Trotter-Kato product formula and fractional powers of self-adjoint generators

Takashi Ichinose*
Department of Mathematics
Faculty of Science
Kanazawa University
Kanazawa, 920-1192
Japan

Hagen Neidhardt†
Weierstrass Institute for
Applied Analysis and Stochastics (WIAS) Berlin
Mohrenstr. 39
10117 Berlin
Germany

Valentin A. Zagrebnov‡
Université de la Méditerranée (Aix-Marseille II)
and
CPT-CNRS-Luminy-Case 907
13288 Marseille Cedex 9
France

October 2, 2002

*Email: ichinose@kappa.s.kanazawa-u.ac.jp
†Email: neidhard@wias-berlin.de
‡Email: zagrebnov@cpt.univ-mrs.fr

Abstract

Let A and B be non-negative self-adjoint operators in a Hilbert space such that their densely defined form sum $H = A \dot{+} B$ obeys

$$\mathrm{dom}(H^\alpha) \subseteq \mathrm{dom}(A^\alpha) \cap \mathrm{dom}(B^\alpha),$$

for some $\alpha \in (1/2, 1)$. It is proved that if, in addition, A and B satisfy $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$, then the symmetric and non-symmetric Trotter-Kato product formula converges in the operator norm:

$$\left\| \left(e^{-tB/2n} e^{-tA/n} e^{-tB/2n}\right)^n - e^{-tH} \right\| = O(n^{-(2\alpha-1)}),$$
$$\left\| \left(e^{-tA/n} e^{-tB/n}\right)^n - e^{-tH} \right\| = O(n^{-(2\alpha-1)})$$

uniformly in $t \in [0, T]$, $0 < T < \infty$ as $n \to \infty$, both with the same optimal error bound. The same is valid if one replaces the exponential function in the product by functions of the Kato class, that is, by real-valued Borel measurable functions $f(\cdot)$ defined on the non-negative real axis obeying $0 \leq f(x) \leq 1$, $f(0) = 1$ and $f'(+0) = -1$, with some additional smoothness property at zero. The present result improves previous ones relaxing the smallness of B^α with respect to A^α to the milder assumption $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$ and extending essentially the admissible class of Kato functions.

1 Introduction

In the present paper we deal with the operator-norm convergence of the Trotter-Kato product formula, which may have applications in quantum and in statistical mechanics.

Let A and B be two non-negative self-adjoint operators in a Hilbert space $\mathcal{H}$ such that $\mathrm{dom}(A^{1/2}) \cap \mathrm{dom}(B^{1/2})$ is dense in $\mathcal{H}$. By H we denote the form-sum of A and B, i.e.

$$H = A \dot{+} B \tag{1.1}$$

which is a non-negative self-adjoint operator in the Hilbert space $\mathcal{H}$. Obviously, one has $\mathrm{dom}(H^{1/2}) = \mathrm{dom}(A^{1/2}) \cap \mathrm{dom}(B^{1/2})$. Further, we consider the Kato functions: they are real-valued Borel measurable functions f on $[0, \infty)$ satisfying

$$0 \leq f(x) \leq 1, \quad x \in [0, \infty), \qquad f(0) = 1, \qquad f'(+0) = -1, \tag{1.2}$$
$$0 \leq g(x) \leq 1, \quad x \in [0, \infty), \qquad g(0) = 1, \qquad g'(+0) = -1. \tag{1.3}$$

Typical examples of the Kato functions are

$$f(x) = e^{-x} \quad \text{and} \quad f(x) = (1 + k^{-1}x)^{-k}, \quad k > 0. \tag{1.4}$$

In two remarkable papers [6], [7], Kato has shown that these assumptions are enough to prove

$$s - \lim_{n\to\infty} \left(f(tA/n) g(tB/n)\right)^n = e^{-tH} \tag{1.5}$$

uniformly in $t \in [0,T]$, $0 < T < \infty$. In the following we call a relation of this type a Trotter-Kato product formula. Naturally the question arises whether under suitable conditions the strong convergence of the Trotter-Kato product formula can be improved to the operator-norm convergence with a convergence rate estimate. Indeed this is possible. Beginning with Rogava [16] the operator-norm convergence with different convergence rates was verified in [8]-[14]. However, all these convergence rates are not optimal except the cases studied in [12] and [14]. In [11],[12] some of ideas of Chernoff [2],[3], have been used to prove that in the case $\mathrm{dom}(H) \subseteq \mathrm{dom}(A) \cap \mathrm{dom}(B)$, which means that the algebraic sum $H = A + B$ is self-adjoint, the optimal error bound is $O(n^{-1})$. In [14] the conditions are formulated on the fractional powers A^α, B^α, for $\alpha \in (1/2, 1]$. They lead to the optimal convergence rate $O(n^{-2(\alpha-1)})$.

The aim of the present paper is to study, in an sense, an intermediate case. We assume

$$\mathrm{dom}(H^\alpha) \subseteq \mathrm{dom}(A^\alpha) \cap \mathrm{dom}(B^\alpha) \tag{1.6}$$

for some $\alpha \in (1/2, 1)$. This assumption is stronger than $\mathrm{dom}(H^{1/2}) \subseteq \mathrm{dom}(A^{1/2}) \cap \mathrm{dom}(B^{1/2})$, which is always satisfied, but weaker than the assumption $\mathrm{dom}(H) \subseteq \mathrm{dom}(A) \cap \mathrm{dom}(B)$ used in [11] and [12]. Notice that comparing to [14] we do not demand the smallness of B^α with respect to A^α. We assume that the Kato functions further fulfill the conditions

$$|f|_{2\alpha} := \sup_{x>0} \frac{|f(x) - 1 + x|}{x^{2\alpha}} < +\infty, \quad \alpha \in (0,1], \tag{1.7}$$

$$|g|_{2\alpha} := \sup_{x>0} \frac{|g(x) - 1 + x|}{x^{2\alpha}} < +\infty, \quad \alpha \in (0,1]. \tag{1.8}$$

It is easily seen that (1.7) and (1.8) are in fact conditions at the neighborhood of zero. We set

$$m_f(x) := \sup_{y \in [x,\infty)} f(y), \quad x > 0. \tag{1.9}$$

Notice that the examples (1.4) satisfy condition (1.7) and $m_f(x) < 1$ for $x > 0$. The aim of this note is to prove the following statement:

Theorem 1.1 *Let A and B be non-negative self-adjoint operators and let $H := A \dot{+} B$ be their form sum. Assume that for some $\alpha \in (1/2, 1)$ the condition (1.6) is satisfied. Further, let f and g be Kato functions which obey conditions (1.7) and (1.8). If in addition one has $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$ and $m_f(x) < 1$ for $x > 0$, then for any finite interval $[0,T]$ there is a constant $C_{T,2\alpha-1} > 0$ such that*

$$\left\| \left(f(tA/2n) g(tB/n) f(tA/2n)\right)^n - e^{-tH} \right\| \leq C_{T,2\alpha-1} \frac{1}{n^{2\alpha-1}} \tag{1.10}$$

for $t \in [0,T]$ and $n = 1, 2, \ldots$.

The estimate (1.10) gives the ultimate error bound for the convergence rate, which can be seen from an example given in [17]. The formula (1.10) remains true with the same error bound, when $f(\tau A/2) g(\tau B) f(\tau A/2)$, where

$\tau = t/n$, is replaced by related families of the form $f(\tau A)^{1/2} g(\tau B) f(\tau A)^{1/2}$, $g(\tau B)^{1/2} f(\tau A) g(\tau B)^{1/2}$, $g(\tau B) f(\tau A)$, $f(\tau A) g(\tau B)$ and $g(\tau B/2) f(\tau A) g(\tau B/2)$, $\tau \geq 0$. We note further that Theorem 1.1 improves the previous result in [14] where the same optimal convergence rate $O(n^{-(2\alpha-1)})$ was obtained but under stronger conditions on the operators A and B and on the Kato functions f and g, for details see Section 7. Notice also that Theorem 1.1 is treating a case which is not covered by [11], [12]. Nevertheless, setting formally $\alpha = 1$ in Theorem 1.1 the assumptions and results of that theorem turn into those ones of [11], [12] except assumption $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$ which is superfluous there. In [8] it is conjectured that this condition can be dropped for $\alpha \in (1/2, 1]$. However, the proof of this conjecture remains still open. By the way condition $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$ implies $\mathrm{dom}(H^{1/2}) = \mathrm{dom}(A^{1/2})$ which guarantees the density of $\mathrm{dom}(H^{1/2})$ in $\mathcal{H}$.

