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NOTE ON BASIC FEATURES OF LARGE TIME BEHAVIOUR OF HEAT KERNELS

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Abstract. Large time behaviour of heat semigroups (and more generally, of positive selfadjoint semigroups) is studied. Convergence of the semigroup to the ground state and of averaged logarithms of kernels to the ground state energy is shown in the general framework of positivity improving selfadjoint semigroups. This framework includes Laplacians on manifolds, metric graphs and discrete graphs.

Introduction

The study of the heat equation has a long history. There is a vast amount of literature devoted to heat kernel estimates under various geometric assumptions. Here, we want to investigate two basic issues concerning long term behaviour of the heat semigroup, which turn out to be rather independent of the underlying geometry. These issues are:

- Convergence of the semigroup to the ground state.
- Convergence of averaged logarithms of the kernels to the infimum of the spectrum.

In differential geometry these topics have been studied both for compact and non-compact manifolds. In the compact case the results are well known. In the general case, the first issue is settled by a result of Chavel and Karp [4] (see Simon [37] for simplification as well) and the second is known as theorem of Li after [31], where a statement can be found. (The paper itself does not seem to contain a proof but rather provides much stronger estimates under additional curvature assumptions). Corresponding results on heat equations with an elliptic generator can also be found in Pinchover's work [34, 35].

In probability theory these points are well known for Markov chains on a finite state space due to the Perron-Frobenius theorem. We are not aware of a treatment for general Markov chains on an infinite state space.

Here, we present a new approach to these two issues in the general framework of arbitrary positivity improving selfadjoint semigroups. This framework covers a large array of examples, among them Laplacians on manifolds, metric graphs and discrete graphs. In particular, we recover the mentioned results of [4, 31, 37] and provide results for Markov chains on infinite state spaces. A short way of phrasing our result would be that existence of kernels alone already implies the above long term behaviour (irrespective of the underlying setting or geometry).

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The crucial new insight for our unified treatment in the mentioned generality is that any positive function completely controls the bottom of the spectrum of a positivity improving selfadjoint semigroup. The proof of this fact is based on the simple observation that for a strictly positive function h on the measure space (X, m) the set

$$\{u \in L^2(X, m) : 0 \leqslant u \leqslant h\}$$

is total in $L^2(X, m)$ (see Lemma 2.1 and its proof for details).

As a consequence of our investigations and earlier results of [38, 39] we can substantially generalize a result of Cabré and Martel [3] on existence of positive weak solutions of the heat equation with a strongly negative potential.

We also note in passing that an application of our results to graphs positively answers a question raised by Weber in [41].

Unlike other basic results of semigroup theory, our results crucially depend on the selfadjointness of the underlying semigroup. In fact, they become wrong for general positivity improving semigroups as we show by an example below (see, however, [34, 35] for a treatment of certain non-selfadjoint semigroups in strongly local situations).

We develop our general results in three steps, first discussing general semigroups of selfadjoint operators in Section 1, then turning to positivity improving semigroups in Section 2 and finally turning to positivity improving semigroups with kernels in Section 3. An application to negative perturbations of positivity improving semigroups is presented in Section 4. This provides the above mentioned generalization of the result of [3]. In Section 5 we discuss examples viz Laplacians on manifolds, metric graphs and discrete graphs. This section contains the answer to the mentioned question of [41]. The (counter)example proving that selfadjointness is needed for our considerations is given at the end of Section 2.

The topic of the paper concerns the intersection of various subjects. Thus, not all readers may be familiar with the general theory of positivity improving semigroups. For this reason we include an appendix gathering various basic pieces of that theory.

1. Framework and basic result

In this section we introduce the framework used throughout the paper. We then present the basic result on convergence concerning the two issues discussed in the introduction.

We consider a selfadjoint operator L on a Hilbert space $\mathcal{H}$. The inner product on $\mathcal{H}$ is denoted by $\langle \cdot, \cdot \rangle$. The operator L is assumed to be bounded below. Hence, the operators e^{-tL}, $t \geqslant 0$ form a semigroup of bounded operators. The behaviour of this semigroup for large t is the focus of attention in the present work. The infimum of the spectrum of L is denoted by $E_0 = E_0(L)$. The projection onto the eigenspace associated to E_0 is denoted by P, i.e.,

$$P := \mathbb{1}_{\{E_0\}}(L),$$

where $\mathbb{1}_X$ denotes the indicator function of the set X. Note that $P = 0$ if E_0 is not an eigenvalue. In any case, we speak about E_0 as the *ground state energy*. The spectral measure of an element $f \in \mathcal{H}$ with respect to L is denoted by ρ_f. It is a finite measure on $[E_0, \infty)$ with the characteristic property that

$$\langle f, e^{-tL} f\rangle = \int_{[E_0,\infty)} e^{-ts}\, d\rho_f(s)$$

for all $t \geqslant 0$.

The topological support of the measure ρ_f is given by

$$\operatorname{spt}(\rho_f) = \big\{E \in \mathbb{R} \;\big|\; \rho_f(E-\delta, E+\delta) > 0 \text{ for all } \delta > 0\big\}.$$

The following is a rather immediate consequence of the spectral theorem (and part (a) is already contained in the considerations of [37]).

Theorem 1.1. *Let L be a selfadjoint operator in the Hilbert space $\mathcal{H}$ with infimum of the spectum $E_0 > -\infty$, and let $P = \mathbb{1}_{\{E_0\}}(L)$. Then the following holds:*

(a) *The operators $e^{tE_0}e^{-tL}$ converge strongly to P for $t \to \infty$, i.e.,*

$$e^{tE_0}e^{-tL} f \to Pf \qquad (t \to \infty)$$

for all $f \in \mathcal{H}$.

