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On the norm convergence of the self-adjoint Trotter–Kato product formula with error bound

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Abstract. The norm convergence of the Trotter–Kato product formula with error bound is shown for the semigroup generated by that operator sum of two nonnegative self-adjoint operators A and B which is self-adjoint.

Keywords. Trotter product formula; Trotter–Kato product formula; norm convergence; self-adjoint operator; semigroup.

1. Introduction and result

It is well-known [23, 15; 19] that the Trotter–Kato product formula for the self-adjoint semigroup holds in strong operator topology. Namely, when A and B are nonnegative self-adjoint operators in a Hilbert space $\mathcal{H}$ with domains $D[A]$ and $D[B]$, then

$$\text{s-lim}_{n\to\infty}(\mathrm{e}^{-tB/2n}\mathrm{e}^{-tA/n}\mathrm{e}^{-tB/2n})^n = \text{s-lim}_{n\to\infty}(\mathrm{e}^{-tA/n}\mathrm{e}^{-tB/n})^n = \mathrm{e}^{-tC}, \tag{1.1}$$

if C is the form sum $A\dot{+}B$ which is self-adjoint, or, in particular, if the operator sum $A+B$ is essentially self-adjoint on $D[A]\cap D[B]$ with C its closure. The convergence is uniform on each compact t-interval in the closed half-line $[0,\infty)$.

The aim of this note is to elucidate some of the main ideas of our recent results on its operator-norm convergence with error bound. In [12] we have shown

Theorem 1.1. *If A and B are nonnegative self-adjoint operators in $\mathcal{H}$ with domains $D[A]$ and $D[B]$ and if their operator sum $C := A + B$ is self-adjoint on $D[C] = D[A]\cap D[B]$, then the product formula in operator norm holds with error bound*:

$$\begin{aligned}&\|(\mathrm{e}^{-tB/2n}\mathrm{e}^{-tA/n}\mathrm{e}^{-tB/2n})^n - \mathrm{e}^{-tC}\| = O(n^{-1/2}),\\ &\qquad\|(\mathrm{e}^{-tA/n}\mathrm{e}^{-tB/n})^n - \mathrm{e}^{-tC}\| = O(n^{-1/2}), \quad n\to\infty.\end{aligned} \tag{1.2}$$

The convergence is uniform on each compact t-interval in the open half-line $(0,\infty)$, and further, if C is strictly positive, uniform on the closed half-line $[T,\infty)$ for every fixed $T > 0$.

One of the typical examples of such a self-adjoint operator $C = A+B$ is the Schrödinger operator

$$H = -\frac{1}{2}\Delta + g|x|^{-1} + o|x|^2 + \frac{a}{12}|x|^{2000}$$

in $L^2(\mathbf{R}^3)$, where $g,\ o$ and a are nonnegative constants.

Remark 1.1. The first result of such a norm convergence of the Trotter–Kato product formula (1.1) was proved by Rogava [20] in the abstract case under an additional condition that B is A-bounded, with error bound $O(n^{-1/2}\log n)$. The next was by Helffer [5] for the Schrödinger operators $H = H_0 + V \equiv -\frac{1}{2}\Delta + V(x)$ with C^∞ nonnegative potentials $V(x)$, roughly speaking, growing at most of order $O(|x|^2)$ for large $|x|$ with error bound $O(n^{-1})$. Each of these two results is independent of the other.

Then under some stronger or more general conditions, several further results are obtained. As for the abstract case, a better error bound $O(n^{-1}\log n)$ than Rogava's is obtained by Ichinose–Tamura [11] (cf. [9]) when B is A^α-bounded for some $0 < \alpha < 1$, even though the $B = B(t)$ may be t-dependent, and by Neidhardt–Zagrebnov [16, 17] (cf. [18]) when B is A-bounded with relative bound less than 1. As for the Schrödinger operators, a different proof to Helffer's result was obtained by Dia–Schatzman [2]. Further, more general results were proved for continuous nonnegative potentials $V(x)$, roughly speaking, growing of order $O(|x|^\rho)$ for large $|x|$ with $\rho > 0$, together with error bounds dependent on the power ρ (for instance, of order $O(n^{-2/\rho})$, if $\rho \geq 2$), by Ichinose–Takanobu [6] (cf. [7]), Doumeki–Ichinose–Tamura [3], Ichinose–Tamura [10], Decombes–Dia [1] and others, although the primary purpose of most of these papers was to prove rather a norm estimate between the Kac transfer operator and its corresponding Schrödinger semigroup. The Schrödinger operators treated in [6] and [3] may even involve bounded magnetic fields $\nabla \times A(x) : H = H_0(A) + V \equiv \frac{1}{2}(-i\nabla - A(x))^2 + V(x)$. In [7] and [8] the relativistic Schrödinger operator was also dealt with.

