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Numerical analysis view on the general Trotter–Kato product formulae

Petra Csomós and Eszter Sikolya

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Abstract. We show that the abstract operator-theoretic (general) Trotter–Kato formulae yield the convergence of numerical methods used for solving differential equations. These methods combine operator splitting procedures with certain time discretisation schemes which should be consistent, strongly A-stable, positive rational approximations of the exponential function. We also show that it is possible to apply more numerical steps in one splitting time step and the convergence results remain true.

1. Introduction

Product formulae like Trotter–Kato provide a way to approximate the solution of an abstract Cauchy problem, hence, they can be studied in the framework of numerical analysis, too. In the present paper we will show the connection between the general Trotter–Kato product formulae and the convergence of the operator splitting procedures introduced by Bagrinovskii and Godunov [2], Marchuk [24] and Strang [29]. These methods are widely used for simplifying models which describe the combined effect of several processes, and involve the solution of the sub-problems corresponding to these processes. The convergence analysis of the methods should be performed also in the case when certain time discretisation schemes are used to solve the sub-problems, since their exact solutions are usually not known in the applications, see, e.g., Bátkai et al. [3], Csomós and Faragó [7], Dujardin and Lafitte [8]. In the present paper we show which properties of the time discretisation schemes ensure the assumptions of the general Trotter–Kato

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product formulae in the results of Ito and Kappel [19], Neidhardt and Zagrebnov [25], Ichinose, Neidhardt and Zagrebnov [16] and Ichinose, Tamura, Tamura and Zagrebnov [17]. In particular, in Propositions 4.11, 4.17 and 4.22 we obtain that the general Trotter–Kato product formulae yield the convergence of the combined numerical methods, that is, when operator splitting procedures are used together with certain time discretisation methods. The latter should satisfy mainly those constrains that are usual in practice, namely, that they are consistent and strongly A-stable rational approximations of the exponential function which preserve the positivity. We also show that the convergence estimates remain true even in the case if we apply sub-stepping, see Corollaries 4.12, 4.18 and 4.23. Our results give then a starting point to the error analysis of this kind of combined numerical methods.

The paper is organised as follows. In Section 2 we briefly summarize the functional-analytic background of our investigations. Section 3 contains the basic notions of numerical analysis, in particular, time discretisation schemes that are used to approximate the solution of differential equations. We also define operator splitting procedures and cite the original Trotter–Kato product formula. Section 4 deals with the general Trotter–Kato formulae and our main results according to their validity for numerical methods.

2. Functional-analytic background

In this section we shortly summarize the concept of an abstract Cauchy problem in view of operator semigroups, and we show how one can define bounded rational functions of semigroup generators. The last method, applied for certain rational approximations of the exponential function that are introduced in Subsection 2.2, yields the time-discretisation schemes that will have a crucial role in the present paper. We note that our main results in Section 4 will be stated in Hilbert spaces for self-adjoint positive operators. However, because the concepts of the following sections can be stated in Banach spaces, too, we do not want to restrict the presentation at this point.

2.1. Semigroups and generators

Our main reference for the concepts below is the monograph of Engel and Nagel [9].

We consider a linear, closed, densely defined operator $(A, D(A))$ on the Banach space $\mathcal{X}$, and the following abstract Cauchy problem for the unknown function

$u\colon [0,\infty) \to \mathcal{X}$:

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}u(t) + Au(t) = 0, \quad t > 0, \\ u(0) = u_0 \in \mathcal{X}, \end{cases} \tag{ACP}$$

where $u_0 \in \mathcal{X}$ is a given element. Since most of the results concerning the convergence of general Trotter–Kato formulae, including the ones referred to in the present work, define the operator A with the opposite sign as it appears in our main reference [9], we will accommodate our formulae and definitions accordingly.

In order to characterise the solution u of problem (ACP), we introduce the following notion.

Definition 2.1. A family $S := (S(t))_{t\geq 0}$ of bounded linear operators on a Banach space $\mathcal{X}$ is called a *strongly continuous semigroup* (C_0-semigroup for short) if it satisfies the following properties:

(a) $S(0) = I$, the identity operator on $\mathcal{X}$,
(b) $S(t+s) = S(t)S(s)$ holds for all $t, s \geq 0$,
(c) for every $x \in \mathcal{X}$, the orbit maps $t \mapsto S(t)x$ are continuous from $[0,\infty)$ into $\mathcal{X}$.

To each strongly continuous semigroup we can associate an operator called generator.

Definition 2.2. Let S be a C_0-semigroup on the Banach space $\mathcal{X}$ and let $D(A)$ be the subspace of $\mathcal{X}$ defined by

$$D(A) := \Big\{ x \in \mathcal{X} \;\Big|\; \lim_{\tau\to 0+} \frac{x - S(\tau)x}{\tau} \text{ exists} \Big\}.$$

For every $x \in D(A)$ we define the operator

$$Ax := \lim_{\tau\to 0+} \frac{x - S(\tau)x}{\tau}.$$

The operator $A\colon D(A) \subseteq \mathcal{X} \to \mathcal{X}$ is called the *generator* of the semigroup S.

The connection between the semigroup, its generator, and the solution of problem (ACP), is given by the following results, see, e.g., in [9, Thm. II.1.4, Prop. I.5.5, Thm. II.1.10, Prop. II.6.4]. We denote the space of bounded linear operators acting on the Banach space $\mathcal{X}$ by $\mathscr{L}(\mathcal{X})$ and the norm on it by $\|\cdot\|_{\mathscr{L}(\mathcal{X})}$.

Theorem 2.3. *Let $(A, D(A))$ be the generator of the C_0-semigroup S on the Banach space $\mathcal{X}$. Then the following assertions are true.*

(i) *The generator is a closed and densely defined operator which determines the semigroup uniquely.*

(ii) *There exist constants* $M \geq 1$, $\omega \in \mathbb{R}$ *such that* $\|S(t)\|_{\mathscr{L}(\mathcal{X})} \leq M\mathrm{e}^{\omega t}$ *holds for all* $t \geq 0$.

(iii) *The left half-plane* $\{\lambda \in \mathbb{C} : \operatorname{Re}\lambda \leq -\omega\}$ *is contained in the resolvent set of* A, *denoted by* $\rho(A)$. *This set is defined by* $\lambda \in \rho(A)$ *if and only if* $\lambda I - A$ *is bijective, hence, the* resolvent operator *of* A, $R(\lambda, A) := (\lambda I - A)^{-1}$ *exists and is bounded by the closed graph theorem.*

(iv) *The unique (mild) solution of the corresponding abstract Cauchy problem* (ACP) *is given as*

$$u(t) = S(t)u_0 \quad \textit{for all} \quad t \geq 0. \tag{1}$$

We note that the semigroup S is called *bounded* if ω can be chosen as zero.

2.2. Rational approximations

We now introduce rational approximations of the exponential function that will be used to define time-discretisation schemes for approximating the solution u of (ACP) being of the form (1).

