $\|f\|_2 \leq \|f\|_1 \leq n^{1/2} \|f\|_2$ for all $f \in \mathbf{C}^n$ and $M_2 = M_2^* \geq 0$. However, this provides no insight into the limiting behaviour as $n \rightarrow \infty$.

Table 1. Values of $\|e^{-M_1 t}\|$ for various n

t	$n = 100$	$n = 200$	$n = 300$
0	1	1	1
100	4.059	4.059	4.059
200	4.824	4.824	4.824
300	5.333	5.337	5.337
400	5.701	5.735	5.735
500	5.945	6.063	6.063
600	6.071	6.346	6.346
700	6.095	6.595	6.595
800	6.036	6.818	6.818
900	5.914	7.022	7.022
1000	5.747	7.208	7.209

For $n = 300$ the maximum value of the norm occurs for $t \sim 6000$. While the increase may not appear very rapid, it should be noted that we have assumed a unit separation of the points on \mathbf{Z}^+ , so the implied time scale is very long by comparison with that of the corresponding differential operator. Table 2 shows how the maximum value of the l^1 norm as t varies depends upon the value of n .

Table 2. $\max_{t \geq 0} \|e^{-M_1 t}\|$ as a function of n .

n	norm max
50	4.33
100	6.10
150	7.46
200	8.60
250	9.61
300	10.53

Since every eigenvalue of M_1 is positive we must have

$$\lim_{t \rightarrow \infty} \|e^{-M_1 t}\| = 0$$

but, still using the l^1 norm, if $n = 300$ the inequality $\|e^{-M_1 t}\| \leq 1$ only holds for $t \geq 4.6 \times 10^4$.

Table 1 suggests the existence of a limit as $n \rightarrow \infty$, and this is proved below. We identify \mathbf{C}^n with the subspace of $l^1(\mathbf{Z}^+)$ consisting of sequences with support in $\{1, \dots, n\}$. We also identify any $n \times n$ matrix X with the operator \tilde{X} on $l^1(\mathbf{Z}^+)$ defined by

$$(\tilde{X}f)_r = \begin{cases} \sum_{s=1}^n X_{r,s} f_s & \text{if } 1 \leq r \leq n \\ 0 & \text{otherwise.} \end{cases}$$

We finally exhibit the n -dependence of the various operators explicitly.

Lemma 24 *There exists a bounded operator $M_{1,\infty}$ on $l^1(\mathbf{Z}^+)$ to which $M_{1,n}$ converge strongly as $n \rightarrow \infty$. For every $t \geq 0$ the operators $e^{-M_{1,n}t}$ increase monotonically to $e^{-M_{1,\infty}t}$, and*

$$\lim_{n \rightarrow \infty} \|e^{-M_{1,n}t}\| = \|e^{-M_{1,\infty}t}\|. \quad (11)$$

Proof The limit operator is given by

$$(M_{1,\infty}f)_r = \begin{cases} (2 - v_1)f_1 - \frac{1}{2}f_2 & \text{if } r = 1 \\ (2 - v_r)f_r - \frac{r}{r-1}f_{r-1} - \frac{r}{r+1}f_{r+1} & \text{if } r \geq 2 \end{cases}$$

and is evidently bounded on $l^1(\mathbf{Z}^+)$. The strong convergence of $M_{1,n}$ to $M_{1,\infty}$ implies the strong convergence of the semigroup operators. We also have

$$(e^{-M_{1,n}t}f)_r = \sum_{s=1}^{\infty} K_n(t, r, s) f_s$$

for all $f \in l^1(\mathbf{Z}^+)$, where $K_n(t, r, s) \geq 0$ is the transition ‘probability’ for a jump process which is killed if it moves outside $\{1, \dots, n\}$ and grows at the rate v_r at each r such that $1 \leq r \leq n$. It follows on probabilistic grounds that $n \rightarrow K_n(t, r, s)$ is monotonic increasing with

$$\lim_{n \rightarrow \infty} K_n(t, r, s) = K_{\infty}(t, r, s).$$

This implies (11).

