

Positivity and Monotonicity Properties of C_0 -Semigroups. I

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Abstract. If $\exp\{-tH\}$, $\exp\{-tK\}$, are self-adjoint, positivity preserving, contraction semigroups on a Hilbert space $\mathcal{H} = L^2(X; d\mu)$ we write

$$e^{-tH} \succcurlyeq e^{-tK} \succcurlyeq 0 \tag{*}$$

whenever $\exp\{-tH\} - \exp\{-tK\}$ is positivity preserving for all $t \geq 0$ and then we characterize the class of positive functions for which (*) always implies

$$e^{-tf(H)} \succcurlyeq e^{-tf(K)} \succcurlyeq 0.$$

This class consists of the $f \in C^\infty(0, \infty)$ with

$$(-1)^n f^{(n+1)}(x) \geq 0, \quad x \in (0, \infty), \quad n = 0, 1, 2, \dots$$

In particular it contains the class of monotone operator functions. Furthermore if $\exp\{-tH\}$ is $L^p(X; d\mu)$ contractive for all $p \in [1, \infty]$ and all $t > 0$ (or, equivalently, for $p = \infty$ and $t > 0$) then $\exp\{-tf(H)\}$ has the same property. Various applications to monotonicity properties of Green's functions are given.

A bounded operator A on the Hilbert space $\mathcal{H} = L^2(X; d\mu)$ is called positivity preserving if

$$(\phi, A\psi) \geq 0$$

for all non-negative ϕ, ψ , and if this is the case we write

$$A \succcurlyeq 0.$$

More generally if $A, B, A - B$, are positivity preserving we write

$$A \succcurlyeq B \succcurlyeq 0.$$

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Our aim is to study pairs of positive self-adjoint operators H, K , such that the associated contraction semigroups satisfy

$$e^{-tH} \succcurlyeq e^{-tK} \succcurlyeq 0$$

for all $t \geq 0$. If the semigroups are given by integral kernels, i.e. Green's functions, this order states that one kernel is pointwise larger than the other.

We demonstrate that the ordering of semigroups can be characterized by a simple ordering of the infinitesimal generators.

Theorem A. *The following conditions are equivalent*

1. $e^{-tH} \succcurlyeq e^{-tK} \succcurlyeq 0$ for all $t \geq 0$.

2. $(\phi, K\psi) \geq (H\phi, \psi)$ for all non-negative ϕ , and ψ , in the domains of H , and K , respectively.

This result is easy to derive but has many immediate implications for monotonicity properties of Green's functions. (It should be emphasized that condition 2 is quite different to the usual operator order $K \geq H$ and in general it neither implies, nor is implied by, this latter order.) This theorem is also of great use in characterizing the class of functions which respect the generator property and the semigroup order relation.

Theorem B, *Let f be a non-negative measurable function on $[0, \infty)$.*

The following conditions are equivalent

1. $e^{-tK} \succcurlyeq e^{-tH} \succcurlyeq 0, \quad t \geq 0,$

implies

$$e^{-tf(K)} \succcurlyeq e^{-tf(H)} \succcurlyeq 0, \quad t \geq 0,$$

for all pairs of contraction semigroups ;

2. *f has a representation*

$$f(x) = \int_0^\infty d\mu(t) \left(\frac{1 - e^{-tx}}{t} \right) + \alpha x + \beta, \quad x > 0$$

$$f(0) \leq \beta$$

where μ is a positive measure such that the integral exists, $\alpha \geq 0$, and

$$\beta = \lim_{x \rightarrow 0^+} f(x) \geq 0 ;$$

3. $f \in C^\infty(0, \infty)$ and

$$(-1)^n f^{(n+1)}(x) \geq 0 \quad x \in (0, \infty), \quad n = 0, 1, 2, \dots .$$

and

$$f(0) \leq \lim_{x \rightarrow 0^+} f(x) .$$

In particular these conditions are satisfied by the monotone operator functions¹.

1 The terminology operator monotone function might be more appropriate but we adopt Löwner's terminology which is now conventional

The equivalence of conditions 2 and 3 is an integrated version of Bernstein's theorem (see, for example, Widder [1], Theorem 12a) but we have included it for two reasons. Firstly condition 3 is particularly easy to verify in applications and secondly the tactic of our proof is to show that $2 \Rightarrow 1 \Rightarrow 3$.

The monotone operator functions mentioned in Theorem B were introduced and characterized by Löwner [2]. Löwner's work was subsequently clarified by Bendat and Sherman [3] and a detailed account of the theory is given in the book by Donoghue [4]. The monotone operator functions are the real positive measurable functions f such that

$$f(A) \geq f(B) \geq 0$$

for every pair of bounded self-adjoint operators A , and B , satisfying

$$A \geq B \geq 0.$$

Löwner's characterizations together with a theorem of Herglotz [5] establish that f is a monotone operator function, if, and only if, it has a representation

$$f(x) = \int_0^{\infty} d\mu(t) \frac{(1+t)x}{t+x} + \alpha x + \beta, \quad x > 0,$$

where μ is a positive finite measure and $\alpha, \beta \geq 0$. From this representation one can check the validity of condition 3 of Theorem B, e.g., for $n \geq 1$

$$(-1)^n f^{(n+1)}(x) = (n+1)! \int_0^{\infty} d\mu(t) \frac{t(1+t)}{(t+x)^{n+2}} \geq 0.$$

Nevertheless the function

$$x \rightarrow (1 - e^{-tx})$$

respects the semigroup ordering although it is not a monotone operator function. Thus the class of functions introduced in Theorem B is strictly larger than the class of monotone operator functions.

Our third result concerns contractivity on the spaces $L^p(X; d\mu)$. The semigroup $\exp\{-tH\}$ is defined to be L -contractive if

$$\|e^{-tH} \phi\|_p \leq \|\phi\|_p$$

for all $\phi \in L^2 \cap L^p$, all $p \in [1, \infty]$, and all $t > 0$. It can be shown for a positivity preserving contraction semigroup that this property of L -contractivity is equivalent to contractivity on $L^\infty(X; d\mu)$ (see, for example, [6], Theorem XIII.51), if $(X; d\mu)$ is σ -finite.