Definition 2.4.

(a) The rational function $r\colon \mathbb{C} \to \mathbb{C}$ is called a *consistent rational approximation* of the exponential function $z \mapsto \mathrm{e}^{-z}$, $z \in \mathbb{C}$, if $r(0) = 1$ and $r'(0) = -1$ hold, that is, their Taylor series around zero coincide up to (at least) the second term.

(b) We say that the consistent rational approximation r of the exponential function is of *order* $p \geq 1$, if $r^{(k)}(0) = (-1)^k$, $k = 0, \dots, p$, that is, their Taylor series around zero coincide up to the $(p+1)$th term.

(c) The rational function r is called *A-stable* if $|r(z)| \leq 1$ holds for all $\operatorname{Re} z \geq 0$.

(d) The rational function r is called *strongly A-stable* if it is A-stable and there exists a constant $c \in [0, 1)$ such that $|r(z)| \to c$ holds as $|z| \to \infty$.

We note that the letter A in the word A-stable does not refer to the operator A in (ACP). After Ehre conjectured in 1973, Wanner, Hairer, and Nørsett proved the following result in 1978.

Theorem 2.5. [31, Thm. 7] *A consistent rational approximation of the exponential function having the form* $r = P/Q$, *where the polynomials* P *and* Q *have no common zeros and* $Q(0) \neq 0$, *is A-stable if and only if* $0 \leq \deg(Q) - \deg(P) \leq 2$ *holds for the degrees of the polynomials.*

Example 2.6. The two most common A-stable consistent rational approximations are

$$r(z) = \frac{1}{1+z} \qquad \text{corresponding to the implicit Euler method and} \tag{2}$$

$$r(z) = \frac{1-\frac{z}{2}}{1+\frac{z}{2}} \qquad \text{corresponding to the Crank–Nicolson method.} \tag{3}$$

More about these methods and their application for solving differential equations will be shown in Section 3.1.

2.3. Functional calculus

Let r be an A-stable rational approximation of the form

$$r(z) = \frac{P(z)}{Q(z)} \tag{4}$$

with polynomials

$$P(z) = a\prod_{k=0}^{n}(z_k - z)^{p_k}, \quad Q(z) = b\prod_{\ell=0}^{m}(z_\ell - z)^{q_\ell}$$

having no common zeros. Further, let $(A, D(A))$ be a semigroup generator with $\sigma(A) = \mathbb{C}\setminus\rho(A) \subset \{\lambda \in \mathbb{C} : \operatorname{Re}\lambda \geq 0\}$. Since by A-stability, Q has no zeros on the right half-plane, for such an operator A we can define the bounded linear operator $r(A)$ by

$$r(A) = \frac{a}{b}\prod_{k=0}^{n}(z_k I - A)^{p_k}\prod_{\ell=0}^{m}R(z_\ell, A)^{q_\ell}. \tag{5}$$

Later, in Section 4, we will deal with operators being self-adjoint, densely defined and bounded from below on some Hilbert space $\mathcal{H}$. Hence, in this case $r(A)$ can be understood in view of (5).

We remark that for an A-stable rational approximation r and a semigroup generator A, the bounded linear operator $r(A)$ can be defined in several ways, yielding the same result. One can use the Hille–Phillips calculus (see, e.g., [5]) or, in the case when A is sectorial (e.g. self-adjoint and bounded from below) the holomorphic functional calculus (see, e.g., [11]).

However, in Section 4 we will also need to plug in self-adjoint operators into (certain) bounded Borel-functions. Here the so-called Borel functional calculus is used, based on the spectral theorem for normal (or self-adjoint) operators, see, e.g., [28, Section 5.3]. One can prove that for an A-stable rational approximation r of the form (4) this also yields the same operator as in (5), see, e.g., [28, Prop. 5.9].

3. Numerical methods for approximating the solution of ACP

We show now how the rational approximations introduced before are used when constructing numerical methods for solving differential equations. First we give an insight to the derivation of time discretisation schemes, then we consider the operator splitting procedures which are applied for problems describing the combined effect of two (or more) phenomena. Our main aim is to use operator splitting procedures together with time discretisation schemes, and to analyse the convergence of the combined numerical method obtained. For a functional analytic introduction to time discretisation schemes we refer to Atkinson and Han [1] and Lax [22], while for even more details we refer to Hairer, Nørsett and Wanner [12] and Hairer and Wanner [13].

3.1. Time discretisation schemes

We aim at approximating the solution u of (ACP) being of the form (1). To this end we choose a time step $\tau > 0$, and approximate the solution $u(n\tau)$ at time levels $t_n = n\tau$ by $u_n(\tau)$ for all $n \in \mathbb{N}$. In the present paper we consider one-step methods where $u_n(\tau)$ depends only on its previous value $u_{n-1}(\tau)$, and the relation between them is given by the formula

$$\begin{cases} u_n(\tau) = E(\tau)u_{n-1}(\tau), \quad n \in \mathbb{N}, \\ u_0(\tau) = u_0, \end{cases} \tag{6}$$

where u_0 is the initial value of (ACP). The operator $E(\tau) \in \mathscr{L}(\mathcal{X})$ is a bounded linear operator for each $\tau > 0$, and the function $E\colon [0,\infty) \to \mathscr{L}(\mathcal{X})$ is strongly continuous with $E(0) = I$. The function E is referred to as *time discretisation scheme*.

If a semigroup generator A can be plugged in a consistent rational approximation r of the exponential function (see Subsection 2.3), we can consider time discretisation schemes of the form (6) with the choice $E(\tau) = r(\tau A)$, $\tau > 0$, hence

$$\begin{cases} u_n(\tau) = r(\tau A)u_{n-1}(\tau), \quad n \in \mathbb{N}, \\ u_0(\tau) = u_0 \end{cases} \tag{7}$$

for a time step $\tau > 0$.

Naturally, we expect that at a certain time level t, the approximate solution $u_n(\tau)$ gets closer to the exact one $u(t)$ when the time step $\tau = t/n$ is decreasing:

$$\lim_{n\to\infty} \Big\| u(t) - u_n\Big(\frac{t}{n}\Big)\Big\|_{\mathcal{X}} = 0.$$

For the time discretisation scheme (6), especially for (7), we arrive at the following definition.

Definition 3.1. Let $(A, D(A))$ be the generator of the C_0-semigroup S on the Banach space $\mathcal{X}$. Suppose that there is a densely and continuously embedded subspace $\mathcal{Y} \subset \mathcal{X}$, which is invariant under the semigroup S, and let $p \geq 1$. The time discretisation scheme (6) is called *convergent* of order p on $\mathcal{Y}$, if for all $T > 0$ there is a constant $C > 0$ such that for all $x \in \mathcal{Y}$ we have

$$\left\| S(t)x - E\Big(\frac{t}{n}\Big)^n x \right\|_{\mathcal{X}} \leq \frac{C}{n^p} \|x\|_{\mathcal{Y}}$$

for all $n \in \mathbb{N}$ with $t \in [0, T]$. The constant C can depend on T but is independent of n.

