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SEMIGROUP GROWTH BOUNDS

E.B. DAVIES

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ABSTRACT. We use the Legendre transform to find a relationship between the norms of a one-parameter semigroup and those of its resolvent operators. The theorems are illustrated with a variety of examples, particularly estimates of the norms of the semigroups associated with Schrödinger operators, considered as acting on the space $L^1(\mathbb{R}^n)$.

KEYWORDS: *One-parameter semigroups, growth bounds, resolvent norms, Schrödinger operators, spectral theory.*

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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 $T_t = \mathrm{e}^{At}$ 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 the spectrum of the operator in question is purely imaginary (Theorem 2.17 of [4] and [36]). 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.

There is an enormous literature studying the asymptotic behaviour of one-parameter semigroups as $t \to \infty$, [10], 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 ([19], pp. 16–19 in [32]; see also [6]). In this case the underlying cause is the non-self-adjointness of the operators concerned, which act in a Hilbert space.

The relevance of such issues to studies of the stability of fixed points of non-linear hydrodynamic equations is still a matter of investigation. Traditionally it was assumed that stability was equivalent to the spectrum of the linearized equation lying in the left-hand half plane. However, Trefethen and others have established that in some problems in hydrodynamics pseudospectral methods provide stability information unavailable by the use of spectral theory alone; see [29], [30] and [9]. On the other hand Renardy has shown that in certain other hydrodynamic problems spectral analysis does indeed suffice to determine stability [21], [22], [23].

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 [28], [29], [33], [32], [34]. 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 6.4) 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 Section 2 and the numerical aspects of Section 5 are, however, new.

2. LOWER BOUNDS

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

$$\begin{aligned}\omega_0 &= \limsup_{t\to+\infty} t^{-1}\log(\|T_t\|),\\ s &= \sup\{\mathrm{Re}\,(\lambda) : \lambda \in \mathrm{Spec}(A)\},\\ s_\varepsilon &= \sup\{\mathrm{Re}\,(z) : \|R_z\| \geqslant \varepsilon^{-1}\},\end{aligned}$$

$$s_0 = \lim_{\varepsilon\to 0} s_\varepsilon,$$
$$\rho = \min\{\omega : \|T_t\| \leqslant e^{\omega t} \text{ for all } t \geqslant 0\},$$

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 2.2. One always has $s \leqslant s_0 \leqslant \omega_0 \leqslant \rho$, and each of these may be a strict inequality. In a Hilbert space $\omega_0 = s_0$ ([10], Theorem 5.1.11). This identity is, however, not always valid in Banach spaces ([10], Counterexample 4.2.7).

The pseudospectra of the operator A are by definition the sets

$$\mathrm{Spec}_\varepsilon(A) = \mathrm{Spec}(A) \cup \{z \in \mathbb{C} : \|R_z\| > \varepsilon^{-1}\},$$

defined for all $\varepsilon > 0$. Determining of the pseudospectra is equivalent to knowing the value of $\|R_z\|$ for all $z \in \mathbb{C}$. Recent computational advances enable the sets to be plotted efficiently even for very large matrices [28], [29], [32], [33], [34]. They provide considerable insights into the behaviour of the operators concerned, and there is an ongoing programme to relate other quantities of interest to these sets.

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

$$\|T_t\| \leqslant M e^{st}$$

for all $t \geqslant 0$. 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 4.1 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 $T_t : \mathcal{D} \to \mathcal{B}$ is a strongly continuous family of operators defined for $t \geqslant 0$, satisfying $\|T_0\| = 1$ and $\|T_t\| \leqslant M e^{\omega t}$ for some M, ω and all $t \geqslant 0$. 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 $\nu(t) \geqslant \log(\|T_t\|)$ for all $t \geqslant 0$. It is immediate that $N(t)$ is continuous for $t > 0$, and that

$$1 = N(0) \leqslant \lim_{t\to 0+} N(t).$$

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 $k \in \mathbb{R}$ 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 $\mathrm{Spec}(A) \subseteq \{z : \mathrm{Re}\,(z) \leqslant 0\}$. It also implies that $\|T_t\| \geqslant 1$ for all $t \geqslant 0$ by Theorem 1.22 of [4]. If we define $R_z : \mathcal{D} \to \mathcal{B}$ by

$$R_z f = \int_0^\infty (T_t f)\mathrm{e}^{-zt}\,\mathrm{d}t$$

then $\|R_z\|$ is uniformly bounded on $\{z : \mathrm{Re}\,(z) \geqslant \gamma\}$ for any $\gamma > 0$, and the norm converges to 0 as $\mathrm{Re}\,(z) \to +\infty$. 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

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

of $\|T_t\|$, which was introduced by Trefethen [31] and implemented in the package Eigtool by Wright ([32], page 82 and [33]).