The proof of Theorem 1.1 relies again on ideas of Chernoff [2], [3] and follows in many aspects [11], [12]. Theorem 2.2 in Section 2 can be regarded as operator-norm variant of Chernoff's approach, which, in contrast to [15], gives error-bound estimates. In particular, it generalizes a result of [11]. In Section 3 we prove some estimates which are necessary in the following using results from [11]. The main theorem announced in the introduction is proved in Section 4. In Section 5 we extend Theorem 1.1 to related families. In Section 6, an example is given which reflects the situation of our main theorem. Finally, in Section 7 we make some remarks on the obtained result.

2 Convergence theorem

We start with a lemma, which is proven using the standard Dunford-Taylor operator calculus.

Lemma 2.1 *Let K and L be non-negative self-adjoint operators on the Hilbert space $\mathcal{H}$. Then*

$$\|e^{-K} - e^{-L}\| \leq N \|(I+K)^{-1} - (I+L)^{-1}\| \tag{2.1}$$

with a constant $N > 0$ independent of operators K and L.

Proof. By the Dunford-Taylor representation for exponentials we find

$$e^{-K} - e^{-L} = \frac{1}{2\pi i} \int_\Gamma dz\, e^{-z} \left((z-K)^{-1} - (z-L)^{-1}\right), \tag{2.2}$$

where the contour Γ is given by $\Gamma = \Gamma_0 \cup \Gamma_\infty$ with

$$\begin{aligned} \Gamma_0 &= \{z \in \mathbb{C} : z = e^{i\varphi}, \quad \pi/4 \leq \varphi \leq 2\pi - \pi/4\}, \\ \Gamma_\infty &= \{z \in \mathbb{C} : z = re^{\pm i\pi/4}, \quad r \geq 1\}. \end{aligned} \tag{2.3}$$

From (2.2) we find the representation

$$\begin{aligned} e^{-K} - e^{-L} = \frac{1}{2\pi i} \int_\Gamma dz\, e^{-z} (I+K)(z-K)^{-1} \cdot \\ \cdot \left((I+L)^{-1} - (I+K)^{-1}\right)(I+L)(z-L)^{-1}. \end{aligned} \tag{2.4}$$

Since

$$(I+K)(z-K)^{-1} = -I + (1+z)(z-K)^{-1} \tag{2.5}$$

one gets the estimate

$$\left\|(I+K)(z-K)^{-1}\right\| \leq 1 + \frac{1+|z|}{\operatorname{dist}(z,\mathbb{R}_+)}. \tag{2.6}$$

Setting

$$N_\Gamma := \sup_{z\in\Gamma} \frac{1+|z|}{\operatorname{dist}(z,\mathbb{R}_+)} < \infty \tag{2.7}$$

we find

$$\sup_{z\in\Gamma} \left\|(I+K)(z-K)^{-1}\right\| \leq (1+N_\Gamma), \tag{2.8}$$

where the constant N_Γ depends only on Γ but not on the operator K. From (2.8) one also gets

$$\sup_{z\in\Gamma} \left\|(I+L)(z-L)^{-1}\right\| \leq (1+N_\Gamma). \tag{2.9}$$

Using these estimates, we find from (2.4) that

$$\left\|e^{-K} - e^{-L}\right\| \leq N \left\|(I+K)^{-1} - (I+L)^{-1}\right\| \tag{2.10}$$

with a constant

$$N := \frac{1}{2\pi}(1+N_\Gamma)^2 \int_\Gamma |dz|\, |e^{-z}| \tag{2.11}$$

depending only on the contour Γ. □

To prove the main theorem we shall use, as in [11] and [12], an operator norm version of Chernoff's theorem with error bound, which partly improves Lemma 2.1 of [11] in the case $\varrho < 1$.

Theorem 2.2 *Let $\{F(\tau)\}_{\tau\geq 0}$ be a family of non-negative self-adjoint contractions on $\mathcal{H}$ such that $F(0) = I$ and let*

$$S(\tau) := \frac{I - F(\tau)}{\tau}, \quad \tau > 0. \tag{2.12}$$

Assume $\varrho \in (0,1)$. Then there is a constant $M_\varrho > 0$ such that

$$\|(I + tS(\tau))^{-1} - (I+tH)^{-1}\| \leq M_\varrho \left(\frac{\tau}{t}\right)^\varrho \tag{2.13}$$

holds for $\tau, t \in (0,1]$ with $0 < \tau \leq t$, if and only if there is a constant $C_\varrho > 0$ such that

$$\|F(\tau)^{t/\tau} - e^{-tH}\| \leq C_\varrho \left(\frac{\tau}{t}\right)^\varrho \tag{2.14}$$

is valid for $\tau, t \in (0,1]$ with $0 < \tau \leq t$.

Proof. Assume (2.13). By Lemma 2.1 there is a constant $N > 0$ such that

$$\|e^{-tS(\tau)} - e^{-tH}\| \leq N\|(I + tS(\tau))^{-1} - (I + tH)^{-1}\| \tag{2.15}$$

for $\tau, t > 0$. Using (2.13) we obtain

$$\left\|e^{-tS(\tau)} - e^{-tH}\right\| \leq N\ M_\varrho \left(\frac{\tau}{t}\right)^\varrho \tag{2.16}$$

for $\tau, t \in (0, 1]$ with $0 < \tau \leq 1$. Since

$$\sup_{x\in[0,1]} \left|x^r - e^{-r(1-x)}\right| \leq \frac{1}{r}, \quad r \geq 1, \tag{2.17}$$

we find

$$\left\|F(\tau)^{t/\tau} - e^{-tS(\tau)}\right\| \leq \frac{\tau}{t} \tag{2.18}$$

for $\tau, t \in (0, 1]$ with $0 < \tau \leq t$. By

$$\left\|F(\tau)^{t/\tau} - e^{-tH}\right\| \leq \left\|F(\tau)^{t/\tau} - e^{-tS(\tau)}\right\| + \left\|e^{-tS(\tau)} - e^{-tH}\right\| \tag{2.19}$$

we finally get

$$\left\|F(\tau)^{t/\tau} - e^{-tH}\right\| \leq \frac{\tau}{t} + N\ M_\varrho \left(\frac{\tau}{t}\right)^\varrho \tag{2.20}$$

for $\tau, t \in (0, 1]$ with $0 < \tau \leq t$. Since $\frac{\tau}{t} \leq \left(\frac{\tau}{t}\right)^\varrho$ for $0 < \tau \leq t$, $\varrho \in [0, 1]$, we obtain

$$\left\|F(\tau)^{t/\tau} - e^{-tH}\right\| \leq (1 + N\ M_\varrho) \left(\frac{\tau}{t}\right)^\varrho \tag{2.21}$$

for $\tau, t \in (0, 1]$ with $0 < \tau \leq t$. Setting $C_\varrho := 1 + N\ M_\varrho$ we have verified (2.14).

To prove the converse we use the representation

$$(I + tS(\tau))^{-1} - (I + tH)^{-1} = \int_0^\infty dx\ e^{-x} \left(e^{-xtS(\tau)} - e^{-xtH}\right) \tag{2.22}$$

for $\tau, t > 0$. We have

$$(I + tS(\tau))^{-1} - (I + tH)^{-1} = \sum_{n=0}^\infty \int_n^{n+1} dx\ e^{-x} \left(e^{-xtS(\tau)} - e^{-xtH}\right) \tag{2.23}$$

for $\tau, t > 0$. By the substitution $x = y + n$ we obtain

$$\begin{aligned}&(I + tS(\tau))^{-1} - (I + tH)^{-1} = \\ &\qquad \sum_{n=0}^\infty e^{-n} \int_0^1 dy\ e^{-y} \left(e^{-(y+n)tS(\tau)} - e^{-(y+n)tH}\right)\end{aligned} \tag{2.24}$$

for $\tau, t > 0$. Since

$$\begin{aligned}&e^{-(y+n)tS(\tau)} - e^{-(y+n)tH} = \\ &\qquad \left(e^{-ntS(\tau)} - e^{-ntH}\right) e^{-ytS(\tau)} + e^{-ntH} \left(e^{-ytS(\tau)} - e^{-ytH}\right)\end{aligned} \tag{2.25}$$

and

$$e^{-ntS(\tau)} - e^{-ntH} = \sum_{k=0}^{n-1} e^{-ktS(\tau)} \left(e^{-tS(\tau)} - e^{-tH}\right) e^{-(n-k-1)tH} \tag{2.26}$$

we get

$$\begin{aligned} &(I + tS(\tau))^{-1} - (I + tH)^{-1} = \\ &\sum_{n=0}^{\infty} e^{-n} \left\{ \sum_{k=0}^{n-1} e^{-ktS(\tau)} \left(e^{-tS(\tau)} - e^{-tH}\right) e^{-(n-k-1)tH} \int_0^1 dy\, e^{-y}\, e^{-ytS(\tau)} + \right. \\ &\left. \int_0^1 dy\, e^{-y}\, e^{-ntH} \left(e^{-ytS(\tau)} - e^{-ytH}\right) \right\}. \end{aligned} \tag{2.27}$$