When considering the special kind of time discretisation scheme (7), the question arises what properties of the rational approximation r ensure the convergence. The answer was given in Brenner and Thomée [5], using the Hille–Phillips calculus that can be applied for any semigroup generator A on a Banach space $\mathcal{X}$.

Theorem 3.2. ([5, Thm. 3]) *Let r be an A-stable rational approximation of the exponential function of order $p \geq 1$, and let $(A, D(A))$ be the generator of the C_0-semigroup S on the Banach space $\mathcal{X}$. Then the time discretisation scheme (7) is convergent of order p on $\mathcal{Y} = D(A^{p+1})$ with $\|x\|_{\mathcal{Y}} := \|A^{p+1}x\|_{\mathcal{X}} + \|x\|_{\mathcal{X}}$.*

We sketch now the formal derivation of the two simplest time discretisation schemes applied to problem (ACP). A nice introduction can be found in [18, Section I.1]. We assume that A is a densely defined self-adjoint operator on the Hilbert space $\mathcal{H}$ that generates a C_0-semigroup. By taking a fixed value $\tau > 0$, when subsituting the time derivative in (ACP) at time $t > \tau$ by the difference quotient, and rearranging the equation, we arrive at the approximations

$$\begin{aligned} \frac{u(t) - u(t-\tau)}{\tau} + Au(t) \approx 0, \\ u(t) + \tau A u(t) \approx u(t-\tau), \\ u(t) \approx (I + \tau A)^{-1} u(t-\tau), \end{aligned}$$

where in the last step we used that $1/\tau$ belongs to the resolvent set of the operator $-A$, which is true for τ small enough, see Theorem 2.3(iii). For $t := t_n = n\tau$, $n \in \mathbb{N}$, this leads to the time discretisation scheme

$$u_n(\tau) = (I + \tau A)^{-1} u_{n-1}(\tau), \quad n \in \mathbb{N}, \tag{8}$$

which is of the form (7) with the corresponding rational approximation $r(z) = 1/(1+z)$ already presented in (2) as the implicit Euler method.

If one takes the operator A at the average of the solutions at time levels t and $t-\tau$, one arrives at the approximations

$$\frac{u(t)-u(t-\tau)}{\tau} + A\Big(\frac{u(t)+u(t-\tau)}{2}\Big) \approx 0,$$
$$u(t) \approx \Big(I+\frac{\tau}{2}A\Big)^{-1}\Big(I-\frac{\tau}{2}A\Big)u(t-\tau)$$

leading to the Crank–Nicolson scheme

$$u_n(\tau) = \Big(I+\frac{\tau}{2}A\Big)^{-1}\Big(I-\frac{\tau}{2}A\Big)u_{n-1}(\tau), \quad n \in \mathbb{N}. \tag{9}$$

This has again the form of (7) with the rational approximation $r(z) = (1+\frac{z}{2})^{-1}(1-\frac{z}{2})$ from (3).

Modelling of physical phenomena often requires the forecast of such quantities which should stay positive during the computation. One may think of mass, pressure, concentration, etc. Then we expect that for any $n \in \mathbb{N}$, $u(t_{n-1}) \geq 0$ implies that $u(t_n) = S(\tau)u(t_{n-1}) \geq 0$ holds as well, that is, the semigroup operators $S(\tau)$ are *positive* for all $\tau \in [0,T]$. For the precise definition of positive operator see [4, Def. 10.17]. We would expect that the time discretisation scheme (7) also *preserves the positivity*, that is, the operators $r(\tau A)$ are positive for all $\tau \in [0,T]$. This property is implied by the Borel functional calculus if r is a bounded rational approximation of the exponential function that satisfies $r(z) \geq 0$ for $z \in [0,\infty)$. Such kind of functions will be needed in Section 4 for our main results.

3.2. Operator splitting procedures

In applied sciences one usually wants to solve problems where the time behaviour of the system's state is determined by the combined effect of several phenomena. By considering two of these phenomena, this kind of systems is modelled by an abstract Cauchy problem (ACP) with the sum of two operators:

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}u(t) + (A+B)u(t) = 0, \quad t>0, \\ u(0) = u_0 \in \mathcal{X}. \end{cases} \tag{10}$$

The solution to problem (10) is usually hard to find. However, in several cases the exact solutions of the sub-problems $\dot{u} + Au = 0$ and/or $\dot{u} + Bu = 0$ are known, or there are efficient time discretisation schemes for approximating them. Then the question arises how to construct an approximate solution from the (approximate) sub-solutions.

In case of the *sequential splitting*, derived in Bagrinovskii and Godunov [2], we solve the sub-problem with operator A on the time interval $[0,\tau]$ for an arbitrary time step $\tau > 0$ with the initial value u_0 given in (10). Then we solve the sub-problem with B also on the time interval $[0,\tau]$ with the same τ as before, but by using the previously obtained solution as initial value. After that we repeat this procedure in a cycle n times, until the solution reaches the time level $t_n = n\tau$. We can change, of course, the order of the operators, and start with B. There is a symmetrised version of this method, called *Strang splitting* introduced by Marchuk [24] and Strang [29].

Assuming that the exact solutions of the sub-problems exist, that is, A and B are generators of the C_0-semigroups S_A and S_B, respectively, the above procedures result in the following formulae for all $n \in \mathbb{N}$ and $\tau > 0$:

$$\begin{aligned} u_n(\tau) = & S_A(\tau)S_B(\tau)u_{n-1}(\tau) = \big(S_A(\tau)S_B(\tau)\big)^n u_0 \qquad (11)\\ \text{or} \quad & S_B(\tau)S_A(\tau)u_{n-1}(\tau) = \big(S_B(\tau)S_A(\tau)\big)^n u_0, \\ u_n(\tau) = & S_A\Big(\frac{\tau}{2}\Big)S_B(\tau)S_A\Big(\frac{\tau}{2}\Big)u_{n-1}(\tau) = \Big(S_A\Big(\frac{\tau}{2}\Big)S_B(\tau)S_A\Big(\frac{\tau}{2}\Big)\Big)^n u_0 \qquad (12)\\ \text{or} \quad & S_B\Big(\frac{\tau}{2}\Big)S_A(\tau)S_B\Big(\frac{\tau}{2}\Big)u_{n-1}(\tau) = \Big(S_B\Big(\frac{\tau}{2}\Big)S_A(\tau)S_B\Big(\frac{\tau}{2}\Big)\Big)^n u_0 \end{aligned}$$

for the sequential splitting and the Strang splitting, respectively. Due to the semigroup law (2.1)(b), if $S(\tau)$ is positive, we have $S(\frac{\tau}{2}) = S(\tau)^{1/2}$. Thus, the Strang splitting (12) can also be written in the following form:

$$\begin{aligned} u_n(\tau) = & S_A(\tau)^{1/2}S_B(\tau)S_A(\tau)^{1/2}u_{n-1}(\tau) = \big(S_A(\tau)^{1/2}S_B(\tau)S_A(\tau)^{1/2}\big)^n u_0 \qquad (13)\\ \text{or} \quad & S_B(\tau)^{1/2}S_A(\tau)S_B(\tau)^{1/2}u_{n-1}(\tau) = \big(S_B(\tau)^{1/2}S_A(\tau)S_B(\tau)^{1/2}\big)^n u_0. \end{aligned}$$

The last method we will call *square-root splitting* to distinguish it from (12). Since later we will use certain approximations of the semigroups S_A, S_B, the methods using (12) and (13) will not be the same any more.