The formula (9) with $N = 3$ suggests that for our example one should have

$$\|e^{-M_{1,\infty}t}\| \sim kt^{1/4}$$

as $t \rightarrow \infty$. For finite n this can only happen for t in the transitory growth interval. Numerical calculations confirm this. If $n = 200$ one has

$$(2.69t)^{1/4} \leq \|e^{-M_1 t}\| \leq (2.71t)^{1/4}$$

for all t satisfying $200 \leq t \leq 1200$. If $n = 300$ the same holds for $200 \leq t \leq 2500$.

We may also investigate the resolvent norms in the l^1 context, or more specifically the function $c(a) = a\|R_a\|$; see Lemma 9. The eigenvalues of M_1 are all positive,

so $\omega_0 \neq 0$, and we must have $\lim_{a \rightarrow 0^+} c(a) = 0$. However, the smallest eigenvalue converges to 0 as $n \rightarrow \infty$, so $c(a)$ may be quite large even for small positive a . The data in Table 3 were obtained for the case $n = 300$, putting $a = 2^{-m}$ and stopping at the value of m for which $c(a)$ takes its maximum value. For $n = 300$ the smallest eigenvalue of M_1 is 6.38×10^{-5} and the largest is 4.00.

Table 3. Dependence of $c(a)$ on $a = 2^{-m}$ for $n = 300$.

m	$c(a)$
1	1.50
2	1.72
4	2.36
6	3.30
8	4.65
10	6.56
12	8.45

For $n = 1000$ the smallest eigenvalue of M_1 is 5.772×10^{-6} and the largest is 4.00. The largest value of $c(a)$ for a of the above form occurs for $a = 2^{-16}$ and is 15.50.

We finally tabulate how the smallest eigenvalue λ of M_1 depends upon n , with the values of the norm of the corresponding spectral projection P_λ , computed using (10). The fact that $\|P_\lambda\|$ grows like $n^{1/2}$ as n increases was expected on the basis of replacing f in (10) by the exact zero energy resonance $g_r = r^{1/2}$ of the operator M_1 acting in $L^1(\mathbf{Z}^+)$.

Table 4. Dependence of λ and $\|P_\lambda\|$ on n .

n	λ	$\ P_\lambda\ $	$\ P_\lambda\ /n^{1/2}$
100	5.669×10^{-4}	11.178	1.1178
200	1.4314×10^{-4}	15.772	1.1152
400	3.597×10^{-5}	22.278	1.1139
600	1.601×10^{-5}	27.274	1.1134
800	9.014×10^{-6}	31.487	1.1132
1000	5.772×10^{-6}	35.199	1.1131

Example 25 In the above study we focussed on the case $N = 3$, but the difference between the l^1 and l^2 theories becomes even more dramatic for larger values of N . The only change needed in our discrete example with the critical value of c in (8), namely $c = (N-2)^2/4$, is to redefine D by $D_{r,s} = r^{(N-1)/2}\delta_{r,s}$ for all r, s . For $N = 6$ the bounds (9) then suggest that $\|e^{-M_1 t}\| \sim t$ as $t \rightarrow \infty$. Numerical calculations yield

$$4.00 t \leq \|e^{-M_1 t}\| \leq 4.02 t$$

for all t satisfying $100 \leq t \leq 2000$, when $n = 300$.

Conjecture Let $N > 2$, let $(Df)_r = r^{(N-1)/2}f_r$ for all $r \geq 1$, and let

$$(M_{2,\infty}f)_r = \begin{cases} (2 - v_1)f_1 - f_2 & \text{if } r = 1 \\ (2 - v_r)f_r - f_{r-1} - f_{r+1} & \text{if } r \geq 2. \end{cases}$$

Then $M_{1,\infty} = DM_{2,\infty}D^{-1}$ is a bounded operator on $l^1(\mathbf{Z}^+)$ with non-negative real spectrum, and there exists a positive constant c such that

$$\lim_{t \rightarrow \infty} t^{-(N-2)/4} \|e^{-M_{1,\infty}t}\| = c.$$

6 Absence of Upper Bounds

In finite dimensions it is also possible to obtain upper bounds on semigroup norms from spectral or pseudospectral information, but the results deteriorate as the dimension increases, [9, 3, 4, 22]. It is therefore not surprising that no such bounds can be obtained in a general Banach space setting. In this section we describe physically important examples to show that this difficulty cannot be evaded.