Hence we obtain the estimate

$$\begin{aligned} &\|(I + tS(\tau))^{-1} - (I + tH)^{-1}\| \le \\ &\quad \sum_{n=0}^{\infty} e^{-n} \left\{ n \left\| e^{-tS(\tau)} - e^{-tH} \right\| + \int_0^1 dy\, e^{-y} \left\| e^{-ytS(\tau)} - e^{-ytH} \right\| \right\} \end{aligned} \tag{2.28}$$

for $\tau, t > 0$. By assumption (2.14) we have the estimate

$$\left\| e^{-tS(\tau)} - e^{-tH} \right\| \le C_\varrho \left(\frac{\tau}{t}\right)^\varrho \tag{2.29}$$

for $\tau, t \in (0, 1]$ with $0 < \tau \le t$. Further, we use the decomposition

$$\begin{aligned} &\int_0^1 dy\, e^{-y} \left\| e^{-ytS(\tau)} - e^{-ytH} \right\| = \\ &\quad \int_{\tau/t}^1 dy\, e^{-y} \left\| e^{-ytS(\tau)} - e^{-ytH} \right\| + \int_0^{\tau/t} dy\, e^{-y} \left\| e^{-ytS(\tau)} - e^{-ytH} \right\| \end{aligned} \tag{2.30}$$

Setting $t' = yt$ one has $\tau \le t'$ if $\tau/t \le y$. Hence by assumption (2.14) we obtain

$$\left\| e^{-ytS(\tau)} - e^{-ytH} \right\| \le C_\varrho \left(\frac{\tau}{ty}\right)^\varrho \tag{2.31}$$

for $\tau, t, y \in (0, 1]$ and $\tau/t \le y$. This yields the estimate

$$\int_{\tau/t}^1 dy\, e^{-y} \left\| e^{-ytS(\tau)} - e^{-ytH} \right\| \le C_\varrho \int_0^1 dy\, e^{-y} y^{-\varrho} \left(\frac{\tau}{t}\right)^\varrho \tag{2.32}$$

for $\tau, t \in (0, 1]$ with $0 < \tau \le t$. For $\varrho < 1$ one obviously has

$$\int_0^{\tau/t} dy\, e^{-y} \left\| e^{-ytS(\tau)} - e^{-ytH} \right\| \le\ 2 \left(\frac{\tau}{t}\right)^\varrho \tag{2.33}$$

for $\tau, t \in [0,1]$ with $0 < \tau \leq t$. Taking into account (2.32) and (2.33) we obtain from (2.30) the estimate

$$\int_0^1 dy\, e^{-y} \left\|e^{-ytS(\tau)} - e^{-ytH}\right\| \leq \left(C_\varrho \int_0^1 dy\, e^{-y} y^{-\varrho} + 2\right) \left(\frac{\tau}{t}\right)^\varrho \tag{2.34}$$

for $\tau, t \in (0,1]$ with $0 < \tau \leq t$. Finally, using (2.29) and (2.34) we get from (2.28) the estimate

$$\begin{aligned} &\|(I+tS(\tau))^{-1} - (I+tH)^{-1}\| \leq \\ &\qquad \sum_{n=0}^{\infty} e^{-n} \left\{n\, C_\varrho + C_\varrho \int_0^1 dy\, e^{-y} y^{-\varrho} + 2\right\} \left(\frac{\tau}{t}\right)^\varrho \end{aligned} \tag{2.35}$$

for $\tau, t \in (0,1]$ with $0 < \tau \leq t$. Setting

$$M_\varrho := \sum_{n=0}^{\infty} e^{-n} \left\{n\, C_\varrho + C_\varrho \int_0^1 dy\, e^{-y} y^{-\varrho} + 2\right\} \tag{2.36}$$

we have verified (2.13). □

We note that in [11] it was shown that for $\varrho = 1$ condition (2.13) implies (2.14). It is unclear whether in this case the converse is also true. Note also that setting $\tau = t/n$, $n = 1, 2, \ldots$, the estimate (2.14) transforms into

$$\|F(t/n)^n - e^{-tH}\| \leq C_\varrho \frac{1}{n^\varrho} \tag{2.37}$$

for $t \in (0,1]$ and $n = 1, 2, \ldots$. However, this is nothing else but an operator norm estimate for a chosen family of contractions $F(\tau)$.

3 Auxiliary estimates

We are going to apply the Theorem 2.2 to the family

$$F(\tau) := f(\tau A/2) g(\tau B) f(\tau A/2), \quad \tau > 0. \tag{3.1}$$

In the following we use notations which essentially go back to [11] and [12] but which are slightly modified. We set

$$A_\tau := \frac{I - f(\tau A)}{\tau}, \qquad \tau > 0, \tag{3.2}$$

$$B_\tau := \frac{I - g(\tau B)}{\tau}, \qquad \tau > 0, \tag{3.3}$$

$$K_\tau := B_\tau + A_{\tau/2} - \frac{\tau}{4} A_{\tau/2}^2, \qquad \tau > 0. \tag{3.4}$$

One has $K_\tau \geq 0$ and

$$S(\tau) = K_\tau + \frac{\tau^2}{4} A_{\tau/2} B_\tau A_{\tau/2} - \frac{\tau}{2}\left(B_\tau A_{\tau/2} + A_{\tau/2} B_\tau\right) \tag{3.5}$$

for $\tau > 0$. We set

$$Q_\tau := \frac{\tau^2}{4}(I+K_\tau)^{-1/2}A_{\tau/2}B_\tau A_{\tau/2}(I+K_\tau)^{-1/2} - \tag{3.6}$$
$$\frac{\tau}{2}(I+K_\tau)^{-1/2}\left(B_\tau A_{\tau/2} + A_{\tau/2}B_\tau\right)(I+K_\tau)^{-1/2}, \quad \tau > 0,$$

so that

$$I + S(\tau) = (I+K_\tau)^{1/2}(I+Q_\tau)(I+K_\tau)^{1/2}, \quad \tau > 0.$$

Our next aim is to prove several estimates which we need for the proof of the main theorem.

Lemma 3.1 *Let A and B be non-negative self-adjoint operators. If f and g are Kato functions, then one has*

$$\left\|B_\tau^{1/2}(I+K_\tau)^{-1/2}\right\| \le \left\|(I+B_\tau)^{1/2}(I+K_\tau)^{-1/2}\right\| \le 1 \tag{3.7}$$

and

$$\left\|A_{\tau/2}^{1/2}(I+K_\tau)^{-1/2}\right\| \le \sqrt{2}\left\|\left(I + \frac{1}{2}A_{\tau/2}\right)^{1/2}(I+K_\tau)^{-1/2}\right\| \le \sqrt{2} \tag{3.8}$$

for $\tau > 0$. Moreover, the operator $I + Q_\tau$ is boundedly invertible for each $\tau > 0$ and the norm of its inverse operator is uniformly estimated by

$$\left\|(I+Q_\tau)^{-1}\right\| \le \frac{1}{2}\left(3+\sqrt{5}\right) \tag{3.9}$$

for $\tau > 0$.

Proof. The proof can be obtained from [11] by making the replacements $A \leftrightarrow B$ and $f \leftrightarrow g$. □

Lemma 3.2 *Let A and B be non-negative self-adjoint operators. If f and g are Kato functions and $m_f(x) < 1$ for $x > 0$, then there are constants $C_A > 0$ and $C_0 > 0$ such that*

$$\|(I+S(\tau))^{-1/2}u\| \le C_A \left\|(I+A)^{-1/2}u\right\| + C_0\,\|u\|\,\tau^{1/2} \tag{3.10}$$

for $u \in \mathcal{H}$ and $\tau > 0$.