By chosing

$$\begin{aligned} E(\tau) &= S_A(\tau)S_B(\tau) \quad \text{or} \quad S_B(\tau)S_A(\tau), \\ E(\tau) &= S_A\Big(\frac{\tau}{2}\Big)S_B(\tau)S_A\Big(\frac{\tau}{2}\Big) \quad \text{or} \quad S_B\Big(\frac{\tau}{2}\Big)S_A(\tau)S_B\Big(\frac{\tau}{2}\Big), \\ E(\tau) &= S_A(\tau)^{1/2}S_B(\tau)S_A(\tau)^{1/2} \quad \text{or} \quad S_B(\tau)^{1/2}S_A(\tau)S_B(\tau)^{1/2}, \end{aligned}$$

respectively, one can see that the operator splittings (11)–(13) are also time discretisation schemes of the form (6). Hence, their convergence can be investigated in view of Definition 3.1. From the numerical analysis point of view, the Trotter–Kato product formula delivers the convergence of the sequential splitting (11) under appropriate conditions.

Theorem 3.3. (Trotter–Kato product formula, [9, Cor. III.5.8]) *Let S_A,S_B be strongly continuous semigroups on $\mathcal{X}$ satisfying the stability condition*

$$\Big\| \Big(S_B\Big(\frac{t}{n}\Big) S_A\Big(\frac{t}{n}\Big)\Big)^n \Big\|_{\mathscr{L}(\mathcal{X})} \le M\mathrm{e}^{\omega t}$$

for all $t \ge 0$, $n \in \mathbb{N}$, and for constants $M \ge 0$, $\omega \in \mathbb{R}$. Consider the sum $A+B$ on $D := D(A) \cap D(B)$ of the generators $(A, D(A))$,$(B, D(B))$ of S_A, S_B, respectively, and assume that D and $(\lambda_0 - A - B)D$ are dense in $\mathcal{X}$ for some $\lambda_0 < -\omega$. Then $C := \overline{A+B}$ generates the strongly continuous semigroup S given by the product formula

$$S(t)x = \lim_{n\to\infty} \Big(S_A\Big(\frac{t}{n}\Big) S_B\Big(\frac{t}{n}\Big)\Big)^n x, \quad x \in \mathcal{X}, \tag{14}$$

with uniform convergence for t in compact intervals.

Since Trotter [30] and Kato [20], product formulae of the above kind have been widely investigated in the literature. Generalisation of Theorem 3.3 leads to product formulae, e.g., like Chernoff's in [6], where the operator in the limit contains no longer the product of C_0-semigroups but some strongly continuous function satisfying certain consistency and stability properties. Another direction of research considers formula (14) with (not just exponential) functions of operators A, B instead of S_A, S_B. In the present paper we deal with the latter case and consider rational approximations of the exponential function. From the numerical point of view this means that the approximate solutions of the corresponding split sub-problems are computed by (even different) time discretisation schemes of the form (7).

4. General Trotter–Kato product formulae

In this section we show convergence results of numerical methods which combine an operator splitting procedure with certain time discretisation schemes used to solve the sub-problems. The proofs use such results from the literature which deal with the convergence of general Trotter–Kato product formulae.

The first result we refer to is from the textbook [19] of Ito and Kappel. Since the authors deal with nonlinear operators, we cite their result in a way which fits into our framework. In any case, their result serves as a good motivation to our next results. The authors consider formulae like Trotter–Kato (14) but with the following terms on the right-hand side:

$$\lim_{n\to\infty}\Big(\Big(I+\frac{t}{n}A\Big)^{-1}\Big(I+\frac{t}{n}B\Big)^{-1}\Big)^{n}x \qquad \text{in [19, Thm. 10.18]}, \tag{15}$$

$$\lim_{n\to\infty}\Big(\Big(2\Big(I+\frac{t}{2n}A\Big)^{-1}-I\Big)\Big(2\Big(I+\frac{t}{2n}B\Big)^{-1}-I\Big)\Big)^{n}x \quad \text{in [19, Thm. 10.20]}. \tag{16}$$

We note that n/t and $2n/t$ are contained in $\rho(-A)$ and $\rho(-B)$ for $n\in\mathbb{N}$ large enough, hence the formulae are right. Formula (15) was first mentioned in [23, Algorithm I] and it represents the Peaceman–Rachford method in the case when the semigroups are changed to the corresponding resolvents. Hence, besides the operator splitting, there appears another approximation which plays an important role in our present paper. Namely, from the numerical analysis point of view (cf. Definition 3.1), formula (15) describes the numerical solution of the problem (10) in the case when the sequential splitting (11) is applied and the sub-problems are solved by using the implicit Euler method (8) with time step $\tau = t/n$. Furthermore, the resolvent identity implies $2(I+\lambda A)^{-1}-I=(I+\lambda A)^{-1}(I-\lambda A)$ for all $1/\lambda\in\rho(-A)$, and similarly for operator B. Thus, formula (16) corresponds to the numerical solution of the problem (10) in the case when the sequential splitting (11) is applied together with the Crank–Nicolson scheme (9) with time step $\tau = t/n$.

Neidhardt and Zagrebnov [25] considered a generalised version of the results above (at least for linear operators), where they treat not only one special time discretisation scheme for solving the sub-problems, but a whole family. We list the assumptions needed on the operators and on the functions appearing in the formulae.

Assumptions 4.1. Let A, B be densely defined self-adjoint operators, bounded from below in the Hilbert space $\mathcal{H}$. Without loss of generality we can assume that

$$\langle Ax, x\rangle \ge \|x\|^2_{\mathcal{H}} \quad \text{for all } x\in D(A),$$
$$\langle Bx, x\rangle \ge \|x\|^2_{\mathcal{H}} \quad \text{for all } x\in D(B).$$

Furthermore, let $D(A)\subset D(B)$ hold and assume that there exists $0\le a<1$ such that

$$\|Bx\|_{\mathcal{H}} \le a\|Ax\|_{\mathcal{H}} \quad \text{for all} \quad x\in D(A). \tag{17}$$

Since A, B are densely defined self-adjoint operators being bounded from below by 1 (hence, $-A$ and $-B$ are dissipative) on the Hilbert space $\mathcal{H}$, it follows by [9, Cor. II.3.17 and Cor. II.4.7] that they generate analytic C_0-semigroups of contractions on $\mathcal{H}$. Hence, using (17), we obtain by [9, Thm. III.2.7] that the self-adjoint operator $(A+B, D(A))$ generates an analytic contraction semigroup that we denote by S.