Theorem C. *If $\exp\{-tH\}$ is a positivity preserving L -contractive semigroup and f is a function of the class described by Theorem B then $\exp\{-tf(H)\}$ is also L -contractive.*

After proving these theorems in Sects. 1–3, we discuss an ordering of semigroups on different Hilbert spaces in Sect. 4. We conclude with various applications to Green's functions in Sect. 5.

1. Generators

If H is a self-adjoint operator on \mathcal{H} we denote its domain by $D(H)$. Moreover if D is a subspace of \mathcal{H} then D_+ will denote the non-negative functions in D .

If H is a positive self-adjoint operator we define the corresponding positive closed quadratic form h by

$$D(h) = D(H^{1/2}), \quad h(\psi) = \|H^{1/2}\psi\|^2.$$

The starting point of our analysis is the following known result which characterizes positivity preserving semigroups by properties of their generators.

Proposition 1. *Let $H \geq 0$ be a positive self-adjoint operator on $\mathcal{H} = L^2(X; d\mu)$ with associated quadratic form h and let $T_t = \exp\{-tH\}$ denote the corresponding C_0 -semigroup of contractions.*

The following conditions are equivalent

1. T_t is positivity preserving for all $t \geq 0$.
2. $(\lambda \mathbf{1} + H)^{-1}$ is positivity preserving for all $\lambda > 0$.
3. For all $\psi \in D(h)$ one has $|\psi| \in D(h)$ and

$$h(|\psi|) \leq h(\psi).$$

The equivalence of conditions 1 and 2 is a standard result of semigroup theory which follows from the relations

$$(\lambda \mathbf{1} + H)^{-1} = \int_0^\infty dt e^{-\lambda t} T_t$$

and

$$T_t = \lim_{n \rightarrow \infty} \left(\mathbf{1} + \frac{t}{n} H \right)^{-n}.$$

The equivalence of conditions 1 and 3 is proved in the book by Reed and Simon [6], Theorem XIII.50; they ascribe the result to Beurling and Deny [7].

Condition 3 immediately implies that the sum of two generators is in fact a generator. To be more precise let H, K , be positive self-adjoint operators and assume that the closed form sum $h+k$ is densely defined. If this is the case then $h+k$ determines a self-adjoint sum of H and K which we denote by $H \dot{+} K$. Now if H and K are both generators of positivity preserving semigroups then it follows immediately from Condition 3 that $H \dot{+} K$ also generates a semigroup of the same type.

Our first result establishes a second simple stability property of such generators which is the key to the subsequent analysis.

Lemma 2. *If $H \geq 0$ is the generator of a C_0 -semigroup of positivity preserving contractions and $\varepsilon > 0$ then*

$$H_\varepsilon = \frac{\mathbf{1} - e^{-\varepsilon H}}{\varepsilon}$$

generates a semigroup of the same type.

Proof. One has $H_\varepsilon \geq 0$ and

$$\begin{aligned} e^{-tH_\varepsilon} &= e^{-t/\varepsilon} e^{te^{-\varepsilon H}/\varepsilon} \\ &\geq e^{-t/\varepsilon} \mathbb{1} . \end{aligned}$$

One can now prove stability of the generator property for the class of functions described in condition 2 of Theorem B by combining Lemma 2 and the observation that the sum of generators is a generator.

Theorem 3. *Let $H \geq 0$ be the generator of a C_0 -semigroup of positivity preserving contractions on $\mathcal{H} = L^2(X; d\mu)$ and f a function of the form described in condition 2 of Theorem B.*

It follows that $f(H)$ generates a C_0 -semigroup of positivity preserving contractions on \mathcal{H} .

Proof. First it is necessary to give a precise definition of the operator $f(H)$ or the associated quadratic form h_f . We will construct the form by a monotone approximation argument.

Lemma 4. *Let h_α be a monotonically increasing net of positive closed densely defined quadratic form on \mathcal{H} and define h by*

$$\begin{aligned} D(h) &= \left\{ \psi ; \psi \in \bigcap_\alpha D(h_\alpha), \sup_\alpha h_\alpha(\psi) < +\infty \right\} \\ h(\psi) &= \sup_\alpha h_\alpha(\psi) = \lim_\alpha h_\alpha(\psi) . \end{aligned}$$

It follows that h is a positive closed quadratic form and hence if it is densely defined it uniquely determines a positive self-adjoint operator H such that $D(h) = D(H^{1/2})$ and

$$h(\psi) = (H^{1/2}\psi, H^{1/2}\psi) .$$

This is a straightforward result in the theory of positive operators and quadratic forms. For a proof see, for example, [8], Lemma 5.2.13.

Now let us return to the proof of Theorem 3.

Let E_H denote the spectral measure associated with H and define the bounded quadratic forms F_n by $D(F_n) = \mathcal{H}$ and

$$F_n(\psi) = \int_0^n d(\psi, E_H(\lambda)\psi) f(\lambda) .$$

Since f is positive these forms are monotone increasing and if we introduce a limit form h_f by

$$\begin{aligned} D(h_f) &= \left\{ \psi ; \sup_n F_n(\psi) < +\infty \right\} \\ h_f(\psi) &= \sup_n F_n(\psi) = \lim_{n \rightarrow \infty} F_n(\psi) \end{aligned}$$

then h_f is positive and closed. But it is densely defined because $D(h_f)$ contains all vectors of the form $E_H(\Delta)\psi$, $\psi \in \mathcal{H}$, with Δ a bounded open set. Thus h_f determines a self-adjoint operator $f(H)$.

