

Recent Results on the Selfadjoint Trotter–Kato Product Formula in Operator Norm with Open Problems*

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Abstract. The norm convergence of the Trotter–Kato product formula with optimal error bound is shown for the semigroup generated by those operator sum and form sum of two nonnegative selfadjoint operators A and B which are selfadjoint.

1. Introduction and Result

Let A and B be nonnegative selfadjoint operators in a Hilbert space $\mathcal{H}$ with domains $D[A]$ and $D[B]$. Consider their operator sum $A+B$ with domain $D[A] \cap D[B]$, and their form sum $A \dot{+} B$ with form domain $D[A^{1/2}] \cap D[B^{1/2}]$. We assume that $D[A^{1/2}] \cap D[B^{1/2}]$ is dense in $\mathcal{H}$. We denote this operator sum as well as the form sum by the same symbol C , i.e. $C := A + B$ and $C := A \dot{+} B$.

In a celebrated paper, Kato [K] proved for the form sum $C := A \dot{+} B$

$$s - \lim_{n \rightarrow \infty} (e^{-tB/2n} e^{-tA/n} e^{-tA/2n})^n = s - \lim_{n \rightarrow \infty} (e^{-tA/n} e^{-tA/n})^n = e^{-tC}, \quad (1.1)$$

in the strong operator topology, uniformly on each compact t -interval in $[0, \infty)$.

In this lecture, I will mainly talk about the following two results on the operator norm convergence of this formula, based on three joint works with Hideo Tamura [IT], with Hideo Tamura, Hiroshi Tamura and V. A. Zagrebnov [ITTZ], and with H. Neidhardt and V. A. Zagrebnov [INZ].

The result of this kind was first proved by Rogava [R], when $C = A + B$ is selfadjoint with $D[A] \subseteq D[B]$, with error bound $O(n^{-1/2} \log n)$, and by Helffer [H] for the Schrödinger operator $H = -\Delta + V(x)$ with nonnegative potential $V(x)$ satisfying $|\partial^\alpha V(x)| \leq C_\alpha$ for $|\alpha| \geq 2$, with error bound $O(n^{-1})$. Since then there have appeared

* Talk given at the Workshop on Harmonic Analysis and Nonlinear Partial Differential Equations, RIMS, Kyoto University, July 7–9, 2003.

many papers, which improve either of these two results (See e.g. references in [IT]). The results presented below extend and properly contain all the so far known results.

First consider the case of the operator sum $C = A + B$.

Theorem 1.1 [IT, ITTZ]. *If the operator sum $C = A + B$ is selfadjoint on their domain $D[A] \cap D[B]$, then it holds in operator norm that*

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

uniformly on each compact t -interval in $[0, \infty)$. The error bound $O(n^{-1})$ is optimal.

Unless the sum $A + B$ is selfadjoint 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 selfadjoint there and B is A -form-bounded with relative bound less than 1. A counterexample is constructed in [Ta].

Next we come to consider the case of the form sum $C = A \dot{+} B$, but this case does not hold in general, as we have just said above.

We need to assume some additional condition on A and B . Namely, we assume that for some γ with $\frac{1}{2} < \gamma < 1$,

$$D[C^\gamma] \subseteq D[A^\gamma] \cap D[B^\gamma]. \quad (1.3)$$

Theorem 1.2 [INZ]. *Let $C = A \dot{+} B$ be the form sum with the relation (1.3) among the fractional powers of A , B and C . Further assume that one of A and B is form-bounded with respect to the other, namely, $D[A^{1/2}] \subseteq D[B^{1/2}]$ or $D[B^{1/2}] \subseteq D[A^{1/2}]$. Then it holds in operator norm that*

$$\begin{aligned} \|(e^{-tB/2n} e^{-tA/n} e^{-tB/2n})^n - e^{-tC}\| &= O(n^{-(2\gamma-1)}), \\ \|(e^{-tA/n} e^{-tB/n})^n - e^{-tC}\| &= O(n^{-(2\gamma-1)}), \quad n \rightarrow \infty, \end{aligned} \quad (1.4)$$

uniformly on each compact t -interval in $[0, \infty)$. The error bound $O(n^{-(2\gamma-1)})$ is optimal.

Notice here that condition (1.3) excludes the case $\gamma = 1$, i.e. the case of Theorem 1.1, so that there is no overlap between Theorems 1.1 and 1.2.