The converse part of the following theorem is a classical result of Hille and Yosida, and has frequently been used to pass from resolvent bounds or from the dissipative property to a one-parameter semigroup, [5, Cor. 2.22]. The smallest possible constant c in (12) is often called the Kreiss constant by numerical analysts, by analogy with the constant of the Kreiss matrix theorem.

Theorem 26 *If T_t is a one-parameter semigroup satisfying $\|T_t\| \leq c$ for all $t \geq 0$ then its generator A satisfies*

$$\text{Spec}(A) \subseteq \{\lambda : \text{Re}(\lambda) \leq 0\}$$

and

$$\|(\lambda I - A)^{-1}\| \leq \frac{c}{\text{Re}(\lambda)} \tag{12}$$

for all λ such that $\text{Re}(\lambda) > 0$. The converse implication holds if $c = 1$.

There are many important examples in which one does not have $c = 1$. The following is typical of semigroups whose generator is an elliptic operator of order greater than 2, and is treated in detail in [6].

Example 27 Let T_t act in $L^1(\mathbf{R}^n)$ for $t \geq 0$ according to the formula

$$T_t f(x) = k_t * f(x)$$

where $*$ denotes convolution and

$$\hat{k}_t(\xi) = e^{-|\xi|^4 t}$$

Formally speaking $T_t = e^{At}$ where $A = -\Delta^2$. It is immediate that k_t lies in Schwartz space for every $t > 0$, and hence that convolution by k_t defines a bounded operator on L^1 . k_t is not a positive function on \mathbf{R}^n , and if we put $c_n = \|k_t\|_1$ then $c_n > 1$ is independent of t by scaling and

$$\|T_t\| = c_n$$

for all $t > 0$. For $n = 1$ we have $c_1 \sim 1.2367$.

The following more general theorem implies that $\rho = +\infty$ for all one-parameter semigroup whose generator is elliptic of order greater than 2, [14].

Theorem 28 *Let Ω be a region in \mathbf{R}^N and let A be an elliptic operator of order greater than two whose domain contains $C_c^\infty(\Omega)$. If A generates a one-parameter semigroup T_t on $L^p(\Omega)$ and $p \neq 2$ then T_t cannot be a contraction semigroup.*

In spite of its great value, we emphasize that the Hille-Yosida theorem is numerically fragile. An estimate which differs from that required by an unmeasurably small amount does not imply the existence of a corresponding one-parameter semigroup. We conjecture that an example with similar properties can be constructed in Hilbert space.

Theorem 29 *For every $\varepsilon > 0$ there exists a reflexive Banach space \mathcal{B} and a closed densely defined operator A on \mathcal{B} such that*

- (i) $\text{Spec}(A) \subseteq i\mathbf{R}$,
- (ii) $\|(\lambda I - A)^{-1}\| \leq (1 + \varepsilon)/|\text{Re}(\lambda)|$ for all $\lambda \notin i\mathbf{R}$,
- (iii) A is not the generator of a one-parameter semigroup.

Proof Given $1 \leq p \leq 2$, we define the operator A on $L^p(\mathbf{R})$ by

$$Af(x) = i \frac{d^2 f}{dx^2}.$$

As initial domain we choose Schwartz space \mathcal{S} , which is dense in $L^p(\mathbf{R})$. The closure of A , which we denote by the same symbol, has resolvent operators given by $R_\lambda f = g_\lambda * f$, where $*$ denotes convolution and

$$\hat{g}_\lambda(\xi) = (\lambda - i\xi^2)^{-1}$$

for all $\lambda \notin i\mathbf{R}$. If $p = 2$ the unitarity of the Fourier transform implies that $\|R_\lambda\| \leq |\text{Re}(\lambda)|^{-1}$. For $p = 1$, however,

$$\|R_\lambda\| = \|g_\lambda\|_{L^1}.$$

Assuming for definiteness that $\text{Re}(\lambda) > 0$ the explicit formula for g_λ yields

$$\|R_\lambda\| = \frac{1}{|\lambda|^{1/2}} \int_0^\infty \exp[-|x|\text{Re}\{(i\lambda)^{1/2}\}] \, dx.$$