Now f can be written as a sum of a function f_1 with the representation

$$f_1(x) = \int_0^\infty d\mu(t) \frac{(1 - e^{-tx})}{t} + \alpha x + \beta, \quad x \in [0, \infty)$$

and a second function f_2 such that

$$\begin{aligned} f_2(0) &= 0 \\ f_2(x) &= c > 0, \quad x > 0. \end{aligned}$$

We will prove that $f_1(H)$ and $f_2(H)$ are both generators and then $f = f_1 + f_2$ is a generator by the discussion preceding Lemma 2

Firstly for $\psi \in D(h_f)$ one has

$$\begin{aligned} h_{f_1}(\psi) &= \int_0^\infty d(\psi, E_H(\lambda)\psi) \left\{ \int_0^\infty d\mu(t) \frac{(1 - e^{-t\lambda})}{t} + \alpha\lambda + \beta \right\} \\ &= \int_0^\infty d\mu(t) \left(\psi, \frac{1 - e^{-tH}}{t} \psi \right) + \alpha h(\psi) + \beta \|\psi\|^2 \\ &\geq \int_0^\infty d\mu(t) \left(|\psi|, \frac{1 - e^{-tH}}{t} |\psi| \right) + \alpha h(|\psi|) + \beta \|\psi\|^2, \end{aligned}$$

where the inequality follows from Proposition 1 and Lemma 2. But this shows that $|\psi| \in h_{f_1}(\psi)$ and

$$h_{f_1}(\psi) \geq h_{f_1}(|\psi|).$$

Hence $f_1(H)$ is a generator by Proposition 1.

Next remark that

$$f_2(H) = s \cdot \lim_{t \rightarrow \infty} c(1 - e^{-tH})$$

by spectral analysis. But $c(1 - \exp\{-tH\})$ is a generator and hence $f_2(H)$ is also a generator by Proposition 1.

At this stage we are prepared to derive the L -contractive statement in Theorem C². For this it is necessary to have a modified version of Proposition 1.

Proposition 1'. *Let $H \geq 0$ be the generator of a C_0 -semigroup of positivity preserving contractions on the Hilbert space $\mathcal{H} = L^2(X; d\mu)$ and let h denote the associated quadratic form. Moreover for each $\psi \in \mathcal{H}_+$ let $(\psi \wedge 1)(x) = \min\{\psi(x), 1\}$.*

The following conditions are equivalent

1. $\exp\{-tH\}$ is a contraction on $L^p(X; d\mu)$ for all $1 \leq p \leq +\infty$ and all $t > 0$.
2. $\exp\{-t(\mathbb{1} - e^{-\varepsilon H})/\varepsilon\}$ is a contraction on $L^p(X; d\mu)$ for all $1 \leq p \leq +\infty$, all $t > 0$ and all $\varepsilon > 0$ (or all $0 < \varepsilon < \varepsilon_0$).
3. If $\psi \in D(h)_+$ then $\psi \wedge 1 \in D(h)_+$ and

$$h(\psi \wedge 1) \leq h(\psi).$$

2 In this discussion we assume $(X; d\mu)$ is σ -finite

4. If $\psi \in \mathcal{H}_+$ then

$$\left(\psi \wedge 1, \frac{\mathbb{1} - e^{-\varepsilon H}}{\varepsilon} \psi \wedge 1 \right) \leq \left(\psi, \frac{\mathbb{1} - e^{-\varepsilon H}}{\varepsilon} \psi \right)$$

for all $\varepsilon > 0$ (for all $0 < \varepsilon < \varepsilon_0$).

This result is essentially Theorem XIII.51 in [6] although it is not stated in the same manner. In this reference the equivalence $1 \Leftrightarrow 3$ is stated but it is established by showing $1 \Rightarrow 4 \Rightarrow 3 \Rightarrow 1$. The equivalence $2 \Leftrightarrow 4$ is of course $1 \Leftrightarrow 3$ with H replaced by $H_\varepsilon = (\mathbb{1} - \exp\{-\varepsilon H\})/\varepsilon$ (which is a generator by Lemma 2).

Once again one remarks that the sum of two generators of positivity preserving L -contractive semigroups is a generator of the same nature. The proof of Theorem C is then a word for word repetition of the proof of Theorem 3 with condition 3 of Proposition 1 replaced by condition 4 of Proposition 1'.

Remark. All the foregoing observations have been based on the fact that the generator property and L -contractivity are invariant under the replacement of H by $H_\varepsilon = (\mathbb{1} - \exp\{-\varepsilon H\})/\varepsilon$. Some of these results can be obtained by remarking that these properties are also invariant under the replacement of H by $H_\varepsilon = H(\mathbb{1} + \varepsilon H)^{-1}$. To see that H_ε generates a positivity preserving semigroup one remarks that

$$\begin{aligned} \exp\{-tH_\varepsilon\} &= \exp\{-t/\varepsilon\} \exp\{(t/\varepsilon)(\mathbb{1} + \varepsilon H)^{-1}\} \\ &\geq \exp\{-t/\varepsilon\} \mathbb{1} \end{aligned}$$

because $(\mathbb{1} + \varepsilon H)^{-1}$ is positivity preserving. Moreover the conditions of Proposition 1' are equivalent to

5. If $\psi \in \mathcal{H}_+$ then

$$(\psi \wedge 1, H(\mathbb{1} + \varepsilon H)^{-1} \psi \wedge 1) \leq (\psi, H(\mathbb{1} + \varepsilon H)^{-1} \psi)$$

for all $\varepsilon > 0$ (for all $0 < \varepsilon < \varepsilon_0$).

Condition 5 follows from Condition 4 by remarking that

$$\int_0^\infty dt e^{-\lambda t} (\psi, \mathbb{1} - e^{-tH} \psi) = \lambda^{-1} (\psi, H(\lambda \mathbb{1} + H)^{-1} \psi)$$

and Condition 3 follows from Condition 5 by taking the limit $\varepsilon \rightarrow 0$.

The operators $H_\varepsilon = H(\mathbb{1} + \varepsilon H)^{-1}$ and the Herglotz representation given in the introduction are particularly useful for discussing positivity monotone operator functions.

2. Ordering of Semigroups

In this section we examine pairs of semigroups ordered in the sense defined in the introduction and prove Theorem A and $2 \Rightarrow 1$ in Theorem B. We begin by characterizing the order relation.