LEMMA 2.1. *If* $\omega_0 = 0$ *then*

$$\|T_t\| \leqslant L(t) \leqslant N(t),$$

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

$$N(t) \leqslant L\Big(\frac{t}{n}\Big)^{n+1}$$

for all positive integers n *and* $t \geqslant 0$.

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 $\|T_t\| \leqslant L(t) \leqslant N(t)$. If T_t is a one-parameter semigroup we note that $s \to L(t/n)^{1+ns/t}$ is a log-concave function which dominates $\|T_s\|$ for all $s \geqslant 0$, and which therefore also dominates $N(s)$. ∎

In the following well-known lemma we put

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

LEMMA 2.2. *The constant* ρ *satisfies*

$$\rho = N'(0+) \geqslant \limsup_{t\to 0} t^{-1}\left\{\|T_t\| - 1\right\}.$$

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

$$\rho = \sup\{\mathrm{Re}\,(z) : z \in \mathrm{Num}(A)\} \tag{2.1}$$

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

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

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

for all $t \geqslant 0$. 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 $\mathrm{Num}(A-\omega I)$ is contained in $\{z : \mathrm{Re}\,(z) \leqslant 0\}$. ∎

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

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

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 $\omega \to +\infty$ to $\limsup_{t\to 0} \|T_t\|$. Hence $M(\omega) \geqslant 1$ for all $\omega > 0$. We also have

$$N(t) = \inf\{M(\omega)\mathrm{e}^{\omega t} : 0 < \omega < \infty\} \tag{2.2}$$

for all $t > 0$ by the theory of the Legendre transform, i.e. simple convexity arguments, due to Young and Fenchel ([27], p. 67).

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

LEMMA 2.3. *If $a > 0$, $b \in \mathbb{R}$, and $a\|R_{a+\mathrm{i}b}\| = c \geqslant 1$ then*

$$M(\omega) \geqslant \widetilde{M}(\omega) := \begin{cases} \frac{(a-\omega)c}{a} & \text{if } 0 < \omega \leqslant r = a\Big(1 - \frac{1}{c}\Big), \\ 1 & \text{otherwise.} \end{cases}$$

Proof. The formula

$$R_{a+\mathrm{i}b} = \int_0^\infty T_t \mathrm{e}^{-(a+\mathrm{i}b)t}\,\mathrm{d}t \tag{2.3}$$

implies that

$$\frac{c}{a} \leqslant \int_0^\infty N(t)\mathrm{e}^{-at}\,\mathrm{d}t \leqslant \int_0^\infty M(\omega)\mathrm{e}^{\omega t - at}\,\mathrm{d}t$$

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 $M(\omega) \geqslant 1$ for all $\omega > 0$.

THEOREM 2.4. *If $a\|R_{a+\mathrm{i}b}\| = c \geqslant 1$ and $r = a(1 - 1/c)$ then*

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

for all $t \geqslant 0$.

Proof. This uses

$$N(t) \geqslant \inf\{\widetilde{M}(\omega)\mathrm{e}^{\omega t} : \omega > 0\},$$

which follows from (2.2). ∎

Trefethen and Wright give a related lower bound in [31] and [32], namely

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

Although these are lower bounds for different quantities and under slightly different conditions, the bound of Theorem 2.4 is better in the following sense. The two sides of (2.4) are asymptotically equal as $t \to 0+$ and $t \to \infty$, but for intermediate t we have:

LEMMA 2.5. *Let $a > 0$, $t \geqslant 0$ and $c \geqslant 1$ then*

$$\frac{e^{at}}{1 + \frac{e^{at}-1}{c}} \leqslant \min\{e^{a(1-1/c)t}, c\}. \tag{2.4}$$

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

$$\frac{e^{s}}{1 + \frac{e^{s}-1}{c}} \leqslant c,$$
$$\frac{e^{s}}{1 + \frac{e^{s}-1}{c}} \leqslant e^{(1-1/c)s}.$$

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

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

are immediately calculable from the pseudospectra. It follows from (2.3) and $\omega_0 = 0$ that $c(a)$ remains bounded as $a \to +\infty$. The transform $\widetilde{c}(\cdot)$ defined below is easily calculated from $c(\cdot)$.