Putting $\lambda = re^{i\theta}$ where $r > 0$ and $-\pi/2 < \theta < \pi/2$, we get

$$\|R_\lambda\| = \frac{1}{r \cos(\theta/2 + \pi/4)} \leq \frac{2}{|\operatorname{Re}(\lambda)|}.$$

Interpolation then implies that if $1 \leq p \leq 2$ and $1/p = \gamma + (1 - \gamma)/2$ then

$$\|R_\lambda\| \leq \frac{2^\gamma}{|\operatorname{Re}(\lambda)|}.$$

By taking p close enough to 2 we achieve the condition (ii).

The operators T_t are given for $t \neq 0$ by $T_t f = k_t * f$ where $*$ denotes convolution and

$$k_t(x) = (4\pi it)^{-1/2} \exp\{-x^2/4it\}.$$

It follows from the formula for the operator norm on $L^1(\mathbf{R})$ that T_t are not bounded operators on $L^1(\mathbf{R})$ for any $t \neq 0$. Suppose next that $1 < p < 2$ and that a semigroup T_t on $L^p(\mathbf{R})$ with generator A does exist; we will derive a contradiction by an argument which goes back at least forty years. If $f \in \mathcal{S}$ and $\hat{f}_t \in \mathcal{S}$ is defined for all $t \in \mathbf{R}$ by

$$\hat{f}_t(\xi) = e^{-i\xi^2 t} \hat{f}(\xi)$$

then f_t is differentiable with respect to the Schwartz space topology, and therefore with respect to the L^p norm topology, with derivative $A f_t$. It follows by [5, Th. 1.7] that $\hat{f}_t = T_t \hat{f}$. Now assume that $a > 0$ and $\hat{f}(\xi) = e^{-a\xi^2}$, so that $\hat{f}_t(\xi) = e^{-(a+it)\xi^2}$. Explicit calculations of f_t and f yield

$$\begin{aligned} \|f\|_p &= (4\pi a)^{1/2p-1/2} p^{-1/2p} \\ \|f_t\|_p &= (4\pi)^{1/2p-1/2} p^{-1/2p} a^{-1/2p} (a^2 + t^2)^{1/2p-1/4}. \end{aligned}$$

Hence

$$\|T_t\| \geq \frac{\|f_t\|_p}{\|f\|_p} = (1 + t^2/a^2)^{(2-p)/4p}.$$

But this diverges to ∞ as $a \rightarrow 0$, so T_t cannot exist as a bounded operator for any $t \neq 0$.

The above theorem implies that one cannot expect to derive upper bounds on semigroup norms from *numerical* resolvent norm estimates, i.e. from pseudospectra, in infinite-dimensional contexts. The Miyadera-Hille-Yosida-Phillips theorem provides a general connection between resolvent and semigroup bounds, [5, Theorem 2.21]. However, it involves obtaining bounds on all powers of the resolvent, and is rarely useful.

7 Special Initial States

It might be hoped that the pathologies described above are a result of applying the semigroup to ‘untypical, badly behaved’ initial vectors f , and that they would

disappear if f is restricted in an appropriate manner. In this section we investigate the consequences of assuming that f lies in the domain of A , so that $t \rightarrow T_t f$ satisfies the Cauchy problem in the classical sense. This amounts to studying the behaviour of T_t regarded as an operator from $\mathcal{D} := \text{Dom}(A)$ to \mathcal{B} , where the former space is provided with the natural Banach space norm