Theorem 5. Let $\exp\{-tH\}$, $\exp\{-tK\}$, be two C_0 -semigroups of self-adjoint positivity preserving contractions on $\mathcal{H} = L^2(X; d\mu)$.

The following conditions are equivalent

1. $e^{-tH} \succcurlyeq e^{-tK} \succcurlyeq 0$ for all $t \geq 0$.
2. $(\lambda \mathbb{1} + H)^{-1} \succcurlyeq (\lambda \mathbb{1} + K)^{-1} \succcurlyeq 0$ for all $\lambda > 0$.
3. $(\phi, K\psi) \geq (H\phi, \psi)$

for all $\phi \in D(H)_+$ and $\psi \in D(K)_+$.

Remark. It is not absolutely necessary that the semigroups $\exp\{-tH\}$, $\exp\{-tK\}$ are contractive. The theorem is valid if H and K are bounded below but then the range of λ in condition 2 must be suitably restricted.

Proof. $1 \Leftrightarrow 2$. This follows directly from the semigroup relations used to prove $1 \Leftrightarrow 2$ in Proposition 1.

$1 \Rightarrow 3$. If $\phi \in D(H)_+$ and $\psi \in D(K)_+$ then condition 1 implies that

$$(\phi, e^{-tH}\psi) \geq (\phi, e^{-tK}\psi).$$

Therefore

$$\left(\phi, \frac{\mathbb{1} - e^{-tK}}{t} \psi \right) \geq \left(\frac{\mathbb{1} - e^{-tH}}{t} \phi, \psi \right)$$

and condition 3 follows by taking the limit $t \rightarrow 0$.

$3 \Rightarrow 2$. Let $\phi, \psi \in \mathcal{H}_+$ then $(\lambda \mathbb{1} + K)^{-1}\psi \in D(K)_+$ and $(\lambda \mathbb{1} + H)^{-1}\phi \in D(H)_+$ by Proposition 1. Therefore

$$((\lambda \mathbb{1} + H)^{-1}\phi, K(\lambda \mathbb{1} + K)^{-1}\psi) \geq (H(\lambda \mathbb{1} + H)^{-1}\phi, (\lambda \mathbb{1} + K)^{-1}\psi).$$

But $H(\lambda \mathbb{1} + H)^{-1} = \mathbb{1} - \lambda(\lambda \mathbb{1} + H)^{-1}$ and hence

$$(\phi, (\lambda \mathbb{1} + H)^{-1}\psi) \geq (\phi, (\lambda \mathbb{1} + K)^{-1}\psi).$$

Remark. If $H = (H_{ij})$, $K = (K_{ij})$, are positive matrices condition 3 of Proposition 1 states that they generate positivity preserving semigroups if, and only if,

$$H_{ij} \leq 0 \quad K_{ij} \leq 0$$

for all $i \neq j$. Condition 3 of Theorem 5 states that

$$e^{-tH} \succcurlyeq e^{-tK}$$

for all $t \geq 0$ if, and only if

$$H_{ij} - K_{ij} \leq 0$$

for all i, j . This will be of importance in Sect. 4.

Theorem 5 is deceptively simple. In applications it is often difficult to decide directly whether one semigroup dominates another, e.g. to decide when a family of semigroups is monotonic in some parameter, but condition 3 of the theorem is, however, often easy to confirm. This condition on the generators is also the key to the following functional analysis of generators. Note for example that if

$$e^{-tH} \succcurlyeq e^{-tK} \succcurlyeq 0$$

for all $t \geq 0$ and if

$$H_\varepsilon = \frac{\mathbb{1} - e^{-\varepsilon H}}{\varepsilon}, \quad K_\varepsilon = \frac{\mathbb{1} - e^{-\varepsilon K}}{\varepsilon}$$

with $\varepsilon > 0$ then

$$(\phi, K_\varepsilon \psi) \geq (\phi, H_\varepsilon \psi)$$

for all $\phi, \psi \in \mathcal{H}_+$. But K_ε and H_ε are generators by Lemma 2 and therefore

$$e^{-tH_\varepsilon} \geq e^{-tK_\varepsilon} \geq 0$$

for all $t \geq 0$. Thus the function $x \rightarrow (1 - e^{-\varepsilon x})/\varepsilon$ respects both the generator property and the semigroup order.

Theorem 6. *Let $\exp\{-tH\}$ and $\exp\{-tK\}$ be two self-adjoint C_0 -semigroups of positivity preserving contractions on $\mathcal{H} = L^2(X; d\mu)$ and f a function satisfying condition 2 of Theorem B.*

If

$$e^{-tH} \geq e^{-tK} \geq 0$$

for all $t \geq 0$ then

$$e^{-tf(H)} \geq e^{-tf(K)} \geq 0$$

for all $t \geq 0$.

Proof. Again one can write $f = f_1 + f_2$ where

$$f_1(x) = \int_0^\infty d\mu(t) \frac{(1 - e^{-tx})}{t} + \alpha x + \beta$$

for all $x \geq 0$ and f_2 is given by

$$f_2(0) = 0$$

$$f_2(x) = c > 0, \quad x > 0.$$

But for $\phi \in D(f_1(H))_+$, $\psi \in D(f_2(H))_+$ one has

$$\begin{aligned} (\phi, f_1(K)\psi) &= \int_0^\infty d\mu(t) \left(\phi, \frac{\mathbb{1} - e^{-tK}}{t} \psi \right) + \alpha(\phi, K\psi) + \beta(\phi, \psi) \\ &\geq \int_0^\infty d\mu(t) \left(\frac{\mathbb{1} - e^{-tH}}{t} \phi, \psi \right) + \alpha(H\phi, \psi) + \beta(\phi, \psi) \\ &= (f_1(H)\phi, \psi) \end{aligned}$$

by the remark preceding the theorem. Moreover

$$\begin{aligned} (\phi, f_2(K)\psi) &= \lim_{t \rightarrow \infty} c(\phi, (1 - e^{-tK})\psi) \\ &\geq \lim_{t \rightarrow \infty} c(\phi, (1 - e^{-tH})\psi) \\ &= (\phi, f_2(H)\psi) \end{aligned}$$

for all $\phi, \psi \in \mathcal{H}_+$. Thus $f_1 + f_2$ satisfies condition 3 of Theorem 5.