Definition 4.2. ([32, Def. 5.4]) The Borel measurable function $f\colon [0,\infty) \to [0,1]$ is called a *generic Kato function* if

$$f(0) = 1 \quad \text{and} \quad \lim_{z\to 0+} f'(z) = -1. \tag{18}$$

Assumptions 4.3. Let f, g be generic Kato functions with

$$\begin{aligned}
F_0 &:= \operatorname{ess\,sup}_{z>0} \frac{z\sqrt{f(z)}}{1-f(z)} < \infty,\\
F_1 &:= \operatorname{ess\,sup}_{z>0} \frac{1-f(z)}{z} < \infty,\\
F_2 &:= \operatorname{ess\,sup}_{z>0} \Big| \Big(f(z) - \frac{1}{1+z}\Big)\frac{1}{z^2}\Big| < \infty,\\
G_1 &:= \operatorname{ess\,sup}_{z>0} \frac{1-g(z)}{z} < \infty,\\
G_2 &:= \operatorname{ess\,sup}_{z>0} \Big| \Big(g(z) - \frac{1}{1+z}\Big)\frac{1}{z^2}\Big| < \infty.
\end{aligned}$$

Assumption 4.4. In the case Assumptions 4.1 and 4.3 hold, we suppose $F_0G_1a < 1$.

Example 4.5. (See, e.g., [25].) Besides the exponential functions $f(z) = g(z) = e^{-z}$, there is a class of Borel functions which satisfy Assumptions 4.3, for instance

$$f(z) = \frac{1}{(1+\frac{z}{2})^2} \quad \text{with} \quad F_0 = 2,$$

which corresponds to two steps with the implicit Euler method defined in (2) with time step $\tau/2$. We remark that the choice $f(z) = \frac{1}{1+z}$ of the same implicit Euler method (2) with time step τ does not satisfy Assumptions 4.3, since in this case F_0 is infinite. On the other hand, the choice $g(z) = \frac{1}{1+z}$ satisfies all conditions, because there is no condition like $F_0 < \infty$ for the function g.

We now cite the convergence result of Neidhardt and Zagrebnov.

Proposition 4.6. ([25, Thm. 2.7 and Cor. 2.8], [32, Prop. 5.8]) *Let the operators A, B satisfy Assumptions 4.1 and the functions f, g satisfy Assumption 4.3 and Assumption 4.4. Let S denote the C_0-semigroup generated by $(A+B, D(A))$. Then there exist positive constants L_1 and L_2 such that the estimates*

$$\Big\| S(t) - \Big(f\Big(\frac{t}{n}A\Big) g\Big(\frac{t}{n}B\Big)\Big)^n \Big\|_{\mathscr{L}(\mathcal{H})} \le \frac{L_1}{(1-F_0G_1a)^2(1-a)} \frac{\ln n}{n}, \tag{19}$$

$$\Big\| S(t) - \Big(f^{1/2}\Big(\frac{t}{n}A\Big) g\Big(\frac{t}{n}B\Big) f^{1/2}\Big(\frac{t}{n}A\Big)\Big)^n \Big\|_{\mathscr{L}(\mathcal{H})} \le \frac{L_2}{(1-F_0G_1a)(1-a)} \frac{\ln n}{n} \tag{20}$$

hold for $n = 3, 4, \dots$ and uniformly in $t \ge 0$.

In view of Definition 3.1, formulae (19) and (20) give the convergence of the time discretisation scheme $E(\tau)$ of $f(\tau A)g(\tau B)$ and $f^{1/2}(\tau A)g(\tau B)f^{1/2}(\tau A)$, respectively. For the choice $f(z) = g(z) = \mathrm{e}^{-z}$, we have $f(\cdot A) = S_A(\cdot)$, $g(\cdot B) = S_B(\cdot)$ by the properties of the functional calculus. Hence, in this case formula (19) corresponds to the sequential splitting, while (20) describes the Strang and square-root splittings. We note that the norm estimates above imply the desired (strong) convergence of the schemes. We aim at showing that the functions f, g can be considered as time discretisation schemes applied to approximate the solutions of the sub-problems. Then formulae (19), (20) describe the convergence of the combined numerical methods, namely, the sequential and the square-root operator splittings used together with time discretisation schemes. We also note that $f^{1/2}(\tau A) = f(\tau A)^{1/2}$ holds due to the Borel functional calculus. In this context we prefer the first notation to be consistent with the literature.

In the rest of the paper, in each result we suppose that f and g satisfy the following.

Main Assumptions. We suppose that f, g are the consistent, strongly A-stable rational approximations of the exponential function. Furthermore, $f(z), g(z) \geq 0$ holds for $z \geq 0$, and $f(z), g(z) < 1$ holds for all $z \in (0, +\infty)$.

Lemma 4.7. *If the functions f, g are consistent A-stable rational approximations of the exponential function with $f(z), g(z) \geq 0$ for $z \geq 0$ – especially, if they satisfy the Main Assumptions –, then they are generic Kato functions.*

Proof. Since $f(z), g(z) \geq 0$ for $z \in [0, +\infty)$ and f, g are A-stable rational approximations of the exponential function, we obtain that f, g are Borel functions mapping $[0, \infty)$ to $[0, 1]$. Moreover, the consistency criterion implies property (18) for both f, g.

■

Proposition 4.8. *Let the Main Assumptions be satisfied for the functions f, g. Further let f be of the form*

$$f(z) = \frac{P(z)}{Q(z)} \quad \text{with} \quad \deg(Q) = \deg(P) + 2 \tag{21}$$

where the polynomials P and Q have no common zeros. Then Assumptions 4.3 hold true.

Proof. Lemma 4.7 implies that f, g are generic Kato functions. In order to prove that the essential supremums in Assumptions 4.3 are finite, we note that by assumption, f, g are continuous on $[0, \infty)$ and $0 \leq f(z), g(z) < 1$ if $z \in (0, +\infty)$.

Hence, the maxima and minima of the functions in Assumptions 4.3 exist on any compact subinterval of $(0, +\infty)$. Therefore, it suffices to study the behaviour of them in the neighbourhoods of zero and infinity. By using the L'Hospital rule and the consistency criterion, we have

$$\lim_{z\to 0+} \frac{1-f(z)}{z} = \lim_{z\to 0} \frac{-f'(z)}{1} = -f'(0) = -(-1) = 1 < \infty.$$

Since f is bounded on the right half-line, we have that

$$\lim_{z\to\infty} \frac{1-f(z)}{z} = 0.$$

The same holds for the function g as well, thus, F_1 and G_1 are finite.