COROLLARY 2.6. *Under the above assumptions one has*

$$N(t) \geqslant \widetilde{c}(t) := \sup_{\{a:c(a)\geqslant 1\}} \{\min\{e^{r(a)t}, c(a)\}\} \tag{2.5}$$

where

$$r(a) = a\Big(1 - \frac{1}{c(a)}\Big).$$

THEOREM 2.7. *If T_t is a one-parameter semigroup and $s_0 = \omega_0 = 0$ then $c(a) \geqslant 1$ for all $a > 0$.*

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

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

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

Examples show that $c(\cdot)$ is often a decreasing function, but this is not true in Example 4.4 below. If $c(\cdot)$ is differentiable then the supremum in (2.5) need only be taken over those a at which $c'(a) \le 0$. The following transform of $c(\cdot)$ may sometimes be easier to compute than $\widetilde{c}(\cdot)$.

LEMMA 2.8. *If $c(\cdot) \geqslant 1$ is a monotonic decreasing function then $N(t) \geqslant \widehat{c}(t)$ for all $t \geqslant 0$, where $\widehat{c}(\cdot)$ is the function inverse to*

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

and $c \to a(c)$ is the function inverse to $a \to c(a)$. The function $\widehat{c}(t)$ 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 $t \to N(t)$ lies above each of the points $(t(c), c)$ by Theorem 2.4. Putting $g(c) = \log(c)/(1-1/c)$ a direct calculation shows that $g'(c) \geqslant 0$ for all $c \geqslant 1$. 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 $\widehat{c}(\cdot)$ is the same as the range of $t(\cdot)$, and one may show that $t(c(a)) \to 0$ as $a \to \infty$, while $t(c(a)) \to \infty$ as $a \to 0$. ∎

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 $f \geqslant 0$ implies $T_t f \geqslant 0$ for all $t \geqslant 0$. 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 [18].

LEMMA 2.9. *Let T_t be a positivity-preserving one-parameter semigroup acting in $L^p(X, \mathrm{d}x)$ for some $1 \leqslant p < \infty$. If $\omega_0 = 0$ then*

$$\|R_{a+\mathrm{i}b}\| \leqslant \|R_a\|$$

for all $a > 0$ and $b \in \mathbb{R}$. 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

$$|\langle R_{a+\mathrm{i}b} f, g\rangle| = \Big| \int_0^\infty \langle T_t f, g\rangle \mathrm{e}^{-(a+\mathrm{i}b)t}\,\mathrm{d}t \Big| \leqslant \int_0^\infty |\langle T_t f, g\rangle| \mathrm{e}^{-at}\,\mathrm{d}t$$
$$\leqslant \int_0^\infty \langle T_t |f|, |g|\rangle \mathrm{e}^{-at}\,\mathrm{d}t = \langle R_a |f|, |g|\rangle \leqslant \|R_a\| \|f\|_p \|g\|_q.$$

By letting f and g vary we obtain the statement of the lemma. (The inequality $|\langle Bf, g\rangle| \leqslant \langle B|f|, |g|\rangle$ for all positivity-preserving operators B 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 $t \geqslant 0$ 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 $1 \leqslant r \leqslant n$. 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

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

for all $t \geqslant 0$. 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(·,1)** routines, and it is easy to confuse the two.

The following standard result is included for completeness.

LEMMA 3.1. *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* $\mathcal{L}_n = \mathrm{lin}\{f_1, \dots, f_n\}$. *Then*

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

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

Proof. Given $\varepsilon > 0$ and $t \geqslant 0$ 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 $\|T_t\| \geqslant \|T_{n,t}\| > \|T_t\| - \varepsilon$.