3. Matrix Semigroups

Theorems 3 and 6 establish that $2 \Rightarrow 1$ in Theorem B. In this section we prove $1 \Rightarrow 3 \Rightarrow 2$. For the implication $1 \Rightarrow 3$ it suffices to consider matrix semigroups and $3 \Rightarrow 2$ follows from Bernstein's theorem.

If H and K are non-negative matrices which generate positivity preserving semigroups then Theorem 5 establishes that

$$e^{-tH} \succcurlyeq e^{-tK} \succcurlyeq 0$$

for all $t > 0$ if, and only if, $K \succcurlyeq H$. With this in mind one sees that the following establishes $1 \Rightarrow 3$ in Theorem B.

Theorem 7. *Let f be a real function on an interval $(a, b) - \infty \leq a < b \leq +\infty$ such that*

$$f(K) \succcurlyeq f(H)$$

for each pair of selfadjoint matrices K, H with spectrum in (a, b) satisfying

$$e^{-tH} \succcurlyeq e^{-tK} \succcurlyeq 0$$

for all $t \geq 0$.

It follows that $f \in C^\infty(a, b)$ and

$$(-1)^n f^{(n+1)}(x) \geq 0, \quad x \in (a, b), \quad n=0, 1, 2, \dots$$

*Proof*³. The hypotheses, applied to 1×1 matrices H and K , imply that f is nondecreasing on (a, b) .

Next, assume that H and K are $n \times n$ matrices with $n \geq 1$ and introduce $2n \times 2n$ matrices H' and K' by

$$H' = \begin{pmatrix} \frac{K+H}{2} + \theta \mathbf{1} & -\frac{K-H}{2} - \theta \mathbf{1} \\ -\frac{K-H}{2} - \theta \mathbf{1} & \frac{K+H}{2} + \theta \mathbf{1} \end{pmatrix}$$

$$K' = \begin{pmatrix} \frac{K+H}{2} + \theta \mathbf{1} & -\frac{K-H}{2} \\ -\frac{K-H}{2} & \frac{K+H}{2} + \theta \mathbf{1} \end{pmatrix},$$

where θ is nonnegative. Then one has

$$H' = HE_+ + (K + 2\theta \mathbf{1})E_-$$

$$K' = (H + \theta \mathbf{1})E_+ + (K + \theta \mathbf{1})E_-,$$

where E_\pm are projection operators defined by

$$E_\pm = \begin{pmatrix} \mathbf{1}/2 & \pm \mathbf{1}/2 \\ \pm \mathbf{1}/2 & \mathbf{1}/2 \end{pmatrix}.$$

³ The present proof of this theorem was suggested to us by H. Araki

It follows from the hypotheses on H, K that the spectra of H', K' are contained in (a, b) for sufficiently small θ . But $K - H \succcurlyeq 0$ by Theorem 5 and H' and K' generate positivity preserving semigroups by the remark following Theorem 5. Moreover, since $K' - H' = \theta(E_+ - E_-) \succcurlyeq 0$ it follows that

$$e^{-tH'} \succcurlyeq e^{-tK'} \succcurlyeq 0.$$

By the hypothesis on f it follows that $f(K') \succcurlyeq f(H')$. But

$$f(K') - f(H') = (f(H + \theta\mathbb{1}) - f(H))E_+ + (f(K + \theta\mathbb{1}) - f(K + 2\theta\mathbb{1}))E_-$$

and considering the diagonal part of the 2×2 matrix representation of this operator one must have

$$f(H + \theta\mathbb{1}) - f(H) \succcurlyeq f(K + 2\theta\mathbb{1}) - f(K + \theta\mathbb{1}). \tag{*}$$

Choosing $H = K = (x - \theta)\mathbb{1}$ this implies

$$f(x) \geq \frac{f(x + \theta) + f(x - \theta)}{2}.$$

Since f is nondecreasing it follows that it is concave in the sense that

$$f(\lambda x + (1 - \lambda)y) \geq \lambda f(x) + (1 - \lambda)f(y)$$

for all $0 \leq \lambda \leq 1$ and $x, y \in (a, b)$ (see, for example, Roberts and Varberg [9], Chap. VII, Theorem C). Thus f is continuous and the right derivative

$$f'_+(x) = \lim_{y \rightarrow 0_+} y^{-1}(f(x + y) - f(x))$$

exists for all $x \in (a, b)$. Moreover f'_+ is nonincreasing and $f \in C^1(a, b)$ if and only if f'_+ is continuous, in which case $f' = f'_+$. But (*) gives

$$-\theta^{-1}(f(K + 2\theta\mathbb{1}) - f(K + \theta\mathbb{1})) \geq -\theta^{-1}(f(H + \theta\mathbb{1}) - f(H))$$

and in the limit $\theta \rightarrow 0$ one finds

$$-f'_+(K) \geq -f'_+(H).$$

Thus $-f'_+$ has the property assumed for f in the theorem. Consequently $-f'_+$ is concave and absolutely continuous on (a, b) . In particular $f \in C^1(a, b)$ and $f'(x) \geq 0$ for all $x \in (a, b)$.

The full statement of the theorem then follows by recursion.

To complete the proof of Theorem B it remains to prove that $3 \Rightarrow 2$. But condition 3 states that f' is completely monotone on $(0, \infty)$ and hence there exists a positive measure μ on $[0, \infty)$ such that

$$f'(x) = \int_0^\infty d\mu(t)e^{-tx}.$$

Thus by integrating and explicitly separating out the contribution of μ at the origin one has

$$f(x) = \int_0^\infty d\mu(t) \left(\frac{1 - e^{-tx}}{t} \right) + \alpha x + \beta,$$

where $\alpha \geq 0$ and $\beta = f(0+) \geq 0$. Finally

$$(1 - e^{-1}) \int_1^{\infty} d\mu(s) \frac{1}{s} \leq \int_1^{\infty} d\mu(s) \left(\frac{1 - e^{-s}}{s} \right) \leq f(1)$$

and

$$e^{-1} \int_0^1 d\mu(s) \leq \int_0^1 d\mu(s) e^{-s} \leq f'(1).$$

Thus

$$\int_0^1 d\mu(s) < +\infty, \quad \int_1^{\infty} d\mu(s) \frac{1}{s} < +\infty.$$

Remark. The arguments of this section establish that the class of functions which respect the generator property and the semigroup ordering for all semigroups coincides with the class that respects these properties for all matrix semigroups.

