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On positivity, shape, and norm-bound preservation of time-stepping methods for semigroups

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Abstract

We use functional calculus methods to investigate qualitative properties of C_0-semigroups that are preserved by time-discretization methods. Preservation of positivity, concavity and other qualitative shape properties which can be described via positivity are treated in a Banach lattice framework. Preservation of contractivity (or norm-bound) of the semigroup is investigated in the Banach space setting. The use of the Hille–Phillips (H–P) functional calculus instead of the Dunford–Taylor functional calculus allows us to extend fundamental qualitative results concerning time-discretization methods and simplify their proofs, including results on multi-step schemes and variable step-sizes. Since the H–P functional calculus is used throughout the paper, we present an elementary introduction to it based on the Riemann–Stieltjes integral.

1. Introduction

In this paper we are interested in certain functions of a generator A of a (linear) strongly continuous semigroup (C_0-semigroup) on a Banach space X. The class of functions under consideration originates from the investigation of numerical methods, in particular time-discretization methods, for differential equations $u'(t) = Au(t)$. Many of the basic methods used to analyse time-discretization schemes in a Banach-space setting go back to Lax and

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Richtmyer [19]. Often, the C_0-semigroup $T(t) = e^{tA}$ generated by A is approximated by a product of operators $\prod_{i=1}^{n} r(\tau_i A)$, $\sum_{i=1}^{n} \tau_i = t$, where the operators $r(\tau_i A)$ are rational functions of the generator. The use of a functional calculus allows us to obtain information about an operator $r(A)$ from a detailed analysis of the function $z \to r(z)$. Probably the best known functional calculus is the Dunford–Taylor functional calculus (see [10]) which was—mainly for analytic semigroups—extensively used by various authors to obtain stability and convergence results for time-discretization schemes (see, for example, [9,21, 23]). When working with general C_0-semigroups, the Hille–Phillips (H–P) functional calculus is a more suitable instrument that leads to stronger results and easier proofs (see, for example, [4,7,15]). Since the H–P functional calculus plays a dominant role in this paper, we give in Section 2 an elementary construction of it via Laplace transforms of functions of bounded variation (as an alternative to the original approach taken by Hille and Phillips in [16] via Laplace transforms of regular Borel-measures). We would like to emphasize that the idea of using functions of bounded variation in the H–P calculus is not new (see, for example, [14]), but we could not find a reference where this approach has been worked out in detail. Thus, we give an elementary construction of the H–P calculus using Riemann integration techniques without any reference to measure theory whatsoever.

In Sections 3–5, we use the H–P functional calculus to investigate the preservation of certain qualitative properties of the semigroup under suitable time-discretization methods. To describe the notion of *positivity preservation* considered in Section 3, let X be a Banach lattice and $T(\cdot)$ a positive (i.e., $T(t)x \geqslant 0$ for all $t \geqslant 0$ if $x \geqslant 0$), C_0-semigroup on X. For any (not necessarily rational) function r for which $\prod_{i=1}^{n} r(\tau_i A)$ with $\sum_{i=1}^{n} \tau_i = t$ converges strongly to $T(t)$ as $\max \tau_i \to 0$, we seek conditions on the time-stepping parameters $\tau_i > 0$ and on the function $z \to r(z)$ which guarantee that $r(\tau_i A)$, and hence $\prod_{i=1}^{n} r(\tau_i A)$, defines a positive operator. If there are no restrictions on the time-steps, then the approximation scheme is said to be *unconditionally positivity preserving*; else we call it *conditionally positivity preserving.* We extend results of Bolley and Crouzeix [5] on positivity preservation

(i) to positive, strongly continuous semigroups on Banach lattices (in the unconditional case),
(ii) to positive, uniformly continuous semigroups on Banach lattices (in the conditional case), and
(iii) to variable step-sizes and multi-step schemes.

In Section 4 we introduce the concept of B-shape preservation. This allows us, among others, to treat *convexity preservation* of time-discretization methods for the heat equation in an abstract setting. A C_0-semigroup $T(\cdot)$ is said to *preserve B-shape* if

(i) B is a closed linear operator with $D(A) \subset D(B) \subset X$ with range is in some Banach lattice Y, and
(ii) if $BT(t)x \geqslant 0$ $(t \geqslant 0)$ for every $x \in D(A)$ with $Bx \geqslant 0$.

In Section 5 we generalize some results in [22] on *contractivity preservation* to general bounded C_0-semigroups. As for positivity preservation, we give a common treatment of conditional and unconditional norm-bound preservation and present results for variable step-sizes and multi-step schemes.

We would like to emphasize that we are looking at preservation properties for time-discretization methods only. It is possible to apply the results to fully discrete solutions (i.e., approximate solutions after both space- and time-discretization). In this case we first do a spatial semi-discretization (like finite element of finite difference methods) which will yield a new semigroup, the solution operator of the semi-discrete problem. Then we apply a time-discretization method and our qualitative analysis will tell us whether the qualitative properties from the semi-discrete solution are inherited by the fully discrete solution. We do not investigate whether the particular properties are preserved under the spatial semi-discretization. We remark that there are examples where certain properties are lost under the spatial semi-discretization (finite element methods with irregular meshes) but reappear after an appropriate time-discretization (see [12]). In this case our methods are not applicable to the fully discrete solution. Finally, we remark that the inverse approach, that is, the investigation of qualitative properties of certain approximations that are inherited by the semigroup are considered, for example, in [1,8].

2. The Hille–Phillips (H–P) functional calculus: an elementary construction without measures

The H–P functional calculus is a useful tool to study functions of the generator of a C_0-semigroup on a Banach space X. The class of functions on which this functional calculus is defined is a Banach algebra of functions r which are analytic on some left half-plane and have a Laplace–Stieltjes representation $r(z) = \int_0^\infty e^{zt}\, d\alpha(t)$ $(\mathrm{Re}(z) \leqslant w)$ for a certain Banach algebra of normalized functions α of bounded variation. To construct this algebra, we recall some facts from the basic theory of the Riemann–Stieltjes integral (for proofs, see [6,16,24]).

