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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 $C := A\dot{+}B$

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

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 convergnce 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 $|\partial^\alpha V(x)| \le C_\alpha$ for $|\alpha| \ge 2$, with error bound $O(n^{-1})$. Since then there have appeared

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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*

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

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 assme that for some γ with $\frac{1}{2} < \gamma < 1$,

$$D[C^\gamma] \subseteq D[A^\gamma] \cap D[B^\gamma]. \tag{1.3}$$

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*

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

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 $0 \le f(s) \le 1$, $f(0) = 1$, $f'(0) = -1$, (ii) that for every small $\varepsilon > 0$ there exists a positive constant $\delta = \delta(\varepsilon) < 1$ such that $f(s) \le 1 - \delta(\varepsilon)$, $s \ge \varepsilon$, 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

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

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 $A_1, \ldots, A_m$.

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 Cwickel–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 memmas, 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 $\tau > 0$

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

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

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

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

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

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*

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

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

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

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

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

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 $D[B] = \{u \in W^2(\Omega); \frac{\partial}{\partial\nu}\Big|_{\partial\Omega} u = 0\}$.

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

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

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

$$D[A^\alpha] = \{u \in W^{2\alpha}(\Omega); u\Big|_{\partial\Omega} = 0\}, \quad \frac{1}{2} < \alpha < 1;$$

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

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 $\kappa := 2\alpha - 1 < \kappa_0 := \frac{1}{2}\,(\alpha = \frac{3}{4})$,

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

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

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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