A FUNCTIONAL CALCULUS APPROACH FOR THE RATIONAL APPROXIMATION WITH NONUNIFORM PARTITIONS

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Abstract. By introducing $\mathcal{M}$-functional calculus we generalize some results of Brenner and Thomée on the stability and convergence of rational approximation schemes of bounded semigroups for nonuniform time steps. We give also the rate of convergence for the approximation of the time derivative of these semigroups.

1. Introduction.

Let A be a closed densely defined linear operator in a Banach space X which generates a strongly continuous semigroup e^{tA}. The purpose of this paper is to approximate e^{tA} by suitable linear operators $P_n(A)$ by using nonuniform partitions of the time-interval $[0, t]$.

If $\tau_1, \dots, \tau_n$ are n positive time steps whose sum equals to t then we will consider approximations of the form

$$P_n(A) = R(\tau_1 A) \dots R(\tau_n A) \tag{1.1}$$

where R is a rational function. Such a choice is motivated by the fact that rational functions of A appear in time discretizations of the initial-value problem

$$\frac{\mathrm{d}}{\mathrm{d}t} u = Au \quad t > 0, \quad u(0) = u_0 \in X. \tag{1.2}$$

Indeed, backward Euler and Crank-Nicholson schemes leads respectively to rational functions of the form $R(z) = (1 - z)^{-1}$ and $R(z) = (1 + z/2)(1 - z/2)^{-1}$.

In the case where R is *p-acceptable* and the semigroup e^{tA} is bounded, the following results can be found in the literature (see Section 2 for notation and definitions).

• If e^{tA} is analytic and the partition is uniform then Brenner and Thomée prove that

$$\|(R(\tfrac{t}{n}A)^n - e^{tA})A^{-p}\| \le C\big(\frac{t}{n}\big)^p.$$

Moreover, if $|R(\infty)| < 1$ then

$$\|R(\tfrac{t}{n}A)^n - e^{tA}\| \le C\frac{1}{n^p}.$$

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• If e^{tA} is analytic and the partition is nonuniform then it is proved in [Yan] that

$$\|(P_n(A) - e^{tA})A^{-p}\| \leq C\tau_{\mathsf{m}}^p,$$

where $\tau_{\mathsf{m}} = \max_k \tau_k$. Moreover, if $|R(\infty)| < 1$ then Saito proves in [Sai] that

$$\|P_n(A) - e^{tA}\| \leq C\big(\frac{\tau_{\mathsf{m}}}{\tau_*}\big)^p \tau_{\mathsf{m}}^p,$$

where $\tau_* = \min_k \tau_k$.

• If e^{tA} is not necessarily analytic and the partition is uniform then Brenner and Thomée prove in [BT2] that

$$\|(P_n(A) - e^{tA})A^{-p}\| \leq Ct^p n^{-\frac{p^2}{p+1}},$$

(see also Remark 5.3 below). Irrespective to the analytic case, $R(\frac{t}{n}A)^n$ may diverges. For example, if $A = \mathrm{d}/\mathrm{d}x$ and $X = L^\infty(\mathbb{R})$ then by [BT1] Theorem 4.2, for every $\varepsilon > 0$ there exists some p-acceptable function R_ε with $R_\varepsilon(\infty) = 0$ such that

$$\|R_\varepsilon(\tfrac{t}{n}A)^n\| \geq Cn^{\frac{1}{2}-\varepsilon}.$$

Without the condition $R_\varepsilon(\infty) = 0$, the value $\varepsilon = 0$ is allowed in the above estimate.

This paper focuses on the case where e^{tA} is not analytic and the partition is nonuniform.

We will now introduce our main results. In Theorem 5.1, we will prove that for $\alpha \in (1/2, p]$, the following holds

$$\|(P_n(A) - e^{tA})(1 - A)^{-\alpha}\| \leq C(t)\tau_{\mathsf{m}}^{(\alpha-1/2)\frac{p}{p+1}}.$$

Thus we obtain convergence on a continuum of intermediate spaces between X and the domain of A^p (see also [Kov]). If $A = \mathrm{d}/\mathrm{d}x$, $X = C_0(\mathbb{R})$, $|R| = 1$ on $\mathrm{i}\mathbb{R}$ and the partition is quasiuniform in the sense of Section 2 then

$$\|P_n(A)(1 - A)^{-\alpha}\| \xrightarrow[n\to\infty]{} \infty \qquad \forall \alpha < 1/2.$$

The reader is refered to Theorem 6.1 and Corollary 6.2 for precise statements. Besides, following [Yan], we study approximations of the time derivative. We prove in Theorem 7.1 that for $\alpha > 3/2$,

$$\frac{1}{\tau_n}\big(P_n(A) - P_{n-1}(A)\big) \to \frac{\mathrm{d}}{\mathrm{d}t}e^{tA} \quad \text{ in } \mathcal{L}(D(A^\alpha), X).$$

It is worthwhile to mention that a similar estimation is obtained in [Yan] only when A generates an analytic C_0-semigroup.

This paper is organized as follows. In Section 2, we fix some notations and state our main assumptions. In Section 3, we introduce the so-called $\mathcal{M}$*-functional calculus* which allows to define operators-valued functionals. This calculus is the main tool for proving, in Section 5 and 7, convergence results toward e^{tA} and $\frac{\mathrm{d}}{\mathrm{d}t}e^{tA}$. In Section 6, we give examples where the Crank-Nicholson scheme diverges.

2. Notation and main assumptions

Though out this paper, t, p, Γ and H will denote respectively a nonnegative time, a positive integer, the Euler function and the Heaviside step function. The notation $[\mathrm{Re}\, z \leq 0]$ and $[\mathrm{Im}\, z \geq 0]$ stand for the left and upper half-complex plane. For every function f defined on a subset of $\mathbb{C}$, $f_{\mathbb{R}}$ denotes the restriction of f to $\mathbb{R}$.

In the sequel, $A : D(A) \subset X \to X$ is a closed densely defined linear operator on the Banach space X. The norm on X and on the space of bounded linear operators acting on X will be both denoting by $\|\cdot\|$. We will further assume that A generates a strongly continuous semigroup of bounded linear operator $\{e^{tA} \mid t \geq 0\}$. Moreover we suppose that this semigroup is bounded i.e.

$$M := \sup_{t\geq 0} \|e^{tA}\| < \infty. \tag{2.1}$$

For any positive integer n, a sequence of positive numbers $(\tau_1, \tau_2, \cdots, \tau_n)$ whose sum equals t is called a *n-grid*. We denote

$$\tau_{\mathsf{m}} := \tau_{\mathsf{m}}^n := \max_{1\leq k\leq n} \tau_k, \qquad \tau_* := \tau_*^n := \min_{1\leq k\leq n} \tau_k.$$

As a simple consequence, $\tau_{\mathsf{m}} \geq t/n$ and $\tau_* \leq t/n$. Moreover, without loss of generality, we may assume $\tau_{\mathsf{m}} \leq 1$. The case $\tau_{\mathsf{m}} = \tau_*$ corresponds to uniform partition of $[0, t]$. According to [Yan], for any positive number μ, a grid $(\tau_1, \tau_2, \cdots, \tau_n)$ is said to be *μ–quasiuniform* if $\tau_{\mathsf{m}}/\tau_* \leq \mu$.

Definition 2.1. *We say that a rational complex function R is p-**acceptable** if*

(a) $|R(z)| \leq 1$ *for all* $Re(z) \leq 0$*;*

(b) $R(\mathrm{i}x) = e^{\mathrm{i}x} + O(x^{p+1})$ *as* $x \to 0$, $x \in \mathbb{R}$.

In this definition, since $p \geq 1$ the condition (b) implies that $R(0) = R'(0) = 1$ and the condition (a) implies that $|R(\mathrm{i}\infty)| \leq 1$, consequently the degree of R is nonpositive, that is

$$R := \frac{P}{Q} \quad \text{and} \quad \operatorname{degree} R := \operatorname{degree} P - \operatorname{degree} Q \leq 0. \tag{2.2}$$

In the sequel, $(\tau_1, \tau_2, \cdots, \tau_n)$ is a n-grid, R a p-acceptable rational function and P_n will denote the function defined for all z in $[\mathrm{Re}\, z \leq 0]$ by

$$P_n(z) = R(\tau_1 z) \dots R(\tau_n z).$$

For simplicity we put $P_{n-1}(z) = R(\tau_1 z) \dots R(\tau_{n-1} z)$ and looking out that in this case $\sum_{k=1}^{n-1} \tau_k \neq t$. Moreover, we define $P_n(A)$ by (1.1). It may be observed that our results extend to the case where $P_n(A) = R_1(\tau_1 A) \dots R_n(\tau_n A)$ provided $R_1, \dots, R_n$ are p-acceptable functions satisfying Definition 2.1 (b) uniformly with respect to n i.e.

$$|R_k(\mathrm{i}x) - e^{\mathrm{i}x}| \leq C|x|^{p+1} \quad \forall x \in [-1, 1],\ k = 1, \dots, n,$$

where C is independent of n.