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 3.2. *If $B_{r,s} = \langle f_s, f_r\rangle$ and $D_{r,s,t} = \mathrm{e}^{\lambda_r t}\delta_{r,s}$ for $1 \leqslant r,s \leqslant n$, then*

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

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

Proof. The $n\times n$ matrix B is readily seen to be self-adjoint and positive. If $S : \mathbb{C}^n \to \mathcal{L}_n$ 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 4.1. Let T_t be the positivity-preserving, one-parameter semigroup acting on $L^2(\mathbb{R}^+)$ with generator

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

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

$$T_t f(x) = \frac{a(x+t)}{a(x)} f(x+t) \tag{4.1}$$

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

$$a(x) = \exp\Big\{ \int_0^x v(s)\,\mathrm{d}s \Big\}.$$

The function a is continuous and satisfies

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

for all x, t; hence $\|T_t\| \leqslant \mathrm{e}^{\|v\|_\infty t}$ for all $t \geqslant 0$.

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

$$a(x) = 1 + (c-1)\sin^2\left(\frac{\pi x}{2b}\right) \tag{4.2}$$

leads to $\|T_{2nb}\| = 1$ and $\|T_{(2n+1)b}\| = c$ for all positive integers n. In the case (4.2), the regularizations $N(t)$ and $L(t)$ are not equal, but both are equal to c for $t \geqslant b$.

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 (4.1), and observe that

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

for all $t \geqslant 0$. 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 $t \to \infty$ 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 $f \in L^2(\mathbb{R}^+)$, because of the uniform boundedness theorem.

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

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

Hence

$$\mathrm{Spec}(A) = \{z : \mathrm{Re}\,(z) \leqslant 0\}.$$

On the other hand $\rho = +\infty$, and $\mathrm{Num}(A)$, which is always a convex set, must equal the entire complex plane by Lemma 2.2.

EXAMPLE 4.2. If we put

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

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

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

so

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

for all $a > 0$. We also have

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

which is log-concave, so $\|T_t\| = N(t)$ for all $t \geqslant 0$. The choice $a = 2$ provides a fairly good lower bound on $N(t)$ for $0 \leqslant t \leqslant 0.5$. 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 4.3. 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 $\mathbb{C}^n$ with the l^1 norm. Then

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

and

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

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

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

for all $t \geqslant 0$, 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 (2.1) 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

$$\rho = \cos\left(\frac{\pi}{n+1}\right) < 1.$$

EXAMPLE 4.4. Given $\gamma > 0$, let

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

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

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

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 $a \to \infty$, 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) $V : \mathbb{R}^N \to \mathbb{R}$ lies in the so-called Kato class of [26], then the formula $H = -\Delta + V$ may be interpreted as a quadratic form sum in $L^2(\mathbb{R}^N)$, and the one-parameter "Schrödinger semigroup" $\{e^{-Ht}\}_{t \geqslant 0}$ on L^2 may be extended consistently to all of the L^p spaces, $1 \leqslant p \leqslant \infty$ ([26], Theorem B.1.1). The domain of the semi-bounded self-adjoint operator H may be hard to specify, but its quadratic form domain is $W^{1,2}(\mathbb{R}^N)$ by p. 459, item (2) of [26]. If V is bounded below and locally L^2 then H is essentially self-adjoint on $C_c^\infty(\mathbb{R}^N)$ by [14]; see also Theorem X.28 of [20].

If H is interpreted as a quantum-mechanical Hamiltonian, then there are good reasons for being interested primarily in the choice $p = 2$: the time-dependent Schrödinger equation $f'(t) = -iHf(t)$ is only soluble in L^p for $p = 2$, and 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

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

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 $L^1(\mathbb{R}^N)$. The point here is that the semigroup e^{-Ht} is positivity-preserving, and $f_t = e^{-Ht}$ describes the distribution of some continuous quantity in $\mathbb{R}^N$ at time $t \geqslant 0$ given its initial distribution f. Assuming $f \geqslant 0$, the total amount of the quantity at time t is given by

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

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, [12]. The operators e^{-Ht} are known to have positive "heat" kernels $K(t,x,y)$ (see Theorem 6.4

of [25] or Lemma B.7.5 of [26]) and

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

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; we do not claim originality for the theorem, which seems to be a part of the folklore.

THEOREM 5.1. *Let $H_1 = -\Delta + V$, where V is continuous and bounded below, with*

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

Then $c = -\rho$.