(b) *For any $f \in \mathcal{H}$ with $f \neq 0$ the equality*

$$\lim_{t\to\infty} \frac{\log\langle f, e^{-tL} f\rangle}{t} = -\inf \operatorname{spt}(\rho_f)$$

holds.

Proof. (a) The spectral theorem gives

$$\|(e^{tE_0}e^{-tL} - P)f\|^2 = \int_{[E_0,\infty)} |e^{tE_0}e^{-ts} - \mathbb{1}_{\{E_0\}}(s)|^2\, d\rho_f(s).$$

Obviously, the integrand is bounded by 1 and tends to zero everywhere. Hence, the Lebesgue convergence theorem gives (a).

(b) Let $E_f := \inf \operatorname{spt}(\rho_f)$, and let $t, \delta > 0$. The spectral theorem easily yields

$$e^{-(E_f+\delta)t}\|\mathbb{1}_{[E_f,E_f+\delta]}(L)f\|^2 \leqslant \int_{[E_f,\infty)} e^{-ts}\, d\rho_f(s) \leqslant e^{-E_f t}\|f\|^2.$$

We can take logarithms in this inequality as

$$\mathbb{1}_{[E_f,E_f+\delta]}(L)f \neq 0$$

by the definition of $\operatorname{spt}\rho_f$, obtaining

$$-(E_f+\delta)t + 2\ln\|\mathbb{1}_{[E_f,E_f+\delta]}(L)f\| \leqslant \ln\langle f, e^{-tL}f\rangle \leqslant -E_f t + 2\ln\|f\|.$$

After division by t, the desired statement then follows by considering first the limit $t \to \infty$ and then $\delta \to 0$. $\square$

For later use we note that any selfadjoint L which is bounded below by, say, C comes with a closed form Q defined by

$$Q(f,g) := \langle (L-C)^{1/2} f, (L-C)^{1/2} g\rangle + C\langle f,g\rangle$$

for $f,g \in D(Q) := D((L-C)^{1/2})$. Note that this definition does not depend on the actual choice of C, provided that $L \geqslant C$.

2. Positivity improving semigroups

In this section we specialize the framework of the last section to positivity improving selfadjoint semigroups. This will allow us to strengthen the result on convergence to the ground state energy of the previous section.

Let $\mathcal{H} = L^2(X,m)$, where X is a measure space with σ-algebra $\mathcal{B}$ and a σ-finite measure m. A function f on X is called *positive* if

$$\langle f,f\rangle > 0 \text{ and } f(x) \geqslant 0 \text{ for } m\text{-almost every } x \in X.$$

A function f on X is called *strictly positive* if $f(x) > 0$ for m-almost every $x \in X$. The semigroup $(e^{-tL})_{t\geqslant 0}$ is called positivity preserving if e^{-tL} maps non-negative functions to non-negative functions for each $t > 0$, it is called *positivity improving* if

$$e^{-tL} f \text{ is strictly positive}$$

for any positive f and all $t > 0$. Note that σ-finiteness of the measure m is a necessary condition for the semigroup to be positivity improving.

Remark. As is well known, the semigroup is positivity preserving if and only if the associated symmetric form Q satisfies the first Beurling-Deny criterium (see e.g. [2, 13]). A positivity preserving semigroup is positivity improving if it has further irreducibility properties; see Appendix A for further details.

The following simple lemma on positivity preserving semigroups contains a crucial new ingredient for the main result of this section.

Lemma 2.1. *Let L be selfadjoint and bounded below in $L^2(X,m)$ with infimum of the spectrum E_0. Assume that the associated semigroup $(e^{-tL})_{t\geqslant 0}$ is positivity preserving. Then*

$$\lim_{t\to\infty} \frac{\log\langle f, e^{-tL} g\rangle}{t} = -E_0$$

for all strictly positive f and g in $L^2(X,m)$.

Proof. Without loss of generality we can assume that $E_0 = 0$. We will show two inequalities:

As e^{-tL} is positivity preserving, we have

$$0 \leqslant \langle f, e^{-tL} g\rangle \leqslant \|e^{-tL}\|\|f\|\|g\|.$$

As $E_0 = 0$, we have $\|e^{-tL}\| \leqslant 1$ for all $t \geqslant 0$ and hence

$$\limsup_{t\to\infty} \frac{\log\langle f, e^{-tL} g\rangle}{t} \leqslant 0$$

follows. To show the reverse inequality we need the assumption that f and g are strictly positive. Thus,

$$h := \min\{f, g\} \text{ satisfies } h(x) > 0 \text{ for } m\text{-almost every } x \in X.$$

Therefore,

$$\mathcal{A} := \{u \in L^2(X, m) \mid 0 \leqslant u \leqslant h\}$$

is total in $L^2(X, m)$ (i.e., the linear span of $\mathcal{A}$ is dense). Thus,

$$0 = E_0 = \inf_{u \in \mathcal{A}} E_u, \qquad (\clubsuit)$$

where $E_u := \inf \operatorname{spt}(\rho_u)$. As e^{-tL} is positivity preserving and obviously

$$f, g \geqslant \min\{f, g\} = h \geqslant u \geqslant 0$$

for any $u \in \mathcal{A}$, we obtain that

$$\langle f, e^{-tL} g\rangle \geqslant \langle h, e^{-tL} h\rangle \geqslant \langle u, e^{-tL} u\rangle$$

for any $u \in \mathcal{A}$. Combined with (b) of Theorem 1.1 this gives

$$\liminf_{t\to\infty} \frac{\log\langle f, e^{-tL} g\rangle}{t} \geqslant \lim_{t\to\infty} \frac{\log\langle u, e^{-tL} u\rangle}{t} = -E_u$$

for any $u \in \mathcal{A}$. By ($\clubsuit$) we obtain the desired inequality

$$\liminf_{t\to\infty} \frac{\log\langle f, e^{-tL} g\rangle}{t} \geqslant 0,$$

and the theorem is proven. □

The following theorem can be seen as an integrated version of Li's theorem. It does not require existence of kernels.