Proof. Using Lemma 3.1 we get

$$\|(I+S(\tau))^{-1/2}u\| \le \sqrt{\frac{3+\sqrt{5}}{2}}\left\|(I+K_\tau)^{-1/2}u\right\| \tag{3.11}$$

for $u \in \mathcal{H}$ and $\tau > 0$. Since $K_\tau \ge \frac{1}{2}A_{\tau/2}$ we find

$$\|(I+S(\tau))^{-1/2}u\| \le \sqrt{3+\sqrt{5}}\left\|(I+A_{\tau/2})^{-1/2}u\right\| \tag{3.12}$$

for $u \in \mathcal{H}$ and $\tau > 0$. Obviously, there is a constant $\delta > 0$ such that $\left|(1 - f(x))x^{-1} - 1\right| > 1/2$ for $x \in (0, \delta)$. Hence

$$1 - f(x) \geq \frac{1}{2} x \tag{3.13}$$

for $x \in (0, \delta)$, which yields

$$1 - f(x) \geq \frac{1}{2} x \, \chi_{(0,\delta)}(x) + (1 - m_f(\delta)) \, \chi_{[\delta,\infty)}(x) \tag{3.14}$$

for $x > 0$, where $\chi_{(0,\delta)}(\cdot)$ and $\chi_{[\delta,\infty)}(\cdot)$ are the characteristic functions of the intervals $(0, \delta)$ and $[\delta, \infty)$, respectively. Hence we find

$$A_{\tau/2} \geq \frac{1}{2} A \, E_A([0, 2\delta/\tau)) + 2\frac{1 - m_f(\delta)}{\tau} \, E_A([2\delta/\tau, \infty)) \tag{3.15}$$

for $\tau > 0$, where $E_A(\cdot)$ is the spectral measure of A. Therefore we obtain

$$\begin{aligned} &\|(I + S(\tau))^{-1/2} u\| \leq \\ &\quad \sqrt{2(3 + \sqrt{5})} \left\|(I + A)^{-1/2} E_A([0, 2\delta/\tau)) u\right\| + \\ &\quad \sqrt{\frac{3 + \sqrt{5}}{2(1 - m_f(\delta))}} \, \|E_A([2\delta/\tau, \infty)) u\| \; \tau^{1/2} \end{aligned} \tag{3.16}$$

for $u \in \mathcal{H}$ and $\tau > 0$. Setting $C_A := \sqrt{2(3 + \sqrt{5})}$ and $C_0 := \sqrt{\frac{3+\sqrt{5}}{2(1-m_f(\delta))}}$ we prove (3.10). $\square$

Lemma 3.3 *Let A and B be non-negative self-adjoint operators such that their form sum obeys (1.6) for some $\alpha \in (1/2, 1)$. Further, let f and g be Kato functions which satisfy (1.7) and (1.8).*

(i) If $p, q \in [0, \alpha]$ and $p + q \geq 1$, then there is a constant $D_{p,q} > 0$ such that

$$\|(I + H)^{-p}(H - S(\tau))(I + H)^{-q}\| \leq D_{p,q} \, \tau^{p+q-1} \tag{3.17}$$

for $\tau > 0$.

(ii) There is a constant $D_\alpha > 0$ such that

$$\|S(\tau)(I + H)^{-\alpha}\| \leq D_\alpha \, \tau^{\alpha-1} \tag{3.18}$$

for $\tau > 0$.

Proof. (i) First we note that if $p \in [0, \alpha]$, then condition (1.6) implies $\mathrm{dom}(H^p) \subseteq \mathrm{dom}(A^p) \cap \mathrm{dom}(B^p)$. Hence $(I+A)^p(I+H)^{-p}$ and $(I+B)^p(I+H)^{-p}$ are bounded operators. Since

$$\begin{aligned} I - F(\tau) \;\; = \;\; & I - f(\tau A/2)^2 + (I - g(\tau B)) + \\ & (I - f(\tau A/2))(I - g(\tau B))(I - f(\tau A/2)) - \\ & (I - f(\tau A/2))(I - g(\tau B)) - (I - g(\tau B))(I - f(\tau A/2)) \, , \end{aligned} \tag{3.19}$$

we find

$$
\begin{aligned}
(I+H)^{-p}(H-S(\tau))(I+H)^{-q} = \qquad\qquad & \qquad\qquad\qquad\qquad\qquad\qquad (3.20)\\
(I+H)^{-p}\left(A-\frac{I-f(\tau A/2)^2}{\tau}\right)(I+H)^{-q} &+ \\
(I+H)^{-p}\left(B-\frac{I-g(\tau B)}{\tau}\right)(I+H)^{-q} &- \\
(I+H)^{-p}(I-f(\tau A/2))(I-g(\tau B))(I-f(\tau A/2))(I+H)^{-q}\ \tau^{-1} &+ \\
(I+H)^{-p}(I-f(\tau A/2))(I-g(\tau B))(I+H)^{-q}\ \tau^{-1} &+ \\
(I+H)^{-p}(I-g(\tau B))(I-f(\tau A/2))(I+H)^{-q}\ \tau^{-1} &,
\end{aligned}
$$

which gives the estimate

$$\|(I+H)^{-p}(H-S(\tau))(I+H)^{-q}\| \leq$$

$$\left\|(I+H)^{-p}\left(A-\frac{I-f(\tau A/2)^2}{\tau}\right)(I+H)^{-q}\right\| + \tag{3.21}$$

$$\left\|(I+H)^{-p}\left(B-\frac{I-g(\tau B)}{\tau}\right)(I+H)^{-q}\right\| + \tag{3.22}$$

$$\|(I-f(\tau A/2))(I+H)^{-p}\|\ \|(I-f(\tau A/2))(I+H)^{-q}\|\ \tau^{-1} + \tag{3.23}$$

$$\|(I-f(\tau A/2))(I+H)^{-p}\|\ \|(I-g(\tau B))(I+H)^{-q}\|\ \tau^{-1} + \tag{3.24}$$

$$\|(I-g(\tau B))(I+H)^{-p}\|\ \|(I-f(\tau A/2))(I+H)^{-q}\|\ \tau^{-1} \tag{3.25}$$

for $\tau > 0$. To estimate (3.21) we use

$$
\begin{aligned}
\left\|(I+H)^{-p}\left(A-\frac{I-f(\tau A/2)^2}{\tau}\right)(I+H)^{-q}\right\| \leq \qquad\qquad & \qquad (3.26)\\
\|(I+A)^p(I+H)^{-p}\|\ \|(I+A)^q(I+H)^{-q}\| \cdot & \\
\left\|(I+A)^{-p}\left(A-\frac{I-f(\tau A/2)^2}{\tau}\right)(I+A)^{-q}\right\| &
\end{aligned}
$$

and the functional calculus which yield

$$
\begin{aligned}
\left\|(I+H)^{-p}\left(A-\frac{I-f(\tau A/2)^2}{\tau}\right)(I+H)^{-q}\right\| \leq \qquad\qquad & \qquad (3.27)\\
\|(I+A)^p(I+H)^{-p}\|\ \|(I+A)^q(I+H)^{-q}\| \cdot & \\
\left\{|f|_{p+q}+\frac{1}{2}\gamma_f((p+q)/2)^2\right\}\ \tau^{p+q-1} &
\end{aligned}
$$

for $\tau > 0$, where

$$\gamma_h(r) := \sup_{x>0}\frac{1-h(x)}{x^r}, \quad r \in (0,1], \tag{3.28}$$

and h is a Kato function. Similarly, one estimates (3.22) to get

$$
\begin{aligned}
\left\|(I+H)^{-p}\left(B-\frac{I-g(\tau B)}{\tau}\right)(I+H)^{-q}\right\| \leq \qquad\qquad & \qquad (3.29)\\
\|(I+B)^p(I+H)^{-p}\|\ \|(I+B)^q(I+H)^{-q}\|\ |g|_{p+q}\ \tau^{p+q-1} &
\end{aligned}
$$

for $\tau > 0$. Since

$$\|(1-f(\tau A/2))(I+H)^{-r}\| \le 2^{-r}\|(I+A)^r(I+H)^{-r}\|\,\gamma_f(r)\,\tau^r \tag{3.30}$$

and

$$\|(I-g(\tau B))(I+H)^{-r}\| \le \|(I+B)^r(I+H)^{-r}\|\,\gamma_g(r)\,\tau^r \tag{3.31}$$

for $\tau > 0$ and $r \in (0,\alpha]$, we finally obtain the estimate

$$\begin{aligned}\|(I+H)^{-p}(H-S(\tau))(I+H)^{-q}\| \;\le\; & \|(I+A)^p(I+H)^{-p}\|\cdot \\ & \|(I+A)^q(I+H)^{-q}\|\left\{|f|_{p+q}+\frac{1}{2}\gamma_f((p+q)/2)^2\right\}\tau^{p+q-1}+ \\ & \|(I+B)^p(I+H)^{-p}\|\;\|(I+B)^q(I+H)^{-q}\|\;|g|_{p+q}\;\tau^{p+q-1}+ \\ & 2^{-(p+q)}\gamma_f(p)\gamma_f(q)\|(I+A)^p(I+H)^{-p}\|\;\|(I+A)^q(I+H)^{-q}\|\;\tau^{p+q-1}+ \\ & 2^{-p}\gamma_f(p)\gamma_g(q)\|(I+A)^p(I+H)^{-p}\|\;\|(I+B)^q(I+H)^{-q}\|\;\tau^{p+q-1}+ \\ & 2^{-q}\gamma_f(q)\gamma_g(p)\|(I+A)^q(I+H)^{-q}\|\;\|(I+B)^p(I+H)^{-p}\|\;\tau^{p+q-1}\end{aligned} \tag{3.32}$$

for $\tau > 0$. Setting

$$\begin{aligned}D_{p,q} := \;& \|(I+A)^p(I+H)^{-p}\|\cdot \\ & \|(I+A)^q(I+H)^{-q}\|\left\{|f|_{p+q}+\frac{1}{2}\gamma_f((p+q)/2)^2\right\}+ \\ & \|(I+B)^p(I+H)^{-p}\|\;\|(I+B)^q(I+H)^{-q}\|\;|g|_{p+q}+ \\ & 2^{-(p+q)}\gamma_f(p)\gamma_f(q)\|(I+A)^p(I+H)^{-p}\|\;\|(I+A)^q(I+H)^{-q}\|+ \\ & 2^{-p}\gamma_f(p)\gamma_g(q)\|(I+A)^p(I+H)^{-p}\|\;\|(I+B)^q(I+H)^{-q}\|+ \\ & 2^{-q}\gamma_f(q)\gamma_g(p)\|(I+A)^q(I+H)^{-q}\|\;\|(I+B)^p(I+H)^{-p}\|\end{aligned} \tag{3.33}$$

for $\tau > 0$ we prove the estimate (3.17).