Remarks. 1. These theorems hold with the exponential function e^{-x} for e^{-tA} and e^{-tB} replaced by the following two different more general real-valued functions f and g on $[0, \infty)$, which are Borel measurable and satisfy (i) that $0 \leq f(s) \leq 1$, $f(0) = 1$, $f'(0) = -1$, (ii) that for every small $\varepsilon > 0$ there exists a positive constant $\delta = \delta(\varepsilon) < 1$ such that $f(s) \leq 1 - \delta(\varepsilon)$, $s \geq \varepsilon$, and (iii) that $[f]_2 := \sup_{s>0} \frac{|f(s)-1+s|}{s^2} < \infty$.

Some examples of functions satisfying these conditions (i), (ii), (iii) are

$$f(s) = e^{-s}, \quad f(s) = (1 + k^{-1}s)^{-k}, \quad k > 0. \quad (1.5)$$

A function $f(s)$ satisfying (i) has property (ii), if it is non-increasing. Condition (ii) is necessary.

2. The symmetric product case of Theorem 1.2 is proved in [ITTZ] also for the operator sum $C := A_1 + \cdots + A_m$ of m nonnegative selfadjoint operators $A_1, \dots, A_m$.

3. We also mention the trace norm case will be derived from these theorems.

As a matter of fact, the Trotter–Kato product formula is a useful tool in quantum mechanics and statistical mechanics. For instance, Brascamp and Lieb [BL] studied the Prékopa–Leindler and Brunn–Minkowski theorems to log concave functions and derived as an application inequalities for the fundamental solution of the diffusion equation with a convex potential. There they are using the Trotter product formula. I should also like to mention it may be used to prove Cwikel–Lieb–Rozenblum estimate giving the asymptotic formula for the number of the negative eigenvalues of the Schrödinger operator [RS].

In [I 1] and its extended version [I 2], we have discussed some aspect of the convergence of the time-sliced approximation to Feynman path integral in imaginary time. For another review about our results on the subject, we also refer to [Z].

In Section 2, to prove the theorems, we describe the key lemmas without proof. Section 3 gives some typical examples for the two theorems. In Section 4 some open problems are presented.

2. How to Prove Theorems

To prove the theorems, we shall establish the following key lemmas, an operator-norm version of Chernoff's theorem with error bounds.

In these lemmas, let C be a nonnegative selfadjoint operator in a Hilbert space $\mathcal{H}$ and let $\{F(\tau)\}_{\tau \geq 0}$ be a family of selfadjoint operators with $0 \leq F(\tau) \leq 1$ with $F(0) = I$. Define for $\tau > 0$

$$S_\tau = \tau^{-1}(1 - F(\tau)). \quad (2.1)$$

Lemma 2.1 [IT]. *Let $0 < \alpha \leq 1$. If it holds that*

$$\|(1 + S_\tau)^{-1} - (1 + C)^{-1}\| \leq C_\alpha \tau^\alpha, \quad \tau \downarrow 0, \quad (2.2)$$

with a constant $C_\alpha > 0$, then it holds that, for any $\delta > 0$ with $0 < \delta \leq 1$,

$$\|F(t/n)^n - e^{-tC}\| \leq M_\alpha t^{-1+\alpha} e^{\delta t} n^{-\alpha}, \quad n \rightarrow \infty, \quad (2.3)$$

for all $t > 0$, with a constant $C_\alpha > 0$.

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 $[0, \infty)$).

Lemma 2.2 [INZ]. *Let $0 < \alpha < 1$. Then it holds that*

$$\|(1 + tS_\tau)^{-1} - (1 + tC)^{-1}\| \leq C_\alpha(\tau/t)^\alpha, \quad 0 < \tau \leq t < 1, \quad (2.4)$$

with a constant $C_\alpha > 0$, if and only if it holds that

$$\|F(\tau)^{t/\tau} - e^{-tC}\| \leq M_\alpha(\tau/t)^\alpha, \quad 0 < \tau \leq t < 1, \quad (2.5)$$

with a constant $M_\alpha > 0$.

Here note that, indeed, Lemma 2.2 is extending Lemma 2.1 for the case $0 < \alpha < 1$ until (2.2) and (2.3) become equivalent assertions, but says nothing for the case $\alpha = 1$.