A function $\alpha : [0, R] \to \mathbb{C}$ is in $NBV[0, R]$ if it is of *bounded variation* ($\alpha \in BV[0, R]$) and *normalized*; i.e., $\alpha(0) = 0$, and $\alpha(u) = (\alpha(u+) + \alpha(u-))/2$ for all $u \in (0, R)$. We define $NBV_{\mathrm{loc}} := \bigcap_{R>0} NBV[0, R]$ and $BV_{\mathrm{loc}} := \bigcap_{R>0} BV[0, R]$. The space NBV_{loc} is an algebra with multiplication defined by the *Stieltjes convolution,*

$$(\alpha * \beta)(t) = \int_0^t \alpha(t-u)\, d\beta(u) = \int_0^t \beta(t-u)\, d\alpha(u) \quad (t \notin P_{\alpha+\beta}), \tag{1}$$

where $P_{\alpha+\beta} := \{t \in \mathbb{R}\colon\ t = t_\alpha + t_\beta,\ t_\alpha \in P_\alpha,\ t_\beta \in P_\beta\}$, and where P_α (and similarly P_β) denotes the countable set of points where α is discontinuous. If P_α or P_β is empty, we define $P_{\alpha+\beta}$ to be the empty set. If $\alpha, \beta \in NBV[0, R]$ have discontinuities in P_α and P_β, respectively, then $\gamma := \alpha * \beta$ exists on $[0, R] \setminus P_{\alpha+\beta}$. Moreover, γ may be defined in the points of $P_{\alpha+\beta}$ so that it becomes normalized (see [24, Theorems 11.1 and 11.2a]). We can extend $\alpha, \beta \in NBV[0, R]$ by defining α, β to be zero in $(-\infty, 0)$ and to be $\alpha(R)$ and $\beta(R)$, respectively, in (R, ∞). Then $\gamma(t) = \int_{-\infty}^{\infty} \alpha(t-u)\, d\beta(u)$ if $t \notin P_{\alpha+\beta}$. To see that γ is again of bounded variation (see [24, Theorem 11.2b]), let $V_\alpha(t)$ denote the *total variation function* of α on the interval $[0,t]$. Then $V_\alpha \in NBV_{\mathrm{loc}}$ and we define

$$\int_a^b f(t)\,\bigl|d\alpha(t)\bigr| := \int_a^b f(t)\,dV_\alpha(t).$$

Let $0 \leqslant a = t_0 < t_1 < \cdots < t_N = b \leqslant R$ with $t_i \notin P_{\alpha+\beta}$. Then, for all $u \geqslant 0$,

$$\sum_{i=0}^{N-1} \bigl|\alpha(t_{i+1}-u) - \alpha(t_i-u)\bigr| \leqslant \sum_{i=0}^{N-1} \int_{t_i-u}^{t_{i+1}-u} \bigl|d\alpha(v)\bigr| \leqslant \int_{-\infty}^{\infty} \bigl|d\alpha(v)\bigr| = V_\alpha(R).$$

Hence,

$$\sum_{i=0}^{N-1} \bigl|\gamma(t_{i+1}) - \gamma(t_i)\bigr| \leqslant \int_{-\infty}^{\infty} V_\alpha(R)\bigl|d\beta(u)\bigr| = V_\alpha(R)V_\beta(R).$$

Since the right-hand side is independent of the points t_i, we may let them approach points of $P_{\alpha+\beta}$, we may let a approach zero and b approach R. The left-hand side can be brought arbitrary close to $V_\gamma(R)$, so that

$$V_\gamma(R) \leqslant V_\alpha(R)V_\beta(R). \tag{2}$$

Thus, $(NBV_{\mathrm{loc}}, +, *)$ is an algebra. A well-known extension (see [24, Theorem 11.3]) of the classical Cauchy theorem regarding the multiplication of absolutely convergent series states that if $\alpha, \beta \in NBV_{\mathrm{loc}}$ with $\lim_{t\to\infty} \alpha(t) := \alpha(\infty)$ and $\lim_{t\to\infty} \beta(t) := \beta(\infty)$, then

$$\lim_{t\to\infty} \gamma(t) = \alpha(\infty)\beta(\infty), \tag{3}$$

where $\gamma = \alpha * \beta$. To see this observe that

$$\gamma(t) - \alpha(\infty)\beta(t) = \int_0^t \bigl[\alpha(t-u) - \alpha(\infty)\bigr]\,d\bigl[\beta(u) - \beta(\infty)\bigr] = \int_0^t \tilde{\alpha}(t-u)\,d\tilde{\beta}(u),$$

with $\tilde{\alpha}(t) := \alpha(t) - \alpha(\infty)$ and $\tilde{\beta}(u) := \beta(u) - \beta(\infty)$. Thus,

$$\begin{aligned}
&\gamma(t) - \alpha(\infty)\beta(t)\\
&\quad = \int_0^{t/2} \tilde{\alpha}(t-u)\,d\tilde{\beta}(u) + \int_{t/2}^{t} \tilde{\alpha}(t-u)\,d\tilde{\beta}(u)\\
&\quad = \int_0^{t/2} \tilde{\alpha}(t-u)\,d\tilde{\beta}(u) - \int_{t/2}^{t} \tilde{\beta}(u)\,d_u\tilde{\alpha}(t-u) + \tilde{\alpha}(0)\tilde{\beta}(t) - \tilde{\alpha}\left(\frac{t}{2}\right)\tilde{\beta}\left(\frac{t}{2}\right)\\
&\quad = \int_0^{t/2} \tilde{\alpha}(t-u)\,d\tilde{\beta}(u) + \int_0^{t/2} \tilde{\beta}(t-u)\,d\tilde{\alpha}(u) + \tilde{\alpha}(0)\tilde{\beta}(t) - \tilde{\alpha}\left(\frac{t}{2}\right)\tilde{\beta}\left(\frac{t}{2}\right).
\end{aligned}$$

To prove (3) it is sufficient to show that $\lim_{t\to\infty}\int_0^{t/2}\tilde{\alpha}(t-u)\,d\tilde{\beta}(u)=0$. If $\tilde{\beta}(t)$ is constant, then the result is trivial. Otherwise, let us denote its total variation on $[0,\infty)$ by $V_{\tilde{\beta}}(\infty)$. For any $\varepsilon>0$ there is a $t_0>0$ such that, for $t>t_0/2$, we have $|\tilde{\alpha}(t)|\leqslant\varepsilon/V_{\beta}(\infty)$ and hence

$$\left|\int_0^{t/2}\tilde{\alpha}(t-u)\,d\tilde{\beta}(u)\right|\leqslant\frac{\varepsilon}{V_{\tilde{\beta}}(\infty)}\int_0^{t/2}\left|d\tilde{\beta}(u)\right|\leqslant\varepsilon.$$

This finishes the proof of (3).

The following statements will play a major role in the proofs of the main results of this section. For their proofs we refer to [24, Theorems 16.4 and 10a].

Proposition 1 (Helly–Bray Theorem). *Let* $\alpha_n\in BV[a,b]$ *be of uniform bounded variation and* $\alpha_n(t)\to\alpha(t)$ *for all* $t\in[a,b]$. *If* $f\in C[a,b]$, *then* $\lim_{n\to\infty}\int_a^b f(t)\,d\alpha_n(t)=\int_a^b f(t)\,d\alpha(t)$.