(ii) Using the decomposition (3.19) we find the estimate

$$\begin{aligned}&\left\|S(\tau)(I+H)^{-\alpha}\right\| \le \\ &\quad 4\left\|(I-f(\tau A/2))(I+H)^{-\alpha}\right\|\;\tau^{-1}+\|(I-g(\tau B))(I+H)^{-\alpha}\|\;\tau^{-1}\end{aligned} \tag{3.34}$$

for $\tau > 0$. Taking into account (3.30) and (3.31) we obtain

$$\begin{aligned}&\left\|S(\tau)(I+H)^{-\alpha}\right\| \le \\ &\quad 2^{2-\alpha}\|(I+A)^\alpha(I+H)^{-\alpha}\|\;\gamma_f(\alpha)\;\tau^{\alpha-1}+ \\ &\quad \|(I+B)^\alpha(I+H)^{-\alpha}\|\;\gamma_g(\alpha)\;\tau^{\alpha-1}\end{aligned} \tag{3.35}$$

for $\tau > 0$. Setting

$$\begin{aligned}D_\alpha := \;& 2^{2-\alpha}\|(I+A)^\alpha(I+H)^{-\alpha}\|\;\gamma_f(\alpha) \\ & +\|(I+B)^\alpha(I+H)^{-\alpha}\|\;\gamma_g(\alpha)\end{aligned} \tag{3.36}$$

we prove (3.18) for $\tau > 0$. □

4 Error estimate

In order to prove the main theorem we need the following two lemmata.

Lemma 4.1 *Let A and B be non-negative self-adjoint operators such that for some $\alpha \in (1/2, 1)$ the condition (1.6) is satisfied. Further, let f and g be Kato functions which obey conditions (1.7) and (1.8). If in addition one has* $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$ *and $m_f(x) < 1$ for $x > 0$, then there is a constant $S_{\alpha-1/2} > 0$ such that*

$$t\|(I + tS(\tau))^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \leq S_{\alpha-1/2}\left(\frac{\tau}{t}\right)^{\alpha-1/2} \tag{4.1}$$

for $t, \tau \in (0, 1]$ with $0 < \tau \leq t$.

Proof. By the functional calculus one has

$$\begin{aligned} t\|(I + tS(\tau))^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \leq \\ t^{1/2}\|(I + S(\tau))^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \end{aligned} \tag{4.2}$$

for $t \in (0, 1]$ and $\tau > 0$. By Lemma 3.2 we find

$$\begin{aligned} t\|(I + tS(\tau))^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \leq \\ C_A\,\|(I + A)^{-1/2}(H - S(\tau))(I + tH)^{-1}\|\,t^{1/2} + \\ C_0\,\|(H - S(\tau))(I + tH)^{-1}\|\,\tau^{1/2}\,t^{1/2} \end{aligned} \tag{4.3}$$

for $t \in (0, 1]$ and $\tau > 0$. Since $\mathrm{dom}(H^{1/2}) = \mathrm{dom}(A^{1/2})$, we get

$$\begin{aligned} \|(I + A)^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \leq \\ \|(I + H)^{1/2}(I + A)^{-1/2}\|\,\|(I + H)^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \end{aligned} \tag{4.4}$$

for $t \in (0, 1]$ and $\tau > 0$. Using again the functional calculus we obtain

$$\begin{aligned} \|(I + A)^{-1/2}(H - S(\tau)(I + tH)^{-1}\| \leq \\ \|(I + H)^{1/2}(I + A)^{-1/2}\|\,\|(I + H)^{-1/2}(H - S(\tau))(I + H)^{-\alpha}\|\,t^{-\alpha} \end{aligned} \tag{4.5}$$

for $t \in (0, 1]$ and $\tau > 0$. By Lemma 3.3(i) there is a constant $D_{\frac{1}{2},\alpha} > 0$ such that

$$\begin{aligned} \|(I + A)^{-1/2}(H - S(\tau)(I + tH)^{-1}\| \leq \\ D_{\frac{1}{2},\alpha}\,\|(I + H)^{1/2}(I + A)^{-1/2}\|\,\tau^{\alpha-1/2}\,t^{-\alpha}, \end{aligned} \tag{4.6}$$

which yields

$$\begin{aligned} \|(I + A)^{-1/2}(H - S(\tau))(I + tH)^{-1}\|\,t^{1/2} \leq \\ D_{\frac{1}{2},\alpha}\,\|(I + H)^{1/2}(I + A)^{-1/2}\|\,\left(\frac{\tau}{t}\right)^{\alpha-1/2} \end{aligned} \tag{4.7}$$

for $t \in (0, 1]$ and $\tau > 0$.

To estimate the second term of the right hand side of (4.3) we use again the functional calculus to find that

$$\|(H - S(\tau))(I + tH)^{-1}\| \le \frac{1}{t} + \|S(\tau)(I + H)^{-\alpha}\|\, t^{-\alpha} \tag{4.8}$$

for $t \in (0,1]$ and $\tau > 0$. By virtue of Lemma 3.3(ii) there is a constant $D_\alpha > 0$ such that

$$\|S(\tau)(I + tH)^{-1}\| \le D_\alpha\, \tau^{\alpha-1}\, t^{-\alpha} \tag{4.9}$$

for $t \in (0,1]$ and $\tau > 0$, which yields

$$\|S(\tau)(I + tH)^{-1}\|\, \tau^{1/2}\, t^{1/2} \le D_\alpha\, \left(\frac{\tau}{t}\right)^{\alpha-1/2} \tag{4.10}$$

for $t \in (0,1]$ and $\tau > 0$. Hence we obtain

$$\|(H - S(\tau))(I + tH)^{-1}\|\, \tau^{1/2}\, t^{1/2} \le (1 + D_\alpha)\, \left(\frac{\tau}{t}\right)^{\alpha-1/2} \tag{4.11}$$

for $t, \tau \in (0,1]$ and $0 < \tau \le t$. Applying the estimates (4.7) and (4.10) we find from (4.3) that

$$\begin{aligned} & t\|(I + tS(\tau))^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \le \\ & \qquad \left\{C_A\, D_{\frac{1}{2},\alpha}\, \|(I + H)^{1/2}(I + A)^{-1/2}\| + C_0(1 + D_\alpha)\right\} \left(\frac{\tau}{t}\right)^{\alpha-1/2} \end{aligned} \tag{4.12}$$

for $t, \tau \in (0,1]$ with $0 < \tau \le t$. Setting

$$S_{\alpha-1/2} := C_A\, D_{\frac{1}{2},\alpha}\, \|(I + H)^{1/2}(I + A)^{-1/2}\| + C_0(1 + D_\alpha) \tag{4.13}$$

we get (4.1). □

Lemma 4.2 *Let A and B be non-negative self-adjoint operators such that for some $\alpha \in (1/2, 1)$ the condition (1.6) is satisfied. Further, let f and g be Kato functions which obey conditions (1.7) and (1.8). Then there is a constant $G_{2\alpha-1} > 0$ such that*

$$t\|(I + tH)^{-1}(H - S(\tau))(I + tH)^{-1}\| \le G_{2\alpha-1}\, \left(\frac{\tau}{t}\right)^{2\alpha-1} \tag{4.14}$$

for $t \in (0,1]$ and $\tau > 0$.

Proof. By the functional calculus we get

$$\begin{aligned} & t\|(I + tH)^{-\alpha}(H - S(\tau))(I + tH)^{-\alpha}\| \le \\ & \qquad \|(I + H)^{-\alpha}(H - S(\tau))(I + H)^{-\alpha}\|\, t^{-(2\alpha-1)} \end{aligned} \tag{4.15}$$

for $t \in (0,1]$ and $\tau > 0$. Applying Lemma 3.3 we find a constant $G_{2\alpha-1} > 0$ such that

$$t\|(I + tH)^{-\alpha}(H - S(\tau))(I + tH)^{-\alpha}\| \le G_{2\alpha-1}\, \left(\frac{\tau}{t}\right)^{2\alpha-1} \tag{4.16}$$

for $t \in (0,1]$ and $\tau > 0$, proving (4.14). $\square$

We are now going to prove the main theorem mentioned in the Introduction.