Theorem 2.2. *Let L be selfadjoint and bounded below in $L^2(X, m)$ with infimum of the spectrum E_0. Assume that the associated semigroup $(e^{-tL})_{t\geqslant 0}$ is positivity improving. Then*

$$\lim_{t\to\infty} \frac{\log\langle f, e^{-tL} g\rangle}{t} = -E_0$$

for all positive f and g in $L^2(X, m)$.

Proof. As e^{-tL} is positivity improving, the functions $e^{-L}f$, $e^{-L}g$ are strictly positive. Clearly,

$$\langle f, e^{-tL} g\rangle = \langle e^{-L} f, e^{-(t-2)L} e^{-L} g\rangle$$

holds for any $t > 2$. Now, the theorem follows easily from Lemma 2.1. □

We note the following consequence of the theorem and part (b) of Theorem 1.1.

Corollary 2.3. *Consider L as in the previous theorem. Let $f \in L^2(X, m)$ be positive. Then*

$$E_0 = \inf \operatorname{spt}(\rho_f),$$

and in particular

$$\mathbb{1}_{[E_0, E_0+\delta)}(L) f \neq 0$$

for any $\delta > 0$.

Remarks. (1) The corollary is well known if E_0 is an eigenvalue. In this case there exists a (unique) almost-everywhere positive normalized eigenfunction to E_0. This eigenfunction has then a non-vanishing inner-product with any positive f and this easily implies the corollary.

(2) For strictly positive f the corollary will also hold if the semigroup is only assumed to be positivity preserving (as can be seen from Lemma 2.1).

(3) If the semigroup is only assumed to be positivity preserving, then the corollary (and the preceeding theorem) will in general be false: consider the direct sum of two positivity improving semigroups on disjoint sets and assume that the infima of the spectra of the two generators are different.

Large parts of the basic theory of positivity preserving semigroups do not depend on the selfadjointness of the generator. For this reason it is remarkable that our results crucially depend on this selfadjointness: In the following example it is shown that Theorem 2.2 is not true in general without the selfadjointness of L.

Example 2.4. Let $\mathbb{N} = \{1, 2, \ldots\}$ be the set of natural numbers and $\ell_2 := \ell^2(\mathbb{N})$ the associated ℓ^2 space (with $m(\{x\}) = 1$ for all $x \in \mathbb{N}$). Let L be the left shift on ℓ_2, i.e, $Lx = (x_2, x_3, \ldots)$ for all $x = (x_1, x_2, x_3, \ldots) \in \ell_2$. Observe that, as a positivity preserving operator, L generates a positivity preserving semigroup $(e^{tL})_{t\geqslant 0}$ on ℓ_2 which, however, is not positivity improving. (Note that here we consider L and not $-L$ as a generator.)

Let $\mu \in (0, 1)$. Then $y_\mu := (\mu^k)_{k\in\mathbb{N}} \in \ell_2$. We define a bounded positivity preserving operator L_1 on ℓ_2 by

$$L_1 x := Lx + x_1 y_\mu;$$

then one easily sees that L_1 generates a positivity improving semigroup $(e^{tL_1})_{t\geqslant 0}$ on ℓ_2. For $\lambda \in (0, 1)$, $\lambda \neq 2\mu$, a straightforward computation shows that the function $f\colon [0, \infty) \to \ell_2$,

$$f(t) := e^{\lambda t} y_\lambda + \frac{\lambda}{\lambda - 2\mu}(e^{\lambda t} - e^{2\mu t}) y_\mu$$

satisfies the differential equation $f'(t) = L_1 f(t)$ for $t \geqslant 0$, and $f(0) = y_\lambda$. Therefore,

$$e^{tL_1} y_\lambda = f(t)$$

for all $t \geqslant 0$.

Now suppose that $\mu < \frac{1}{2}$. Then for $\lambda \in (2\mu, 1)$ and any positive $x \in \ell_2$ we obtain that

$$\lim_{t\to\infty} \frac{\log\langle x, e^{tL_1} y_\lambda\rangle}{t} = \lambda.$$

In particular, the limit depends on the choice of λ, so no analogue of Theorem 2.2 can be true for the operator L_1.

3. Semigroups with kernels

In this section we further specialize the setting of the last section by assuming existence of (pointwise consistent) kernels. More precisely, we assume, for $f \in L^2(X, m)$ and $t > 0$, that

$$e^{-tL} f(x) = \int_X p_t(x, y) f(y)\, dm(y) \text{ for } m\text{-almost every } x \in X,$$

for a measurable function

$$p\colon (0,\infty)\times X\times X \longrightarrow (0,\infty)$$

satisfying

(K1) $p_t(x,y) = p_t(y,x)$ for all $x,y\in X$,
(K2) $p_t(x,\cdot)\in L^2(X,m)$ for any $x\in X$ and $t>0$,
(K3) $p_{t+s}(x,y) = \int_X p_t(x,z)p_s(z,y)\,dm(z)$ for all $x,y\in X$ and $t,s>0$.

Note that p is positive everywhere and accordingly e^{-tL} is positivity improving.

In this situation we can combine the result of the previous section with ideas developed in the context of manifolds in [4, 37] to obtain the following result. In fact, part (a) of the result is a rather direct adaption of the proof in [37]. Part (b) is then a consequence of (a) combined with Theorem 2.2. Note that part (b) is a rather general version of Li's theorem [31] (cf. the introduction).