The space of all continuous linear operators defined on a normed vector space Y with values in X will be denoted by $\mathcal{L}(Y, X)$. Regarding functions spaces, the Lebesgue spaces of complex-valued functions defined on $\mathbb{R}$ are denoted by $L^q(\mathbb{R})$ $(1 \leq q \leq \infty)$, with norm $\|\cdot\|_q$. Besides

$$W^{1,q}(\mathbb{R}) = \{f : \mathbb{R} \to \mathbb{C} \mid f \text{ and } f' \in L^q(\mathbb{R})\},$$
$$C(\mathbb{R}) = \{f : \mathbb{R} \to \mathbb{C} \mid f \text{ is continuous on } \mathbb{R}\}.$$

Let

$$\mathcal{M}_+ = \{f \in C(\mathbb{R}) \mid \mathcal{F}f \in L^1(\mathbb{R}) \text{ and } \mathcal{F}f \text{ is supported in } [0,\infty)\} \tag{2.3}$$

where $\mathcal{F}f$ is the Fourier transform of f, i.e.

$$\mathcal{F}f(s) = \int_{-\infty}^{\infty} e^{-\mathrm{i}xs} f(x)\,\mathrm{d}x \qquad \forall s \in \mathbb{R}.$$

In the sequel we will use the following inequality, known as *Carlson's inequality* (see [Car]):

$$\|\mathcal{F}f\|_1 \leq 2\sqrt{2}\pi \|f\|_2^{\frac{1}{2}} \|f'\|_2^{\frac{1}{2}} \qquad \forall f \in W^{1,2}(\mathbb{R}). \tag{2.4}$$

Let also $\mathcal{H}_+$ be the set of all $f : [\operatorname{Im} z \geq 0] \to \mathbb{C}$ holomorphic in $[\operatorname{Im} z \geq 0]$ (i.e. f has an holomorphic extension in a neighborhood of $[\operatorname{Im} z \geq 0]$) and converging to zero as $|z| \to \infty$.

Finally, various constants independent of t, n and the grid $(\tau_1, \tau_2, \cdots, \tau_n)$ will be generically denoted by the letters C or K. In order to emphasize the dependence of C on some parameters $\alpha_1, \ldots, \alpha_m$, we will use the notation $C_{\alpha_1,\ldots,\alpha_m}$ and we keep the same notation even if the values of $C_{\alpha_1,\ldots,\alpha_m}$ are not the same in different formulae.

3. $\mathcal{M}$-functional calculus

Under notation and assumptions of Section 2, for any f in $\mathcal{M}_+$, we define a $\mathcal{M}$-functional calculus by

$$f(-\mathrm{i}A)u = \int_0^{\infty} e^{sA} u \mathcal{F}f(s)\,ds \qquad \text{for all } u \in X. \tag{3.1}$$

This defines a bounded linear operator $f(-\mathrm{i}A)$ satisfying

$$\|f(-\mathrm{i}A)\| \leq M \|\mathcal{F}f\|_1. \tag{3.2}$$

Let $\alpha > 0$ and $\lambda \in [\operatorname{Re} z > 0]$. By choosing the principal determination of the complex logarithm, the function

$$f_{\alpha,\lambda} : \mathbb{R} \to \mathbb{C}, \qquad x \mapsto (\lambda - \mathrm{i}x)^{-\alpha}$$

is well defined and belongs to $\mathcal{M}_+$ since it is well known that

$$\mathcal{F}f_{\alpha,\lambda}(s) = \frac{1}{\Gamma(\alpha)} H(s) s^{\alpha-1} e^{-s\lambda} \qquad \forall s \in \mathbb{R}, \tag{3.3}$$

where H denotes the Heaviside step function. Consequently,

$$f_{1,\lambda}(-\mathrm{i}A) = \int_0^{\infty} e^{sA} e^{-s\lambda} ds = (\lambda - A)^{-1}. \tag{3.4}$$

Here we want to generalize this formula to any entire power of $(\lambda - A)^{-1}$.

Lemma 3.1. *Under the above assumptions and notation, if $\alpha = m$ is a positive integer then*

$$f_{m,\lambda}(-\mathrm{i}A) = (\lambda - A)^{-m},$$

i.e. for any $m \in \mathbb{N}$,

$$\frac{1}{(m-1)!}\int_0^\infty e^{sA}s^{m-1}e^{-s\lambda}\,\mathrm{d}s = (\lambda - A)^{-m}. \tag{3.5}$$

Proof. We proceed by induction. The case $m = 1$ is given in (3.4), suppose $m \geq 1$. Then, from the identity $\mathcal{F}(fg) = \mathcal{F}f * \mathcal{F}g$, we deduce

$$\int_0^\infty e^{sA}\mathcal{F}f_{m,\lambda}(s)\,\mathrm{d}s = \int_0^\infty e^{sA}\int_{\mathbb{R}}\mathcal{F}f_{1,\lambda}(y)\mathcal{F}f_{m-1,\lambda}(s-y)\,\mathrm{d}y\,\mathrm{d}s.$$

By using the fact that these Fourier transforms are supported in $[0,\infty)$, we obtain (3.5) as desired. □

This formula can also be generalized for any fractional power of $(\lambda - A)^{-1}$. If $\alpha > 0$ is not an integer then, in accordance with Lemma 3.1, the bounded linear operator $f_{\alpha,\lambda}(-\mathrm{i}A)$ will be denoted by $(\lambda - A)^{-\alpha}$ i.e.

$$(\lambda - A)^{-\alpha} := \frac{1}{\Gamma(\alpha)}\int_0^\infty e^{sA}s^{\alpha-1}e^{-\lambda s}\,\mathrm{d}s. \tag{3.6}$$

Since we can prove in a standard way that $(1 - A)^{-\alpha}$ is one-to-one, we put $D(A^\alpha) := (1 - A)^{-\alpha}X$ and define the unbounded operator $(1 - A)^\alpha$ with domain $D(A^\alpha)$ by $(1 - A)^\alpha := [(1 - A)^{-\alpha}]^{-1}$, which is valid in the intermediate space $D(A^\alpha)$ equipped with the norm

$$\|u\|_{A^\alpha} = \|(1 - A)^\alpha u\|. \tag{3.7}$$

The following lemmas give criteria for functions to belong to $\mathcal{M}_+$. First we have

Lemma 3.2. *Let $f \in \mathcal{H}_+$ be such that $\mathcal{F}f_{\mathbb{R}}$ belongs to $L^1(\mathbb{R})$. Then $f_{\mathbb{R}}$ lies in $\mathcal{M}_+$.*

Proof. It is enough to show that $\mathcal{F}f_{\mathbb{R}}$ is supported in $[0,\infty)$. For every positive r, let $\gamma_r = \{re^{\mathrm{i}\theta} \mid 0 \leq \theta \leq \pi\}$. Due to the residue formula,

$$\mathcal{F}f_{\mathbb{R}}(s) = \int_{\mathbb{R}} e^{-\mathrm{i}sx}f(x)\,\mathrm{d}x = -\lim_{r\to\infty}\int_{\gamma_r} e^{-\mathrm{i}sz}f(z)\,\mathrm{d}z.$$

Since $f \in \mathcal{H}_+$, this limit is zero for any negative s. □

Lemma 3.3. *Let $g, h : [\operatorname{Im} z \geq 0] \to \mathbb{C}$ be continuous functions in $[\operatorname{Im} z \geq 0]$ such that*

(a) *the product gh belongs to $\mathcal{H}_+$;*
(b) *$g_{\mathbb{R}}$ and $h_{\mathbb{R}}$ belong to $W^{1,\infty}(\mathbb{R})$ and $W^{1,2}(\mathbb{R})$ respectively.*

Then $gh_{\mathbb{R}}$ belongs to $\mathcal{M}_+$ and

$$\|\mathcal{F}(gh_{\mathbb{R}})\|_1 \leq C\|g_{\mathbb{R}}\|_{W^{1,\infty}}\|h_{\mathbb{R}}\|_{W^{1,2}}.$$

Proof. The above estimate follows from Carlson's inequality (2.4). Thus Lemma 3.2 yields $gh_{\mathbb{R}} \in \mathcal{M}_+$. □

The following statement will be used later.