Proof. The inequality $\rho \leqslant -c$, or equivalently

$$\|e^{-H_1 t}\| \leqslant e^{-ct} \quad \text{for all } t \geqslant 0$$

may be proved by the use of functional integration ([25], p. 459).

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

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

This implies that $\rho \geqslant -c$. ∎

COROLLARY 5.2. *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 [16], [17] and by Davies and Simon [7] using the concepts of criticality, subcriticality and zero energy resonance. The most general results which we know about are by Zhang [37].

EXAMPLE 5.3. Let $N \geqslant 3$ and let

$$\alpha_\pm = \frac{N-2}{2} \pm \sqrt{\frac{(N-2)^2}{4} - c}, \quad 0 < c < \frac{(N-2)^2}{4}, \tag{5.1}$$

so that

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

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

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

It is known that the operator H_p has spectrum $[0, \infty)$ for all $1 \leqslant p \leqslant \infty$, and that $c = (N-2)^2/4$ is a critical value for the emergence of a negative eigenvalue [12], [7].

The operator H_p possesses a zero energy resonance η (i.e. a positive eigenfunction associated with the eigenvalue 0, which decays at infinity but not rapidly enough to lie in $L^2(\mathbb{R}^N)$) given by

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

where

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

The operator $-H_p$ generates a positivity-preserving one-parameter semigroup acting in $L^p(\mathbb{R}^N)$ for all $1 \leqslant p \leqslant \infty$, and for $p = 2$ it is a self-adjoint contraction semigroup. On the other hand it is proved in Theorem 14 of [7] 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

$$c_1(1+t)^{\sigma_1} \leqslant \|\mathrm{e}^{-H_1 t}\| \leqslant c_2(1+t)^{\sigma_2} \tag{5.2}$$

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

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

THEOREM 5.4. *For every $\gamma > 0$ there exists a Schrödinger semigroup $\mathrm{e}^{-K_p t}$ acting in $L^p(\mathbb{R}^N)$ for all $1 \leqslant p \leqslant \infty$ such that*

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

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

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

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

The bounds are proved by reducing to the case $\gamma = 1$ by using the scaling transformation $(U_\gamma f)(x) = \gamma^{N/2} f(\gamma x)$. See [7] for details. ∎

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 5.5. *Let the potential V be rotationally invariant and bounded below on $\mathbb{R}^N$. 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 $t \geqslant 0$ by $T_t = \mathrm{e}^{-Ht}$ acts consistently on $L^p(\mathbb{R}^N)$ for all $1 \leqslant p < \infty$ and commutes with rotations. If we identify the rotationally invariant subspace of $L^2(\mathbb{R}^N)$ with $L^2((0,\infty), \mathrm{d}r)$ in the usual way, then the restriction of H_2 to this subspace is given by*

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

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

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

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

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

$$H_2 f(r) = -\frac{1}{r^{N-1}} \frac{\mathrm{d}}{\mathrm{d}r}\Big\{ r^{N-1} \frac{\mathrm{d}f}{\mathrm{d}r} \Big\} + V(r) f(r).$$

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

We have already commented that the operator H is essentially self-adjoint on $C_c^\infty(\mathbb{R}^N)$, but since $N \geqslant 3$, the origin has zero capacity, and $C_c^\infty(\mathbb{R}^N \backslash \{0\})$ is a quadratic form core for H. On restricting to the rotationally invariant subspace it follows that $C_c^\infty(0,\infty)$ is a quadratic form core for L_2. If $N = 3$ then one imposes Dirichlet boundary conditions at 0 in the traditional sense, but if $N > 3$ then L_2 is in the limit point case at both 0 and ∞ because of the singularity of the potential at the origin. Technically speaking there is no choice of boundary conditions to be made, but one might also say that Dirichlet boundary conditions are forced.