Theorem 3.1. *Let L be a selfadjoint operator in $L^2(X,m)$ with infimum of the spectrum given by $E_0>-\infty$. Assume that the semigroup $(e^{-tL})_{t\geqslant 0}$ has a kernel p as above. Then the following holds:*

(a) *There exists a unique measurable function $\Phi\colon X\to[0,\infty)$ such that*

$$e^{tE_0}p_t(x,y)\to \Phi(x)\Phi(y) \qquad (t\to\infty)$$

for all $x,y\in X$. If E_0 is an eigenvalue, then the function Φ is a strictly positive normalized eigenfunction to E_0. If E_0 is not an eigenvalue, then the function Φ vanishes everywhere.

(b) *For all $x,y\in X$ the convergence*

$$\frac{\log p_t(x,y)}{t}\to -E_0 \qquad (t\to\infty)$$

holds.

Proof. Note that the uniqueness in (a) follows immediately from the convergence statement and non-negativity of Φ by considering $x=y$.

Without loss of generality assume that $E_0=0$. For any $x\in X$ we define the function $g_x\in L^2(X,m)$ via the kernel at $t=1$ by

$$g_x(y) = p_1(x,y).$$

Note that g_x is positive everywhere by assumption on p. Moreover, the assumption (K3) on p immediately gives

$$p_{t+2}(x,y) = \langle g_x, e^{-tL}g_y\rangle. \quad (\spadesuit)$$

We now distinguish two cases:

Case 1: $E_0=0$ is not an eigenvalue. As E_0 is not an eigenvalue, the projection P is zero. We set $\Phi\equiv 0$. Then by ($\spadesuit$) and (a) of Theorem 1.1 we obtain that

$$p_t(x,y) = \langle g_x, e^{-(t-2)L}g_y\rangle \to \langle g_x, Pg_y\rangle = 0 = \Phi(x)\Phi(y)$$

as $t \to \infty$, for all $x, y \in X$. This gives (a) of the theorem in this case. Moreover, (♠) and Theorem 2.2 give

$$\frac{\log p_t(x,y)}{t} = \frac{\log\langle g_x, e^{-(t-2)L} g_y\rangle}{t} \to -E_0.$$

This shows the desired statements in this case.

Case 2: $E_0 = 0$ is an eigenvalue. By general principles (see e.g. Section XIII.12 of [36]), there exists then a unique normalized eigenfunction Ψ that is positive m-almost everywhere and satisfies

$$P = \langle \Psi, \cdot \rangle \Psi.$$

Observe that

$$\Phi(x) := \langle g_x, \Psi \rangle = \int p_1(x,y)\Psi(y)\, dm(y) = e^{-L}\Psi(x) = \Psi(x)$$

for m-almost every $x \in X$, so Φ is a representative of Ψ. Moreover, by the assumption on p the function g_x is strictly positive for all $x \in X$ and hence $\Phi(x) > 0$ for all $x \in X$. Finally, (♠) and (a) of Theorem 1.1 give

$$p_t(x,y) = \langle g_x, e^{-(t-2)L} g_y \rangle \to \langle g_x, P g_y \rangle = \langle g_x, \Psi\rangle\langle g_y, \Psi\rangle = \Phi(x)\Phi(y)$$

for all $x, y \in X$. This proves part (a) of the theorem in this case. Given strict positivity of Φ, the convergence of the kernels gives easily part (b) of the theorem in this case. □

Note that the theorem gives a characterisation of whether E_0 is an eigenvalue:

Corollary 3.2. *Let L be as in the theorem. Let $\Phi_t(x) := \left(e^{-tE_0} p_t(x,x)\right)^{1/2}$ Then the following are equivalent:*

(i) *E_0 is an eigenvalue.*
(ii) *The pointwise limit (for $t \to \infty$) of the Φ_t is not the zero function in $L^2(X, m)$.*
(iii) *There exists an $x \in X$ such that $\lim_{t\to\infty} \Phi_t(x) \neq 0$.*

4. Admissible potentials

In this section we assume that we are given a positivity preserving selfadjoint semigroup. In this situation one can then try and study perturbations by potentials $V : X \to \mathbb{R}$. Here, two types of perturbations are of particular interest. These are perturbations that are positive (or more generally bounded below) and perturbations that are negative (or more generally bounded above). It turns out that perturbations which are bounded below are 'essentially harmless'. Details providing a more precise version of this statement are discussed in the appendix.

Here, we consider the much more subtle situation of perturbations arising from negative potentials. Our theorem below generalises a result from Cabré and Martel [3] for the heat equation on smooth bounded subdomains of Euclidean space to all selfadjoint positivity improving semigroups. Note that below the addition of a negative potential is performed by subtracting a positive potential.

Let L be a selfdadjoint operator in $L^2(X,m)$ that is bounded below, and assume that the semigroup $(e^{-tL})_{t\geqslant 0}$ is positivity preserving. Let $V\colon X \to [0,\infty)$ be a measurable potential. We then define the "generalised ground state energy" of $L-V$ by

$$\lambda_1(L,V) := \inf\bigl\{Q(u,u) - \|V^{1/2}u\|_2^2 \bigm| u \in D(Q),\ \|u\|_2^2 = 1\bigr\}.$$

Also, then for every $t \geqslant 0$, the sequence $(e^{-t(L-V\wedge k)})$ of positive operators is increasing, i.e., $(e^{-t(L-V\wedge k)}f)$ is an increasing sequence in $L^2(X,m)$, for each positive $f \in L^2(X,m)$. (This is an easy consequence of the Trotter product formula.) The potential V is called *admissible* if the strong limits

$$S_V(t) := \operatorname*{s-lim}_{k\to\infty} e^{-t(L-V\wedge k)}$$

exist and form a C_0-semigroup, i.e., satisfy

- $S_V(t+s) = S_V(s)S_V(t)$ for all $s,t > 0$ and
- $S_V(t) \to I$ strongly for $t \to 0$.