Theorem 3.4. *Let $\alpha > 0$ and R be a rational function bounded on $[\mathrm{Re} z \leq 0]$ with non positive degree. Then the following functions of the real variable x,*

$$x \mapsto e^{\mathrm{i}tx}(1-\mathrm{i}x)^{-\alpha}, \quad x \mapsto R(x)(1-\mathrm{i}x)^{-\alpha}$$

belong to $\mathcal{M}_+$ and

$$e^{tA}(1-A)^{-\alpha} = \int_0^\infty e^{sA}\,\mathcal{F}(e^{itx}(1-ix)^{-\alpha})(s)\,\mathrm{d}s, \tag{3.8}$$

$$= \frac{1}{\Gamma(\alpha)}\int_0^\infty e^{(t+s)A}\,s^{\alpha-1}e^{-s}\,\mathrm{d}s \tag{3.9}$$

$$R(A)(1-A)^{-\alpha} = \int_0^\infty e^{sA}\,\mathcal{F}(R(ix)(1-ix)^{-\alpha})(s)\,\mathrm{d}s. \tag{3.10}$$

Proof. Since $\mathcal{F}(e^{\mathrm{i}tx}(1-\mathrm{i}x)^{-\alpha})(s) = \mathcal{F}((1-\mathrm{i}x)^{-\alpha})(s-t)$, we deduce with (3.3) that $x \mapsto e^{\mathrm{i}tx}(1-\mathrm{i}x)^{-\alpha}$ belongs to $\mathcal{M}_+$. Hence

$$\begin{aligned}\int_0^\infty e^{sA}\,\mathcal{F}(e^{itx}(1-ix)^{-\alpha})(s)\,\mathrm{d}s &= \frac{1}{\Gamma(\alpha)}\int_0^\infty e^{(t+s)A}s^{\alpha-1}e^{-s}\,\mathrm{d}s\\ &= \frac{e^{tA}}{\Gamma(\alpha)}\int_0^\infty e^{sA}s^{\alpha-1}e^{-s}\,\mathrm{d}s\\ &= e^{tA}(1-A)^{-\alpha},\end{aligned}$$

in view of (3.6). We prove (3.10) by using partial fractions decomposition for R: we first show with Lemma 3.3 that $x \mapsto R(\mathrm{i}x)(1-\mathrm{i}x)^{-\alpha}$ is in $\mathcal{M}_+$, secondly, by using Lemma 3.1, we arrive at (3.10). □

4. Some estimates on P_n

The $\mathcal{M}$-functional calculus allows to reduce our problem to one dimensional analysis. In this section, we will give some technical results regarding the rational function P_n. With the notation of Section 2, we have

Lemma 4.1. *Suppose that R is a p–acceptable rational function. Then there exists a constant C such that for all x in $\mathbb{R}$,*

$$\left|P_n(\mathrm{i}x) - e^{\mathrm{i}tx}\right| \leq C\tau_{\mathsf{m}}^p t|x|^{p+1} \tag{4.1}$$

$$\left|\frac{\mathrm{d}}{\mathrm{d}x}\big(P_n(\mathrm{i}x) - e^{\mathrm{i}tx}\big)\right| \leq C(t+1)^2\min\big(1, \tau_{\mathsf{m}}^p(|x|^p + |x|^{p+1})\big) \tag{4.2}$$

$$\sup_{x\in\mathbb{R}} |(P_n(\mathrm{i}x) - e^{\mathrm{i}tx})(1-\mathrm{i}x)^{-s}| \leq C(t+1)\tau_{\mathsf{m}}^{\frac{sp}{p+s+1}}. \tag{4.3}$$

Proof. For every $x \in \mathbb{R}$, $P_n(\mathrm{i}x) - e^{\mathrm{i}tx}$ is equal to

$$\begin{aligned}&R(\mathrm{i}\tau_1 x)\prod_{k=2}^n R(\mathrm{i}\tau_k x) - e^{\mathrm{i}\tau_1 x}\prod_{k=2}^n e^{\mathrm{i}\tau_k x}\\ &\qquad = (R(\mathrm{i}\tau_1 x) - e^{\mathrm{i}\tau_1 x})\prod_{k=2}^n R(\mathrm{i}\tau_k x) + e^{\mathrm{i}\tau_1 x}\Big(\prod_{k=2}^n R(\mathrm{i}\tau_k x) - \prod_{k=2}^n e^{\mathrm{i}\tau_k x}\Big).\end{aligned}$$

Since R is p–acceptable, $|R(i\tau_1 x) - e^{\mathrm{i}\tau_1 x}| \le C|\tau_1 x|^{p+1}$. Using also the boundedness of R on $\mathrm{i}\mathbb{R}$, we get

$$
\begin{aligned}
\left|P_n(\mathrm{i}x) - e^{\mathrm{i}tx}\right| &\le C|\tau_1 x|^{p+1} + \left|\prod_{k=2}^{n} R(\mathrm{i}\tau_k x) - \prod_{k=2}^{n} e^{\mathrm{i}\tau_k x}\right| \\
&\le C\sum_{k=1}^{n} |\tau_k x|^{p+1}, \qquad (4.4)
\end{aligned}
$$

by induction. Recalling that $\tau_k \le \tau_{\mathsf{m}}$ and $\sum \tau_k = t$, we obtain (4.1).

To prove (4.2), we write $\frac{\mathrm{d}}{\mathrm{d}x}\big(P_n(\mathrm{i}x) - e^{\mathrm{i}tx}\big)$ in the form

$$
\begin{aligned}
&\mathrm{i}\sum_{k=1}^{n}\left(\tau_k R'(\mathrm{i}\tau_k x)\prod_{\ell\ne k} R(\mathrm{i}\tau_\ell x) - \tau_k e^{\mathrm{i}\tau_k x}\prod_{\ell\ne k} e^{\mathrm{i}\tau_\ell x}\right) = \\
&\quad \mathrm{i}\sum_{k=1}^{n}\left(\tau_k\big(R'(\mathrm{i}\tau_k x) - e^{\mathrm{i}\tau_k x}\big)\prod_{\ell\ne k} R(\mathrm{i}\tau_\ell x) + \tau_k e^{\mathrm{i}\tau_k x}\big(\prod_{\ell\ne k} R(\mathrm{i}\tau_\ell x) - \prod_{\ell\ne k} e^{\mathrm{i}\tau_\ell x}\big)\right). \qquad (4.5)
\end{aligned}
$$

Since R' and R are bounded on $\mathrm{i}\mathbb{R}$, we deduce that

$$
\left|\frac{\mathrm{d}}{\mathrm{d}x}\big(P_n(\mathrm{i}x) - e^{\mathrm{i}tx}\big)\right| \le Ct. \qquad (4.6)
$$

Furthermore by Definition 2.1 (b) and (4.4), we have $|R'(\mathrm{i}x) - e^{\mathrm{i}x}| \le C|x|^p$ and

$$
\left|\prod_{\ell\ne k} R(\mathrm{i}\tau_\ell x) - \prod_{\ell\ne k} e^{\mathrm{i}\tau_\ell x}\right| \le Ct|x|^{p+1}\tau_{\mathsf{m}}^{p},
$$

thus going back to (4.5), we deduce

$$
\begin{aligned}
\left|\frac{\mathrm{d}}{\mathrm{d}x}\big(P_n(\mathrm{i}x) - e^{\mathrm{i}tx}\big)\right| &\le C\sum_{k=1}^{n} \tau_k^{p+1}|x|^p + \tau_k t\tau_{\mathsf{m}}^{p}|x|^{p+1} \\
&\le C(t+1)^2\tau_{\mathsf{m}}^{p}(|x|^p + |x|^{p+1}).
\end{aligned}
$$

Then using also (4.6), (4.2) follows.

In order to show (4.3), for any $r \in \mathbb{R}$ there are two alternatives:
(i) If $|x| \le \tau_{\mathsf{m}}^{r}$ then according to (4.1)

$$
\begin{aligned}
|(P_n(\mathrm{i}x) - e^{\mathrm{i}tx})(1-\mathrm{i}x)^{-s}| &\le |P_n(\mathrm{i}x) - e^{\mathrm{i}tx}| \\
&\le C\tau_{\mathsf{m}}^{p} t|x|^{p+1} \\
&\le Ct\tau_{\mathsf{m}}^{r(p+1)+p}.
\end{aligned}
$$

(ii) If $|x| > \tau_{\mathsf{m}}^{r}$ then by Definition 2.1 (a),

$$
|(P_n(\mathrm{i}x) - e^{\mathrm{i}tx})(1-\mathrm{i}x)^{-s}| \le 2|x|^{-s} \le 2\tau_{\mathsf{m}}^{-rs}.
$$

Next by choosing $r = -\frac{p}{p+s+1}$, we get (4.3) which completes the proof of the lemma. $\square$

Lemma 4.2. *Let R be a p-acceptable rational function. Then for any positive s and τ, we have*

$$\sup_{x\in\mathbb{R}} \left|\big(R'(\mathrm{i}\tau x) - e^{\mathrm{i}\tau x}\big)(1-\mathrm{i}x)^{-s}\right| \leq C\tau^{\frac{sp}{s+p}}. \tag{4.7}$$

Proof. Let $r<0$. (i) If $|x| \leq \tau^r$ then since $R'(\mathrm{i}\tau x) - e^{\mathrm{i}\tau x} = O\big((\tau x)^p\big)$,

$$\left|\big(R'(\mathrm{i}\tau x) - e^{\mathrm{i}\tau x}\big)(1-\mathrm{i}x)^{-s}\right| \leq C|\tau x|^p \leq C\tau^{(1+r)p}.$$