For the proof of the theorems, take $F(\tau) := e^{-\tau B/2} e^{-\tau A} e^{-\tau B/2}$ and apply these key lemmas, then we get the symmetric product case in (1.2)/(1.4). The nonsymmetric product case follows from the symmetric one, because we can show $\|F(t/n)^n - G(t/n)^n\| = O(n^{-1})$, where $G(\tau) := e^{-\tau A} e^{-\tau B}$.

3. Examples

Example for Theorem 1.1 :

Consider the Schrödinger operator

$$C = -\frac{1}{2}(-i\nabla - A(x))^2 + \frac{k}{|x|} + \frac{y_o}{7}|x|^2 + \frac{t_o}{7}|x|^{2003} \quad (3.1)$$

in $L^2(\mathbf{R}^3)$ with magnetic fields $\nabla \times A(x)$ bounded, where k, y_o, t_o are nonnegative constants.

It is known that this C is selfadjoint in $L^2(\mathbf{R}^3)$. Theorem 1.1 applies with error bound $O(n^{-1})$.

Example for Theorem 1.2 :

Let Ω be a bounded domain in $\mathbf{R}^d$ with smooth boundary $\partial\Omega$. Let A and B be the Dirichlet Laplacian and Neumann Laplacian in Ω , respectively. Namely, put $A := -\frac{1}{2}\Delta_D$ with domain $D[A] = W^2(\Omega) \cap W_0^1(\Omega)$, and $B := -\frac{1}{2}\Delta_N$ with domain $D[B] = \{u \in W^2(\Omega); \frac{\partial}{\partial \nu} u|_{\partial\Omega} = 0\}$.

Then $D[A^{1/2}] = W_0^1(\Omega) \subseteq W^1(\Omega) = D[B^{1/2}]$, and hence

$$D[C^{1/2}] = D[A^{1/2}] \cap D[B^{1/2}] = D[A^{1/2}] = W_0^1(\Omega),$$

so that $C = A \dot{+} B$ becomes

$$-\Delta_D = (-\frac{1}{2}\Delta_D) \dot{+} (-\frac{1}{2}\Delta_N). \quad (3.2)$$

It is known ([F], [G]) that

$$\begin{aligned} D[A^\alpha] &= \{u \in W^{2\alpha}(\Omega); u|_{\partial\Omega} = 0\}, \quad \frac{1}{2} < \alpha < 1; \\ D[B^\alpha] &= \begin{cases} W^{2\alpha}(\Omega), & \frac{1}{2} < \alpha < \frac{3}{4}, \\ \{u \in W^{2\alpha}(\Omega); \frac{\partial}{\partial \nu} u|_{\partial\Omega} = 0\}, & \frac{3}{4} < \alpha < 1. \end{cases} \end{aligned}$$

Consequently, for $\frac{1}{2} < \alpha < \frac{3}{4}$,

$$D[C^\alpha] = D[A^\alpha] \subseteq D[B^\alpha].$$

Thus by Theorem 1.2, we have for every $\kappa := 2\alpha - 1 < \kappa_0 := \frac{1}{2}$ ($\alpha = \frac{3}{4}$),

$$\| [e^{t\Delta_D/2n} e^{t\Delta_N/2n}]^n - e^{t\Delta_D} \| = O(n^{-\kappa}), \quad (3.3)$$

uniformly on each compact t -interval in $[0, \infty)$ as $n \rightarrow \infty$.

However, for $\frac{3}{4} \leq \alpha \leq 1$, Theorem 1.2 does not apply.

4. Some Open Problems.

1. Theorem 1.1 is a final result in a sense, but Theorem 1.2 not yet, for its statement is not symmetric with respect to two selfadjoint operators A and B . Namely, so as to make it symmetric, can we not remove the condition that “one of A and B is form-bounded with respect to the other, i.e. $D[A^{1/2}] \subseteq D[B^{1/2}]$ or $D[B^{1/2}] \subseteq D[A^{1/2}]$ ” ?

In other words, can we not prove Theorem 1.2 without this condition ?

2. How about the case where one of A and B is not bounded below, though we are assuming the sum $C = A + B$ in a form sense is bounded below ?

3. Doesn't the pointwise convergence of the integral kernels hold in Theorems 1.1 and 1.2 or don't the theorems imply it, when these semigroups have their integral kernels ?

4. How about the case where one of A and B is m -accretive ?

5. How about the nonlinear analogue ? Note that in the strong operator topology case, Kato and Masuda [KM] extended Kato's result [K] to the nonlinear semigroups with subdifferential generators.

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