It is well known that admissibility of V follows if the $S_V(t)$ are exponentially bounded. We refer to [38, 39] for the notion of admissibility.

Theorem 4.1. *Let L be a selfadjoint operator in $L^2(X,m)$ that is bounded below, and assume that the semigroup $(e^{-tL})_{t\geqslant 0}$ is positivity improving. Let $V\colon X \to [0,\infty)$ be measurable, and let $E \in \mathbb{R}$. Then the following assertions are equivalent:*

(i) *V is admissible, and $\|S_V(t)\| \leqslant e^{-Et}$ for all $t \geqslant 0$.*

(ii) *There exist $M > 0$ and positive functions $f,g \in L^2(X,m)$ such that*

$$\langle f, e^{-t(L-V\wedge k)}g\rangle \leqslant Me^{-Et}$$

for all $t \geqslant 0$ and $k \in \mathbb{N}$.

(iii) *The inequality $\lambda_1(L,V) \geqslant E$ holds, i.e., the inequality $V + E \leqslant L$ holds in the sense that*

$$\|V^{1/2}u\|_2^2 + E\|u\|_2^2 \leqslant Q(u,u)$$

for all $u \in D(Q)$.

Proof. Obviously $V \wedge k$ is bounded and nonnegative for any $k \in \mathbb{N}$. The assumptions on L then give that the operator $L - V\wedge k$ is bounded below and generates a positivity improving semigroup. Thus, if $f,g \in L^2(X,m)$ are positive and $k \in \mathbb{N}$, then

$$E_0(L - V\wedge k) = -\lim_{t\to\infty} \frac{\log\langle f, e^{-t(L-V\wedge k)}g\rangle}{t}$$

by Theorem 2.2. Therefore, property (ii) holds if and only if $E_0(L-V\wedge k) \geqslant E$ for all $k \in \mathbb{N}$, and the latter is equivalent to

(ii') $L - V\wedge k \geqslant E$ in the form sense for all $k \in \mathbb{N}$.

Now the equivalence of (i), (ii') and (iii) is shown in Proposition 5.7 of [38]. There the proof is given for the heat semigroup on $\mathbb{R}^n$ only, but literally the same proof carries over to the general case. This proves the desired equivalence.

For illustration purposes we actually give a proof of "(iii)⇒(i)" here. While slightly longer than the proof in [38], our proof seems to be more elementary: If (iii) holds, it will also hold with V replaced by $V \wedge k$ for any $k \in \mathbb{N}$. As $V \wedge k$ is bounded, this gives

$$\|e^{-t(L-V\wedge k)}\| \leqslant e^{-Et}$$

for all $t \geqslant 0$ and $k \in \mathbb{N}$. Since for every positive $f \in L^2(X,m)$ the sequence $(e^{-t(L-V\wedge k)}f)$ is increasing, it follows that the limit in the definition of $S_V(t)$ exists for each $t \geqslant 0$, and $\|S_V(t)\| \leqslant e^{-Et}$ for all $t \geqslant 0$. It remains to show that $S_V(t)f \to f$ in $L^2(X,m)$ as $t \to 0$, for all $f \in L^2(X,m)$. By linearity we can assume without loss of generality that $f \geqslant 0$. Note that $0 \leqslant u(t) := e^{-tL}f \leqslant S_V(t)f =: u_V(t)$ for all $t \geqslant 0$. It follows that

$$\|u_V(t) - u(t)\|_2^2 = \|u_V(t)\|_2^2 + \|u(t)\|_2^2 - 2\langle u_V(t), u(t)\rangle \leqslant \|u_V(t)\|_2^2 - \|u(t)\|_2^2$$

for all $t \geqslant 0$. Moreover, $\|u(t)\|_2 \to \|f\|_2$ as $t \to 0$ (since $u(t) \to f$ in $L^2(X,m)$) and $\|u_V(t)\|_2 \leqslant e^{-Et}\|f\|_2$ for all $t \geqslant 0$. We conclude that $u_V(t) - u(t) \to 0$ and hence $u_V(t) \to f$ in $L^2(X,m)$ as $t \to 0$. □

It is possible to reformulate (parts of) the preceding theorem in terms of solutions of a corresponding abstract Cauchy problem. This is done in the following corollary. Let $\rho \in L^2(X,m)$ be strictly positive, and let $u_0 \in L^1(X,\rho m)$. We say that $u\colon [0,\infty) \to L^1(X,\rho m)$ is an *approximated solution* of the initial value problem

$$u'(t) + Lu(t) = Vu(t) \quad (t > 0), \qquad u(0) = u_0 \qquad (\heartsuit)$$

if there exists a sequence $(u_{0,k})$ in $L^2(X,m)$ such that $0 \leqslant u_{0,k} \uparrow u_0$ m-almost everywhere, $e^{-t(L-V\wedge k)}u_{0,k} \to u(t)$ in $L^1(X,\rho m)$ as $k \to \infty$, for all $t \geqslant 0$, and $u(t) \to u_0$ as $t \to 0$. We note that $L^2(X,m) \subseteq L^1(X,\rho m)$ since $\rho \in L^2(X,m)$.