(ii) If $|x| > \tau^r$ then since R' is bounded on $\mathrm{i}\mathbb{R}$, we have

$$\left|\big(R'(\mathrm{i}\tau x) - e^{\mathrm{i}\tau x}\big)(1-\mathrm{i}x)^{-s}\right| \leq C|x|^{-s} \leq C\tau^{-rs}.$$

Now, by choosing $r = -\frac{p}{p+s}$, we get (4.7). $\square$

Lemma 4.3. *Under the assumptions of Lemma 4.2, we have*

$$\sup_{x\in\mathbb{R}} \left|\Big\{\frac{\mathrm{d}}{\mathrm{d}x}(P_n(\mathrm{i}x) - e^{\mathrm{i}tx})\Big\}(1-\mathrm{i}x)^{-s}\right| \leq C(t^2+1)\tau_{\mathsf{m}}^{\frac{sp}{p+s+1}}. \tag{4.8}$$

Proof. By differentiation,

$$\Big\{\frac{\mathrm{d}}{\mathrm{d}x}(P_n(\mathrm{i}x) - e^{\mathrm{i}tx})\Big\}(1-\mathrm{i}x)^{-s} = \sum_{k=1}^{n} \mathrm{i}\tau_k(A_1+A_2),$$

with

$$A_1 = \big(R'(\mathrm{i}\tau_k x) - e^{\mathrm{i}\tau_k x}\big)\prod_{\ell\neq k} R(\mathrm{i}\tau_\ell x)(1-\mathrm{i}x)^{-s}$$

$$A_2 = e^{\mathrm{i}\tau_k x}\Big(\prod_{\ell\neq k} R(\mathrm{i}\tau_\ell x) - \prod_{\ell\neq k} e^{\mathrm{i}\tau_\ell x}\Big)(1-\mathrm{i}x)^{-s}.$$

By (4.7), $|A_1| \leq C\tau_{\mathsf{m}}^{sp/(p+s)} \leq C\tau_{\mathsf{m}}^{sp/(p+s+1)}$, while $\tau_{\mathsf{m}} \leq 1$. For estimating A_2, let $r<0$. (i) If $|x| \leq \tau^r$ then by (4.4), $|A_2| \leq Ct\tau_{\mathsf{m}}^{p+r(p+1)}$. (ii) If $|x| > \tau^r$ then since R is bounded, $|A_2| \leq C|x|^{-s} \leq C\tau_{\mathsf{m}}^{-rs}$. Now by choosing $r = -\frac{p}{p+s+1}$, we obtain $|A_2| \leq C(t+1)\tau_{\mathsf{m}}^{sp/(p+s+1)}$. Then (4.8) follows. $\square$

5. On the rate of convergence

We would like to estimate the rate of convergence of the approximation scheme. For this, we will use the notation and assumptions of Section 2. In particular, $\tau_{\mathsf{m}} \leq 1$.

Theorem 5.1. *If R is a p-acceptable rational function and $\alpha \in (1/2, p]$ is given, then*

$$\|(P_n(A) - e^{tA})(1-A)^{-\alpha}\| \leq MC_{p,\alpha}(t+1)^{3/2}\tau_{\mathsf{m}}^{(\alpha-1/2)\frac{p}{p+1}}. \tag{5.1}$$

Proof. We adapt the method developed by Brenner and Thomée in [BT2] to nonuniform partitions. We use the $\mathcal{M}$-functional calculus introduced in Section 3 which gives simpler computations. For every positive integer n and $\alpha > 0$, we define

$$f_n : \mathbb{R} \to \mathbb{C}, \quad x \mapsto (1-\mathrm{i}x)^{-\alpha}(P_n(\mathrm{i}x) - e^{\mathrm{i}tx})$$

and $g_n(\cdot) := f_n(\tau^{-1}\cdot)$ where $\tau := \tau_{\mathsf{m}}^{p/(p+1)}$. According to Theorem 3.4, f_n is in $\mathcal{M}_+$ and $(P_n(A) - e^{tA})(1 - A)^{-\alpha}$ is equal to $f_n(-\mathrm{i}A)$. By (3.2) and Carlson's inequality (2.4), we have

$$\begin{aligned} \|f_n(-\mathrm{i}A)\| &\leq M\|\mathcal{F}f_n\|_1 = M\|\mathcal{F}g_n\|_1 \\ &\leq MC\|g_n\|_2^{1/2}\,\|g_n'\|_2^{1/2}. \end{aligned} \tag{5.2}$$

Moreover by Lemma 4.1,

$$|P_n(\mathrm{i}\tfrac{x}{\tau}) - e^{\mathrm{i}\frac{t}{\tau}x}| \leq Ct|x|^{p+1}$$

with our choice for τ. Therefore

$$|P_n(\mathrm{i}\tfrac{x}{\tau}) - e^{\mathrm{i}\frac{t}{\tau}x}| \leq C\min(t|x|^{p+1}, 1). \tag{5.3}$$

We deduce that $|g_n(x)| \leq C\tau^\alpha|x|^{-\alpha}\min(t|x|^{p+1}, 1)$ and since $\alpha \in (1/2, p]$,

$$\|g_n\|_2 \leq C_{p,\alpha}(t+1)\tau^\alpha. \tag{5.4}$$

Let us now estimate $\|g_n'\|_2$. We have

$$g_n'(x) = \underbrace{\tfrac{\mathrm{i}\alpha}{\tau}(1 - \mathrm{i}\tfrac{x}{\tau})^{-\alpha-1}(P_n(\mathrm{i}\tfrac{x}{\tau}) - e^{\mathrm{i}\frac{t}{\tau}x})}_{=A} + \underbrace{(1 - \mathrm{i}\tfrac{x}{\tau})^{-\alpha}(P_n(\mathrm{i}\tfrac{x}{\tau}) - e^{\mathrm{i}\frac{t}{\tau}x})'}_{=B}$$

By (5.3),

$$\begin{aligned} |A| &\leq \alpha\tau^\alpha|x|^{-\alpha-1}C\min(t|x|^{p+1}, 1) \\ &\leq \alpha C(t+1)\tau^\alpha\min(|x|^{p-\alpha}, |x|^{-\alpha-1}). \end{aligned} \tag{5.5}$$

In order to bound $|B|$ from above, we first consider its second factor. According to (4.2),

$$\left|\tfrac{\mathrm{d}}{\mathrm{d}x}(P_n(\mathrm{i}\tfrac{x}{\tau}) - \mathrm{e}^{\mathrm{i}\frac{t}{\tau}x})\right| \leq \tau^{-1}C(t+1)^2\min(1, |x|^p + |x|^{p+1}),$$

since $\tau = \tau_{\mathsf{m}}^{p/(p+1)}$ and $\tau \leq 1$. Thus

$$|B| \leq C(t+1)^2\tau^{\alpha-1}\min(|x|^{-\alpha}, |x|^{p-\alpha} + |x|^{p+1-\alpha}). \tag{5.6}$$

From (5.5) and (5.6), we obtain since $\alpha \in (1/2, p]$ and $\tau \leq 1$,

$$\|g_n'\|_2 \leq C_{p,\alpha}(t+1)^2\tau^{\alpha-1}. \tag{5.7}$$

Going back to (5.2), we finally get in view of (5.4) and (5.7),

$$\|f_n(-\mathrm{i}A)\| \leq MC_{p,\alpha}(t+1)^{3/2}\tau^{\alpha-1/2},$$

which proves (5.1). □

Remark 5.2. Inequality (5.1) may be restated as

$$\|(P_n(A) - e^{tA})u\| \leq MC_{p,\alpha}(t+1)^{3/2}\tau_{\mathsf{m}}^{(\alpha-1/2)\frac{p}{p+1}}\|u\|_{A^\alpha} \quad \forall u \in D(A^\alpha).$$

Consequently, for every sequence $(\tau_k^n)_{1\leq k\leq n}$, $n \geq 1$ of grids satisfying $\tau_{\mathsf{m}} \to 0$ as $n \to \infty$, we have

$$P_n(A) \xrightarrow[n\to\infty]{} e^{tA} \quad \text{in } \mathcal{L}(D(A^\alpha), X).$$

Remark 5.3. In the case of constant time steps, the best convergence exponent for $\alpha = 0, ..., p+1$, $\alpha \neq (p+1)/2$ is

$$\beta(s) = \alpha \frac{p}{p+1} + \min\Big(0, \frac{\alpha}{p+1} - \frac{1}{2}\Big).$$

See [BT2] Theorem 4.

In general, we have the following upper bound for the best convergence exponent.