Proposition 2 (Mean Value Theorem). *If* $\alpha\in BV[a,b]$ *is nondecreasing* (*or nonincreasing*) *and* $f\in C([a,b])$ *is real valued, then there exists* $\zeta\in[a,b]$ *such that* $\int_a^b f(t)\,d\alpha(t)=f(\zeta)[\alpha(b)-\alpha(a)]$.

If $\alpha\in NBV_{\mathrm{loc}}$ and if

$$f(z):=\int_0^{\infty}e^{zt}\,d\alpha(t):=\lim_{R\to\infty}\int_0^{R}e^{zt}\,d\alpha(t)\tag{4}$$

exists for some $z\in\mathbb{C}$, then f is called the *Laplace–Stieltjes transform of* α. We will sometimes refer to α as the *generating function* and to f as the *determining function*. This terminology is adopted from [24]. It is well known that the *region of convergence* of (4) is an appropriate left half-plane; i.e., if (4) converges for some $z_0\in\mathbb{C}$, then it converges for all $z\in\mathbb{C}$ with $\operatorname{Re}z<\operatorname{Re}z_0$ (see [2, Chapter 1] or [24, Chapter II]). We call

$$\operatorname{abs}(\alpha):=\sup\left\{\operatorname{Re}z\colon\int_0^{\infty}e^{zt}\,d\alpha(t)\text{ converges}\right\}$$

the *abscissa of convergence* of (4). As shown by Widder in [24], if $\int_0^\infty e^{zt}\,d\alpha(t)$ converges for $z=\gamma+i\delta$ with $\gamma<0$, then

$$\alpha(t)=o\big(e^{-\gamma t}\big)\quad\text{as }t\to\infty;\tag{5}$$

if $\int_0^\infty e^{zt}\,d\alpha(t)$ converges for $z=\gamma+i\delta$ with $\gamma>0$, then $\alpha(\infty)$ exists and

$$\alpha(t)-\alpha(\infty)=o\big(e^{-\gamma t}\big)\quad\text{as }t\to\infty.\tag{6}$$

It is well known that the function $f:z\to\int_0^\infty e^{zt}\,d\alpha(t)$ is an analytic function on the open left half-plane $\{z\in\mathbb{C}\colon\operatorname{Re}z<\operatorname{abs}(\alpha)\}$. We say that the integral (4) *converges absolutely* at $z=z_0=\gamma+i\delta$ if $\int_0^\infty e^{\gamma t}\,|d\alpha(t)|:=\int_0^\infty e^{\gamma t}\,dV_\alpha(t)$ converges. Let $\alpha,\beta\in NBV_{\mathrm{loc}}$ and

$\gamma := \alpha * \beta$. If the integrals $f(z) := \int_0^\infty e^{zt}\,d\alpha(t)$ and $g(z) := \int_0^\infty e^{zt}\,d\beta(t)$ converge absolutely at $z_0 := \omega + i\delta$, then

$$f(z_0)g(z_0) = \int_0^\infty e^{z_0 t}\,d\gamma(t) \tag{7}$$

and

$$\int_0^\infty e^{\omega t}\,\bigl|d\gamma(t)\bigr| \leqslant \int_0^\infty e^{\omega t}\,\bigl|d\alpha(t)\bigr| \int_0^\infty e^{\omega t}\,\bigl|d\beta(t)\bigr|. \tag{8}$$

For the proof see [24, Chapter II, Section 11]. Now, we are in the position to prove the first main result of this section.

Theorem 3. *Let $\omega \in \mathbb{R}$. Then $NBV^\omega := \{\alpha \in NBV_{\mathrm{loc}}\colon \int_0^\infty e^{\omega t}\,|d\alpha(t)| < +\infty\}$ is a Banach algebra with Stieltjes-convolution as multiplication and norm $\|\alpha\|_\omega := \int_0^\infty e^{\omega t}\,|d\alpha(t)|$.*

Proof. Clearly, NBV^ω is a vector space and $\|\cdot\|_\omega$ defines a norm. By (2), $\gamma := \alpha * \beta \in NBV_{\mathrm{loc}}$ if $\alpha, \beta \in NBV^\omega$. By (8), $\|\gamma\|_\omega \leqslant \|\alpha\|_\omega \|\beta\|_\omega$. Thus, NBV^ω is a normed algebra with unit $e = \chi_{(0,\infty)}$ (the characteristic function of the interval $(0,\infty)$). To show that NBV^ω is complete, we prove first that a Cauchy sequence $\alpha_n \in NBV^\omega$ converges uniformly on compacts. Let $\varepsilon > 0$ and $k := \min_{t\in[0,R]}(e^{\omega t})$. Then there is $N \in \mathbb{N}$ such that $\int_0^\infty e^{\omega t}\,|d(\alpha_n - \alpha_m)(t)| = \|\alpha_n - \alpha_m\|_\omega < \varepsilon \cdot k$ for all $n, m \geqslant N$. Let $t_0 \in [0, R]$. Then $\int_0^{t_0} e^{\omega t}\,|d(\alpha_n - \alpha_m)(t)| < \varepsilon \cdot k$. Therefore, by Proposition 2, there exists $\zeta \in [0, t_0]$ such that $\int_0^{t_0} e^{\omega t}\,|d(\alpha_n - \alpha_m)(t)| = e^{\omega\zeta} V_{\alpha_n - \alpha_m}(t_0) < \varepsilon \cdot k$. Thus,

$$V_{\alpha_n-\alpha_m}(t_0) < \varepsilon \quad \text{for all } n, m \geqslant N \text{ and } t_0 \in [0, R], \tag{9}$$

which implies that $|\alpha_m(t_0) - \alpha_n(t_0)| < \varepsilon$ for all $n, m \geqslant N$ and $t_0 \in [0, R]$, since $\alpha_m(0) - \alpha_n(0) = 0$. Thus, the functions α_n converge uniformly on compacts to a function α. Therefore, α is normalized and from (9) we see that $|V_{\alpha_n}(t_0) - V_{\alpha_m}(t_0)| \leqslant V_{\alpha_n-\alpha_m}(t_0) < \varepsilon$ for all $t_0 \in [0, R]$. This implies that the sequence α_n is of uniform bounded variation on every interval $[0, R]$, i.e., there is $M_R > 0$ such that $V_{\alpha_n}(R) \leqslant M_R$ for all $n \in \mathbb{N}$. Let $0 = t_0 < t_1 < t_2 < \cdots < t_N = R$ be a subdivision of $[0, R]$. Let $\varepsilon > 0$ and let us choose α_n so that $|\alpha(t) - \alpha_n(t)| \leqslant \frac{\varepsilon}{2N}$ for all $t \in [0, R]$. Then

$$\begin{aligned}\sum_{i=1}^N \bigl|\alpha(t_i) - \alpha(t_{i-1})\bigr| &\leqslant \sum_{i=1}^N \bigl|\alpha(t_i) - \alpha_n(t_i)\bigr| + \bigl|\alpha_n(t_i) - \alpha_n(t_{i-1})\bigr| \\ &\quad + \bigl|\alpha(t_{i-1}) - \alpha_n(t_{i-1})\bigr| \\ &\leqslant \varepsilon + V_{\alpha_n}(R) < \varepsilon + M_R.\end{aligned}$$

