TROTTER-KATO PRODUCT FORMULA: SOME RECENT RESULTS

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Recently new results about the operator-norm and the trace-norm convergences of the Trotter-Kato product formulae with ultimate optimal error-bound estimates have been established. They concern the self-adjoint strongly continuous and Gibbs semigroups on Hilbert spaces. Explicit dependence of the rate of convergence on the generators domains is found.

1. Operator-Norm Convergence and Optimal Error Bound

1.1. *Operator-Norm Convergence*

Consider real-valued, Borel measurable functions f on $[0,\infty)$ satisfying

$$0 \leq f(s) \leq 1, \quad f(0) = 1, \quad f'(0) = -1. \tag{1}$$

Some examples of functions satisfying (1) are

$$f(s) = e^{-s}, \quad f(s) = (1 + k^{-1}s)^{-k}, \quad k > 0. \tag{2}$$

We are interested in those functions f which satisfy not only (1) but also that for every small $\varepsilon > 0$ there exists a positive constant $\delta = \delta(\varepsilon) < 1$ such that

$$f(s) \leq 1 - \delta(\varepsilon), \quad s \geq \varepsilon, \tag{3}$$

and that for some fixed constant κ with $1 < \kappa \leq 2$,

$$[f]_\kappa := \sup_{s>0} \frac{|f(s) - 1 + s|}{s^\kappa} < \infty. \tag{4}$$

A function $f(s)$ satisfying (1) has property (3), if it is non-increasing. Of course, the functions in (2) have properties (3) and (4). Condition (3) is necessary. For this account and some further remarks on conditions (3) and (4) we refer to [1] and [2].

The following theorem is proved by Ichinose-Tamura-Tamura-Zagrebnov in [2].

Theorem 1.1. *Let f and g be functions having properties (3) and (4) with $\kappa = 2$ as well as (1). If A and B are non-negative self-adjoint operators in a Hilbert space $\mathcal{H}$ with domains $dom(A)$ and $dom(B)$ such that the operator sum $C := A + B$ is self-adjoint on domain*

$dom(C) = dom(A) \cap dom(B)$, then the Trotter-Kato product formulae converge in operator norm with the error bound $O(n^{-1})$:

$$\|[g(tB/2n)f(tA/n)g(tB/2n)]^n - e^{-tC}\| = O(n^{-1}),$$
$$\|[f(tA/n)g(tB/n)]^n - e^{-tC}\| = O(n^{-1}), \quad n \to \infty. \tag{5}$$

The convergence is uniform on each compact t-interval in the half-line $[0, \infty)$. If the operator C is strictly positive, i.e. $C \geq \eta I$ for some constant $\eta > 0$, the convergence is uniform on the whole half-line $[0, \infty)$.

Taking in (2) the exponential functions $f(s) = g(s) = e^{-s}$, one gets the following operator-norm converging *symmetric* and *nonsymmetric* Trotter formulae :

Corollary 1.1. *For non-negative self-adjoint operators A and B whose operator sum $C := A + B$ is self-adjoint on $dom(C) = dom(A) \cap dom(B)$ we have*

$$\|(e^{-tB/2n}e^{-tA/n}e^{-tB/2n})^n - e^{-tC}\| = O(n^{-1}),$$
$$\|(e^{-tA/n}e^{-tB/n})^n - e^{-tC}\| = O(n^{-1}), \quad n \to \infty, \tag{6}$$

uniformly on each compact t-interval in $[0, \infty)$, and uniformly on $[0, \infty)$, if C is strictly positive.

In [2] it is also shown that Theorem 1.1 allows a generalization to the case, when $C := A_1 + \cdots + A_m$ is self-adjoint on $dom(C) = dom(A_1) \cap \cdots \cap dom(A_m)$.

1.2. *Optimality of the Error Bound*

Notice that the results of the paper [2] are wonderfully optimal in many respects.

Remark 1.1. One can *not* relax the self-adjointness of the sum $C := A + B$ to *essential* self-adjointness, since in this case there is an example of a couple of non-negative self-adjoint operators A and B such that

$$\liminf_{n\to\infty} \|(e^{-tA/n}e^{-tB/n})^n - e^{-tC}\| \geq D(t), \tag{7}$$

where $D(t)$ is positive and continuous function of $t > 0$. This example is due to [3].