Proof of Theorem 1.1. By the resolvent identities

$$\begin{aligned}(I+tS(\tau))^{-1}-(I+tH)^{-1} &= t\,(I+tS(\tau))^{-1}(H-S(\tau))(I+tH)^{-1}\\ &= t\,(I+tH)^{-1}(H-S(\tau))(I+tS(\tau))^{-1}\end{aligned}$$

one gets

$$\begin{aligned}(I+tS(\tau))^{-1}-(I+tH)^{-1} = t(I+tH)^{-1}(H-S(\tau))(I+tH)^{-1}+\\ t^2(I+tH)^{-1}(H-S(\tau))(I+tS(\tau))^{-1}(H-S(\tau))(I+tH)^{-1}\end{aligned} \tag{4.17}$$

for $\tau, t > 0$. Hence we find the estimate

$$\begin{aligned}&\|(I+tS(\tau))^{-1}-(I+tH)^{-1}\| \le\\ &\quad t\|(I+tH)^{-1}(H-S(\tau))(I+tH)^{-1}\| +\\ &\quad t^2\|(I+tH)^{-1}(H-S(\tau))(I+tS(\tau))^{-1}(H-S(\tau))(I+tH)^{-1}\|\end{aligned} \tag{4.18}$$

for $\tau, t > 0$, which can be written as

$$\begin{aligned}&\|(I+tS(\tau))^{-1}-(I+tH)^{-1}\| \le\\ &\quad t\|(I+tH)^{-1}(H-S(\tau))(I+tH)^{-1}\| +\\ &\quad t^2\|(I+tS(\tau))^{-1/2}(H-S(\tau))(I+tH)^{-1}\|^2.\end{aligned} \tag{4.19}$$

Taking into account Lemma 4.1 and Lemma 4.2 we get

$$\|(I+tS(\tau))^{-1}-(I+tH)^{-1}\| \le G_{2\alpha-1}\left(\frac{\tau}{t}\right)^{2\alpha-1} + S^2_{\alpha-1/2}\left(\frac{\tau}{t}\right)^{2\alpha-1} \tag{4.20}$$

for $t, \tau \in (0,1]$ with $0 < \tau \le t$. Setting $M_{2\alpha-1} := G_{2\alpha-1} + S^2_{\alpha-1/2}$ one gets a constant such that the condition (2.13) holds for $\tau, t \in (0,1]$ with $0 < \tau \le t$. By Theorem 2.2 there is a constant $C_{2\alpha-1} > 0$ such (2.14) is valid for $\varrho = 2\alpha - 1$ and $\tau, t \in (0,1]$ and $0 < \tau \le t$. Setting $C_{1,2\alpha-1} := C_{2\alpha-1}$ and $\tau = t/n$, $n = 1, 2, \ldots$, we immediately verify (1.10) for $t \in [0,1]$.

To extend the result to $t \in [0,T]$, $0 < T < \infty$, we set $A_s := s\;A$ and $B_s := s\;B$ where $s > 0$. Obviously, one has $H_s := A_s \dot{+} B_s = s\;H$. If A and B are non-negative self-adjoint operators such that for some $\alpha \in (1/2, 1)$ condition (1.6) is satisfied, then, of course, one has $\mathrm{dom}(H_s^\alpha) \subseteq \mathrm{dom}(A_s^\alpha) \cap \mathrm{dom}(B_s^\alpha)$ for $s > 0$. Similarly, the condition $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$ implies $\mathrm{dom}(A_s^{1/2}) \subseteq \mathrm{dom}(B_s^{1/2})$ for $s > 0$. Hence, there is a constant $C_{2\alpha-1}(s) > 0$ such that

$$\left\|(f(tA_s/2n)g(tB_s/n)f(tA_s/2n))^n - e^{-tH_s}\right\| \le C_{2\alpha-1}(s)\frac{1}{n^{2\alpha-1}} \tag{4.21}$$

for $t \in [0,1]$ and $n = 1, 2, \ldots$, which yields

$$\left\|(f(tA/2n)g(tB/n)f(tA/2n))^n - e^{-tH}\right\| \le C_{2\alpha-1}(s)\frac{1}{n^{2\alpha-1}} \tag{4.22}$$

for $t \in [0,s]$ and $n = 1, 2, \ldots$. Choosing $s = T$ and setting $C_{T,2\alpha-1} := C_{2\alpha-1}(T)$ we get that for any finite interval $[0,T]$ there is a constant $C_{T,2\alpha-1} > 0$ such that (1.10) holds. $\square$

5 Related families

Let us show that the estimate (1.10) holds not only for the family $F(\tau) = f(\tau A/2)g(\tau B)f(\tau A/2)$ but also for the families

$$
\begin{aligned}
F_1(\tau) &:= f(\tau A)^{1/2} g(\tau B) f(\tau A)^{1/2}, && (5.1)\\
F_2(\tau) &:= g(\tau B)^{1/2} f(\tau A) g(\tau B)^{1/2}, && (5.2)\\
F_3(\tau) &:= g(\tau B) f(\tau A), && (5.3)\\
F_4(\tau) &:= f(\tau A) g(\tau B), && (5.4)\\
F_5(\tau) &:= g(\tau B/2) f(\tau A) g(\tau B/2), && (5.5)
\end{aligned}
$$

where $\tau \geq 0$. To this end we prove the following:

Lemma 5.1 *Let A and B be non-negative self-adjoint operators such that for some $\alpha \in (1/2, 1)$ the condition (1.6) is satisfied. Further, let f and g be Kato functions which obey (1.7) and (1.8). Then there is a constant $C_F > 0$ such that*

$$\left\|(I - F(t/n))e^{-tH}\right\| \leq C_F \frac{e^t}{n^\alpha} \tag{5.6}$$

for $t \geq 0$ and $n = 1, 2, \ldots$.

Proof. We use the representation

$$
\begin{aligned}
&(I - F(t/n))e^{-tH} = \qquad (5.7)\\
&\quad f(tA/2n)g(\tau B)(I - f(tA/2n))e^{-tH} + f(tA/2n)(I - g(tB/n))e^{-tH} + \\
&\quad (I - f(tA/2n))e^{-tH},
\end{aligned}
$$

which yields the estimate

$$
\begin{aligned}
&\|(I - F(t/n))e^{-tH}\| \leq \qquad (5.8)\\
&\qquad 2\|(I - f(tA/2n))e^{-tH}\| + \|(I - g(tB/n))e^{-tH}\|.
\end{aligned}
$$

Since

$$
\begin{aligned}
&(I - f(tA/2n))e^{-tH} = \qquad (5.9)\\
&\quad (I - f(tA/2n))(I + A)^{-\alpha}(I + A)^\alpha (I + H)^{-\alpha}(I + H)^\alpha e^{-(I+H)t} e^t ,
\end{aligned}
$$

we find the estimate

$$
\begin{aligned}
&\|(I - f(tA/2n))e^{-tH}\| \leq \qquad (5.10)\\
&\quad \|(I - f(tA/2n))(I + A)^{-\alpha}\| \, \|(I + A)^\alpha (I + H)^{-\alpha}\| \, \|(I + H)^\alpha e^{-(I+H)t}\| e^t.
\end{aligned}
$$

Since

$$
\begin{aligned}
&\|(I - f(tA/2n))(I + A)^{-\alpha}\| \leq \qquad (5.11)\\
&\quad \sup_{\lambda \geq 0} \frac{1 - f(t\lambda/2n)}{(1 + \lambda)^\alpha} \leq \sup_{\lambda > 0} \frac{1 - f(\lambda)}{\lambda^\alpha} \left(\frac{t}{2n}\right)^\alpha \leq \gamma_f(\alpha) \left(\frac{t}{2n}\right)^\alpha ,
\end{aligned}
$$

we obtain the estimate

$$\|(I - f(tA/2n))e^{-tH}\| \le 2^{-\alpha}\gamma_f(\alpha)b(\alpha)\|(I+A)^\alpha(I+H)^{-\alpha}\|\frac{e^t}{n^\alpha} \tag{5.12}$$

for $n = 1, 2, \ldots$, where $b(\alpha) := \sup_{\lambda>0} \lambda^\alpha e^{-\lambda}$. Similarly, we prove that

$$\|(I - g(tB/n))e^{-tH}\| \le \gamma_g(\alpha)b(\alpha)\|(I+B)^\alpha(I+H)^{-\alpha}\|\frac{e^t}{n^\alpha} \tag{5.13}$$

for $n = 1, 2, \ldots$. Setting

$$C_F := \tag{5.14}$$
$$2^{1-\alpha}\gamma_f(\alpha)b(\alpha)\|(I+A)^\alpha(I+H)^{-\alpha}\| + \gamma_g(\alpha)b(\alpha)\|(I+B)^\alpha(I+H)^{-\alpha}\|$$

one gets the estimate (5.6). □

Theorem 5.2 *Let A and B be non-negative self-adjoint operators such that for some $\alpha \in (1/2, 1)$ the condition (1.6) is satisfied. Further, let f and g be Kato functions which satisfy conditions (1.7) and (1.8). If in addition one has* $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$ *and $m_f(x) < 1$ for $x > 0$, then for any finite interval $[0, T]$ there are constants $C^{(j)}_{T,2\alpha-1} > 0$, $j = 1, 2, 3, 4, 5$, such that*

$$\left\|F_j(t/n)^n - e^{-tH}\right\| \le C^{(j)}_{T,2\alpha-1}\frac{1}{n^{2\alpha-1}}, \quad j = 1, 2, 3, 4, 5 \tag{5.15}$$

for $t \in [0, T]$ and $n = 1, 2, \ldots$.