Corollary 4.2. *Let L be a selfadjoint operator in $L^2(X,m)$ that is bounded below, and assume that the semigroup $(e^{-tL})_{t\geqslant 0}$ is positivity improving. Let $V\colon X \to [0,\infty)$ be measurable. Then $\lambda_1(L,V) > -\infty$ if and only if $(\heartsuit)$ has an approximated solution that is exponentially bounded in $L^1(X,\rho m)$ for some strictly positive $\rho \in L^2(X,m)$ and some positive $u_0 \in L^1(X,\rho m)$. Moreover, if $\lambda_1(L,V) > -\infty$, then there exists an approximated solution for any positive $u_0 \in L^2(X,m)$.*

Proof. For the proof of sufficiency, let u be the presumed approximated solution. Let $(u_{0,k})$ be the sequence in $L^2(E,m)$ approximating u_0, with $u_{0,1} \neq 0$ without loss of generality, and let $M > 0$ and $E \in \mathbb{R}$ such that $\|u(t)\|_{L^1(X,\rho m)} \leqslant Me^{-Et}$ for all $t \geqslant 0$. Then from the monotonicity of $(e^{-t(L-V\wedge k)})$ it follows that

$$\langle \rho, e^{-t(L-V\wedge k)}u_{0,1}\rangle \leqslant \langle \rho, u(t)\rangle = \|u(t)\|_{L^1(X,\rho m)} \leqslant Me^{-Et}$$

for all $t \geqslant 0$ and $k \in \mathbb{N}$. Since $u_{0,1}$ is positive, it follows from Theorem 4.1 that $\lambda_1(L,V) \geqslant E > -\infty$.

Necessity is clear: If $\lambda_1(L,V) > -\infty$, then V is admissible by Theorem 4.1, and $(\heartsuit)$ has an approximated solution that is exponentially bounded even in $L^2(X,m)$, for every positive $u_0 \in L^2(X,m)$. □

The previous corollary can be understood as an abstract version of a result due to Cabré and Martel [3]. This is discussed next.

Example 4.3. In [3], Cabré and Martel study existence of positive exponentially bounded solutions of the heat equation with a potential in the following setting: Let X be a smooth bounded subdomain of $\mathbb{R}^n$, let Δ_D be the Dirichlet Laplacian in $L^2(X)$, and let $L := -\Delta_D$. Then $-L$ generates a positivity improving semigroup on $L^2(X)$. Let $V\colon X \to [0,\infty)$ be measurable, and let $u_0\colon X \to [0,\infty)$ be locally integrable. As is discussed in [3], bottom of p. 976, the initial value problem

$$\partial_t u - \Delta_D u = Vu, \quad u(0) = u_0 \qquad (\diamondsuit)$$

has an approximated solution if and only if it has a positive weak solution (and if positive weak solutions exist, then the approximated solution is the minimal one).

Let now $\delta \in L^2(X)$ be defined by $\delta(x) = \mathrm{dist}(x, \partial X)$. Then we obtain the following:

(a) If $(\diamondsuit)$ has a positive weak solution that is exponentially bounded in $L^1(X, \delta m)$, for some positive $u_0 \in L^1(X, \delta m)$, then $\lambda_1(-\Delta_D, V) > -\infty$.
(b) If $\lambda_1(-\Delta_D, V) > -\infty$, then $(\diamondsuit)$ has a positive weak solution that is exponentially bounded in $L^2(X)$, for every positive $u_0 \in L^2(X)$.

Indeed, we have just recalled the equivalence between existence of approximated solutions and existence of positive weak solutions. Given this, (a) is immediate from the Corollary 4.2 and so is (b).

With (a) and (b) we have obtained Theorem 1 of [3] as a special case of Corollary 4.2.

5. Examples

In this section we want to present some examples for which all the assumptions of Section 3 are satisfied and hence all results of the previous sections hold.

We emphasize that nonnegative potentials (satisfying some weak growth conditions) could be added to all the operators L below and the resulting operators would still generate positivity improving semigroups, see Corollary A.3. In particular, Theorem 2.2 would still be valid.

5.1. **The Laplace-Beltrami operator on an manifold.** The Laplace-Beltrami operator on a connected Riemannian manifold gives rise to a positivity improving semigroup with a continuous (and even C^∞) kernel and the results of the previous sections hold. For this example, validity (a) of Theorem 3.1 had already been discussed by Chavel/Karp in [4] with substantial later simplifications by Simon in [37]. In fact, as mentioned already, part of our treatment in Section 3 is a rather direct adaption of these treatments. Part (b) of Theorem 3.1 has been obtained by Li [31]. We refrain from discussing further details and refer to the mentioned literature.

5.2. **Laplacians on metric graphs.** Laplacians on metric graphs (also known as quantum graphs) have attracted considerable interest in both physics and mathematics in recent years (see e.g. the articles [26, 27, 24, 25] and the conference proceedings [1, 12] and the references therein). While several variants and notations can be found in the literature, the basic setting is as follows (see [29] for further details and proofs):

Definition 5.1. A *metric graph* is a quintuple $\Gamma = (E, V, i, j, l)$ where

- E (edges) and V (vertices) are countable sets,
- $l\colon E \to (0, \infty)$ defines the length of the edges,
- $i\colon E \to V$ defines the initial point of an edge, and $j\colon \{e \in E | l(e) < \infty\} \to V$ the end point for edges of finite length.

For $e \in E$ we set $X_e := \{e\} \times (0, l(e))$. Moreover, we set $\overline{X_e} := X_e \cup \{i(e), j(e)\}$ ($\overline{X_e} := X_e \cup \{i(e)\}$ if $l(e) = \infty$) and $X := X_\Gamma = V \cup \bigcup_{e \in E} X_e$.