Since f is twice differentiable, we can use its Taylor expansion around $z = 0$ and the consistency criterion to obtain

$$\begin{aligned}
\lim_{z\to 0+} \left| \left(f(z) - \frac{1}{1+z} \right) \frac{1}{z^2} \right| &= \lim_{z\to 0+} \left| \left(1 + f'(0)z + \frac{1}{2} f''(\xi(z))z^2 - \frac{1}{1+z} \right) \frac{1}{z^2} \right| \\
&= \lim_{z\to 0+} \left| \left(1 - z + \frac{1}{2} f''(\xi(z))z^2 - \frac{1}{1+z} \right) \frac{1}{z^2} \right| \\
&= \lim_{z\to 0+} \left| \frac{-1}{1+z} + \frac{1}{2} f''(\xi(z)) \right| \\
&= \lim_{z\to 0+} \left| \frac{1}{2} f''(\xi(z)) - 1 \right|
\end{aligned}$$

where $\xi(z) \in [0, 1]$. Since f'' is continuous and $\xi(z) \to 0+$ if $z \to 0+$, the limit obtained exists and is finite. For the limit in infinity we obtain by the boundedness of f that

$$\lim_{z\to\infty} \left| \left(f(z) - \frac{1}{1+z} \right) \frac{1}{z^2} \right| = \lim_{z\to\infty} \left| \frac{f(z)}{z^2} - \frac{1}{(1+z)z^2} \right| = 0 < \infty.$$

The same holds for the function g as well, thus, F_2 and G_2 are finite.

We still have to show that $F_0 < \infty$. We use again L'Hospital's rule and the consistency criterion to obtain

$$\lim_{z\to 0+} \frac{z\sqrt{f(z)}}{1-f(z)} = \lim_{z\to 0+} \frac{\sqrt{f(z)} + \frac{z}{2} \frac{1}{\sqrt{f(z)}} f'(z)}{-f'(z)} = \frac{1 + \frac{0}{2} \cdot 1 \cdot (-1)}{-(-1)} = 1 < \infty.$$

For the limit in infinity we will use formula (21) of f. Rewriting it as

$$\lim_{z\to\infty} \frac{z\sqrt{f(z)}}{1-f(z)} = \lim_{z\to\infty} \frac{\sqrt{z^2 f(z)}}{1-f(z)},$$

the denominator is bounded by strong A-stability. By condition (21), the term $z^2 f(z)$ tends to a constant in infinity. Thus, the limit of the fraction, hence F_0 is finite.

■

We can even generalise the result above by considering $k \in \mathbb{N}$ numerical steps in one splitting time step $\tau = t/n$, called sub-stepping. Then the properties of the new rational approximation $f_k(z) = f(\frac{z}{k})^k$ are inherited from the properties of f, and similarly to g.

Lemma 4.9. *Let f, g satisfy the Main Assumptions. Then the functions*

$$f_k(z) = f\Big(\frac{z}{k}\Big)^k \quad \text{and} \quad g_\ell(z) = g\Big(\frac{z}{\ell}\Big)^\ell \quad \text{for any} \quad k, \ell \in \mathbb{N}$$

also satisfy the Main Assumptions.

Proof. We observe first that f_k, g_ℓ are also rational functions for any $k, \ell \in \mathbb{N}$. Since $f(z) \in [0,1]$, $f_k(z) = f(\frac{z}{k})^k \in [0,1]$ holds for all $z \in [0, +\infty)$, and $f_k(z) < 1$ if $z \in (0, +\infty)$. Clearly, $f_k(0) = 1$. Furthermore, for arbitrary $k \in \mathbb{N}$ we have

$$f_k'(z) = \left(f\Big(\frac{z}{k}\Big)^k\right)' = k f\Big(\frac{z}{k}\Big)^{k-1} f'\Big(\frac{z}{k}\Big)\frac{1}{k} = f\Big(\frac{z}{k}\Big)^{k-1} f'\Big(\frac{z}{k}\Big),$$

that is, $f_k'(0) = -1$. The same arguments hold for g_ℓ. Hence, f_k, g_ℓ are consistent, A-stable rational approximations of the exponential function. The strong A-stability of f_k follows from the strong A-stability of f as

$$\lim_{z\to\infty} f_k(z) = \lim_{z\to\infty} f\Big(\frac{z}{k}\Big)^k = c^k < 1,$$

because $c < 1$, and similarly for g_ℓ.

■

We note that Proposition 4.8 and therefore Lemma 4.9 hold under weaker assumptions, too. More precisely, one does not need to exclude the cases $f(z) = 1$ or $g(z) = 1$ for $z \in (0, +\infty)$. However, the main aim of the paper is to enlighten the relation between the constraints appearing in the functional-analytic results and the properties in numerical analysis which ensure them. Hence, to be consequent, we aim at referring to the same Main Assumptions throughout the paper (even if some of our results hold under weaker assumptions, too).

We present now important examples for rational approximations satisfying the Main Assumptions and the degree condition (21) in Proposition 4.8.

Example 4.10.

(i) The implicit Euler method where two steps are made in one splitting time step:

$$f(z) = \frac{1}{(1+\frac{z}{2})^2}.$$

(ii) The method with two implicit Euler steps and $k-2$ Crank–Nicolson steps in one splitting time step:

$$f(z) = \frac{\left(1-\frac{z}{k}\right)^{k-2}}{\left(1+\frac{z}{k}\right)^{k-2}\left(1+\frac{z}{k}\right)^{2}} \quad \text{for all } k=2,3,4,\dots$$

More details on this method can be found in Hansbo [14], Faragó and Kovács [10].

(iii) The family of Padé approximations named Lobatto IIIC methods, see, e.g., in Hairer and Wanner [13, Chapter IV.5].

We now state the first result regarding the convergence of combined numerical methods.

Proposition 4.11. *Let the operators A, B satisfy Assumptions 4.1 and f, g satisfy the Main Assumptions. Further, let f be of the form $f(z) = P(z)/Q(z)$, where the polynomials P and Q have no common zeros and $\deg(Q) = \deg(P) + 2$. Moreover, let Assumption 4.4 be satisfied. Then the error estimates (19) and (20) hold true for the semigroup S generated by $(A+B, D(A))$.*

Proof. Due to Proposition 4.8, the functions f, g satisfy the assumptions of Proposition 4.6. Hence, the assertion is true. ■

Moreover, Lemma 4.9 leads to the following generalisation.