Therefore, $V_\alpha(R) \leqslant M_R$ and thus $\alpha \in NBV_{\mathrm{loc}}$. Finally, we prove that $\int_0^\infty e^{\omega t}\,|d\alpha(t)| < +\infty$ and that $\lim_{n\to\infty} \alpha_n = \alpha$ in NBV^ω. Again, let $R > 0$ be fixed and $0 = t_0 < t_1 < t_2 < \cdots < t_N = R$ be a subdivision of $[0, R]$. Then, by Proposition 1,

$$\begin{aligned}
&\sum_{i=1}^{N}\bigl|(\alpha-\alpha_n)(t_i)-(\alpha-\alpha_n)(t_{i-1})\bigr|\\
&\quad=\sum_{i=1}^{N}\left|\int_{t_{i-1}}^{t_i} d\alpha(t)-\int_{t_{i-1}}^{t_i} d\alpha_n(t)\right|=\lim_{m\to\infty}\sum_{i=1}^{N}\left|\int_{t_{i-1}}^{t_i} d\alpha_m(t)-\int_{t_{i-1}}^{t_i} d\alpha_n(t)\right|\\
&\quad\leqslant\lim_{m\to\infty}\sum_{i=1}^{N}\int_{t_{i-1}}^{t_i}\bigl|d(\alpha_m-\alpha_n)(t)\bigr|=\lim_{m\to\infty}V_{\alpha_n-\alpha_m}(R).
\end{aligned}$$

Therefore, $V_{\alpha-\alpha_n}(R)\leqslant\lim_{m\to\infty}V_{\alpha_n-\alpha_m}(R)$, and by (9), $\lim_{n\to\infty}V_{\alpha-\alpha_n}(R)=0$. Note that this holds uniformly for $t_0\in[0,R]$. We also have that $|V_{\alpha_n-\alpha_m}(t_0)-V_{\alpha_n-\alpha}(t_0)|\leqslant V_{\alpha-\alpha_m}(R)\to 0$ as $m\to\infty$ for $t_0\in[0,R]$ uniformly. Using Proposition 1 for the sequence $(V_{\alpha_m-\alpha_n}(\cdot))_{m\in\mathbb{N}}$, we see that

$$\int_0^R e^{\omega t}\,\bigl|d(\alpha-\alpha_n)(t)\bigr|=\lim_{m\to\infty}\int_0^R e^{\omega t}\,\bigl|d(\alpha_m-\alpha_n)(t)\bigr|\leqslant\lim_{m\to\infty}\|\alpha_m-\alpha_n\|_\omega.$$

Thus,

$$\|\alpha-\alpha_n\|_\omega=\int_0^\infty e^{\omega t}\,\bigl|d(\alpha-\alpha_n)(t)\bigr|\leqslant\lim_{m\to\infty}\|\alpha_m-\alpha_n\|_\omega. \tag{10}$$

If we write $\alpha=(\alpha-\alpha_n)+\alpha_n$, we can immediately conclude that $\int_0^\infty e^{\omega t}\,|d\alpha(t)|<+\infty$. Finally, from (10) it follows that $\lim_{n\to\infty}\alpha_n=\alpha$ in NBV^ω. Thus NBV^ω is complete. □

We are now in the position to define the algebra of functions, isomorphic to NBV^ω, on which the Hille–Phillips functional calculus will be defined.

Corollary 4. *Let* $\mathcal{F}_\omega:=\{f_\alpha\colon\ f_\alpha(z)=\int_0^\infty e^{zt}\,d\alpha(t)$ *if* $\operatorname{Re}z\leqslant\omega,\ \alpha\in NBV^\omega\}$. *Then the operator* $\Phi: NBV^\omega\to\mathcal{F}_\omega$ *defined by* $\Phi(\alpha):=f_\alpha$ *is an algebra isomorphism. If we set* $\|f_\alpha\|:=\|\alpha\|_\omega$, *then* $\mathcal{F}_\omega$ *becomes a Banach algebra and, for* $\omega\geqslant\kappa$, *the inclusion* $\mathcal{F}_\omega\subset\mathcal{F}_\kappa$ *holds.*

Proof. The map Φ is clearly linear. If we define multiplication in $\mathcal{F}_\omega$ as pointwise multiplication, then (7) shows that Φ preserves multiplication. Also, it maps the unit of NBV^ω to the unit of $\mathcal{F}_\omega$ which is $e_{\mathcal{F}_\omega}(z):=1$ for $\operatorname{Re}z\leqslant\omega$. From Theorem 3 it follows that NBV^ω is an algebra and therefore $\mathcal{F}_\omega$, the image of Φ, is also an algebra. By definition, Φ is onto and the injectivity follows from the uniqueness theorem for the Laplace–Stieltjes transform (see, e.g., [24, Chapter II, Theorem 6.3]). The completeness of NBV^ω implies the completeness of $\mathcal{F}_\omega$. Finally, the inclusion $\mathcal{F}_\omega\subset\mathcal{F}_\kappa$ for $\omega\geqslant\kappa$ follows immediately from the definition of $\mathcal{F}_\omega$. □

Recall that a rational function r is called *A-stable* if $|r(z)|\leqslant 1$ for $\operatorname{Re}z\leqslant 0$. Next, we show that this important class of functions is in $\mathcal{F}_0$ and hence in all $\mathcal{F}_\omega$ with $\omega\leqslant 0$ (cf. [16, p. 441]).

Proposition 5. *If a rational function r satisfies $|r(z)| \leqslant M$ for some $M > 0$ and for* $\operatorname{Re} z \leqslant \omega$*, then $r \in \mathcal{F}_\omega$.*

Proof. Clearly, constant functions and the functions $z \to 1/(a-z)$ belong to the algebra $\mathcal{F}_\omega$ for $\operatorname{Re} a > \omega$. Therefore, by developing r into partial fractions, we see that $r \in \mathcal{F}_\omega$. □

Another important example is the function $z \mapsto e^{zt}$ for fixed $t > 0$. It belongs to the algebra $\mathcal{F}_\omega$ since

$$e^{zt} = \int_0^\infty e^{zs}\, dH_t(s),$$

where the normalized Heaviside function H_t is defined as

$$H_t(s) := \begin{cases} 0 & \text{if } 0 \leqslant s < t, \\ \frac{1}{2} & \text{if } s = t, \\ 1 & \text{if } s < t. \end{cases}$$

We define H_0 by setting set $H_0(s) = 0$ for $s = 0$ and $H_0(s) = 1$ for $s > 0$.