$$\|f\| = k(\|f\|^2 + \|Af\|^2)^{1/2},$$

and k is chosen so that the embedding operator from \mathcal{D} to \mathcal{B} has norm 1. Almost equivalently one can study the regularized operators $\tilde{T}_t = hT_t R_a$ on \mathcal{B} for some $a \notin \text{Spec}(A)$, where $h = \|R_a\|^{-1}$. The lower bounds of Section 2 are applicable to either of these families of operators, the appropriate ‘resolvent’ operators in the second case being

$$\tilde{R}_z = hR_z R_a = \frac{h}{a-z} (R_z - R_a). \quad (13)$$

In the first case the resolvent operators are unchanged, but the values of their norms change. It follows immediately from (13) that $b \rightarrow \|\tilde{R}_{a+ib}\|$ is bounded if and only if $b \rightarrow (1 + |b|)\|R_{a+ib}\|$ is bounded.

Lemma 30 *The operators \tilde{T}_t depend norm continuously on t and satisfy the short time growth condition*

$$\|\tilde{T}_t\| \leq 1 + tL(t)(a + \|R_a\|^{-1}). \quad (14)$$

Proof The norm continuity of $t \rightarrow \tilde{T}_t$ follows from the formula

$$\begin{aligned} (\tilde{T}_t - \tilde{T}_s) f &= h \int_s^t T_x (AR_a) f \, dx \\ &= h \int_s^t T_x (aR_a - 1) f \, dx, \end{aligned}$$

proved using [5, Lemma 1.2]. This implies (14) by putting $s = 0$. The following theorem is similar to a result in [12], and both are implied by Theorem 32 below.

Theorem 31 *Assuming that A is unbounded, one has*

$$\text{Spec}(\tilde{T}_t) = \{0\} \cup \{he^{\lambda t}(a - \lambda)^{-1} : \lambda \in \text{Spec}(A)\}$$

for all $t > 0$ and $a > \omega_0$.

Proof We normalize the problem by putting $\hat{A} = A - \gamma I$ where $\omega_0 < \gamma < a$, $\hat{a} = a - \gamma$ and $\hat{T}_t = e^{-\gamma t} T_t$, so that

$$T_t R_a = e^{\gamma t} \hat{T}_t \hat{R}_{\hat{a}}.$$

The semigroup \hat{T}_t is uniformly bounded since $\hat{\omega}_0 = \omega_0 - \gamma < 0$. Moreover

$$\hat{T}_t \hat{R}_{\hat{a}} = \int_0^\infty f(s) \hat{T}_s \, ds$$

where

$$f(s) = \begin{cases} 0 & \text{if } 0 \leq s < t \\ e^{-\hat{a}(s-t)} & \text{if } s \geq t. \end{cases}$$

Since $f \in L^1(0, \infty)$, the stated result is implied by our next, more general, theorem, which appears to be new.

Theorem 32 *Let T_t be a uniformly bounded one-parameter semigroup acting on \mathcal{B} , with an unbounded generator A . Let $f \in L^1(0, \infty)$ and*

$$X_f = \int_0^\infty f(t)T_t \, dt,$$

where the integral converges strongly in $\mathcal{L}(\mathcal{B})$. Put

$$\hat{f}(z) = \int_0^\infty f(t)e^{zt} \, dt$$

for all z satisfying $\operatorname{Re}(z) \leq 0$. Then

$$\operatorname{Spec}(X_f) = \{0\} \cup \{\hat{f}(\lambda) : \lambda \in \operatorname{Spec}(A)\}.$$

Proof We follow the approach of [5, Th. 2.15]. Let \mathcal{A} be a maximal abelian subalgebra of $\mathcal{L}(\mathcal{B})$ which contains T_t for all $t \geq 0$ and R_a for all $a \notin \operatorname{Spec}(A)$. Let M denote its maximal ideal space of \mathcal{A} and $\hat{\cdot}$ the Gelfand transform. Then \mathcal{A} is closed under the taking of inverses and strong operator limits. Hence $X_f \in \mathcal{A}$ and

$$\operatorname{Spec}(D) = \{\hat{D}(m) : m \in M\}$$

for all $D \in \mathcal{A}$.