The operator H_1 acts on the space $L^1((0,\infty), r^{N-1}\,\mathrm{d}r)$ of rotationally invariant functions according to the same formula as for H_2. We transfer H_1 to $L^1((0,\infty), \mathrm{d}r)$ 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 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

$$L_1 f(r) = r^{(N-1)/2} L_2 \{ r^{-(N-1)/2} f(r) \}.$$

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

LEMMA 5.6. *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 $\mathrm{e}^{-M_1 t}$ is positivity-preserving for all $t \geqslant 0$. If also $M_1^* 1 \geqslant 0$ then $\mathrm{e}^{-M_1 t}$ is a contraction semigroup on $\mathbb{C}^n$ 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

$$\|P_\lambda\| = \frac{\|Df\|_1 \, \|(D^{-1})^* f\|_\infty}{\langle f, f\rangle} \tag{5.3}$$

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

Proof. See Theorem 7.14 of [4] or the proof of Lemma 5.9 for the positivity-preservation. The second statement is also classical, but we include a proof for completeness. Since the coefficients of the matrix $\mathrm{e}^{-M_1 t}$ are non-negative, we have

$$\begin{aligned}
\|\mathrm{e}^{-M_1 t} f\|_1 - \|f\|_1 &= \sum_{r=1}^{n} \{ |(\mathrm{e}^{-M_1 t} f)_r| - |f_r| \} \leqslant \sum_{r=1}^{n} \{ (\mathrm{e}^{-M_1 t}|f|)_r - |f_r| \} \\
&= \langle \mathrm{e}^{-M_1 t}|f| - |f|, 1\rangle = -\int_0^t \langle M_1 \mathrm{e}^{-M_1 s}|f|, 1\rangle \,\mathrm{d}s \\
&= \int_0^t \langle \mathrm{e}^{-M_1 s}|f|, M_1^* 1\rangle \,\mathrm{d}s \leqslant 0.
\end{aligned}$$

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

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

EXAMPLE 5.7. We describe a discretization of the operator L_1, with the critical value of the parameter c in (5.1), namely $c = (N-2)^2/4$, and with $N = 3$, acting in the space $\mathbb{C}^n$ of finite sequences. We put

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

We choose

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

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

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

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

THEOREM 5.8. *The matrix M_2 is non-negative and self-adjoint. The operators $\mathrm{e}^{-M_1 t}$ on $\mathbb{C}^n$ are positivity-preserving for all $t \geqslant 0$, and their eigenvalues $\lambda_{r,t}$ all satisfy $0 < \lambda_{r,t} \leqslant 1$. If we replace v_r by 0 in the above definitions, then $\mathrm{e}^{-M_1 t}$ is a one-parameter contraction semigroup on $\mathbb{C}^n$ 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

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

Since M_1 and M_2 are similar, the comments about the eigenvalues of $\mathrm{e}^{-M_1 t}$ follow immediately. The fact that $\mathrm{e}^{-M_1 t}$ is positivity preserving for $t \geqslant 0$ follows using Lemma 5.6, as does the final statement of the theorem. ∎

In spite of the above, Theorem 5.4 suggests that the norm of $\mathrm{e}^{-M_1 t}$, considered as an operator on $\mathbb{C}^n$ 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

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

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

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

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

Table 1. Values of $\|\mathrm{e}^{-M_1 t}\|$ 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 $\mathbb{Z}^+$, 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. $\max_{t\geqslant 0} \|\mathrm{e}^{-M_1 t}\|$ 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

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

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

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

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

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

LEMMA 5.9. *There exists a bounded operator $M_{1,\infty}$ on $l^1(\mathbb{Z}^+)$ to which $M_{1,n}$ converge strongly as $n \to \infty$. For every $t \geqslant 0$ the operators $\mathrm{e}^{-M_{1,n}t}$ increase monotonically to $\mathrm{e}^{-M_{1,\infty}t}$, and*

$$\lim_{n\to\infty} \|\mathrm{e}^{-M_{1,n}t}\| = \|\mathrm{e}^{-M_{1,\infty}t}\|. \tag{5.4}$$

Proof. The limit operator is given by

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

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

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

for all $f \in l^1(\mathbb{Z}^+)$, where $K_n(t,r,s) \geqslant 0$ 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 $1 \leqslant r \leqslant n$. It follows on probabilistic grounds that $n \to K_n(t,r,s)$ is monotonic increasing with

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

This implies (5.4). ∎

The formula (5.2) with $N = 3$ suggests that for our example one should have

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

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

$$(2.69t)^{1/4} \leqslant \|\mathrm{e}^{-M_1t}\| \leqslant (2.71t)^{1/4}$$

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

We may also investigate the resolvent norms in the l^1 context, or more specifically the function $c(a) = a\|R_a\|$; see Lemma 2.9. The eigenvalues of M_1 are all positive, so $\omega_0 \neq 0$, and we must have $\lim_{a\to 0+} c(a) = 0$. However, the smallest eigenvalue converges to 0 as $n \to \infty$, 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 (5.3). The fact that $\|P_\lambda\|$ grows like $n^{1/2}$ as n increases was expected on the basis of replacing f in (5.3) by the exact zero energy resonance $g_r = r^{1/2}$ of the operator M_1 acting in $L^1(\mathbb{Z}^+)$.