Let X be a Banach space and let $A : X \supset \mathcal{D}(A) \to X$ generate a C_0-semigroup $T(\cdot)$ of type (M, ω); i.e., there exists $M \geqslant 1$ and $\omega \in \mathbb{R}$ such that $\|T(t)\| \leqslant Me^{\omega t}$ for all $t \geqslant 0$. For $f \in \mathcal{F}_\omega$ with $f(z) := \int_0^\infty e^{zt}\, d\alpha(t)$ $(\operatorname{Re} z \leqslant \omega)$ let us define

$$f(A)x := \int_0^\infty T(t)x\, d\alpha(t). \tag{11}$$

In order to justify this definition, we show that the map $f \to f(A)$ defined in (11) is an algebra homomorphism.

Theorem 6 (Hille–Phillips Functional Calculus). *If A generates a C_0-semigroup $T(\cdot)$ of type (M, ω), then $\Psi : \mathcal{F}_\omega \to \mathcal{B}(X)$ defined by $\Psi(f) := f(A)$ is an algebra homomorphism. Moreover,*

$$\big\| f(A) \big\| \leqslant M \|\alpha\|_\omega, \tag{12}$$

where $\alpha \in NBV^\omega$ is such that $f(z) = \int_0^\infty e^{zt}\, d\alpha(t)$, $\operatorname{Re} z \leqslant \omega$*.*

Proof. It is clear that the map Ψ is linear and that $\Psi(e_{\mathcal{F}_\omega}) = I \in \mathcal{B}(X)$. Also the range of Ψ is a subset of $\mathcal{B}(X)$ since

$$\big\| f(A)x \big\| = \left\| \int_0^\infty T(t)x\, d\alpha(t) \right\| \leqslant M \int_0^\infty e^{\omega t} \big| d\alpha(t) \big| \|x\| = M \|\alpha\|_\omega \|x\|.$$

This shows that Ψ is continuous and $\|\Psi(f)\| \leqslant M\|f\|$. If $\omega < 0$, it follows from (5) that

$$\lim_{t\to\infty} e^{\omega t}\alpha(t) = 0. \tag{13}$$

If $\omega > 0$, then by (6), we have that

$$\lim_{t\to\infty} e^{\omega t}\bigl(\alpha(t)-\alpha(\infty)\bigr)=0. \tag{14}$$

If $\alpha \in NBV^0$, then $\alpha(\infty)$ exists. This shows that (14) holds for $\omega = 0$, too. We show now that Ψ preserves products, that is

$$\left(\int_0^\infty T(s)\,d\alpha(s)\right)\left(\int_0^\infty T(t)\,d\beta(t)\right)x=\int_0^\infty T(u)x\,d\gamma(u)\quad \text{for all } x\in X, \tag{15}$$

where $\gamma = \alpha * \beta$ is the Stieltjes convolution of α and β defined in (1). Observe first that

$$Sx := \left(\int_0^\infty T(s)\,d\alpha(s)\right)\left(\int_0^\infty T(t)\,d\beta(t)\right)x=\int_0^\infty\int_t^\infty T(u)x\,d\alpha(u-t)\,d\beta(t).$$

If we apply an arbitrary $x^* \in X^*$, then

$$\langle Sx, x^*\rangle = \int_0^\infty\int_t^\infty \bigl\langle T(u)x,x^*\bigr\rangle\,d\alpha(u-t)\,d\beta(t). \tag{16}$$

First assume that $\omega < 0$. Since $\alpha \in NBV_{\mathrm{loc}}$ and $u \to \langle T(u)x, x^*\rangle$ is continuous, we can integrate by parts and obtain

$$\langle Sx, x^*\rangle = \int_0^\infty\left\{\bigl[\bigl\langle T(u)x,x^*\bigr\rangle\alpha(u-t)\bigr]_{u=t}^{u=\infty}-\int_t^\infty \alpha(u-t)\,d\bigl\langle T(u)x,x^*\bigr\rangle\right\}d\beta(t).$$

Since $\alpha(0) = 0$ and $\lim_{u\to\infty}\alpha(u-t)\langle T(u)x, x^*\rangle = 0$ (by (13)), the first term in the integral equals to 0. Therefore,

$$\begin{aligned}\langle Sx, x^*\rangle &= -\int_0^\infty\int_t^\infty \alpha(u-t)\,d\bigl\langle T(u)x,x^*\bigr\rangle\,d\beta(t)\\ &= -\int_0^\infty\int_0^u \alpha(u-t)\,d\beta(t)\,d\bigl\langle T(u)x,x^*\bigr\rangle\\ &= -\int_0^\infty \gamma(u)\,d\bigl\langle T(u)x,x^*\bigr\rangle = \int_0^\infty \bigl\langle T(u)x,x^*\bigr\rangle\,d\gamma(u)\\ &= \left\langle \int_0^\infty T(u)x\,d\gamma(u),x^*\right\rangle.\end{aligned}$$

The above calculation is true for all $x^* \in X^*$ and hence (15) is established. If $\omega \geqslant 0$, then we can write (16) as follows:

$$\begin{aligned}\langle Sx, x^*\rangle &= \int_0^\infty \int_t^\infty \langle T(u)x, x^*\rangle\, d\big(\alpha(u-t)-\alpha(\infty)\big)\, d\beta(t)\\ &= \int_0^\infty \Bigg\{ \big[\langle T(u)x, x^*\rangle\big(\alpha(u-t)-\alpha(\infty)\big)\big]_{u=t}^{u=\infty}\\ &\quad - \int_t^\infty \alpha(u-t)-\alpha(\infty)\, d\langle T(u)x, x^*\rangle \Bigg\}\, d\beta(t),\end{aligned}$$

where the first term in the integral equals to $\langle T(t)x, x^*\rangle\alpha(\infty)$ since $\alpha(0)=0$ and $\lim_{u\to\infty}(\alpha(u-t)-\alpha(\infty))\langle T(u)x, x^*\rangle = 0$ by (14). Therefore,

$$\begin{aligned}\langle Sx, x^*\rangle &= \int_0^\infty \Bigg[\langle T(t)x, x^*\rangle\alpha(\infty) - \int_t^\infty \alpha(u-t)-\alpha(\infty)\, d\langle T(u)x, x^*\rangle\Bigg]\, d\beta(t)\\ &= \int_0^\infty \langle T(t)x, x^*\rangle\alpha(\infty)\, d\beta(t) - \int_0^\infty\int_t^\infty \alpha(u-t)-\alpha(\infty)\, d\langle T(u)x, x^*\rangle\, d\beta(t)\\ &= \int_0^\infty \langle T(t)x, x^*\rangle\alpha(\infty)\, d\beta(t) - \int_0^\infty\int_0^u \alpha(u-t)-\alpha(\infty)\, d\beta(t)\, d\langle T(u)x, x^*\rangle\\ &= \int_0^\infty \langle T(t)x, x^*\rangle\alpha(\infty)\, d\beta(t) - \int_0^\infty \gamma(u)-\alpha(\infty)\beta(u)\, d\langle T(u)x, x^*\rangle. \qquad (17)\end{aligned}$$