Proof. We set

$$f_0(x) := f(2x)^{1/2}, \quad x \ge 0. \tag{5.16}$$

The function $f_0(x)$ is also a Kato function which satisfies $|f_0|_{2\alpha} < \infty$ and $m_{f_0}(x) < 1$ for $x > 0$. One has

$$f_0(\tau A/2) = f(\tau A)^{1/2}, \quad \tau \ge 0. \tag{5.17}$$

We set

$$F_0(\tau) := f_0(\tau A/2)g(\tau B)f_0(\tau A/2), \quad \tau \ge 0. \tag{5.18}$$

By Theorem 1.1 there is a constant $C^{(0)}_{T,2\alpha-1} > 0$ such that

$$\|F_0(t/n)^n - e^{-tH}\| \le C^{(0)}_{T,2\alpha-1}\frac{1}{n^{2\alpha-1}} \tag{5.19}$$

for $t \in [0, T]$ and $n = 1, 2, \ldots$. By (5.17) one has $F_0(\tau) = F_1(\tau)$ for $\tau \ge 0$, which proves the assertion for $j = 1$. We note that

$$F_4(\tau)^n = f(\tau A)^{1/2}F_1(\tau)^{n-1}f(\tau A)^{1/2}g(\tau B), \quad \tau \ge 0, \quad n = 1, 2, \ldots. \tag{5.20}$$

Using the representation

$$F_4(\tau)^n - e^{-tH} = \tag{5.21}$$
$$f(\tau A)^{1/2}\left(F_1(\tau)^{n-1}(I - F_1(\tau))\right) f(\tau A)^{1/2} g(\tau B) +$$
$$f(\tau A)^{1/2}\left(F_1(\tau)^{n} - e^{-tH}\right) f(\tau A)^{1/2} g(\tau B) +$$
$$\left(f(\tau A)^{1/2} - I\right) e^{-tH} f(\tau A)^{1/2} f(\tau A)^{1/2} g(\tau B) +$$
$$e^{-tH}\left(f(\tau A)^{1/2} - I\right) g(\tau B) + e^{-tH}\left(g(\tau B) - I\right)$$

where $\tau = t/n$, $t \geq 0$ and $n = 1, 2 \ldots$, we find the estimate

$$\|F_4(\tau)^n - e^{-tH}\| \leq \left\|F_1(\tau)^{n-1}(I - F_1(\tau)\right\| + \tag{5.22}$$
$$\left\|F_1(\tau)^n - e^{-tH}\right\| + 2\left\|(I - f(\tau A)^{1/2})e^{-tH}\right\| + \left\|(I - g(\tau B))e^{-tH}\right\|.$$

Since

$$\left\|(I - f(\tau A)^{1/2})e^{-tH}\right\| \leq \gamma_f(\alpha) b(\alpha) \|(I + A)^{\alpha}(I + H)^{-\alpha}\| \frac{e^t}{n^{\alpha}} \tag{5.23}$$

and

$$\left\|(I - g(\tau B)^{1/2})e^{-tH}\right\| \leq \gamma_g(\alpha) b(\alpha) \|(I + B)^{\alpha}(I + H)^{-\alpha}\| \frac{e^t}{n^{\alpha}} \tag{5.24}$$

as well as the estimate $\|F_1(\tau)^{n-1}(I - F_1(\tau)\| \leq \frac{1}{n}$, $n = 1, 2, \ldots$, we obtain from the statement for $j = 1$ the existence of a constant $C^{(4)}_{T,2\alpha-1} > 0$ such that (5.15) holds for $j = 4$, $t \in [0, T]$ and $n = 1, 2, \ldots$. Next, using

$$F_3(\tau)^n = g(\tau B) F_4(\tau)^{n-1} f(\tau A) \tag{5.25}$$

and

$$F_2(\tau)^n = g(\tau B)^{1/2} F_4(\tau)^{n-1} f(\tau A) g(\tau B)^{1/2} \tag{5.26}$$

$\tau \geq 0$, $n = 1, 2, \ldots$, as well as the estimates (5.23) and (5.24) one verifies (5.15) for $j = 2, 3$ in the same way as above. To prove the statement for $j = 5$ we introduce the function

$$g_0(x) := g(x/2)^2, \quad x \geq 0. \tag{5.27}$$

Then one gets $F_5(\tau) = g_0(\tau B)^{1/2} f(\tau A) g_0(\tau B)^{1/2}$ for $\tau \geq 0$. The function g_0 is again a Kato function which satisfies (1.8). Hence, applying here the result for $F_2(\tau)$ we prove the case $j = 5$. □

6 Example

Let $\mathcal{H} := L_2(\Omega)$ where Ω is a bounded domain in $\mathbb{R}^l$, $l = 1, 2, \ldots$, with boundary $\partial\Omega$ of C^{∞}-class. By A we denote the negative half Laplacian with Dirichlet boundary conditions on $L_2(\Omega)$, i.e $A = -\frac{1}{2}\Delta_D$. The domain is given by

$$\mathrm{dom}(A) := H^2_2(\Omega) \cap \overset{\circ}{H}{}^1_2(\Omega) \tag{6.1}$$

where $\overset{\circ}{H}{}_2^1(\Omega)$ is the closure of $C_0^\infty(\Omega)$ in the Lebesgue space $H_2^1(\Omega)$, cf. Definitions 4.2.1/1 and 4.2.1/2 of [18]. Using the space $H^2_{2,B_D}(\Omega)$,

$$H^2_{2,B_D}(\Omega) := \{u \in H_2^2(\Omega) : B_D u|_{\partial\Omega} = 0\}, \tag{6.2}$$

cf. Definition 4.3.3/2 of [18], where B_D is given by

$$B_D u := u|_{\partial\Omega} \tag{6.3}$$

for $u \in H_2^2(\Omega)$, we obtain

$$\mathrm{dom}(A) := H^2_{2,B_D}(\Omega). \tag{6.4}$$

Further, let B be the negative half Laplacian with Neumann boundary conditions, i.e $B := -\frac{1}{2}\Delta_N$. One has

$$\mathrm{dom}(B) := H^2_{2,B_N}(\Omega) \tag{6.5}$$

where

$$H^2_{2,B_N}(\Omega) := \{u \in H_2^2(\Omega) : B_N u|_{\partial\Omega} = 0\}, \tag{6.6}$$

cf. Definition 4.3.3/2 of [18]. The boundary operator B_N is given by

$$(B_N u)(x) = \frac{\partial}{\partial\nu(x)} u(x), \quad x \in \partial\Omega, \tag{6.7}$$

for $u \in H_2^2(\Omega)$ where $\nu(x)$ is the outer unit normal to the boundary $\partial\Omega$ at the point $x \in \partial\Omega$. Since $\mathrm{dom}(A^{1/2}) = \overset{\circ}{H}{}_2^1(\Omega)$ and $\mathrm{dom}(B^{1/2}) = H_2^1(\Omega)$ one gets

$$\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2}). \tag{6.8}$$

Hence

$$\mathrm{dom}(H^{1/2}) = \mathrm{dom}(A^{1/2}) \cap \mathrm{dom}(B^{1/2}) = \overset{\circ}{H}{}_2^1(\Omega). \tag{6.9}$$

and $H := A \dot{+} B = 2A = -\Delta_D$. Therefore $\mathrm{dom}(H^\alpha) = \mathrm{dom}(A^\alpha)$ for arbitrary $\alpha \in [0,1]$.