It should be noted (see [4, 21]) that in all these cases of the Schrödinger operators the sum $H = H_0 + V$ (resp. $H = H_0(A) + V$) is self-adjoint on the domain $D[H] = D[H_0] \cap D[V]$ (resp. $D[H] = D[H_0(A)] \cap D[V]$).

Thus the present theorem not only extends Rogava's result, but can also extend and contain all the results mentioned above, inclusive of better error bounds in some cases.

Remark 1.2. Unless the sum $A + B$ is self-adjoint on $D[A] \cap D[B]$, the norm convergence of the Trotter–Kato product formula does not always hold, even though the sum is essentially self-adjoint there and B is A-form-bounded with relative bound less than 1. A counterexample is due to Hiroshi Tamura [22].

The theorem also holds with the exponential function e^{-s} replaced by real-valued, Borel measurable functions f and g on $[0, \infty)$ satisfying

$$0 \leq f(s) \leq 1, \;\; f(0) = 1, \;\; f'(0) = -1, \tag{1.3}$$

that for every small $\varepsilon > 0$ there exists a positive constant $\delta = \delta(\varepsilon) < 1$ such that

$$f(s) \leq 1 - \delta(\varepsilon), \quad s \geq \varepsilon, \tag{1.4}$$

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

$$[f]_\kappa := \sup_{s>0} s^{-\kappa}|f(s) - 1 + s| < \infty, \tag{1.5}$$

and the same for g. Of course, the functions $f(s) = \mathrm{e}^{-s}$ and $f(s) = (1 + k^{-1}s)^{-k}$ with $k > 0$ are examples of functions having these properties.

Theorem 1.3. *If* $3/2 \leq \kappa \leq 2$, *it holds in operator norm that*

$$\begin{aligned} &\|[g(tB/2n)f(tA/n)g(tB/2n)]^n - \mathrm{e}^{-tC}\| = O(n^{-1/2}), \\ &\qquad \|[f(tA/n)g(tB/n)]^n - \mathrm{e}^{-tC}\| = O(n^{-1/2}), \quad n \to \infty. \end{aligned} \tag{1.6}$$

2. Outline of proof

To prove the theorem, it is crucial to show the following operator-norm version of Chernoff's theorem with error bounds. The case without error bounds was noted by Neidhardt–Zagrebnov [18].

Lemma 2.1. *Let C be a nonnegative self-adjoint operator in a Hilbert space $\mathcal{H}$ and let $\{F(t)\}_{t\geq 0}$ be a family of self-adjoint operators with $0 \leq F(t) \leq 1$. Define $S_t = t^{-1}(1 - F(t))$. Then in the following two assertions, for $0 < \alpha \leq 1$,* (a) *implies* (b).

(a)

$$\|(1+S_t)^{-1} - (1+C)^{-1}\| = O(t^\alpha), \quad t \downarrow 0. \tag{2.1}$$

(b) *For any $\delta > 0$ with $0 < \delta \leq 1$,*

$$\|F(t/n)^n - \mathrm{e}^{-tC}\| = \delta^{-2} t^{-1+\alpha} \mathrm{e}^{\delta t} O(n^{-\alpha}), \quad n \to \infty, \tag{2.2}$$

for all $t > 0$.