Corollary 4.12. *Let the assumptions of Proposition 4.11 be satisfied for the operators A, B and the functions f, g. Then there exist constants $L_3, L_4 > 0$ such that the following estimates hold true for the semigroup S generated by $(A+B, D(A))$:*

$$\left\| S(t) - \left(f\left(\frac{t}{nk}A\right)^k g\left(\frac{t}{n\ell}B\right)^\ell \right)^n \right\|_{\mathscr{L}(\mathcal{H})} \le \frac{L_3}{(1-F_0G_1a)^2(1-a)} \frac{\ln n}{n},$$

$$\left\| S(t) - \left(f^{1/2}\left(\frac{t}{nk}A\right)^k g\left(\frac{t}{n\ell}B\right)^\ell f^{1/2}\left(\frac{t}{nk}A\right)^k \right)^n \right\|_{\mathscr{L}(\mathcal{H})} \le \frac{L_4}{(1-F_0G_1a)(1-a)} \frac{\ln n}{n}$$

for $k, \ell \in \mathbb{N}$, $n = 3, 4, \dots$ and uniformly for $t \ge 0$.

Proof. For all $\tau > 0$, the operators in the assertion can be rewritten as

$$f\Big(\frac{\tau}{k}A\Big)^k = f_k(\tau A) \quad \text{and} \quad g\Big(\frac{\tau}{\ell}B\Big)^\ell = g_\ell(\tau B).$$

Then Lemma 4.9 implies that f_k, g_ℓ satisfy the Main Assumptions for all $k, \ell \in \mathbb{N}$. Moreover, formula (21) holds trivially for f_k. Hence, Proposition 4.8 implies the assertion. ∎

The next result is based on the work of Ichinose, Tamura, Tamura and Zagrebnov [17]. Besides being generic Kato functions, we assume the following conditions for the functions f, g.

Assumption 4.13. Let $f, g\colon [0,\infty) \to [0,1]$ be generic Kato functions with

$$\sup_{z>0} \frac{|f(z) - 1 + z|}{z^{2\alpha}} < \infty \quad \text{and} \quad \sup_{z>0} \frac{|g(z) - 1 + z|}{z^{2\alpha}} < \infty \tag{22}$$

for some $\alpha \in (0,1]$.

Assumption 4.14. For all $\varepsilon > 0$ there exists $0 < \delta(\varepsilon) < 1$ such that $f(z), g(z) \le 1 - \delta(\varepsilon)$ if $z \ge \varepsilon$.

Proposition 4.15. *Let the Main Assumptions be satisfied for the functions f, g. Then Assumption 4.13 holds true for any $\alpha \in (1/2, 1]$ and Assumption 4.14 is satisfied.*

Proof. Lemma 4.7 implies that f, g are generic Kato functions. For the inequalities (22) notice that the fractions are bounded on any compact interval not containing zero, hence, it suffices to investigate them in the neighbourhoods of 0 and ∞. Since f, g are bounded and $2\alpha \in (1,2]$, the fractions are bounded on any interval $[K,\infty)$ if $K > 0$. Using that f, g are consistent rational approximations of the exponential function, in a small neighbourhood of 0 the relations

$$f(z) = 1 - z + \mathcal{O}(z^2) \quad \text{and} \quad g(z) = 1 - z + \mathcal{O}(z^2)$$

are satisfied. Since $2\alpha \in (1,2]$, this yields the boundedness of the fractions in neighbourhoods of 0, namely, Assumption 4.13.

In order to show Assumption 4.14 we denote the limit $\lim_{z\to\infty} f(z) =: c$ which exists and belongs to $[0,1)$ by the strong A-stability of f. We further denote $\delta_1 := \frac{1}{2}(1-c) \in (0,1)$. Due to the strong A-stability, for this $\delta_1 \in (0,1)$ there exists $K = K(\delta_1) > 0$ such that $f(z) \le 1 - \delta_1$ for all $z \in [K, +\infty)$. Thus, we have

$$\sup_{z\in[K,+\infty)} f(z) \le 1 - \delta_1.$$

We fix this $K > 0$ and take any $\varepsilon > 0$. Then we have two cases. If $\varepsilon \geq K$ then we can choose $\delta(\varepsilon) := \delta_1$.

Furthermore, if $\varepsilon < K$, we define

$$\delta_2(\varepsilon) := 1 - \max_{z\in[\varepsilon,K]} f(z) \in (0,1],$$

since, by assumption, $f(z) < 1$ if $z \in (0,+\infty)$. In this case the choice $\delta(\varepsilon) := \min\{\delta_1, \delta_2(\varepsilon)\} \in (0,1)$ yields the desired bound $f(z) \leq 1 - \delta(\varepsilon)$ for all $z \in [\varepsilon,+\infty)$. The same holds for the function g as well, which implies Assumption 4.14. ■

We now cite the result of Ichinose et al. and remark that operator positivity is here meant in the Hilbert space sense, that is, that the corresponding quadratic form is non-negative.

Proposition 4.16. ([17, Thm. 1], [32, Prop. 5.25]) *Let A, B be positive self-adjoint operators in the Hilbert space $\mathcal{H}$ such that $A + B$ is self-adjoint on the domain $D(A) \cap D(B)$, and denote by S the semigroup generated by $(A + B, D(A) \cap D(B))$. Let f, g be generic Kato functions which satisfy Assumptions 4.13 and 4.14 with $\alpha = 1$. Then there exist constants $C_1, C_2 > 0$ such that*

$$\Big\|S(t) - \Big(f\Big(\frac{t}{n}A\Big)g\Big(\frac{t}{n}B\Big)\Big)^n\Big\|_{\mathscr{L}(\mathcal{H})} \leq \frac{C_1}{n}, \tag{23}$$

$$\Big\|S(t) - \Big(f\Big(\frac{t}{2n}A\Big)g\Big(\frac{t}{n}B\Big)f\Big(\frac{t}{2n}A\Big)\Big)^n\Big\|_{\mathscr{L}(\mathcal{H})} \leq \frac{C_2}{n} \tag{24}$$

hold for n big enough and uniformly in $t \geq 0$.

We show that if f, g satisfy the Main Assumptions, then the above convergence estimates hold for the sequential and Strang splitting applied together with the time discretisation schemes f, g.

Proposition 4.17. *Let A, B be positive self-adjoint operators in the Hilbert space $\mathcal{H}$ such that $A + B$ is self-adjoint on the domain $D(A) \cap D(B)$, and denote by S the semigroup generated by $(A+B, D(A)\cap D(B))$. Let f, g satsify the Main Assumptions. Then the error estimates (23) and (24) hold true for the semigroup S.*

Proof. Using Proposition 4.15 we have that f, g satisfy Assumptions 4.13 and 4.14 for $\alpha = 1$. Hence, Proposition 4.16 can be applied and the convergence estimates (23) and (24) hold true. ■

In view of Propositions 4.11 and 4.17, estimates (19), (23) and (20), (24) give the convergence of the approximate solutions to the exact one of problem (10) when

f, g are certain rational approximations, and the sequential and Strang splittings, respectively, are applied.

We now show that the above result holds true also for numerical methods using sub-stepping.