Now we are going to calculate the domains $\mathrm{dom}(A^\alpha)$ and $\mathrm{dom}(B^\alpha)$ for $\alpha \in (1/2, 1)$. By Theorem 1 and Theorem 2 of [4] and Theorem 8.1 of [5] (see also Theorem 4.3.3 of [18]) we find

$$\mathrm{dom}(A^\alpha) = H^{2\alpha}_{2,B_D}(\Omega), \quad \alpha \in (1/2, 1), \tag{6.10}$$

and

$$\mathrm{dom}(B^\alpha) = \begin{cases} H_2^{2\alpha}(\Omega), & \alpha \in (1/2, 3/4), \\ H^{2\alpha}_{2,B_N}(\Omega), & \alpha \in (3/4, 1). \end{cases} \tag{6.11}$$

Since $H^{2\alpha}_{2,B_D}(\Omega) \subseteq H_2^{2\alpha}(\Omega)$ one gets

$$\mathrm{dom}(H^\alpha) = \mathrm{dom}(A^\alpha) \subseteq \mathrm{dom}(B^\alpha) \tag{6.12}$$

for $\alpha \in (1/2, 3/4)$. Applying now Theorem 5.2 we find that

$$\left\| \left(e^{-t(-\Delta_D)/2n} e^{-t(-\Delta_N)/2n} \right)^n - e^{-t(-\Delta_D)} \right\| = O(n^{-\kappa}) \qquad (6.13)$$

for any $\kappa := 2\alpha - 1 < \kappa_0 := \frac{1}{2}$ $(\alpha < \frac{3}{4})$ uniformly in $t \in [0, T]$ as $n \to \infty$.

If $\alpha \in (3/4, 1)$, then

$$\begin{aligned} \mathrm{dom}(A^\alpha) \cap \mathrm{dom}(B^\alpha) = H^{2\alpha}_{2,\{B_D, B_N\}}(\Omega) := \\ \{u \in H^{2\alpha}_2(\Omega) : B_D u|_{\partial\Omega} = 0, B_N u|_{\partial\Omega} = 0\} \subseteq H^{2\alpha}_{2,B_D}(\Omega). \end{aligned}$$

which yields that $\mathrm{dom}(A^\alpha) \cap \mathrm{dom}(B^\alpha)$ is a proper subset of $\mathrm{dom}(H^\alpha)$ which does not allow to apply Theorem 5.2, either.

If $\alpha = 1$, then one gets that $\mathrm{dom}(A) \cap \mathrm{dom}(B)$ is a proper subset of $\mathrm{dom}(H)$ too which yields $H \neq A + B$. Therefore the results of [11] and [12] are not applicable.

Notice that in contrast to [14] and to examples given there, here we have given an example when the operator B^α is not small with respect to A^α for $\alpha \in (1/2, 3/4)$.

7 Remarks

Let us make the following remarks:

(i) By an example given in [17] the error bound estimate $O(n^{-(2\alpha-1)})$ in Theorem 1.1 and Theorem 5.2 cannot be improved, i.e. it is the *ultimate optimal* one.

(ii) This optimal error bound was already found in [14] see Theorem 5.3 and Theorem 5.5. Comparing with [14] the conditions on the operators A and B are relaxed here. There it was assumed that B^α is small with respect to A^α, i.e. $\mathrm{dom}(A^\alpha) \subseteq \mathrm{dom}(B^\alpha)$ and

$$||B^\alpha u|| \leq a||A^\alpha u|| + b||u||, \quad u \in \mathrm{dom}(A^\alpha), \qquad (7.1)$$

for some $\alpha \in (1/2, 1)$ and $a \in (0, 1)$, $b > 0$. This condition is reduced in the present paper to the mild subordination condition $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$, which (7.1) obviously implies. The yet open problem is to eliminate completely this subordination condition.

(iii) The conditions on the Kato functions f and g are essentially relaxed comparing with [14]. Indeed, in [14] the Kato functions f and g have to satisfy at zero a smoothness condition of the type $|f|_2, |g|_2 < \infty$ which is replaced here by $|f|_{2\alpha}, |g|_{2\alpha} < \infty$, $\alpha \in (1/2, 1)$. A behaviour at infinity like $f(x) \sim x^{-2\alpha}$ is also demanded there.

(iv) Theorem 1.1 shows that only relations between certain domains related to A, B and H are decisive for the *convergence rate* of the Trotter-Kato product formula.

(v) Theorem 1.1 holds for $\alpha \in (1/2, 1)$. The method of the proof does not allow to include the case $\alpha = 1$. However, this case was considered in [11] and [12]. It is remarkable that one does not need any subordination condition there.

(vi) For $\alpha = 1/2$ we cannot expect operator-norm convergence in general, see [17]. However, if there is a subordination such that the operator B is relatively compact with respect to A, then operator-norm convergence holds, see [15].

The first version of this result was announced in [8] with a sketch of a proof which relies on an operator-norm estimate proved by Birman and Solomyak in [1]. In the present paper we have improved this previous result, by removing some restrictive condition on the Kato functions f and g imposed there as well as by giving a different, simpler proof which does not make use of operator-norm inequalities à la Birman-Solomyak.

Acknowledgements

T.I. and H.N. are grateful to the Université de la Méditerranée and Centre de Physique Théorique-CNRS-Luminy, Marseille (France), for hospitality extended to them and financial support. H.N. and V.Z. thank Department of Mathematics, Faculty of Science, Kanazawa University, Kanazawa (Japan), for hospitality and for financial support extended to them during their visit there. T.I. is supported by the Japan Society of the Promotion of Science (Grand-in-Aid for Scientific Researches (B) No. 11440040, 13440044). We would like to thank Prof. D. Fujiwara and Prof. H. Triebel who helped us to clarify the relation of the domains of fractional powers of Dirichlet and Neumann Laplacians.

References

[1] M. S. Birman and M. Z. Solomyak, Estimates for the difference of fractional powers of self-adjoint operators in case of unbounded perturbations, *Zap. Nauchn. Semin. Leningr. Otd. Mat. Inst. Steklova* **178**(1989), 120-145 (Russian), translated in *J. Soviet Math.* **61** (1992), No. 2, 2018-2034.

[2] P. R. Chernoff, Note on product formulas for operator semigroups, *J. Funct. Anal.* **2**(1968), 238-242.

[3] P. R. Chernoff, Semigroup product formulas and addition of unbounded operators, *Bull. Amer. Math. Soc.* **76** (1970), 395-398.

[4] D. Fujiwara, Concrete characterization of the domains of fractional powers of some elliptic differential operators of the second order. *Proc. Japan Acad.* **43** (1967), 82-86.

[5] P. Grisvard, Caractérisation de quelques espaces d'interpolation. *Arch. Rational Mech. Anal.* **25** (1967), 40-63.

[6] T. Kato, On the Trotter-Lie product formula. *Proc. Japan Acad.* **50** (1974), 694-698.

[7] T. Kato, Trotter's product formula for an arbitrary pair of self-adjoint contraction semigroups. *Topics in Funct. Anal., Ad. Math. Suppl. Studies* Vol **3**, 185-195 (I.Gohberg and Mc.Kac, eds.). Acad. Press, New York, 1978.

[8] T. Ichinose, H. Neidhardt and V. A. Zagrebnov, Operator norm convergence of Trotter-Kato product formula. Proceedings of the International Conference on Functional Analysis. Kiev, 2001. To appear.

[9] T. Ichinose and Hideo Tamura, Error estimates in the operator norm for Trotter-Kato product formula, *Integr. Equ. Oper. Theory.* **27** (1997), 195-207.

[10] T. Ichinose and Hideo Tamura, Error estimate in operator norm of exponential product formulas for propagators of parabolic evolution equations, *Osaka J. Math.* **35** (1998), 751-770.

[11] T. Ichinose and Hideo Tamura, The norm convergence of the Trotter-Kato product formula with error bound. *Commun. Math. Phys.* **217** (2001), 489–502.

[12] T. Ichinose, Hideo Tamura, Hiroshi Tamura and V. A. Zagrebnov, Note on the paper "The norm convergence of the Trotter-Kato product formula with error bound" by Ichinose and Tamura. *Commun. Math. Phys.* **221** (2001), 499–510.

[13] H. Neidhardt and V. A. Zagrebnov, On error estimates for the Trotter-Kato product formula. *Lett. Math. Phys.* **44** (1998), 169-186.

[14] H. Neidhardt and V. A. Zagrebnov, Fractional powers of self-adjoint operators and Trotter-Kato product formula. *Intger. Equ. Oper. Theory.* **35** (1999), 209-231.

[15] H. Neidhardt and V. A. Zagrebnov, Trotter-Kato product formula and operator-norm convergence. *Commun. Math. Phys.* **205** (1999), 129-159.

[16] D. L. Rogava, Error bounds for the Trotter-type formulas for self-adjoint operators. *Funct. Anal. Application* **27** (1993), No. 3, 217-219.

[17] Hiroshi Tamura, A remark on operator-norm convergence of Trotter-Kato product formula. *Integr. Equ. Oper. Theory* **37** (2000), 350-356.

[18] H. Triebel, Interpolation theory. Function spaces. Differential operators. Deutscher Verlag des Wissenschaften, Berlin, 1978.