4. Different Spaces

For at least one application, Green's functions with Dirichlet boundary conditions, it is useful to compare semigroups on different spaces. Let $\mathcal{H} = L^2(X; d\mu)$, take $Y \subset X$, $\nu = \mu|_Y$, and consider the subspace $\mathcal{K} = L^2(Y; d\nu) \subset \mathcal{H}$. If $\exp\{-tH\}$ and $\exp\{-tK\}$ are positivity preserving semigroups on \mathcal{H} and \mathcal{K} respectively we define

$$e^{-tH} \succcurlyeq e^{-tK} \succcurlyeq 0, \quad t \geq 0$$

whenever

$$(\phi, e^{-tH}\psi) \geq (\phi, e^{-tK}\psi) \geq 0, \quad t \geq 0,$$

for all $\phi \in \mathcal{H}_+$ and $\psi \in \mathcal{K}_+$. This definition is appropriate because it coincides with the requirement that

$$(\phi, e^{-tH}\psi) \geq (\phi, e^{-tK}\psi) \geq 0, \quad t \geq 0,$$

for all $\phi, \psi \in \mathcal{K}_+$. To see this remark that if $\phi \in \mathcal{H}_+$ then it has a decomposition $\phi = \phi_1 + \psi_1$ with $\phi_1 \in (\mathcal{K}^\perp)_+$ and $\psi_1 \in \mathcal{K}_+$.

Therefore

$$\begin{aligned} (\phi, e^{-tH}\psi) &\geq (\psi_1, e^{-tH}\psi) \\ &\geq (\psi_1, e^{-tK}\psi) \\ &= (\phi, e^{-tK}\psi) \geq 0, \end{aligned}$$

where the first inequality uses the positivity preservation of $\exp\{-tH\}$, the second uses the order property for $\psi_1, \psi \in \mathcal{K}_+$, and the conclusion follows because $\exp\{-tK\}\psi \in \mathcal{K}_+$ and $\phi_1 \in (\mathcal{K}^\perp)_+$.

Now one has direct analogues of Theorems 5 and 6.

Theorem 5'. Let $\exp\{-tH\}$, $\exp\{-tK\}$, be two C_0 -semigroups of self-adjoint positivity preserving contractions on the Hilbert space $\mathcal{H} = L^2(X; d\mu)$, $\mathcal{K} = L^2(Y; d\nu)$ where $Y \subset X$ and $\nu = \mu|_Y$.

The following conditions are equivalent

1. $e^{-tH} \succcurlyeq e^{-tK} \succcurlyeq 0$ for all $t \geq 0$.
2. $(\phi, (\lambda \mathbb{1} + H)^{-1} \psi) \geq (\phi, (\lambda \mathbb{1} + K)^{-1} \psi)$ for all $\lambda > 0$ and all $\phi \in \mathcal{H}_+$, $\psi \in \mathcal{K}_+$ (or for all $\phi, \psi \in \mathcal{H}_+$).
3. $(\phi, K\psi) \geq (H\phi, \psi)$ for all $\phi \in D(H)_+$, and $\psi \in D(K)_+$.

The proof is a word for word repetition of the proof of Theorem 5.

Theorem 6'. Let $\exp\{-tH\}$ and $\exp\{-tK\}$ be two C_0 -semigroups of self-adjoint positivity preserving contractions $\mathcal{H} = L^2(X; d\mu)$, $\mathcal{K} = L^2(Y; d\nu)$ where $Y \subset X$ and $\nu = \mu|_Y$.

If

$$e^{-tH} \succcurlyeq e^{-tK} \succcurlyeq 0$$

for all $t \geq 0$ then

$$e^{-t f(H)} \succcurlyeq e^{-t f(K)} \succcurlyeq 0$$

for all $t \geq 0$ where f is any function satisfying condition 2 (or condition 3) of Theorem B.

Again the proof is identical to that of Theorem 6 but now one uses Theorem 5'.

5. Applications

In this section we give several simple illustrations of results obtainable from Theorems A, B, and C, applied to Green's functions. If not specified H is assumed to be the self-adjoint generator of a C_0 -semigroup of positivity preserving contractions.

A. Relativistic Greens Functions

The functions $x \rightarrow x + m^2$ and $x \rightarrow x^\alpha$, $0 \leq \alpha \leq 1$ are monotone operator functions. Hence

$$e^{-t(H+m_1^2)^\alpha} \succcurlyeq e^{-t(H+m_2^2)^\alpha} \succcurlyeq 0$$

for all $t \geq 0$ whenever $m_2^2 \geq m_1^2$ by Theorem B. In particular if $K = -\nabla^2$ is the self-adjoint Laplacian on $L^2(\mathbb{R}^v)$ one concludes that the Green's function

$$G_t(x) = \int d^v p e^{-ipx} e^{-(p^2+m^2)^\alpha t}$$

are positive and pointwise decreasing as m^2 increases. The case $\alpha = 1/2$ corresponds to the evolution semigroup for a relativistic particle of mass m . Note that $\exp\{t\nabla^2\}$ is L -contractive (by verification of condition 3 in Proposition 1') and hence all the associated semigroups are L -contractive.

B. Multiplicative Potentials

If V is a positive function on $(X, d\mu)$ we define an associated multiplication operator V by

$$(V\psi)(x) = V(x)\psi(x)$$

with

$$D(V) = \{\psi; \int dx |V(x)|^2 |\psi(x)|^2 < +\infty\}.$$

In the following we always assume that the V, V_1, V_2 , are densely defined.