Notice that in this case we still have the *strong* convergence of the Trotter product formula (see, e.g. [4]):

$$\lim_{n\to\infty} (e^{-tA/n}e^{-tB/n})^n u = e^{-t\tilde{C}}u, \tag{8}$$

for any $u \in \mathcal{H}$. Here $\tilde{C}$ is the closure of operator $C := A + B$ with domain $dom(C) = dom(A) \cap dom(B)$.

Remark 1.2. Let operators A and B verify the conditions of Theorem 1.1. If they do not commute, then it is easy to check that in the *nonsymmetric* case (see (6)) the error bound can not be improved. Hence, in this case the estimate $O(n^{-1})$ is *ultimate optimal.* It is much less evident for case of symmetric Trotter product formula (see (6)). One of the important result of the paper [2] is the construction of *a couple* of *unbounded* operators A and B verifying conditions of Corollary 1.1 such that

$$\|(e^{-tB/2n}e^{-tA/n}e^{-tB/2n})^n - e^{-tC}\| \geq L(t)n^{-1}, \tag{9}$$

where $L(t)$ is positive and continuous function of $t > 0$. This proves optimality of the error bound $O(n^{-1})$ in Theorem 1.1 (and Corollary 1.1) in the *symmetric* case.

Remark 1.3. We would like to warn the reader against the conclusion that for *any* two noncommutative operators A and B verifying conditions of Theorem 1.1 the error bound estimate $O(n^{-1})$ is the best possible for the *symmetric* Trotter-Kato product formula. Whereas for *nonsymmetric* case it is true.

Remark 1.4. The paper [2] covers the most of the known results concerning the operator-norm convergence of the Trotter-Kato product formula for self-adjoint semigroups. Moreover, this paper proves that $O(n^{-1})$ is optimal error bound estimate in the above sense. See discussion in [2].

2. Operator-Norm Convergence and Fractional Power of Self-Adjoint Generators

2.1. *Fractional Power and Convergence Rate*

The results of [2] show how decisive is the relation between operators A and B for the convergence of the product formula. A recent Ichinose-Neidhardt-Zagrebnov theorem [5] extends [6], where the problem of relation between domains of self-adjoint non-negative operators A and B and the bound on the convergence rate in the Trotter-Kato product formula was considered for the first time.

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

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

which is in turn a non-negative self-adjoint operator in $\mathcal{H}$. By definition $dom(H^{1/2}) = dom(A^{1/2}) \cap dom(B^{1/2})$. In [5] we assume that

$$dom(H^{\alpha}) \subseteq (dom(A^{\alpha}) \cap dom(B^{\alpha})), \tag{10}$$

for some $\alpha \in (1/2, 1)$. This assumption is *stronger* than $dom(H^{1/2}) \subseteq dom(A^{1/2}) \cap dom(B^{1/2})$, but *weaker* than the assumption $dom(H) \subseteq dom(A) \cap dom(B)$ used in [1] and [2]. Notice that comparing to our paper [6], in [5] we do not demand *smallness* of the operator B^{α} with respect to A^{α}. We assume that the Kato functions further fulfill the conditions similar to those of [2]:

$$[f]_{2\alpha} := \sup_{s>0} \frac{|f(s) - 1 + s|}{s^{2\alpha}} < +\infty, \quad \alpha \in (0, 1], \tag{11}$$

$$[g]_{2\alpha} := \sup_{s>0} \frac{|g(s) - 1 + s|}{s^{2\alpha}} < +\infty, \quad \alpha \in (0, 1]. \tag{12}$$

It is easily seen that (11) and (12) are in fact conditions at the neighborhood of zero. We set

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

Notice that the examples (2) satisfy condition (11) and $m_f(x) < 1$ for $x > 0$. Then the main statement of the [5] is the following

Theorem 2.1. *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 (10) is satisfied. Further, let f and g be Kato functions which obey conditions (11) and (12). If in addition one has $dom(A^{1/2}) \subseteq dom(B^{1/2})$ 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*

$$\left\|(f(tA/2n)g(tB/n)f(tA/2n))^n - e^{-tH}\right\| \leq C_{T,2\alpha-1}\frac{1}{n^{2\alpha-1}} \tag{13}$$