Therefore, for $0 < \alpha < 1$ (resp. $\alpha = 1$), the convergence in (2.2) *is uniform on each compact t-interval in the open half line $(0, \infty)$ (resp. in the closed half line $[0, \infty)$).*

Moreover, if C is strictly positive, i.e. $C \geq \eta$ for some constant $\eta > 0$, the error bound on the right-hand side of (2.2) *can also be replaced by $(1 + 2/\eta)^2 t^{-1+\alpha} O(n^{-\alpha})$, so that, for $0 < \alpha < 1$ (resp. $\alpha = 1$), the convergence in* (2.2) *is uniform on the closed half line $[T, \infty)$ for every fixed $T > 0$ (resp. on the whole closed half line $[0, \infty)$).*

Sketch of Proof of Lemma 2.1. Put

$$F(t/n)^n - \mathrm{e}^{-tC} = (F(t/n)^n - \mathrm{e}^{-tS_{t/n}}) + (\mathrm{e}^{-tS_{t/n}} - \mathrm{e}^{-tC}).$$

For the first term on the right we have by the spectral theorem

$$\|F(t/n)^n - \mathrm{e}^{-tS_{t/n}}\| = \|F(t/n)^n - \mathrm{e}^{-n(1-F(t/n))}\| \leq \mathrm{e}^{-1} n^{-1},$$

because

$$0 \leq \mathrm{e}^{-n(1-\lambda)} - \lambda^n \leq \mathrm{e}^{-1}/n, \quad \text{for } 0 \leq \lambda \leq 1.$$

For the second term, we use

$$\begin{aligned}
&(1+S_\varepsilon)^{-1}[\mathrm{e}^{-t(\delta+S_\varepsilon)} - \mathrm{e}^{-t(\delta+C)}](1+C)^{-1} \\
&\quad = \int_0^t \mathrm{e}^{-(t-s)(\delta+S_\varepsilon)}[(1+S_\varepsilon)^{-1} - (1+C)^{-1}]\mathrm{e}^{-s(\delta+C)}\mathrm{d}s \\
&\quad = \int_0^{t/2} + \int_{t/2}^t,
\end{aligned}$$

where $0 < \delta \leq 1$ and $\varepsilon > 0$, to bound these two integrals on the right by $(\delta^2 t)^{-1} \mathrm{e}^{\delta t} O(\varepsilon^\alpha)$. Taking $\varepsilon = t/n$, we have

$$\|\mathrm{e}^{-tS_{t/n}} - \mathrm{e}^{-tC}\| \leq (\delta^2 t)^{-1} \mathrm{e}^{\delta t} O((t/n)^\alpha) = \delta^{-2} t^{-1+\alpha} \mathrm{e}^{\delta t} O(n^{-\alpha}).$$

This proves the lemma.

Sketch of Proof of Theorems 1.1. First note that since $C = A + B$ is itself self-adjoint and so a closed operator, by the closed graph theorem there exists a constant a such that

$$\|(1 + A)u\| + \|(1 + B)u\| \le a\|(1 + C)u\|, \quad u \in D[C] = D[A] \cap D[B]. \tag{2.3}$$

The proof of the theorem is divided into two cases: (a) the symmetric product case

$$F(t) = \mathrm{e}^{-tB/2}\mathrm{e}^{-tA}\mathrm{e}^{-B/2}, \tag{2.4}$$

and (b) the non-symmetric product case

$$G(t) = \mathrm{e}^{-tA}\mathrm{e}^{-tB}. \tag{2.5}$$

(a) In the symmetric case we put

$$S_t = t^{-1}(1 - F(t)) = t^{-1}(1 - \mathrm{e}^{-tB/2}\mathrm{e}^{-tA}\mathrm{e}^{-tB/2})$$

and use Lemma 2.1 to show that

$$\|(1 + S_t)^{-1} - (1 + C)^{-1}\| = O(t^{1/2}), \quad t \downarrow 0. \tag{2.6}$$

Put

$$A_t = t^{-1}(1 - \mathrm{e}^{-tA}), \quad B_t = t^{-1}(1 - \mathrm{e}^{-tB}), \quad C_t = t^{-1}(1 - \mathrm{e}^{-tC}).$$

We have

$$\begin{aligned} 1 + S_t &= 1 + A_t + B_{t/2} - \frac{t}{4}B_{t/2}^2 + \frac{t^2}{4}B_{t/2}A_tB_{t/2} - \frac{t}{2}(A_tB_{t/2} + B_{t/2}A_t) \\ &= K_t^{1/2}(1 + Q_t)K_t^{1/2}, \end{aligned}$$

where

$$\begin{aligned} K_t &= 1 + A_t + B_{t/2} - \frac{t}{4}B_{t/2}^2 \ge 1, \\ Q_t &= \frac{t^2}{4}K_t^{-1/2}B_{t/2}A_tB_{t/2}K_t^{-1/2} - \frac{t}{2}K_t^{-1/2}(A_tB_{t/2} + B_{t/2}A_t)K_t^{-1/2}. \end{aligned}$$