Now V is clearly the generator of a positivity preserving contraction semigroup. Thus if H is also a generator of this type and if V_1 and V_2 are bounded it follows that $H + V_1$ and $H + V_2$ are generators and

$$e^{-t(H+V_1)} \succcurlyeq e^{-t(H+V_2)} \succcurlyeq 0 \quad t \geq 0$$

whenever $V_2 \geq V_1$. This follows from Theorem A because $D(H + V_1) = D(H + V_2) = D(H)$ and

$$((H + V_2)\phi, \psi) - (\phi, (H + V_1)\psi) = (\phi, (V_2 - V_1)\psi) \geq 0$$

for all $\phi, \psi \in D(H)_+$.

This conclusion can be extended to much more general V . It suffices to assume that the forms $h + v_1$ and $h + v_2$ are densely defined and then one can conclude for the associated form sums $H + V_1$ and $H + V_2$ that

$$e^{-t(H+V_1)} \succcurlyeq e^{-t(H+V_2)} \succcurlyeq 0, \quad t \geq 0$$

whenever $V_2 \geq V_1$. One way to deduce this is to replace V_i by the bounded approximants $V_i^\varepsilon = (1 - \exp\{-\varepsilon V_i\})/\varepsilon$ and note that the nets $\{h + v_i^\varepsilon\}_{\varepsilon > 0}$, converge monotonically upwards as $\varepsilon \rightarrow 0$ in the sense of Lemma 4 to the forms $\{h + v_i\}$. But it is known in this case (see, for example, [8], Lemma 5.2.13) that the semigroups $\exp\{-t(H + V_i^\varepsilon)\}$ converge strongly to the semigroups $\exp\{-t(H + V_i)\}$ and hence the ordering follows from the case of bounded V_i .

C. Classical Boundary Conditions

Let $\mathcal{H} = L^2(\Omega)$ where Ω is a bounded open subset of \mathbb{R}^v with boundary $\partial\Omega$ which for simplicity we assume to be smooth. Define the quadratic form h_0 by $D(h_0) = H^{2,1}(\Omega)$, the Sobolev space, and

$$h_0(\psi) = \|\nabla\psi\|^2.$$

The positive self-adjoint operator H_0 associated with h_0 is the Laplace operator satisfying the Neumann boundary condition $\partial\psi/\partial n = 0$ on the boundary $\partial\Omega$ of Ω where $\partial/\partial n$ denotes the inward normal derivative. It is readily verified that h_0 satisfies condition 3 of Proposition 1 and hence H_0 generates a positivity preserving contraction semigroup.

Next let $\sigma \in C(\partial\Omega)$ and define a corresponding form h_σ by $D(h_\sigma) = D(h_0)$ and

$$h_\sigma(\psi) = h_0(\psi) + \int_{\partial\Omega} dS \sigma(x) |\psi(x)|^2.$$

The second term is known to be h_0 -bounded with h_0 -bound less than one and hence h_σ is a lower semi-bounded closed quadratic form. If $\sigma \geq 0$ then $h_\sigma \geq 0$. The self-adjoint operator H_σ associated with h_σ is the Laplacian operator which satisfies $\partial\psi/\partial n = \sigma\psi$ on $\partial\Omega$ in the sense of distributions. Since $h_\sigma(\psi) - h_0(\psi)$ depends only on $|\psi|$ one sees that h_σ also satisfies condition 3 of Proposition 1 and hence H_σ generates a positivity preserving semigroup. If $\sigma \geq 0$ this semigroup is contractive but if σ takes negative values one must add a suitable multiple of the identity to obtain the contraction property.

Now if $\sigma_1, \sigma_2 \in C(\partial\Omega)$ and $\phi \in D(H_{\sigma_1})_+$, and $\psi \in D(H_{\sigma_2})_+$ one calculates by approximation with smooth functions and an application of Green's theorem that

$$(\phi, H_{\sigma_2}\psi) - (H_{\sigma_1}\phi, \psi) = \int_{\partial\Omega} dS(\sigma_2(x) - \sigma_1(x))\phi(x)\psi(x).$$

Thus if $\sigma_2 \geq \sigma_1$ one concludes from Theorem A that

$$e^{-t(H_{\sigma_1} + c\mathbb{1})} \geq e^{-t(H_{\sigma_2} + c\mathbb{1})} \geq 0$$

for c sufficiently large that $H_{\sigma_1} + c\mathbb{1} \geq 0$ (in particular $c=0$ if $\sigma_1 \geq 0$). Thus the Green's functions associated with the semigroups $\exp\{-tH_\sigma\}$ are pointwise monotonically decreasing with σ . This conclusion is then valid with $H_\sigma + c\mathbb{1}$ replaced by $f(H_\sigma + c\mathbb{1})$ where f is one of the functions characterized by Theorem B. But $\exp\{-t(H_\sigma + c\mathbb{1})\}$ is also L -contractive (by verification of condition 3 of Proposition 1' for h_0 and hence for h_σ) and consequently all these associated semigroups are L -contractive.

D. Volume Dependence of Dirichlet Functions

Next we give an illustration of Theorem 5' and 6'.

Let $\mathcal{H} = L^2(\Omega)$ and define a quadratic form h_Ω by $D(h_\Omega) = H_0^{-1}(\Omega)$, the Sobolev space, and

$$h_\Omega(\psi) = \|\nabla\psi\|^2.$$

The associated self-adjoint operator H_Ω is just the Laplacian with the Dirichlet boundary condition $\psi=0$ on $\partial\Omega$ and it generates a positivity preserving contraction semigroup by condition 3 of Proposition 1.