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

The estimate (13) gives the ultimate optimal error bound for the convergence rate, which can be seen from the example given in [3]. Theorem 2.1 improves our previous result [6], 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. Notice also that Theorem 2.1 treats a case which is not covered by [1], [2]. Nevertheless, setting formally $\alpha = 1$ in Theorem 2.1 the assumptions and results of that theorem turn into those ones of [1], [2] except that assumption $dom(A^{1/2}) \subseteq dom(B^{1/2})$ becomes *superfluous*. In [7] it is conjectured that this condition is *superfluous* not only for $\alpha = 1$ but also for $\alpha \in (1/2, 1)$. However, the proof of this conjecture remains still an open problem. Notice that condition $dom(A^{1/2}) \subseteq dom(B^{1/2})$ implies $dom(H^{1/2}) = dom(A^{1/2})$ which guarantees the density of $dom(H^{1/2})$ in $\mathcal{H}$. The proof of Theorem 2.1 relies on some ideas of Chernoff [8], [9] and of the Neidhardt-Zagrebnov paper [10]. In many aspects it follows the line of reasoning of [1] and [2].

Remark 2.1.

(i) By example given in [3] the error bound estimate $O(n^{-(2\alpha-1)})$ in Theorem 2.1 cannot be improved, i.e. it is the *ultimate optimal* one.

(ii) This optimal error bound was already found in [6]. In [6] it was assumed that B^α is *small* with respect to A^α, i.e. $dom(A^\alpha) \subseteq dom(B^\alpha)$ and

$$\|B^\alpha u\| \leq a\|A^\alpha u\| + b\|u\|, \quad u \in dom(A^\alpha), \tag{14}$$

for some $\alpha \in (1/2, 1)$ and $a \in (0, 1)$, $b > 0$. This condition is reluxed in [5] to the mild subordination condition $dom(A^{1/2}) \subseteq dom(B^{1/2})$, which is obviously implied by (14). The yet *open problem* is to eliminate completely this subordination condition.

(iii) The conditions on the Kato functions f and g in [5] are essentially relaxed compared to [6].

(iv) Theorem 2.1 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 2.1 holds for $\alpha \in (1/2, 1)$. The method of the proof does not allow one to include the case $\alpha = 1$. We considered it separately in [2]. It is remarkable that one does not need any *subordination* condition in this case.

(vi) For $\alpha = 1/2$ we cannot expect operator-norm convergence in general, see [3]. However, if there is a *subordination* such as, for example, operator B is relatively compact with respect to A, then operator-norm convergence holds, see [10].

2.2. *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 in $L_2(\Omega)$, i.e $A = -\frac{1}{2}\Delta_D$. The domain is given by $dom(A) := H_2^2(\Omega) \cap \overset{\circ}{H}{}_2^1(\Omega)$, where $\overset{\circ}{H}{}_2^1(\Omega)$ is the closure of $C_0^\infty(\Omega)$ in the Lebesgue space $H_2^1(\Omega)$. Using the space $H_{2,B_D}^2(\Omega)$,

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

where B_D is given by $B_D u := u|_{\partial\Omega}$ for $u \in H_2^2(\Omega)$, we obtain $dom(A) := H_{2,B_D}^2(\Omega)$.

Further, let B be the negative half Laplacian with Neumann boundary conditions, i.e., $B := -\frac{1}{2}\Delta_N$. One has $dom(B) := H_{2,B_N}^2(\Omega)$, where

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

The boundary operator B_N is given by $(B_N u)(x) = \frac{\partial}{\partial\nu(x)}u(x), \quad x \in \partial\Omega$, 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 $dom(A^{1/2}) = \overset{\circ}{H}{}_2^1(\Omega)$ and $dom(B^{1/2}) = H_2^1(\Omega)$, one gets $dom(A^{1/2}) \subseteq dom(B^{1/2})$. Hence

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

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

Now we calculate the domains $dom(A^\alpha)$ and $dom(B^\alpha)$ for $\alpha \in (1/2, 1)$. By [11] and [12] one finds : $dom(A^\alpha) = H_{2,B_D}^{2\alpha}(\Omega), \quad \alpha \in (1/2, 1)$, and

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

Since $H_{2,B_D}^{2\alpha}(\Omega) \subseteq H_2^{2\alpha}(\Omega)$, one gets $dom(H^\alpha) = dom(A^\alpha) \subseteq dom(B^\alpha)$ for $\alpha \in (1/2, 3/4)$. Applying now Theorem 2.1 we find that

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

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 $\alpha = 3/4$, then it does not hold that $dom(A^{3/4}) \subseteq dom(B^{3/4})$. Hence $dom(A^{3/4}) \cap dom(B^{3/4})$ is a proper subset of $dom(H^{3/4})$ which *does not* allow one to apply Theorem 2.1.