Then we can show that $(Q_tu, u) \ge -\frac{\sqrt{5}-1}{2}\|u\|^2$ for $u \in \mathcal{H}$, so that

$$\|(1 + Q_t)^{-1}\| \le 2/(3 - \sqrt{5}), \tag{2.7}$$

$$\|(1 + S_t)^{-1}K_t^{1/2}\| = \|K_t^{-1/2}(1 + Q_t)^{-1}\| \le 2/(3 - \sqrt{5}). \tag{2.8}$$

Then we have

$$\begin{aligned} &(1 + S_t)^{-1} - (1 + C)^{-1} \\ &\quad = (1 + S_t)^{-1}\Bigg[A + B - \left(A_t + B_{t/2} - \frac{t}{4}B_{t/2}(1 - tA_t)\right)B_{t/2} \\ &\qquad\qquad - \frac{t}{2}(A_tB_{t/2} + B_{t/2}A_t))\Bigg](1 + C)^{-1} \\ &\quad = (1 + S_t)^{-1}(A - A_t)(1 + C)^{-1} + (1 + S_t)^{-1}(B - B_{t/2})(1 + C)^{-1} \\ &\qquad + (1 + S_t)^{-1}\left[\frac{t}{4}B_{t/2}(1 - tA_t)B_{t/2} + \frac{t}{2}(A_tB_{t/2} + B_{t/2}A_t)\right](1 + C)^{-1} \\ &\quad \equiv R_1(t) + R_2(t) + R_3(t). \end{aligned} \tag{2.9}$$

We can show the bounds

$$\|R_i(t)\| \le cat^{1/2}, \quad i = 1, 2, 3, \tag{2.10}$$

with some constant $c > 0$.

Indeed, for $R_1(t)$, rewriting as

$$R_1(t) = [(1+S_t)^{-1}K_t^{1/2}][K_t^{-1/2}(1+A_t)^{1/2}] \\ \times [(1+A_t)^{-1/2} - (1+A_t)^{1/2}(1+A)^{-1}](1+A)(1+C)^{-1},$$

we have by (2.3) and (2.8) and the spectral theorem

$$\|R_1(t)\| \le \frac{2}{3-\sqrt{5}} a \|(1+A_t)^{-1/2} - (1+A_t)^{1/2}(1+A)^{-1}\| \le cat^{1/2}.$$

The proof for $R_2(t)$ is the same as for $R_1(t)$ above. We have to only replace $A_t,\ A$ and f by $B_{t/2},\ B$ and g, and note that

$$R_2(t) = [(1+S_t)^{-1}K_t^{1/2}]\left[K_t^{-1/2}\left(1+\frac{1}{2}B_{t/2}\right)^{1/2}\right] \\ \times \left[\left(1+\frac{1}{2}B_{t/2}\right)^{-1/2}(1+B_{t/2})^{1/2}\right] \\ \times [(1+B_{t/2})^{-1/2} - (1+B_{t/2})^{1/2}(1+B)^{-1}](1+B)(1+C)^{-1}.$$

For $R_3(t)$ we have

$$R_3(t) = \frac{\sqrt{2}}{4}t^{1/2}[(1+S_t)^{-1}K_t^{1/2}][K_t^{-1/2}B_{t/2}^{1/2}]\left[\left(\frac{t}{2}B_{t/2}\right)^{1/2}(1-tA_t)\right] \\ \times [B_{t/2}(1+B)^{-1}](1+B)(1+C)^{-1} \\ + \left(\frac{1}{2}t^{1/2}[(1+S_t)^{-1}K_t^{1/2}][K_t^{-1/2}A_t^{1/2}][(tA_t)^{1/2}B_{t/2}(1+B)^{-1}]\right. \\ \times (1+B)(1+C)^{-1} + \frac{\sqrt{2}}{2}t^{1/2}[(1+S_t)^{-1}K_t^{1/2}][K_t^{-1/2}B_{t/2}^{1/2}] \\ \left. \times \left[\left(\frac{t}{2}B_{t/2}\right)^{1/2}A_t(1+A)^{-1}\right](1+A)(1+C)^{-1}\right).$$