We claim that $\lim_{t\to\infty}(\gamma(t)-\alpha(\infty)\beta(t))\langle T(t)x, x^*\rangle = 0$. To see this let us write

$$\begin{aligned}&\big|\big(\gamma(t)-\alpha(\infty)\beta(t)\big)\langle T(t)x, x^*\rangle\big|\\ &\quad\leqslant \big|\big(\gamma(t)-\gamma(\infty)\big)\langle T(t)x, x^*\rangle\big| + \big|\big(\gamma(\infty)-\alpha(\infty)\beta(t)\big)\langle T(t)x, x^*\rangle\big|\\ &\quad= \big|\big(\gamma(t)-\gamma(\infty)\big)\langle T(t)x, x^*\rangle\big| + \big|\big(\alpha(\infty)\beta(\infty)-\alpha(\infty)\beta(t)\big)\langle T(t)x, x^*\rangle\big|\\ &\quad= \big|\big(\gamma(t)-\gamma(\infty)\big)\langle T(t)x, x^*\rangle\big| + \big|\alpha(\infty)\big(\beta(\infty)-\beta(t)\big)\langle T(t)x, x^*\rangle\big| \to 0\end{aligned}$$

as $t\to\infty$. The last two steps follow from (3) and (14). Finally, we continue where we left off in (17) and obtain for all $x^*\in X^*$,

$$\begin{aligned}\langle Sx, x^*\rangle &= \int_0^\infty \langle T(t)x, x^*\rangle\alpha(\infty)\, d\beta(t) - \int_0^\infty \gamma(u)-\alpha(\infty)\beta(u)\, d\langle T(u)x, x^*\rangle\\ &= \int_0^\infty \langle T(t)x, x^*\rangle\alpha(\infty)\, d\beta(t) - \big[\big(\gamma(u)-\alpha(\infty)\beta(u)\big)\langle T(u)x, x^*\rangle\big]_{u=0}^{u=\infty}\\ &\quad + \int_0^\infty \langle T(u)x, x^*\rangle\, d\big(\gamma(u)-\alpha(\infty)\beta(u)\big)\end{aligned}$$

$$= \int_0^\infty \langle T(u)x, x^* \rangle \, d\gamma(u) = \left\langle \int_0^\infty T(u)x \, d\gamma(u), x^* \right\rangle.$$

Thus,

$$Sx = \left(\int_0^\infty T(s)\, d\alpha(s) \right) \left(\int_0^\infty T(t)\, d\beta(t) \right) x = \int_0^\infty T(u)x \, d\gamma(u)$$

for all $x \in X$. □

3. Positivity preserving schemes

In this section we consider problems concerning positivity preservation under time-discretization of the semigroup. With the H–P functional calculus tool at hand, we can easily generalize some known results to arbitrary Banach lattices and arbitrary semigroups and simplify earlier proofs significantly. Absolutely monotonic functions will play a central role in the remaining sections. Recall that a function f is *absolutely monotonic* (*a.m.*) at $u \in \mathbb{R}$ if $f^{(k)}(u) \geqslant 0$ for all $k \in \mathbb{N}$. A function f is a.m. on an interval $I \subset \mathbb{R}$ if f is absolutely monotonic at each $u \in I$. Later on in this section we will need the following technical proposition. The proof can be found in [24, Chapter I, Theorem 8a].

Proposition 7. *If f is continuous on $[0, \infty)$, if $\alpha \in BV_{\mathrm{loc}}$ and if α^* is the normalized function of α, then $\int_0^\infty f(t)\, d\alpha(t) = \int_0^\infty f(t)\, d\alpha^*(t)$ provided the first integral converges.*

The following theorem plays a major role when proving positivity preservation without any restriction on the time-step. For the proof see, for example, [3].

Theorem 8 (Bernstein). *A function f is a.m. on $(-\infty, 0]$ if and only if $f(u) = \int_0^\infty e^{ut}\, d\alpha(t)$ for $u \leqslant 0$, where α is a bounded, nondecreasing function.*

Corollary 9. *Let $\omega \in \mathbb{R}$. A function f is a.m. on $(-\infty, \omega]$ if and only if $f(u) = \int_0^\infty e^{ut}\, d\beta(t)$ for $u \leqslant \omega$, where $\beta \in NBV^\omega$ and β is nondecreasing.*

Proof. It is clear that if $f(u) = \int_0^\infty e^{ut}\, d\beta(t)$ with β nondecreasing, then f is a.m. on $(-\infty, \omega]$. Conversely, let f be a.m. on $(-\infty, \omega]$. Then $g(\cdot) := f(\cdot + \omega)$ is a.m. on $(-\infty, 0]$. Therefore, by Theorem 8, $g(u) = \int_0^\infty e^{ut}\, d\alpha(t)$, where α is bounded and nondecreasing (and thus of bounded variation). By Proposition 7, we can replace α with $\alpha^* \in NBV^0$. Thus,

$$f(u) = g(u - \omega) = \int_0^\infty e^{(u-\omega)t}\, d\alpha^*(t) = \int_0^\infty e^{ut}\, d\beta(t),$$

where $\beta(t)=\int_0^t e^{-\omega s}\,d\alpha^*(s)$. Since $\alpha^*\in NBV^0$, it follows that $\beta\in NBV_{\mathrm{loc}}$ and

$$\int_0^\infty e^{\omega t}\left|d\beta(t)\right|=\int_0^\infty \left|d\alpha^*(t)\right|<+\infty.$$

Thus, $\beta\in NBV^\omega$ and, since α^* is nondecreasing, β is also nondecreasing. □

The following theorem is due to Bolley and Crouzeix [5] for generators of positive contraction semigroups on $L_2(\mathbb{R})$ and rational functions r. We generalize this to arbitrary Banach lattices, arbitrary generators of positive C_0-semigroups and get rid of the requirement that r is rational.