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

$$\begin{aligned} &dom(A^\alpha) \cap dom(B^\alpha) = \\ &H_{2,\{B_D,B_N\}}^{2\alpha}(\Omega) := \{u \in H_2^{2\alpha}(\Omega) : B_D u|_{\partial\Omega} = 0, B_N u|_{\partial\Omega} = 0\} \subseteq H_{2,B_D}^{2\alpha}(\Omega). \end{aligned}$$

This yields that $dom(A^\alpha) \cap dom(B^\alpha)$ is a proper subset of $dom(H^\alpha)$ which *does not* allow one to apply Theorem 2.1, either.

If $\alpha = 1$, then one gets that $dom(A) \cap dom(B)$ is a proper subset of $dom(H)$ too which yields $H \neq A + B$. Therefore the results of [2] are not applicable.

Notice that in contrast to [6] and to examples given there, here we have an example, when the operator B^α is *not small* with respect to A^α for $\alpha \in (1/2, 3/4)$.

3. Trotter Product Formula for Gibbs Semigroups

3.1. *Trace-Norm Convergence Rate*

Let $\mathcal{H}$ be a separable Hilbert space with $\mathcal{B}(\mathcal{H})$ the algebra of all bounded operators on $\mathcal{H}$. Let $\mathcal{C}_\infty(\mathcal{H})$ denote the ideal of compact operators in $\mathcal{B}(\mathcal{H})$. Then the eigenvalues $\{\lambda_k(|C|)\}_{k=1}^\infty$ of the compact self-adjoint operator $|C| = \sqrt{C^*C}$ are known as the singular values $\{s_k(C)\}_{k=1}^\infty$ of the operator C. We denote by $\mathcal{C}_p(\mathcal{H})$ $(1 \leq p < \infty)$ the ideals in $\mathcal{B}(\mathcal{H})$ consisting of all compact operators C such that

$$\sum_{k=1}^\infty s_k(C)^p < \infty.$$

Then each ideal $\mathcal{C}_p(\mathcal{H})$ is a Banach space with the norm:

$$\|C\|_p = \left(\sum_{k=1}^\infty s_k(C)^p\right)^{1/p}.$$

In particular the ideal $\mathcal{C}_1(\mathcal{H})$ is called the *trace-class*, with the trace-norm $\|C\|_1 = Tr|C|$.

Definition 3.1. A strongly continuous one-parameter semigroup $\{U_t\}_{t\geq 0}$ is called a Gibbs semigroup if $U_t \in \mathcal{C}_1(\mathcal{H})$ for any $t > 0$ (see e.g. [13]).

There are several results on the trace-norm convergence of the Trotter product formula for self-adjoint Gibbs semigroups, see e.g. [14]-[17]. A recent result by Zagrebnov [18] is related to the above optimal operator-norm convergence of the Trotter-Kato product formula.

Theorem 3.1. *Let A and B be non-negative self-adjoint operators such that :*
(i) the operator sum $C := A + B$ is self-adjoint on $dom(C) = dom(A) \cap dom(B)$;
(ii) either $e^{-\tau A} \in \mathcal{C}_1(\mathcal{H})$, or $e^{-\tau B} \in \mathcal{C}_1(\mathcal{H})$, for $\tau > 0$.
Then
(a) the Trotter product formula converge in the trace-norm with error bound $O(n^{-1})$:

$$\|(e^{-tA/n}e^{-tB/n})^n - e^{-tC}\|_1 = O(n^{-1}), \quad n \to \infty, \tag{15}$$

uniformly on each compact t-interval in $[0, \infty)$. Further, if C is strictly positive, then (15) holds uniformly on $[0, \infty)$;
(b) the error bound $O(n^{-1})$ is ultimate optimal.