With

$$a_0 := \|A_t(1+A)^{-1}\| = \sup_{\lambda\ge 0}\frac{1-\mathrm{e}^{-\lambda}}{t(1+\lambda)} < \infty,$$
$$b_0 := \|B_{t/2}(1+B)^{-1}\| = \sup_{\lambda\ge 0}\frac{1-\mathrm{e}^{-t\lambda/2}}{t(1+\lambda)/2} < \infty, \tag{2.11}$$

it follows from (2.3) and (2.8) that

$$\begin{aligned}\|R_3(t)\| &\le \left[\frac{\sqrt{2}}{4}\frac{2\sqrt{2}}{3-\sqrt{5}}b_0 + \left(\frac{1}{2}\frac{2}{3-\sqrt{5}}b_0 + \frac{\sqrt{2}}{2}\frac{2\sqrt{2}}{3-\sqrt{5}}\right)a_0\right]at^{1/2}\\ &\le \frac{2}{3-\sqrt{5}}(a_0+b_0)at^{1/2}.\end{aligned}$$

(b) The non-symmetric case will follow from the symmetric case. We use the commutator argument to observe that

$$\begin{aligned}\|G(t/n)^n - F(t/n)^n\| &= \|(\mathrm{e}^{-tA/n}\mathrm{e}^{-tB/n})^n - (\mathrm{e}^{-tB/2n}\mathrm{e}^{-tA/n}\mathrm{e}^{-tB/2n})^n\|\\ &= O(1/n).\end{aligned}$$

This proves Theorem 1.1.

The proof of Theorem 1.2 will be done in the same way as with $F(t) = g(tB/2)f(tA)g(tB/2)$ and $G(t) = g(tB)f(tA)$.

3. The final result

In a recent preprint [14], we have shown that if $\kappa = 2$, then Theorem 1.2 holds with optimal error bound $O(n^{-1})$. Further, the convergence is uniform on each compact t-interval in the closed half-line $[0, \infty)$, and further, if C is strictly positive, uniform on the whole closed half-line $[0, \infty)$.

In fact, we can show (2.6) with error bound $O(t)$ in place of $O(t^{1/2})$. The idea of the proof is to simply iterate the resolvent equation of the first identity in (2.9) with the help of its adjoint form to get

$$\begin{aligned}&(1+S_t)^{-1} - (1+C)^{-1}\\ &= ((1+C)^{-1} + [(1+S_t)^{-1} - (1+C)^{-1}])(C-S_t)(1+C)^{-1}\\ &= (1+C)^{-1}(C-S_t)(1+C)^{-1} + [(C-S_t)(1+C)^{-1}]^*\\ &\qquad\qquad (1+S_t)^{-1}(C-S_t)(1+C)^{-1}\\ &\equiv R_1'(t) + R_2'(t).\end{aligned}$$

Then by the same arguments together with (2.8) we can show the bounds

$$\|R_i'(t)\| = O(t), \quad i = 1, 2,$$

noting that what is actually proved in §2 is

$$\|K_t^{-1/2}(C-S_t)(1+C)^{-1}\| = O(t^{1/2}).$$

It is here that we need $\kappa = 2$ in the general case $F(t) = g(tB/2)f(tA)g(tB/2)$ and $G(t) = g(tB)f(tA)$.

Therefore we can apply Lemma 2.1 with $\alpha = 1$. Thus it turns out that the product formula (1.2) in Theorem 1.1 holds, with ultimate error bound $O(n^{-1})$, properly extending and containing all the known previous related results.

Finally, we comment about optimality of the error bound $O(n^{-1})$. We know that if both A and B are bounded operators, then we have, in the symmetric product case (2.4),

$\|F(t/n)^n - e^{-tC}\| = O(n^{-2})$, while, in the non-symmetric product case (2.5), $\|G(t/n)^n - e^{-tC}\| = O(n^{-1})$. Also in the symmetric product case, we can give an example of two unbounded self-adjoint operators A and B whose operator sum $C = A + B$ is self-adjoint on $D[A] \cap D[B]$ such that $\|F(t/n)^n - e^{-tC}\| \geq L(t)n^{-1}$, with a positive continuous function $L(t)$ of $t > 0$ independent of n.

Part of the present results were also briefly announced in [13].

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