If $a, b \notin \operatorname{Spec}(A)$ then the identity

$$\hat{R}_a(m) - \hat{R}_b(m) = (b - a)\hat{R}_a(m)\hat{R}_b(m) \tag{15}$$

implies that the closed set

$$N = \{m \in M : \hat{R}_a(m) = 0\}$$

is independent of the choice of a . Since A is unbounded N must be non-empty. If $m \in M \setminus N$ then

$$\hat{R}_a(m) \in \operatorname{Spec}(R_a) \setminus \{0\} = (a - \lambda_m)^{-1}$$

for some $\lambda_m \in \operatorname{Spec}(A)$. A second application of (15) implies that λ_m does not depend upon a . The definition of the topology of M implies that $\lambda : M \setminus N \rightarrow \operatorname{Spec}(A)$ is continuous.

Let \mathcal{P} denote the set of all functions $f : (0, \infty) \rightarrow \mathbf{C}$ of the form

$$f(t) = \sum_{r=1}^n \alpha_r e^{-\beta_r t}$$

where $\operatorname{Re}(\beta_r) > 0$ for all r . For such a function

$$X_f = \sum_{r=1}^n \alpha_r R_{\beta_r}.$$

Therefore

$$\begin{aligned} \operatorname{Spec}(X_f) &= \{\hat{X}_f(m) : m \in M\} \\ &= \{0\} \cup \left\{ \sum_{r=1}^n \alpha_r \hat{R}_{\beta_r}(m) : m \in M \setminus N \right\} \\ &= \{0\} \cup \left\{ \sum_{r=1}^n \alpha_r (\beta_r - \lambda_m)^{-1} : m \in M \setminus N \right\} \\ &= \{0\} \cup \left\{ \sum_{r=1}^n \alpha_r (\beta_r - \lambda)^{-1} : \lambda \in \operatorname{Spec}(A) \right\} \\ &= \{0\} \cup \left\{ \int_0^\infty f(t) e^{\lambda t} dt : \lambda \in \operatorname{Spec}(A) \right\} \\ &= \{0\} \cup \{\hat{f}(\lambda) : \lambda \in \operatorname{Spec}(A)\}. \end{aligned}$$

Finally let f be a general element of $L^1(0, \infty)$. There exists a sequence $f_n \in \mathcal{P}$ which converges in L^1 norm to f , and this implies that X_{f_n} converges in norm to X_f , and that \hat{f}_n converges uniformly to \hat{f} . Hence

$$\begin{aligned} \operatorname{Spec}(X_f) &= \lim_{n \rightarrow \infty} \operatorname{Spec}(X_{f_n}) \\ &= \{0\} \cup \lim_{n \rightarrow \infty} \{\hat{f}_n(\lambda) : \lambda \in \operatorname{Spec}(A)\} \\ &= \{0\} \cup \{\hat{f}(\lambda) : \lambda \in \operatorname{Spec}(A)\}. \end{aligned}$$

In this final step we used the fact that $\{0\} \cup \{\hat{f}(\lambda) : \lambda \in \operatorname{Spec}(A)\}$ is a closed set. This is because $\operatorname{Spec}(A)$ is a closed subset of $\{z \in \mathbf{C} : \operatorname{Re}(z) \leq 0\}$, and $\hat{f}(z) \rightarrow 0$ as $|z| \rightarrow \infty$ within this set.

In spite of Theorem 31, Wrobel's modification of the example of Zabczyk shows that the long time growth properties of \tilde{T}_t cannot be deduced from its spectral behaviour, [33, Ex. 4.1]; a special case is described in [2, Ex. 5.1.10]. We follow the standard convention of putting $\omega_1 = \tilde{\omega}_0$, that is

$$\omega_1 = \inf\{\omega : \|\tilde{T}_t\| \leq M_\omega e^{\omega t} \text{ for all } t \geq 0\}.$$

Theorem 33 *For any $0 < \sigma < 1$ there exists a one-parameter semigroup T_t acting on a Hilbert space \mathcal{H} such that $s = 0$, $\omega_0 = 1$ and $\omega_1 = \sigma$.*

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