The proof of the theorem is based on

Lemma 3.1. *Let A be a self-adjoint operator such that $e^{-tA} \in \mathcal{C}_1(\mathcal{H})$ for $t > 0$. Let B be generator of a contraction semigroup and let $\{e^{-tH}\}_{t>0}$ be a Gibbs semigroup with*

$\|e^{-tH}\| \leq 1$. *Let*

$$\epsilon(s,t) := \sup_{\frac{2s}{2s+1}t \leq \tau \leq \frac{2s}{2s-1}t} \left\| \left(e^{-\tau A/s} e^{-\tau B/s}\right)^s - e^{-\tau H} \right\|, \tag{16}$$

for $s \in \mathbb{N}$, $s > 1$ *and* $t > 0$. *Then for each* $t_0 > 0$ *there exist* $l(t_0)$ *and* $l'(t_0)$ *such that:*

$$\left\| \left(e^{-tA/n} e^{-tB/n}\right)^n - e^{-tH} \right\|_1 \leq l(t_0)\epsilon([n/2], t/2) + l'(t_0)\epsilon([(n+1)/2], t/2) \tag{17}$$

for all $n > 1$ *and* $t \geq t_0$,

see [17] and [19]. Now conditions of the Theorem 3.1 and the mini-max principle imply that the operator C is generator of the contracting Gibbs semigroup with $\left\|e^{-tC}\right\| \leq 1$ for $t > 0$. On the other hand, by Theorem 1.1 one gets that $\epsilon(s,t) = O(1/s)$ in (16). Then the conditions of Lemma 3.1 are verified for $C = H$ and $\epsilon(k_n, t/2) = O(1/n)$, $\epsilon(m_n, t/2) = O(1/n)$, where $k_n = [n/2]$ and $m_n = [(n+1)/2]$. This proves the assertion (a) of the Theorem 3.1.

3.2. *Optimality of the Error Bound*

Similar to Sec. 1.2 it is enough to produce two operators A and B such that one can find a *positive* $L_1(t)$ ensuring in (15) for $t > 0$ the lower estimate :

$$\|(e^{-tA/n} e^{-tB/n})^n - e^{-tC}\|_1 \geq L_1(t) n^{-1}. \tag{18}$$

To this end let $\mathcal{H}$ be *finite-dimensional*. Then by the Baker–Campbell–Hausdorff formula we have for small $|t|$

$$e^{-tA} e^{-tB} = \exp\left[-t(A+B) + \tfrac{t^2}{2}[A,B] - \tfrac{t^3}{6}[A-B, \tfrac{1}{2}[A,B]] + O_p(|t|^4)\right],$$

with $[A,B] = AB - BA$, where and below $O_p(|t|^k)$, for $k > 0$, means some bounded operator with norm of order $O(|t|^k)$. Then

$$N(t) := (e^{-tA} e^{-tB})^{1/t} = \exp\left[-(A+B) + \tfrac{t}{2}[A,B] + O_p(|t|^2)\right].$$

We understand $N(0) = e^{-(A+B)}$ and have

$$E_1(A;B) := \frac{d}{dt} N(t)|_{t=0} = \frac{1}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k!} \prod_{j=1}^{k} (A+B)^{j-1} [A,B] (A+B)^{k-j}, \tag{19}$$

of which the right-hand side is norm-convergent and can be a non-zero operator with bound $2^{-1}\|[A,B]\| e^{\|A+B\|}$, if A and B do not commute with each other. It follows that

$$N(t) = e^{-(A+B)} + tE_1(A;B) + O_p(t^2),$$

so that with $t = 1/n$

$$(e^{-A/n} e^{-B/n})^n = N(1/n)^n = e^{-(A+B)} + n^{-1} E_1(A;B) + O_p(n^{-2}). \tag{20}$$

Since for *finite-dimensional* Hilbert space $\mathcal{H}$ one has $\|\cdot\|_1 = \|\cdot\|$, the error bound $O(n^{-1})$ is optimal for *nonsymmetric* Trotter product formula for Gibbs semigroups.

Remark 3.1. The proof that the *symmetric* Trotter product formula converges in the trace-norm with error bound $O(n^{-1})$:

$$\|(e^{-tB/2n}e^{-tA/n}e^{-tB/2n})^n - e^{-tC}\|_1 = O(n^{-1}), \quad n \to \infty, \tag{21}$$

follows along the same line of reasoning as in the proof of assertion (a) of Theorem 3.1. The proof of existence of the couple of unbounded operators A and B such that one can find a *positive* $L_2(t)$ ensuring in (21) for $t > 0$ the lower estimate :

$$\|(e^{-tB/2n}e^{-tA/n}e^{-tB/2n})^n - e^{-tC}\|_1 \geq L_2(t)n^{-1}, \quad n \to \infty, \tag{22}$$

needs a more subtle reasoning based on the example [3].

Notice that Remark 1.3 about optimality is also valid in the case of *symmetric* Trotter product formula for Gibbs semigroups.

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