Corollary 4.18. *Let the assumptions of Proposition 4.17 be satisfied for the operators A, B and the functions f, g. Then there exist constants $C_3, C_4 > 0$ such that*

$$\Big\| S(t) - \Big(f\Big(\frac{t}{nk}A\Big)^k g\Big(\frac{t}{n\ell}B\Big)^\ell \Big)^n \Big\|_{\mathscr{L}(\mathcal{H})} \le \frac{C_3}{n},$$

$$\Big\| S(t) - \Big(f\Big(\frac{t}{2nk}A\Big)^k g\Big(\frac{t}{n\ell}B\Big)^\ell f\Big(\frac{t}{2nk}A\Big)^k \Big)^n \Big\|_{\mathscr{L}(\mathcal{H})} \le \frac{C_4}{n}$$

hold for $k, \ell \in \mathbb{N}$ and n big enough and uniformly in $t \ge 0$.

Proof. For all $\tau > 0$, the operators in the assertion can be rewritten as

$$f\Big(\frac{\tau}{k}A\Big)^k = f_k(\tau A) \quad \text{and} \quad g\Big(\frac{\tau}{\ell}B\Big)^\ell = g_\ell(\tau B).$$

Then Lemma 4.9 implies that f_k, g_ℓ satisfy the Main Assumptions for all $k, \ell \in \mathbb{N}$. Thus, the proof is the same as for Proposition 4.17. ∎

Ichinose, Neidhardt and Zagrebnov in [16] investigated the convergence of all general Trotter–Kato product formulae (i.e. numerical methods) treated above, under assumption (22). In this case, however, we should consider the form-sum of the operators in problem (10).

Definition 4.19. Let A, B be positive self-adjoint operators in a Hilbert space $\mathcal{H}$ such that $D(A^{1/2}) \cap D(B^{1/2})$ is dense in $\mathcal{H}$. By H we denote the form-sum of A and B, i.e. $H := A \dot{+} B$ which is a positive self-adjoint operator in $\mathcal{H}$, generating the semigroup S.

Definition 4.20. ([16, Section 5]) For any $\tau > 0$, we define the operator families

$$\begin{aligned}
E_1(\tau) &:= f(\tau A) g(\tau B),\\
E_2(\tau) &:= g(\tau B) f(\tau A),\\
E_3(\tau) &:= f\Big(\frac{\tau}{2}A\Big) g(\tau B) f\Big(\frac{\tau}{2}A\Big),\\
E_4(\tau) &:= g\Big(\frac{\tau}{2}B\Big) f(\tau A) g\Big(\frac{\tau}{2}B\Big),\\
E_5(\tau) &:= f(\tau A)^{1/2} g(\tau B) f(\tau A)^{1/2},\\
E_6(\tau) &:= g(\tau B)^{1/2} f(\tau A) g(\tau B)^{1/2}.
\end{aligned}$$

We present now the result of Ichinose, Neidhardt and Zagrebnov.

Proposition 4.21. ([16, Thm. 5.1]) *Let A, B be positive self-adjoint operators such that $D(H^\alpha) \subset D(A^\alpha) \cap D(B^\alpha)$ holds for some $\alpha \in (1/2, 1)$. Further, let f, g satisfy Assumption 4.13 for this α. If in addition one has $D(A^{1/2}) \subset D(B^{1/2})$ and*

$$\sup_{z \geq x} f(z) < 1, \quad \sup_{z \geq x} g(z) < 1 \quad \textit{for} \quad x > 0 \tag{25}$$

then for any $T > 0$ there are constants $C_{T,\alpha}^{(j)} > 0$, $j = 1, 2, \ldots, 6$, such that with the notations of Definition 4.20, we have

$$\left\| S(t) - E_j\left(\frac{t}{n}\right)^n \right\|_{\mathscr{L}(\mathcal{H})} \leq \frac{C_{T,\alpha}^{(j)}}{n^{2\alpha-1}}, \quad j = 1, 2, \ldots, 6, \tag{26}$$

for any $t \in [0, T]$ and $n \in \mathbb{N}$.

We have then its direct consequence by using Proposition 4.15.

Proposition 4.22. *Let A, B be positive self-adjoint operators such that for some $\alpha \in (1/2, 1)$ $D(H^\alpha) \subset D(A^\alpha) \cap D(B^\alpha)$ holds. Further, let f, g satisfy the Main Assumptions. If in addition one has $D(A^{1/2}) \subset D(B^{1/2})$ then the convergence estimates (26) hold true for all operator families E_j defined in Definiton 4.20.*

Proof. We note that condition (25) is equivalent to Assumption 4.14. Then using Proposition 4.15 we have that f, g satisfy Assumptions 4.13 and 4.14 for $\alpha \in (1/2, 1)$. Hence, we can apply Proposition 4.21 and obtain the desired result. ∎

For $j = 1, 2$, estimate (26) describes the convergence of the sequential splitting when the sub-problems are solved by using rational approximations. The cases $j = 3, 4$ yield the same for the Strang splitting, and the estimates for $j = 5, 6$ correspond to the square-root splitting. Moreover, the result holds true for the sub-stepping as well.

Corollary 4.23. *Let the assumptions of Proposition 4.22 be satisfied for the operators A, B and the functions f, g. Then for any $T > 0$ there are constants $C_{T,\alpha,k,\ell}^{(j)} > 0$, $j = 1, 2, \ldots, 6$, such that we have*

$$\left\| S(t) - E_j^{(k,\ell)}\left(\frac{t}{n}\right)^n \right\|_{\mathscr{L}(\mathcal{H})} \leq \frac{C_{T,\alpha,k,\ell}^{(j)}}{n^{2\alpha-1}}, \quad j = 1, 2, \ldots, 6,$$

for any $t \in [0, T]$ and $k, \ell, n \in \mathbb{N}$, where $E_j^{(k,\ell)}(\tau)$ denote the operators $E(\tau)$ as in Definition 4.20 but with $A/k, B/\ell$ instead of A, B.

Proof. For all $\tau > 0$, the operators appearing in $E_j^{(k,\ell)}(\tau)$ can be rewritten as

$$f\Big(\frac{\tau}{k}A\Big)^k = f_k(\tau A) \quad \text{and} \quad g\Big(\frac{\tau}{\ell}B\Big)^\ell = g_\ell(\tau B).$$

Then Lemma 4.9 implies that f_k, g_ℓ satisfy the Main Assumptions for all $k, \ell \in \mathbb{N}$. Hence, they also satisfy Assumptions 4.13 and 4.14 (equivalent to (25)) by Proposition 4.15. Then the proof is the same as for Proposition 4.22. ∎

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P. Csomós, Eötvös Loránd University, Institute of Mathematics, and MTA-ELTE Numerical Analysis and Large Networks Research Group, Pázmány Péter st. 1/C, H-1117 Budapest, Hungary; *e-mail*: csomos@cs.elte.hu

E. Sikolya, Eötvös Loránd University, Institute of Mathematics, Pázmány Péter st. 1/C, H-1117 Budapest, Hungary; and Alfréd Rényi Institute of Mathematics, Reáltanoda u. 13-15., H-1053 Budapest, Hungary; *e-mail*: eszter.sikolya@ttk.elte.hu