Thus, X_e is essentially just the interval $(0, l(e))$, and the first component is only added to force mutual disjointness of the X_e's. Then, $\overline{X_e}$ can be identified with $[0, l(e)]$ and this will be done tacitly in the following. For simplicity, we will assume that all lengths $l(e)$ are uniformly bounded away from zero.

To introduce a metric structure, we say that $x \in X^N$ is a *good polygon* if for every $k \in \{1, \ldots, N-1\}$ there is a unique edge $e \in E$ such that $\{x_k, x_{k+1}\} \subset \overline{X_e}$. Using the usual distance in $[0, l(e)]$ we get a distance d on $\overline{X_e}$ and define

$$L(x) = \sum_{k=1}^{N} d(x_k, x_{k+1}).$$

Provided the graph is connected and that the degree d_v of every vertex $v \in V$ defined as

$$d_v := \big|\big\{e \in E \bigm| v \in \{i(e), j(e)\}\big\}\big|$$

is finite, a metric on X is given by

$$d(p, q) := \inf\big\{L(x) \bigm| x \text{ is a good polygon with } x_0 = p \text{ and } x_N = q\big\}.$$

The Laplacian L with Kirchhoff boundary conditions is now defined as the operator corresponding to the form Q with

$$D(Q) := W_0^{1,2}(X), \;\; Q(u, v) := \sum_e (u_e' | v_e'),$$

where $u_e := u \circ \pi_e^{-1}$ is defined on $(0, l(e))$, with $\pi_e\colon X_e \to (0, l(e))$ defined by $\pi_e((e, s)) := s$, and

$$W^{1,2}(X) := \left\{ u \in C(X) \;\middle|\; \sum_{e \in E} \|u_e\|_{W^{1,2}}^2 =: \|u\|_{W^{1,2}}^2 < \infty \right\},$$

$$W_0^{1,2}(X) := W^{1,2}(X) \cap C_0(X).$$

Then Q is a Dirichlet form, and $-L$ generates a positivity preserving semigroup (see, e.g., [15, 29]; we refer to [19] for more general boundary conditions in the case of finite graphs).

Proposition 5.2. *(Characterisation of positivity improvement) Let Q be as above, and let L be the associated operator. Then the semigroup $(e^{-tL})_{t\geqslant 0}$ is positivity improving if and only if X is connected.*

Proof. It is clear that e^{-tL} cannot be positivity improving if Γ is not connected. The other implication (and much stronger results) follow immediately from the Harnack inequality presented in [15] for connected graphs. □

Moreover, existence of consistent kernels is known in this situation; see, e.g., [15, 29].

Proposition 5.3. *Let Q be as above, and let L be the associated operator. If X is connected, then e^{-tL} possesses a kernel p satisfying the conditions* (K1), (K2), (K3) *of Section 3.*

Given the previous propositions, as a consequence from Theorem 3.1 we obtain the following result for quantum graphs with Kirchhoff boundary conditions.

Corollary 5.4. *Let Γ be a connected metric graph, and let L be the associated operator with Kirchhoff boundary conditions. Then the kernel p of e^{-tL} satisfies*

$$p_t(x, y) \to \Phi(x)\Phi(y) \ \text{and}\ \frac{\log p_t(x, y)}{t} \to -E_0 \qquad (t \to \infty)$$

for a unique non-negative Φ on X.

5.3. **Laplacians on graphs.** The study of Laplacians on graphs has a long history (see, e.g., the monographs [5, 7] and the references therein). In recent years issues such as essential self-adjointness [18, 42, 40], stochastic (in)completeness and suitable isoperimetric inequalities for infinite graphs have attracted particular attention, see e.g. [6, 9, 10, 11, 14, 18, 20, 21, 22, 23, 42, 43, 40] and the references therein. Theses issues can be studied in various settings. The most general setting seems to be the one introduced in [21] (see [16, 17] as well), which we now recall:

Let V be a countable set. Let m be a measure on V with full support, i.e., m is a map on V taking values in $(0, \infty)$. A *symmetric weighted graph over V* or a *symmetric Markov chain on V* is a pair (b, c) consisting of a map $c\colon V \to [0, \infty)$ and a map $b\colon V \times V \to [0, \infty)$ with $b(x, x) = 0$ for all $x \in V$ satisfying the following two properties:

(b1) $b(x, y) = b(y, x)$ for all $x, y \in V$.
(b2) $\sum_{y\in V} b(x, y) < \infty$ for all $x \in V$.

Then $x, y \in V$ with $b(x, y) > 0$ are called neighbors and thought to be connected by an edge with weight $b(x, y)$. More generally, $x, y \in V$ are called connected if there exist $x_0, x_1, \ldots, x_n \in V$ with $b(x_i, x_{i+1}) > 0$ for $i = 0, \ldots, n$ and $x_0 = x$, $x_n = y$. If any two $x, y \in V$ are connected then (V, b, c) is called connected. To (V, b, c) we associate the form $Q^{\text{comp}} = Q^{\text{comp}}_{b,c}$ defined on the set $C_{\mathrm{c}}(V)$ of functions on V with finite support by

$$Q^{\text{comp}}\colon C_{\mathrm{c}}(V) \times C_{\mathrm{c}}(V) \longrightarrow [0, \infty)$$

$$Q^{\mathrm{comp}}(u,v)=\frac{1}{2}\sum_{x,y\in V}b(x,y)(u(x)-u(y))\overline{(v(x)-v(y))}+\sum_{x}c(x)u(x)\overline{v(x)}.$$

The form Q^{comp} is closable in $\ell^2(V,m)$ and the closure will be denoted by $Q=Q_{b,c,m}$ and its domain by $D(Q)$. Thus, there exists a unique selfadjoint operator $L=L_{b,c,m}$ in $\ell^2(V,m)$ such that

$$D(Q)=\text{Domain of definition of } L^{1/2}$$

and

$$Q(u)=\langle L^{1/2}u,L^{1/2}u\rangle_m$$

for all $u\in D(Q)$. Note that L consists of essentially two parts, viz, a Laplacian type operator encoded by b and a nonnegative potential encoded by c.