Now let $\Omega_1 \supset \Omega_2$ and consider the operators H_{Ω_1} and H_{Ω_2} on $L^2(\Omega_1)$ and $L^2(\Omega_2)$. If $\phi \in D(H_{\Omega_1})_+$ and $\psi \in D(H_{\Omega_2})_+$ one calculates by Green's theorem that

$$(\phi, H_{\Omega_2}\psi) - (H_{\Omega_1}\phi, \psi) = \int_{\partial\Omega_2} dS\phi(x) \frac{\partial\psi}{\partial n}(x) \geq 0.$$

The positivity follows because $\phi \geq 0$ on $\Omega_1 \supset \Omega_2$ and $\psi \geq 0$ in Ω_2 which implies that $\partial\psi/\partial n \geq 0$ on $\partial\Omega_2$. Thus $\Omega_1 \supset \Omega_2$ implies

$$e^{-tH_{\Omega_1}} \geq e^{-tH_{\Omega_2}} \geq 0$$

i.e. the Green's functions associated with the Dirichlet semigroups $\exp\{-tH_\Omega\}$ are pointwise increasing with Ω . It follows from Theorem 6' that the same conclusion is valid for the semigroups $\exp\{-tf(H_\Omega)\}$ where f is a function of the class characterized by Theorem B.

Of course these illustrative examples can be combined, e.g. the Green's function associated with the semigroup

$$\exp \{ -t(\sqrt{H_\Omega + m^2} + V) \}$$

is pointwise monotonically increasing with Ω , and pointwise monotonically decreasing with m and V .

6. Conclusion

The foregoing investigation raises a number of questions, some of which we will answer in subsequent papers.

Firstly we have characterized a class of functions which respect an order property of all pairs of self-adjoint contraction semigroups but it is also natural to ask which functions f respect this order for the $n \times n$ matrix semigroups. (In the context of monotone operator functions the analogous question has been answered by Löwner [2].) Necessary conditions can be deduced from the proof of Theorem 7. By more refined matrix calculations one can in fact show that if $n \geq 2$ then f must be $(2n - 3)$ -times differentiable, $f^{(2n - 3)}$ must be convex and monotone decreasing, and one must have

$$(-1)^m f^{(m+1)}(x) \geq 0, \quad m = 0, 1, \dots, 2n - 4.$$

It is possible that these conditions are also sufficient.

Secondly several of our results extend to more general contexts, semigroups on Banach space, non-self-adjoint semigroups on Hilbert space, or more general cones. The main problem in obtaining such extensions is the absence of quadratic form characterizations of generators, and quadratic form approximation techniques. Nevertheless Theorems 3, 5, and 6, with slight modifications, can be extended to semigroups on Banach space [13] by use of the techniques of Bochner [14] and Phillips [15]. In [15] Phillips constructs the semigroup S^f from the semigroup S by a method which is very suited to the discussion of order properties. This construction is valid for those f in the class we have considered which are right continuous at the origin. On certain Banach spaces, e.g. L^p -spaces with $1 < p < \infty$, general f can be handled by a limiting process.

Thirdly one can introduce a strict order relation \succ on the bounded self-adjoint positivity preserving operators by defining $A \succ 0$ if

$$(\phi, A\psi) > 0$$

for all non-negative ϕ, ψ , which are not identically zero. If $A \succ 0$ then it is said to be positivity improving. Thus for semigroups

$$e^{-tH} \succ e^{-tK} \succ 0$$

if $\exp \{ -tK \}$ and $\exp \{ -tH \} - \exp \{ -tK \}$ are both positivity improving. In a second paper we examine the stability of this strict order property when H and K are replaced by $f(H)$ and $f(K)$.

Finally we remark that Simon [10, 11] and Hess et al. [12], have considered a different but related domination condition between pairs of contraction semigroups S and T on \mathcal{H} . They define S to dominate T if

$$S_t|\psi| \geq |T_t\psi|$$

for all $\psi \in \mathcal{H}$ and $t > 0$. Note that this automatically implies S_t is positivity preserving but this is not necessarily the case for T . If, however, $S_t \geq T_t \geq 0$ then S dominates T in this manner because

$$S_t|\psi| \geq T_t|\psi| \geq |T_t\psi| .$$

It is of interest that this domination relation is also stable under the replacement of the generators H and K of S and T by $f(H)$ and $f(K)$. This follows from the characterization, given in [11, 12], of the domination property by conditions on H and K .

These conditions are

1. $\psi \in D(K)$ implies $|\psi| \in D(h)$.
2. $\text{Re}((\text{sign } \psi)\phi, K\psi) \geq h(\phi, |\psi|)$

for all $\psi \in D(K)$ and $\phi \in D(h)_+$.

But if S dominates T then

$$\text{Re}((\text{sign } \psi)\phi, T_t\psi) \leq (\phi, S_t|\psi|)$$

for all $\phi \in \mathcal{H}_+$, $\psi \in \mathcal{H}$. Therefore

$$\text{Re} \left((\text{sign } \psi)\phi, \frac{(\mathbb{1} - T_t)}{t} \psi \right) \geq \left(\phi, \frac{(\mathbb{1} - S_t)}{t} |\psi| \right)$$

and conditions 1 and 2 above for $f(H)$ and $f(K)$ are verified by integration with μ . (To verify 1 it suffices to first consider the special case $\phi = |\psi|$.) Thus if $S_t^f = \exp \{-tf(H)\}$ and $T_t^f = \exp \{-tf(K)\}$ then S^f dominates T^f whenever S dominates T .

It is also natural to pose the converse question.

Which f are such that S^f dominates T^f whenever S dominates T ? Again it is the class of functions characterized in this paper. Sufficiency follows from the foregoing and for necessity we first remark that if S is positivity preserving

$$\text{Re } S_t(|\psi| \pm \psi) \geq 0$$

and hence

$$S_t|\psi| \geq |S_t\psi| ,$$

i.e. S dominates itself. Thus if we choose semigroups S and T such that

$$S_t \geq T_t \geq 0$$

then the images S^f and T^f are positivity preserving. But if S^f dominates T^f then by choosing $\psi = |\psi|$ in the domination relation one sees that

$$S_t^f|\psi| \geq |T_t^f|\psi| = T_t^f|\psi| .$$

Thus the replacement of H by $f(H)$ also respects the order relation \succcurlyeq . Hence f is necessarily in the class we have characterized. These remarks allow one to generalize the examples given in [11, 12]. Note that in this context of domination it is not necessary that T is self-adjoint but the foregoing remarks also apply in the more general context of [12]

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