Theorem 5.4. *Let $C, C_1, \mu \geq 1$ be given. Let also $(\tau_k^n)_{1\leq k\leq n}$, $n \geq 1$ be a sequence of grids satisfying*

$$\frac{\tau_{\mathsf{m}}}{\tau_*} \leq \mu C_1^n, \quad \tau_{\mathsf{m}} \leq \frac{Ct}{n} \quad \forall n \geq 1.$$

Moreover assume that

$$\limsup_{n\to\infty} \|(P_n(A) - e^{tA})(1-A)^{-\alpha}\| > 0,$$

for every positive α strictly less than a certain threshold α_c. If for some real $\alpha > \alpha_c$ there exists $\beta(\alpha) > 0$ such that

$$\|(P_n(A) - e^{tA})(1-A)^{-\alpha}\| \leq C_{\alpha,t,p} \tau_{\mathsf{m}}^{\beta(\alpha)} \tag{5.8}$$

then $\alpha_c \leq 1/2$ and

$$\beta(\alpha) \leq \begin{cases} \frac{3\alpha}{2\alpha_c} & \text{if } C_1 > 1, \\ \frac{\alpha}{2\alpha_c} & \text{if } C_1 = 1. \end{cases}$$

If the grid $(\tau_1, \ldots, \tau_n)$ is μ-quasiuniform (i.e. $C_1 = 1$) and $\alpha_c = 1/2$ then the above theorem expresses that the optimal rate of convergence on $D(A^\alpha)$ is less or equal to α. Section 6 presents situations where α_c is indeed equal to $1/2$.

The proof of Theorem 5.4 relies on the following Lemma.

Lemma 5.5. *Let $\gamma \in (0,1]$ and u be in $D(A^\gamma)$. Then*

$$\|e^{tA}u - u\| \leq K_{M,\gamma} \|u\|_{A^\gamma} t^\gamma \quad \forall t \geq 0. \tag{5.9}$$

Moreover if $v := v_{\tau,\alpha} := (1-\tau A)^{-\alpha} u$ with $\tau, \alpha > 0$ then

$$\|u - v\| \leq \frac{\Gamma(\alpha+\gamma)}{\Gamma(\alpha)} K_{M,\gamma} \|u\|_{A^\gamma} \tau^\gamma. \tag{5.10}$$

Remark 5.6. Inequality (5.9) yields the continuous injection of the interpolation space $D(A^\alpha)$ into the so-called *Favard space* of order γ,

$$F_\gamma = \Big\{u \in X \mid \sup_{t>0} \|\tfrac{1}{t^\gamma}(e^{tA}u - u)\| < \infty\Big\}$$

endowed with the norm

$$\|u\|_{F_\gamma} = \sup_{t>0} \|\tfrac{1}{t^\gamma}(e^{tA}u - u)\|.$$

We refer the reader to [EN] for more details on Favard spaces.

Proof of Lemma 5.5. According to (3.9) and the boundedness of e^{tA}, we have

$$\|e^{tA}u - u\| \le 2M\|u\|_{A^\gamma}.$$

As a consequence, (5.9) holds true for $t \ge 1$. If $t < 1$ then Theorem 3.4 yields

$$e^{tA}(1-A)^{-\gamma} = \frac{1}{\Gamma(\gamma)}\int_t^\infty e^{sA}(s-t)^{\gamma-1}e^{-s+t}\,\mathrm{d}s.$$

Hence

$$\begin{aligned}
&\Gamma(\gamma)\big(e^{tA}(1-A)^{-\gamma} - (1-A)^{-\gamma}\big)\\
&= \int_t^\infty e^{sA}\big\{(s-t)^{\gamma-1}e^{-s+t} - s^{\gamma-1}e^{-s}\big\}\,\mathrm{d}s - \int_0^t e^{sA}s^{\gamma-1}e^{-s}\,\mathrm{d}s\\
&=: \qquad I_1 \qquad + \qquad I_2.
\end{aligned} \tag{5.11}$$

We bound I_2 as follows:

$$\|I_2\| \le M\int_0^t s^{\gamma-1}e^{-s}\,\mathrm{d}s \le \frac{M}{\gamma}t^\gamma. \tag{5.12}$$

Regarding I_1, the identity

$$(s-t)^{\gamma-1}e^t - s^{\gamma-1} = \big\{(s-t)^{\gamma-1} - s^{\gamma-1}\big\}e^t + (e^t-1)s^{\gamma-1},$$

leads to the decomposition of I_1 into the sum $J_1 + J_2$ where

$$\begin{aligned}
J_1 &:= \int_t^\infty e^{sA}e^{-s+t}\big\{(s-t)^{\gamma-1} - s^{\gamma-1}\big\}\,\mathrm{d}s,\\
J_2 &:= (e^t-1)\int_t^\infty e^{sA}s^{\gamma-1}e^{-s}\,\mathrm{d}s.
\end{aligned}$$

Furthermore, $M^{-1}\|J_1\|$ is bounded by

$$\begin{aligned}
&\int_t^\infty e^{-s+t}\big\{(s-t)^{\gamma-1} - s^{\gamma-1}\big\}\,\mathrm{d}s\\
&\qquad = \int_0^\infty e^{-s}s^{\gamma-1}\,\mathrm{d}s - \int_0^\infty e^{-s+t}s^{\gamma-1}\,\mathrm{d}s + \int_0^t e^{-s+t}s^{\gamma-1}\,\mathrm{d}s\\
&\qquad = (1-e^t)\int_0^\infty e^{-s}s^{\gamma-1}\,\mathrm{d}s + e^t\int_0^t e^{-s}s^{\gamma-1}\,\mathrm{d}s\\
&\qquad \le \frac{e}{\gamma}t^\gamma,
\end{aligned}$$

since $t < 1$ and $1 - e^t \le 0$. Thus $\|J_1\| \le K_{\gamma,M}t^\gamma$. Since $\|J_2\|$ is easily estimated by $Me\Gamma(\gamma)t$ and $t, \gamma \le 1$, we deduce that $\|I_1\| \le K_{\gamma,M}t^\gamma$. With (5.11) and (5.12), it results that

$$\|e^{tA}(1-A)^{-\gamma} - (1-A)^{-\gamma}\| \le K_{\gamma,M}t^\gamma \qquad \forall t \in [0,1)$$

and (5.9) follows.

We now prove (5.10). For u, v as in the statement of the lemma, we have

$$u - v = \frac{1}{\Gamma(\alpha)}\int_0^\infty (u - e^{s\tau A}u)s^{\alpha-1}e^{-s}\,\mathrm{d}s.$$

Hence with (5.9),

$$\begin{aligned}\|u-v\| &\leq \frac{K_{\gamma,M}}{\Gamma(\alpha)}\int_0^\infty (s\tau)^\gamma s^{\alpha-1}e^{-s}\,\mathrm{d}s\|u\|_{A^\gamma}\\ &\leq \frac{\Gamma(\alpha+\gamma)}{\Gamma(\alpha)}K_{\gamma,M}\|u\|_{A^\gamma}\tau^\gamma,\end{aligned}$$

which completes the proofs of the lemma. □

Proof of Theorem 5.4. Let $\tau\in(0,1]$, $\gamma\in(0,\alpha_c)$ and $\alpha>\alpha_c$. By Theorem 5.1, we know that $\alpha_c\leq 1/2$. Besides, according to [BO, Corollary 2.1] $\|P_n(A)\|\leq C\ln(1+\frac{\tau_{\mathsf{m}}}{\tau_*})n^{1/2}$. Thus using also (5.10), we obtain for u and v as in Lemma 5.5,

$$\begin{aligned}\|P_n(A)(u-v)\| &\leq \|P_n(A)\|\,\|u-v\|\\ &\leq C_{M,\alpha,\gamma}\ln(1+\frac{\tau_{\mathsf{m}}}{\tau_*})n^{1/2}\|u\|_{A^\gamma}\tau^\gamma.\end{aligned}$$

By (2.1) and (5.10), $\|e^{tA}(u-v)\|\leq C_{M,\alpha,\gamma}\|u\|_{A^\gamma}\tau^\gamma$, thus

$$\|(P_n(A)-e^{tA})(u-v)\|\leq C_{M,\alpha,\gamma}\ln(1+\frac{\tau_{\mathsf{m}}}{\tau_*})n^{1/2}\tau^\gamma\|u\|_{A^\gamma}. \tag{5.13}$$

Let $\alpha=m+\beta$ where m is the integral part of α and $\beta\in[0,1)$. Since $D((1-A)^\alpha)=(1-\tau A)^{-\alpha}X$, the operator $(1-A)^\alpha(1-\tau A)^{-\alpha}$ is well defined and satisfies

$$(1-A)^\alpha(1-\tau A)^{-\alpha}=\tau^{-\alpha}(1-A)^m(\tau^{-1}-A)^{-m}(1-A)^\beta(\tau^{-1}-A)^{-\beta}.$$