The form Q is a regular Dirichlet form on (V,m) (and any regular Dirichlet form on (V,m) arises in this way). Thus, the operator $-L$ generates a positivity preserving semigroup.

It is not hard to characterise when the semigroup is positivity improving.

Proposition 5.5. *(Characterisation of positivity improvement) Let (V,b,c) be as above, and let L be the associated operator. Then the semigroup $(e^{-tL})_{t\geqslant 0}$ is positivity improving if and only if (V,b,c) is connected.*

Proof. It is clear the the semigroup cannot be positivity improving if the graph is not connected. The other implication has been shown in [21] (see as well [40, 42, 8] for earlier results in special cases). □

As the underlying space is discrete, existence of kernels is obvious. Thus, the results of the previous sections apply. We note in particular the following consequence of Theorem 3.1.

Corollary 5.6. *Let (V,m) be a discrete measure space and (b,c) a graph on V. Let L be the associated operator. Then the kernel p of e^{-tL} satisfies*

$$e^{tE_0}p_t(x,y)\to\Phi(x)\Phi(y)\ \ \textit{and}\ \ \frac{\log p_t(x,y)}{t}\to -E_0\qquad(t\to\infty)$$

for a unique non-negative Φ on V.

Remark. The result of the corollary positively answers a question of Weber in [41].

Appendix A. Irreducibility and positivity preserving semigroups

The crucial assumption in our results is that e^{-tL} is positivity improving. It turns out that this condition is essentially equivalent to irreducibility combined with preservation of positivity. This allows one to set up a stability theory for positivity improving semigroups. For semigroups with E_0 being an eigenvalue this is discussed in XIII.12 of [36]. The general case is treated, e.g., in [30, 33]. For completeness reasons we shortly collect here a few items from [30, 33] to which we refer for further details and results.

We start with the definition of irreducibility for positivity preserving semigroups. Let us emphasize that our definition is the usual one in this context. It differs from the standard definition of irreducibility in the context of selfadjoint operators by an additional assumption on invariance under multiplication by L^∞ functions.

Definition A.1. Let L be a selfadjoint operator in $L^2(X,m)$, and assume that $-L$ generates a positivity preserving semigroup $(e^{-tL})_{t\geqslant 0}$. Then L is called *irreducible* if any closed subspace of $L^2(X,m)$ which is

- invariant under multiplication by bounded measurable functions and
- invariant under the semigroup,

agrees with $\{0\}$ or $L^2(X,m)$.

The following is well known. It can be found in Section C-III.3 of [33] (see [30, 36] as well).

Theorem A.2. *Let L be a selfadjoint operator in $L^2(X,m)$ which is bounded below. Assume that the semigroup $(e^{-tL})_{t\geqslant 0}$ is positivity preserving. Then the following assertions are equivalent:*

(i) *e^{-tL} is positivity improving for one (all) $t>0$.*
(ii) *$(L+\alpha)^{-1}$ is positivity improving for one (all) $\alpha > -E_0(L)$.*
(iii) *L is irreducible.*

Given this theorem we can now discuss stability of improvement of positivity: By the first Beurling-Deny criterium the semigroup $(e^{-tL})_{t\geqslant 0}$ is positivity preserving if and only if the associated form Q satisfies

$$Q(|u|,|u|) \leqslant Q(u,u)$$

for all $u \in D(Q)$. Now, obviously this condition is preserved when Q is replaced by $Q+V$ with $V\colon X\to\mathbb{R}$ measurable and bounded below such that the domain of definition

$$D(Q+V) := \left\{f\in D(Q) \;\Big|\; \int_X V|f|^2\,dm < \infty\right\}$$

is still dense. In particular, the operator $L \dotplus V$ associated to $Q+V$ (the *form sum* of L and V) is minus the generator of a positivity preserving semigroup.

Now, we can present the following variant of Theorem in XIII.12 of [36] and its proof.

Corollary A.3. *Let L be a selfadjoint operator in $L^2(X,m)$ with positivity improving semigroup $(e^{-tL})_{t\geqslant 0}$. Let $V\colon X\to\mathbb{R}$ be measurable and bounded below satisfying the following:*

- *$D(Q+V)$ is dense in $L^2(X,m)$.*
- *There exists a sequence of bounded V_n on X such that $L\dotplus V - V_n$ converges to L in the strong resolvent sense.*

Then, $L\dotplus V$ is the generator of a positivity improving semigroup.

Proof. Set $L_1 := L\dotplus V$. By denseness of $D(Q+V)$ in $L^2(X,m)$ and the preceding discussion, the semigroup e^{-tL_1} is positivity preserving. By Theorem A.2 it now suffices to show irreducibility. Let U be a closed subspace of $L^2(X,m)$ invariant under multiplication by bounded functions and e^{-tL_1} for each $t>0$. Then, by the Trotter product formula, the subspace U will be invariant under $e^{-t(L_1-V_n)}$ as well for each $n\in\mathbb{N}$. Then, by strong resolvent convergence, the subspace U will then be invariant under e^{-tL} as well. As the latter semigroup is positivity improving the subspace U must be trivial. $\square$

Note that the corollary obviously applies to bounded V (see C-III.3.3 of [33] for this case as well). Moreover, if $D(Q+V)$ is a core for $D(Q)$, then one can apply Proposition 5.8(b) of [38] to obtain that the assumptions of the corollary are satisfied with $V_n = V \wedge n$.

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