Theorem 10. *Let X be a Banach lattice. If A generates a positive C_0-semigroup $T(\cdot)$ of type (M,ω) and r is a.m. on $(-\infty,\tau\omega]$ for $\tau>0$, then $r(\tau A)\geqslant 0$.*

Proof. By Corollary 9, we have that $r\in\mathcal{F}_{\tau\omega}$ and $r(u)=\int_0^\infty e^{ut}\,d\beta(t)$ $(u\in(-\infty,\tau\omega])$ with β constructed in the previous proof. Since $T(t)\geqslant 0$ for all $t\geqslant 0$ and β is nondecreasing using the H–P functional calculus, we have $r(\tau A)x=\int_0^\infty T(\tau t)x\,d\beta(t)\geqslant 0$ for all $x\geqslant 0$, $x\in X$. □

Remark 11. The conditions of Theorem 10 are also necessary in the sense that if r is not a.m. on $(-\infty,\tau\omega]$, then we can always find a Banach lattice X and positive semigroup on X generated by A such that $r(\tau A)$ fails to be a positive operator for some $\tau>0$ (see [5] and [17, Theorem 4.1.7]). On the other hand, if we fix the space X and the operator A, the assumptions of the theorem might not be necessary (for example, take $r(z):=\left(\frac{2+z}{2-z}\right)^2$, $X:=\mathbb{R}$, $A:=1$).

Corollary 12 (Variable step-size). *Let X be a Banach lattice. Assume that A generates a positive C_0-semigroup $T(\cdot)$ of type (M,ω). Let τ_i, $i=1,\dots,n$, be positive numbers. If r is a.m. on $(-\infty,\tau_i\omega]$, $i=1,\dots,n$, then $\prod_{i=1}^n r(\tau_i A)\geqslant 0$.*

Proof. The statement follows from Theorem 10 and the fact that product of positive operators is positive. □

Next, recall that a general k-step scheme is of the form

$$u_n=\sum_{i=1}^k r_i(\tau A)u_{n-i},\quad \text{where } n\geqslant k,\ r_i\in\mathcal{F}_{\tau\omega},\ i=1,\dots,n. \tag{18}$$

Corollary 13 (Multi-step schemes). *Let X be a Banach lattice. Assume that A generates a positive C_0-semigroup $T(\cdot)$ of type (M,ω). If r_i, $i=1,\dots,k$, are a.m. on $(-\infty,\tau\omega]$ for some $\tau>0$ and $u_i\geqslant 0$ $(i=0,\dots,k-1)$, then $u_n\geqslant 0$ $(n\geqslant k)$.*

Proof. The statement follows from Theorem 10 and the fact that sum of positive operators is positive. □

Unfortunately, Theorem 10 and its corollaries have a serious practical deficiency. In most cases we would like to use a function r that approximates the exponential $z \to e^z$ at $z = 0$. Recall that a function r *approximates the exponential to order* $q \geqslant 1$ if $r(z) = \exp(z) + O(z^{q+1})$ as $z \to 0$. This, together with absolute monotonicity on $(-\infty, 0]$ leads to an order-barrier which was first observed by Bolley and Crouzeix [5]. We present a short proof for the convenience of the reader.

Theorem 14. *If r is a.m. on $(-\infty, 0]$ and approximates the exponential to order $q > 1$, then $r(z) = e^z$ for* $\operatorname{Re} z \leqslant 0$.

Proof. Using Bernstein's theorem and the fact that r approximates the exponential function to order $q > 1$, it follows that

$$1 = r(0) = r'(0) = r''(0) = \int_0^\infty d\alpha(t) = \int_0^\infty t\, d\alpha(t) = \int_0^\infty t^2\, d\alpha(t),$$

with α bounded and nondecreasing. Hence, $\int_0^\infty (t-1)^2\, d\alpha(t) = 0$. Since the integrand is continuous on $[0, \infty)$, strictly positive except for an arbitrary neighborhood of $t = 1$ and α is nondecreasing, we conclude that the only possible point of increase of α is $t = 1$. Since $1 = \int_0^\infty d\alpha(t)$, we see that α can be chosen to be $\alpha = \chi_{[1,\infty)}$, where $\chi_{[1,\infty)}$ denotes the characteristic function of the interval $[1, \infty)$. Therefore, $r(z) = \int_0^\infty e^{zt}\, d\alpha(t) = e^z$, $\operatorname{Re} z \leqslant 0$. □

If $A \in \mathcal{B}(X)$, then we can extend Theorem 10 to functions that are no longer absolutely monotonic on a half line but in an interval. The idea to preserve positivity under some restrictions on the time-step (conditional positivity) for rational functions can be found in [5] for the finite dimensional situation $X = \mathbb{R}^n$ and A an M-matrix. There, the requirement on the function was absolute monotonicity on an interval. We can generalize this to arbitrary Banach-lattices and arbitrary positive semigroups generated by bounded linear operators. We will require that $r \in \mathcal{F}_{\tau\omega}$ (r does not have to be a rational function), and that r is a.m. at a suitable point depending on A and the time-step τ. We also show that if $r \in \mathcal{F}_{\tau\omega}$ and r is a.m. at $-\tau c$, then r is a.m. on $[-\tau c, \tau\omega]$, automatically. We begin with the characterization of positive semigroups $T(t) = e^{tA}$ with bounded generators A; see [20, C-II, Theorem 1.11].

Lemma 15. *Let $A \in \mathcal{B}(X)$, X Banach lattice. Then $T(t) \geqslant 0$ if and only if $A + \|A\| I \geqslant 0$.*

Lemma 15 is not optimal in the sense that if $A \in \mathcal{B}(X)$ generates a positive semigroup, then there is often a constant $c \geqslant 0$ with $c < \|A\|$ such that $A + cI \geqslant 0$. With this in mind we prove a theorem on conditional positivity.