Since

$$(1-A)^m(\tau^{-1}-A)^{-m}=\Big(1+(\tau-1)(1-\tau A)^{-1}\Big)^m,$$

we have $\|(1-A)^m(\tau^{-1}-A)^{-m}\|\leq(1+M)^m$. Moreover by [Hen, Theorem 1.4.6] , for every $\varepsilon\in(0,1]$ there holds

$$\begin{aligned}\|(1-A)^\beta(\tau^{-1}-A)^{-\beta}\| &\leq 1+C_{\alpha,M,\varepsilon}\tau^{-1}\|(\tau^{-1}-A)^{-1+\varepsilon}\|\\ &\leq(1+C_{\alpha,M,\varepsilon})\tau^{-\varepsilon},\end{aligned}$$

since $\|(\tau^{-1}-A)^{-1+\varepsilon}\|\leq M\tau^{1-\varepsilon}$ and $\tau\leq 1$. Finally we obtain

$$\|(1-A)^\alpha(1-\tau A)^{-\alpha}\|\leq C_{\alpha,M,\varepsilon}\tau^{-\alpha-\varepsilon}.$$

Then, using (5.8), we arrive at the following estimate

$$\begin{aligned}\|(P_n(A)-e^{tA})v\| &\leq \|(P_n(A)-e^{tA})(1-A)^{-\alpha}\|\,\|(1-A)^\alpha(1-\tau A)^{-\alpha}\|\,\|u\|\\ &\leq C_{t,\alpha,p,M,\varepsilon}\tau_{\mathsf{m}}^{\beta(\alpha)}\tau^{-\alpha-\varepsilon}\|u\|.\end{aligned} \tag{5.14}$$

Combining (5.13) and (5.14), we deduce by the triangle inequality,

$$\|(P_n(A)-e^{tA})u\|\leq C\Big(\ln(1+\frac{\tau_{\mathsf{m}}}{\tau_*})n^{1/2}\tau^\gamma+\tau_{\mathsf{m}}^{\beta(\alpha)}\tau^{-\alpha-\varepsilon}\Big)\|u\|_{A^\gamma},$$

where the positive constant C depends on $t, \alpha, \gamma, p, M, \varepsilon$. For n large enough (depending only on α and γ), the optimal choice

$$\tau := \left[\frac{(\alpha+\varepsilon)\tau_{\mathsf{m}}^{\beta(\alpha)}}{\gamma \ln(1+\frac{\tau_{\mathsf{m}}}{\tau_*})n^{1/2}} \right]^{1/(\alpha+\varepsilon+\gamma)}$$

stays in $(0,1]$ and gives

$$\|(P_n(A)-e^{tA})(1-A)^{-\gamma}\| \leq C \left[\ln^{\alpha+\varepsilon}(1+\frac{\tau_{\mathsf{m}}}{\tau_*})n^{(\alpha+\varepsilon)/2}\tau_{\mathsf{m}}^{\beta(\alpha)\gamma} \right]^{1/(\alpha+\varepsilon+\gamma)}.$$

From our assumptions on $(\tau_k)_{1\leq k\leq n}$, we deduce in the case $C_1 > 1$,

$$\|(P_n(A)-e^{tA})(1-A)^{-\gamma}\| \leq C \left[\tau_{\mathsf{m}}^{-3(\alpha+\varepsilon)/2+\beta(\alpha)\gamma} \right]^{1/(\alpha+\varepsilon+\gamma)}.$$

Since

$$\limsup_{n\to\infty} \|(P_n(A)-e^{tA})(1-A)^{-\gamma}\| > 0,$$

we must have $-3(\alpha+\varepsilon)/2+\beta(\alpha)\gamma \leq 0$ which yields $\beta(\alpha) \leq 3\alpha/(2\alpha_c)$. The case $C_1 = 1$ is similar and even simpler. This achieves the proof. □

6. Sharpness of the Convergence Theorem

As a consequence of Theorem 5.1, if $\alpha > \frac{1}{2}$ and $\tau_{\mathsf{m}} \to 0$ then

$$\|(P_n(A)-e^{tA})(1-A)^{-\alpha}\| \xrightarrow[n\to\infty]{} 0.$$

In this section we show that $P_n(A)(1-A)^{-\alpha}$ may diverges in the particular case where $A = \frac{\mathrm{d}}{\mathrm{d}x}$ if $\alpha < 1/2$. This is a consequence of the following result which gives a lower bound for $\|P_n(A)(1-A)^{-\alpha}\|$.

Theorem 6.1. *Let A be the generator of the translation group on $X := C_0(\mathbb{R})$, the space of continuous functions converging to zero at infinity,*

$$e^{tA}u(x) := u(x+t), \ \ u \in C_0(\mathbb{R}), x, t \in \mathbb{R}.$$

Let R be a p-acceptable function satisfying $|R| = 1$ on $\mathrm{i}\mathbb{R}$. Then, if $\tau_{\mathsf{m}} \leq 1$, there exist smooth positive functions $K, L : (0,\infty) \to (0,\infty)$ independent of n and t such that

(i) L is non increasing on $(1,\infty)$, $L(\infty) = 0$;

(ii) for every nonnegative exponent α, there holds

$$\|P_n(A)(1-A)^{-\alpha}\| \geq K(\alpha)n^{\frac{1}{2}}\tau_*^{\alpha}L(\tfrac{\tau_{\mathsf{m}}}{\tau_*}).$$

In particular,

$$\|P_n(A)\| \geq K(0)n^{\frac{1}{2}}L(\tfrac{\tau_{\mathsf{m}}}{\tau_*}).$$

As a consequence, the following statement holds.

Corollary 6.2. *Under the assumptions of Theorem 6.1, assume in addition that the grid $(\tau_k)_{1\leq k\leq n}$ is μ-quasiuniform and $0 \leq \alpha < 1/2$. Then*

$$\lim_{n\to\infty} \|P_n(A)(1-A)^{-\alpha}\| \geq C_{\alpha,t,\mu}n^{\frac{1}{2}-\alpha} \xrightarrow[n\to\infty]{} \infty.$$

Proof. By definition of a μ–quasiuniform grid,

$$\tau_* \geq \mu^{-1}\tau_{\mathsf{m}} \geq \mu^{-1}\frac{t}{n}.$$

So thanks to Theorem 6.1,

$$\|P_n(A)(1-A)^{-\alpha}\| \geq K(\alpha)\big(\frac{t}{\mu}\big)^{\alpha}L(\mu)n^{1/2-\alpha}.$$

□

Remark 6.3. By the convergence results of Section 5, if the conclusion of the above corollary holds then α must be less or equal to $1/2$. To our knowledge, the convergence of $P_n(A)$ on $D(A^{1/2})$ remains to be determinated even for uniform grids.

This result gives rise to the following conjecture: let $(\tau_k^n)_{1\leq k\leq n}$, $n \geq 1$ be a sequence of grids such that $\tau_{\mathsf{m}}^n \to 0$ as $n \to \infty$. Let A be any operator satisfying the assumptions of Section 2. Then there exists a threshold $\alpha_c \in [0, 1/2)$ such that
(i) $\|P_n(A)(1-A)^{-\alpha}\| \to \infty$ as $n \to \infty$ if $\alpha < \alpha_c$;
(ii) $P_n(A) \to e^{tA}$ in $\mathcal{L}(D(A^{\alpha}), X)$ for $\alpha > \alpha_c$.

As quoted in the introduction, $\alpha_c = 0$ for analytic semigroups. If $A = \frac{\mathrm{d}}{\mathrm{d}x}$ then $\alpha_c = 1/2$ under the assumptions of Corollary 6.2; so is it possible to find a sequence of grids with $\alpha_c < 1/2$? Do they exist operators A such that $\alpha_c \in (0, 1/2)$ for (quasi)-uniform grid ?

The proof of Theorem 6.1 is a slight modification of Section 2 in [CLPT]. First we will need the following lemmas.

Lemma 6.4. *Let A be the generator of the translation group on $X = C_0(\mathbb{R})$ and f be a function in $\mathcal{M}_+$. Then*

$$\|f(-\mathrm{i}A)\| = \|\mathcal{F}f\|_1.$$

Proof. For every (u, x) in $C_0(\mathbb{R}) \times \mathbb{R}$, we have $e^{s\frac{\mathrm{d}}{\mathrm{d}x}}u(x) = u(x+s)$ and

$$f(-\mathrm{i}A)u(x) = \int_0^{\infty} u(x+s)\mathcal{F}f(s)\,\mathrm{d}s = \int_{\mathbb{R}} u(s)\mathcal{F}f(s-x)\,\mathrm{d}s. \tag{6.1}$$

Moreover

$$\begin{aligned}\|f(-\mathrm{i}A)\| &= \sup_{\|u\|_\infty\leq 1}\|f(-\mathrm{i}A)u\|_\infty = \sup_{\|u\|_\infty\leq 1}\sup_{x\in\mathbb{R}}|f(-\mathrm{i}A)u(x)| \\ &= \sup_{x\in\mathbb{R}}\sup_{\|u\|_\infty\leq 1}|f(-\mathrm{i}A)u(x)|. \end{aligned}\tag{6.2}$$