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 5.10. In the above study we focused 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 (5.1), 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 (5.2) then suggest that $\|e^{-M_1 t}\| \sim t$ as $t \to \infty$. Numerical calculations yield

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

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

CONJECTURE 5.11. Let $N > 2$, let $(Df)_r = r^{(N-1)/2} f_r$ for all $r \geqslant 1$, and let

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

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

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

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 [8], [2], [3], [24]. 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 ([4], Corollary 2.22). The smallest possible constant c in (6.1) is often called the Kreiss constant by numerical analysts, by analogy with the constant of the Kreiss matrix theorem.

THEOREM 6.1. *If T_t is a one-parameter semigroup satisfying $\|T_t\| \leqslant c$ for all $t \geqslant 0$ then its generator A satisfies*

$$\mathrm{Spec}(A) \subseteq \{\lambda : \mathrm{Re}\,(\lambda) \leqslant 0\}$$

and

$$\|(\lambda I - A)^{-1}\| \leqslant \frac{c}{\mathrm{Re}\,(\lambda)} \tag{6.1}$$

for all λ such that $\mathrm{Re}\,(\lambda) > 0$. *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 [5].

EXAMPLE 6.2. Let T_t act in $L^1(\mathbb{R}^n)$ for $t \geqslant 0$ according to the formula

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

where $*$ denotes convolution and

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

Formally speaking $T_t = \mathrm{e}^{At}$ 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 $\mathbb{R}^n$, 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, [15].

THEOREM 6.3. *Let Ω be a region in $\mathbb{R}^N$ 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 a natural example (i.e. an example arising from a genuine problem in physics) with similar properties can be constructed in Hilbert space. The following theorem, involving the Schrödinger equation, is due to Hörmander [13].

THEOREM 6.4. *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) $\mathrm{Spec}(A) \subseteq \mathrm{i}\mathbb{R}$;
(ii) $\|(\lambda I - A)^{-1}\| \leqslant (1+\varepsilon)/|\mathrm{Re}\,(\lambda)|$ *for all* $\lambda \notin \mathrm{i}\mathbb{R}$;
(iii) *A is not the generator of a one-parameter semigroup.*

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

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

As initial domain we choose Schwartz space $\mathcal{S}$, which is dense in $L^p(\mathbb{R})$. 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

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

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

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

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

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

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

$$\|R_\lambda\| = \frac{1}{r\cos(\frac{\theta}{2} + \frac{\pi}{4})} \leqslant \frac{2}{|\mathrm{Re}\,(\lambda)|}.$$

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

$$\|R_\lambda\| \leqslant \frac{2^\gamma}{|\mathrm{Re}\,(\lambda)|}.$$

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

$$k_t(x) = (4\pi \mathrm{i} t)^{-1/2} \exp\Big\{ -\frac{x^2}{4\mathrm{i}t} \Big\}.$$

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

$$\widehat{f_t}(\xi) = \mathrm{e}^{-\mathrm{i}\xi^2 t} \widehat{f}(\xi)$$

then f_t is differentiable with respect to the Schwartz space topology, and therefore with respect to the L^p norm topology, with derivative Af_t. It follows by Theorem 1.7 of [4] that $f_t = T_t f$. Now assume that $a > 0$ and $\widehat{f}(\xi) = \mathrm{e}^{-a\xi^2}$, so that $\widehat{f_t}(\xi) = \mathrm{e}^{-(a+\mathrm{i}t)\xi^2}$. 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

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

But this diverges to ∞ as $a \to 0$, 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 ([4], Theorem 2.21). However, it involves obtaining bounds on all powers of the resolvent, and is rarely used.

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E.B. DAVIES, DEPARTMENT OF MATHEMATICS, KING'S COLLEGE LONDON, STRAND, LONDON WC2R 2LS, ENGLAND

E-mail address: E.Brian.Davies@kcl.ac.uk

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