Now for every x in $\mathbb{R}$, we define the bounded linear functional ϕ_x on $C_0(\mathbb{R})$ by (see (6.1)),

$$\phi_x(u) = f(-\mathrm{i}A)u(x) = \int_{\mathbb{R}} u(s)\mathcal{F}f(s-x)\,\mathrm{d}s.$$

According to the Riesz representation theorem,

$$\sup_{\|u\|_\infty\leq 1}|\phi_x(u)| = \|\mathcal{F}f(\cdot - x)\|_1 = \|\mathcal{F}f\|_1.$$

Thus by (6.2), $\|f(-\mathrm{i}A)\| = \|\mathcal{F}f\|_1$. □

Lemma 6.5 (Van der Corput's Lemma, see [BT1, Lemma 2.4])**.** *Suppose $g \in C_c^1(\mathbb{R})$, and ψ a real-valued function in $C^2(\mathbb{R})$ such that $|\psi''(x)| \geq \delta > 0$ for all x in the support of g. Then*

$$\|\mathcal{F}(e^{i\psi} g)\|_\infty \leq \frac{8}{\sqrt{\delta}} \|g'\|_1.$$

We are now in position to give the

Proof of Theorem 6.1. Let us first assume that α is positive. According to Lemma 6.4

$$\|P_n(A)(1-A)^{-\alpha}\| = \|\mathcal{F}\left(P_n(ix)(1-ix)^{-\alpha}\right)\|_1. \tag{6.3}$$

Since $|R| = 1$ on $\mathrm{i}\mathbb{R}$, there exists a smooth function $\psi : \mathbb{R} \to \mathbb{R}$ such that

$$R(\mathrm{i}x) = e^{\mathrm{i}\psi(x)} \qquad \text{for all } x \in \mathbb{R}.$$

Therefore, $\psi'(x) = [R'/R](\mathrm{i}x)$ and, as a consequence, ψ'' is a real rational function whose degree does not exceed -2. Since ψ'' has a finite number of zeros and converges to zero as $x \to \infty$, we deduce that there exists a enough large ($a > 2$) such that ψ'' has constant sign on $[a-1, \infty)$ and $|\psi''|$ is non increasing on $[a-1, \infty)$.

Choose $\phi \in C_c^\infty(a-1, a)$ and set

$$g(x) := \phi(x)(1 - \mathrm{i}\tfrac{x}{\tau_*})^{-\alpha}, \qquad \psi_n(x) = \sum_{k=1}^{n} \psi(\tfrac{\tau_k}{\tau_*} x).$$

Then by the Plancherel theorem,

$$\begin{aligned}
\|g\|_2^2 &= \|\mathrm{e}^{\mathrm{i}\psi_n(x)} g(x)\|_2^2 = \|\mathcal{F}\big(\mathrm{e}^{\mathrm{i}\psi_n(x)} g(x)\big)\|_2^2 \\
&\leq \|\mathcal{F}\big(\mathrm{e}^{\mathrm{i}\psi_n(x)} g(x)\big)\|_1 \|\mathcal{F}\big(\mathrm{e}^{\mathrm{i}\psi_n(x)} g(x)\big)\|_\infty \\
&\leq \|\mathcal{F}\big(\mathrm{e}^{\mathrm{i}\psi_n(x)} (1 - \mathrm{i}\tfrac{x}{\tau_*})^{-\alpha}\big)\|_1 \|\mathcal{F}\left(\phi(x)\right)\|_1 \|\mathcal{F}\big(\mathrm{e}^{\mathrm{i}\psi_n(x)} g(x)\big)\|_\infty.
\end{aligned} \tag{6.4}$$

Now, recalling that $\tau_* \leq 1$, we have

$$\begin{aligned}
\|g\|_2^2 &= \int_{a-1}^{a} |\phi(x)|^2 |(1 - \mathrm{i}\tfrac{x}{\tau_*})^{-\alpha}|^2 dx \\
&\geq \left(1 + \tfrac{a^2}{\tau_*^2}\right)^{-\alpha} \|\phi\|_2^2 \geq (1 + a^2)^{-\alpha} \tau_*^{2\alpha} \|\phi\|_2^2.
\end{aligned} \tag{6.5}$$

By differentiating g and using $a > 2$, one finds a positive constant C_ϕ depending only on ϕ such that

$$\|g'\|_1 \leq C_\phi (1 + \alpha) \tau_*^\alpha. \tag{6.6}$$

Moreover, for every x in $(a-1, a)$, there holds

$$\begin{aligned}
|\psi_n''(x)| &= \sum_{k=1}^{n} \left(\tfrac{\tau_k}{\tau_*}\right)^2 |\psi''\left(\tfrac{\tau_k}{\tau_*} x\right)| \\
&\geq |\psi''\left(\tfrac{a\tau_{\mathrm{m}}}{\tau_*}\right)| \sum_{k=1}^{n} \left(\tfrac{\tau_k}{\tau_*}\right)^2 \geq n |\psi''\left(\tfrac{a\tau_{\mathrm{m}}}{\tau_*}\right)|,
\end{aligned}$$

since, as stated above, ψ'' does not change its sign on $[a-1, \infty)$, $|\psi''|$ is non increasing on this interval and $\frac{\tau_k}{\tau_*} x$ belongs to $(a-1, \frac{a\tau_{\mathrm{m}}}{\tau_*})$ for all x in $(a-1, a)$ and k in $[1, n]$.

Lemma 6.5 and the above estimates tell us that there exists a new positive constant C_ϕ such that

$$\|\mathcal{F}\left(\mathrm{e}^{\mathrm{i}\psi_n} g\right)\|_\infty \leq C_\phi(1+\alpha)\frac{\tau_*^\alpha}{\sqrt{n|\psi''\big(\frac{a\tau_{\mathsf{m}}}{\tau_*}\big)|}}. \tag{6.7}$$

Now, using (6.3) and $P_n(\mathrm{i}x) = e^{\mathrm{i}\psi_n(\tau_* x)}$, it follows that

$$\begin{aligned}\|P_n(A)(1-A)^{-\alpha}\| &= \|\mathcal{F}\left(\mathrm{e}^{\mathrm{i}\psi_n(\tau_* x)}(1-\mathrm{i}x)^{-\alpha}\right)\|_1 \\ &= \|\mathcal{F}\left(\mathrm{e}^{\mathrm{i}\psi_n(y)}(1-\mathrm{i}\tfrac{y}{\tau_*})^{-\alpha}\right)\|_1. \end{aligned}\tag{6.8}$$

Going back to (6.4) and using (6.8), (6.7), (6.5), we derive

$$\|P_n(A)(1-A)^{-\alpha}\| \geq C'_\phi(1+a^2)^{-\alpha}(1+\alpha)^{-1} n^{\frac{1}{2}}\tau_*^\alpha|\psi''\big(\tfrac{a\tau_{\mathsf{m}}}{\tau_*}\big)|^{1/2}. \tag{6.9}$$

There remains to consider the case $\alpha = 0$. According to the functional calculus of Section 2, for every α in $(0,\infty)$, we have

$$\|(1-A)^{-\alpha}\| = \frac{1}{\Gamma(\alpha)}\left\|\int_0^\infty e^{sA}s^{\alpha-1}e^{-s}\,\mathrm{d}s\right\| \leq M.$$

Hence

$$\|P_n(A)(1-A)^{-\alpha}\| \leq \|P_n(A)\|\,\|(1-A)^{-\alpha}\| \leq M\|P_n(A)\|$$

and with (6.9),

$$\|P_n(A)\| \geq \frac{C'_\phi}{M}(1+a^2)^{-\alpha}(1+\alpha)^{-1}n^{\frac{1}{2}}\tau_*^\alpha|\psi''\big(\tfrac{a\tau_{\mathsf{m}}}{\tau_*}\big)|^{1/2}.$$

We conclude by letting $\alpha \to 0$ in the above inequality and setting $K(\alpha) = \frac{C'_\phi}{M}(1+a^2)^{-\alpha}(1+\alpha)^{-1}$, $L(\cdot) = |\psi''(a\,\cdot)|^{1/2}$ which achieves the proof of the theorem. □

7. Approximation of the time derivative

We consider the Cauchy problem

$$\begin{cases}\frac{\mathrm{d}}{\mathrm{d}t}u = Au & t>0 \\ u(0) = v.\end{cases}$$

We would like to approach $\frac{\mathrm{d}}{\mathrm{d}t}u$ at time t by

$$\frac{1}{\tau_n}\big(P_n(A) - P_{n-1}(A)\big)v$$

for any $v \in X$ smooth enough. Indeed, for large n, $P_n(A)v$ and $P_{n-1}(A)v$ are closed to $u(t)$ and $u(t-\tau_n)$ respectively. Thus it may be expected that the above finite difference approaches $\frac{\mathrm{d}}{\mathrm{d}t}u$.

Theorem 7.1. *Suppose R is a 1-acceptable rational function. Let $\alpha > 3/2$ be given. Then for every $s \in (1, \alpha - 1/2)$, there exists some constant C depending on α and s such that*

$$\left\|\Big\{\frac{1}{\tau_n}\big(P_n(A) - P_{n-1}(A)\big) - \frac{\mathrm{d}}{\mathrm{d}t}e^{tA}\Big\}(1-A)^{-\alpha}\right\| \leq C(t^2+1)\tau_{\mathsf{m}}^{\frac{s-1}{s+1}}. \tag{7.1}$$

We start with a simple lemma.

Lemma 7.2. *For any* 1*–acceptable rational function* R*, we have for all* x *in* $\mathbb{R}$

$$|(1-\mathrm{i}x)R(\mathrm{i}x)-1| \le C\min(|x|,x^2). \tag{7.2}$$

Proof. Since $R(\mathrm{i}x)=1+\mathrm{i}x+O(x^2)$, (7.2) holds for x in $[-1,1]$. Besides for $|x|>1$, we have

$$|(1-\mathrm{i}x)R(\mathrm{i}x)-1| \le (2\|R\|_\infty+1)|x|.$$

Hence (7.2) follows. □

Proof of Theorem 7.1. Once more, without loss of generality we assume $\tau_{\mathsf{m}}\le 1$. According to Lemma 3.3, by taking $g:=g_n$ and $h:=(1-\mathrm{i}x)^{-(\alpha-s)}$, for obtaining (7.1) it is enough to estimate the $W^{1,\infty}(\mathbb{R})$ norm of the function g_n defined by

$$g_n(x)=\frac{1}{\tau_n}\big(P_n(\mathrm{i}x)-P_{n-1}(\mathrm{i}x)-\mathrm{i}\tau_n x e^{\mathrm{i}tx}\big)(1-\mathrm{i}x)^{-s}.$$

Let us first estimate the L^∞ norm of g_n. Remark that

$$g_n(x)=\underbrace{\tau_n^{-1}\big((1-\mathrm{i}\tau_n x)R(\mathrm{i}\tau_n x)-1\big)P_{n-1}(\mathrm{i}x)(1-\mathrm{i}x)^{-s}}_{=A} + \underbrace{\mathrm{i}x\big(P_n(\mathrm{i}x)-e^{\mathrm{i}tx}\big)(1-\mathrm{i}x)^{-s}}_{=B}.$$

For the term A, let $r<0$.

(i) If $|x|\le\tau_{\mathsf{m}}^r$ then by Lemma 7.2

$$|A|\le C\tau_n x^2|1-\mathrm{i}x|^{-s}\le C\tau_{\mathsf{m}}^{2r+1}.$$

(ii) If $|x|>\tau_{\mathsf{m}}^r$ then by Lemma 7.2

$$|A|\le C|x|^{-s+1}\le C\tau_{\mathsf{m}}^{-r(s-1)}.$$

Next by choosing $r=-1/(s+1)$ in any case we obtain

$$|A|\le C\tau_{\mathsf{m}}^{\frac{s-1}{s+1}}. \tag{7.3}$$

For estimating B, we use (4.3) which yields

$$|B|\le |(P_n(\mathrm{i}x)-e^{\mathrm{i}tx})(1-\mathrm{i}x)^{-(s-1)}|\le C(t+1)\tau_{\mathsf{m}}^{\frac{(s-1)p}{s+p}}.$$

Since, for $s>1$, $\frac{(s-1)p}{s+p}\ge\frac{s-1}{s+1}$, we get

$$\sup_{x\in\mathbb{R}}|g_n(x)|\le C(t+1)\tau_{\mathsf{m}}^{\frac{s-1}{s+1}}. \tag{7.4}$$

Let us now estimate the derivative of g_n. We write

$$g_n'(x)=\underbrace{\tau_n^{-1}\big(P_n(\mathrm{i}x)-P_{n-1}(\mathrm{i}x)-\mathrm{i}\tau_n x e^{\mathrm{i}tx}\big)'(1-\mathrm{i}x)^{-s}}_{=A'} + \underbrace{\mathrm{i}s\tau_n^{-1}\big(P_n(\mathrm{i}x)-P_{n-1}(\mathrm{i}x)-\mathrm{i}\tau_n x e^{\mathrm{i}tx}\big)(1-\mathrm{i}x)^{-(s+1)}}_{=B'}.$$

Arguing as in the proof of (7.4), we find

$$|B'| \le C(t+1)s\tau_{\mathsf{m}}^{\frac{s}{s+2}}. \tag{7.5}$$

Thus, there remains to estimate A' which is equal to

$$\begin{aligned}
&\tau_n^{-1}\Big(\big((1-\mathrm{i}\tau_n x)R(\mathrm{i}\tau_n x)-1\big)P_{n-1}(\mathrm{i}x)+\mathrm{i}\tau_n x(P_n(\mathrm{i}x)-e^{\mathrm{i}tx})\Big)'(1-\mathrm{i}x)^{-s}\\
&=\underbrace{\tau_n^{-1}\Big(\big((1-\mathrm{i}\tau_n x)R(\mathrm{i}\tau_n x)-1\big)P_{n-1}(\mathrm{i}x)\Big)'(1-\mathrm{i}x)^{-s}}_{=A_1'}\\
&\qquad\qquad+\underbrace{\mathrm{i}\Big(x\big(P_n(\mathrm{i}x)-e^{\mathrm{i}tx}\big)\Big)'(1-\mathrm{i}x)^{-s}}_{=A_2'}.
\end{aligned}$$

By Lemma 4.3 and (4.3),

$$|A_2'| \le C(t^2+1)\tau_{\mathsf{m}}^{\frac{s-1}{s+1}}, \tag{7.6}$$

since $\tau_{\mathsf{m}} \le 1$ and $\frac{sp}{p+s+1} \ge \frac{(s-1)p}{p+s} \ge \frac{s-1}{s+1}$. Regarding A_1', it is equal to

$$\begin{aligned}
&\tau_n^{-1}\Big((1-\mathrm{i}\tau_n x)R(\mathrm{i}\tau_n x)-1\Big)'P_{n-1}(\mathrm{i}x)(1-\mathrm{i}x)^{-s}\\
&\qquad\qquad+\tau_n^{-1}\big((1-\mathrm{i}\tau_n x)R(\mathrm{i}\tau_n x)-1\big)P_{n-1}'(\mathrm{i}x)(1-\mathrm{i}x)^{-s}.
\end{aligned}$$

Remark that

$$\big((1-\mathrm{i}\tau_n x)R(\mathrm{i}\tau_n x)-1\big)' = O(\tau_n^2 x) \tag{7.7}$$

and for estimating $P_n'(\mathrm{i}x)$, we write

$$P_{n-1}'(\mathrm{i}x) = \sum_{k=1}^{n-1}\mathrm{i}\tau_k R'(\mathrm{i}\tau_k x)\prod_{\substack{\ell=1\\ \ell\ne k}}^{n-1}R(\mathrm{i}\tau_\ell x).$$

The rational functions R and R' being bounded on $\mathrm{i}\mathbb{R}$, we get

$$|P_{n-1}'(\mathrm{i}x)| \le Ct. \tag{7.8}$$

Now, let $r<0$. (i) If $|x| \le \tau_{\mathsf{m}}^r$ then (7.7), (7.2) and (7.8) imply

$$|A_1'| \le C\tau_n|x| + C\tau_n|x|^2 t \le C(t+1)\tau_{\mathsf{m}}^{2r+1}.$$

(ii) If $|x| > \tau_{\mathsf{m}}^r$. First we remark that by derivating

$$\left|\frac{\mathrm{d}}{\mathrm{d}x}\big((1-\mathrm{i}\tau_n x)R(\mathrm{i}\tau_n x)-1\big)\right| \le C\tau_n$$

since R is bounded on $\mathrm{i}\mathbb{R}$ and the degree of R' is negative. Using also Lemma 7.2, we deduce

$$|A_1'| \le C|x|^{-s} + C^2t|x|^{-s+1} \le C\tau_{\mathsf{m}}^{-rs} + C^2\tau_{\mathsf{m}}^{-r(s-1)} \le C^2t\tau_{\mathsf{m}}^{-r(s-1)}.$$

Next by choosing $r=-1/(s+1)$, we get $|A_1'| \le C(t+1)\,(\tau_{\mathsf{m}})^{(s-1)/(s+1)}$ uniformly for x in $\mathbb{R}$.

Now using also (7.6), it results that

$$|A'| \leq C(t^2+1)\tau_{\mathsf{m}}^{\frac{s-1}{s+1}}. \tag{7.9}$$

Compiling (7.5) and (7.9) we deduce

$$\sup_{x\in\mathbb{R}} |g_n'(x)| \leq C(t^2+1)\tau_{\mathsf{m}}^{\frac{s-1}{s+1}}.$$

Finally by (7.4)

$$\|g_n\|_{W^{1,\infty}} \leq C(t^2+1)\tau_{\mathsf{m}}^{\frac{s-1}{s+1}},$$

which completes the proof of the theorem. □

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