Theorem 16. *Let X be a Banach lattice, let $A \in \mathcal{B}(X)$ generate the positive semigroup $T(\cdot)$ of type (M, ω) and let $c \geqslant \max\{0, -\omega\}$, such that $A + cI \geqslant 0$. If $r \in \mathcal{F}_{\tau\omega}$ and r is a.m. at $-\tau c$ for some $\tau > 0$, then $r(\tau A) \geqslant 0$.*

Proof. Since $r \in \mathcal{F}_{\tau\omega}$, there exists $\alpha \in NBV^{\tau\omega}$ such that $r(z) = \int_0^\infty e^z t\, d\alpha(t)$ for $\operatorname{Re} z \leqslant \tau\omega$. Then,

$$\begin{aligned} r(\tau A) &= \int_0^\infty T(\tau t)\, d\alpha(t) = \int_0^\infty e^{c\tau t} T(\tau t) e^{-c\tau t}\, d\alpha(t) \\ &= \int_0^\infty \sum_{n=0}^\infty \frac{(t\tau(A+cI))^n}{n!} e^{-c\tau t}\, d\alpha(t) = \sum_{n=0}^\infty \frac{\tau^n (A+cI)^n}{n!} \int_0^\infty t^n e^{-c\tau t}\, d\alpha(t) \\ &= \sum_{n=0}^\infty \frac{\tau^n (A+cI)^n}{n!} r^{(n)}(-c\tau) \geqslant 0, \end{aligned}$$

provided we can interchange summation and integration. To see this, first note that since $A + cI \geqslant 0$, we have that

$$\sum_{n=N+1}^\infty \frac{(t\tau(A+cI))^n}{n!} e^{-c\tau t} \leqslant \sum_{n=0}^\infty \frac{(t\tau(A+cI))^n}{n!} e^{-c\tau t} = T(\tau t).$$

Thus,

$$\left\| \sum_{n=N+1}^\infty \frac{(t\tau(A+cI))^n}{n!} e^{-c\tau t} \right\| \leqslant \left\| T(\tau t) \right\| \leqslant M e^{\omega\tau t} \tag{19}$$

for every $N \geqslant 0$. We are going to show that

$$\begin{aligned} &\left\| \int_0^\infty \sum_{n=0}^\infty \frac{(t\tau(A+cI))^n}{n!} e^{-c\tau t}\, d\alpha(t) - \sum_{n=0}^N \int_0^\infty \frac{(t\tau(A+cI))^n}{n!} e^{-c\tau t}\, d\alpha(t) \right\| \\ &\quad = \left\| \int_0^\infty \sum_{n=N+1}^\infty \frac{(t\tau(A+cI))^n}{n!} e^{-c\tau t}\, d\alpha(t) \right\| \end{aligned} \tag{20}$$

is arbitrary small if N is large enough. Let $\varepsilon > 0$. Since $r \in \mathcal{F}_{\tau\omega}$, there is $t_0 > 0$ such that

$$\int_{t_0}^\infty M e^{\omega\tau t} \left| d\alpha(t) \right| \leqslant \frac{\varepsilon}{2}. \tag{21}$$

Since $\sum_{n=0}^N \frac{(t\tau(A+cI))^n}{n!} e^{-c\tau t} \to T(\tau t)$ as $N \to \infty$ uniformly on $[0, t_0]$, choose $N \geqslant 0$ such that

$$\left\| \sum_{n=N+1}^\infty \frac{(t\tau(A+cI))^n}{n!} e^{-c\tau t} \right\| \leqslant \frac{\varepsilon}{2 \int_0^{t_0} |d\alpha(t)|} \tag{22}$$

for all $t \in [0, t_0]$. Then, by (19), (21) and (22) we have

$$\left\| \int_0^\infty \sum_{n=N+1}^\infty \frac{(t\tau(A+cI))^n}{n!} e^{-c\tau t}\, d\alpha(t) \right\|$$
$$\leqslant \int_0^{t_0} \frac{\varepsilon}{2\int_0^{t_0} |d\alpha(t)|} \left|d\alpha(t)\right| + \int_{t_0}^\infty M e^{\omega\tau t} \left|d\alpha(t)\right| \leqslant \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon,$$

which shows that the norm in (20) tends to 0 as $N \to \infty$. $\square$

Corollary 17 (Variable step-size). *Let X be a Banach lattice, let $A \in \mathcal{B}(X)$ generate the positive semigroup $T(\cdot)$ of type (M, ω) and let $c \geqslant 0$ $(c \geqslant -\omega)$, such that $A + cI \geqslant 0$. Let τ_i, $i = 1, \ldots, n$, be positive numbers. If $r \in \mathcal{F}_{\tau_i\omega}$ and r is a.m. at $-\tau_i c$, $i = 1, \ldots, n$, then $\prod_{i=1}^n r(\tau_i A) \geqslant 0$.*

For the corollary on multi-step schemes recall its definition from (18).

Corollary 18 (Multi-step schemes). *Let X be a Banach lattice, let $A \in \mathcal{B}(X)$ generate the positive semigroup $T(\cdot)$ of type (M, ω) and let $c \geqslant 0$ $(c \geqslant -\omega)$, such that $A + cI \geqslant 0$. If $r_i \in \mathcal{F}_{\tau\omega}$, r_i are a.m. at $-\tau c$ and $u_i \geqslant 0$ $(i = 0, \ldots, k-1)$, then $u_n \geqslant 0$ $(n \geqslant k)$.*

Remark 19. The converse of Theorem 16 is also true in the same sense as in Remark 11. Also, for a particular Banach lattice and bounded operator generating a positive semigroup the time-step might sometimes be chosen from a larger set than the set determined by the absolute monotonicity of the function (see, for example, [18]).

We conclude this section by showing that absolute monotonicity at one point is just a formally weaker condition than absolute monotonicity on an interval if $r \in \mathcal{F}_\omega$. Let $r \in \mathcal{F}_\omega$ and assume that r is a.m. at $c < \omega$. Since $r \in \mathcal{F}_\omega$ it follows that $r(z) = \int_0^\infty e^{zt}\, d\alpha(t)$, $\operatorname{Re} z \leqslant \omega$, for some $\alpha \in NBV^\omega$. Let $k \in \mathbb{N}$, and $s \in [c, \omega]$. Then

$$r^{(k)}(s) = \int_0^\infty t^k e^{st}\, d\alpha(t) = \int_0^\infty t^k e^{(s-c)t} e^{ct}\, d\alpha(t) = \int_0^\infty \sum_{n=0}^\infty \frac{(s-c)^n t^n}{n!} t^k e^{ct}\, d\alpha(t)$$
$$= \sum_{n=0}^\infty \frac{(s-c)^n}{n!} \int_0^\infty t^{k+n} e^{ct}\, d\alpha(t) = \sum_{n=0}^\infty \frac{(s-c)^n}{n!} r^{(k+n)}(c) \geqslant 0.$$

Thus, r is a.m. on $[c, \omega]$. The interchange of the sum and integral can be justified with a similar argument as in the proof of Theorem 16.

4. Shape preserving schemes

In this section we introduce a class of qualitative properties which can be described via positivity and illustrate the usefulness of these concepts in the context of the heat equation.

Definition 20. Let X be a Banach space, Y a Banach lattice, A the generator of a C_0-semigroup $T(\cdot)$ on X, and let $B : X \supset \mathcal{D}(B) \to Y$ be a closed linear operator with $\mathcal{D}(A) \subset \mathcal{D}(B)$. The semigroup $T(\cdot)$ preserves shape associated with the operator B (preserves B-shape) if for any $x \in \mathcal{D}(A)$ with $Bx \geqslant 0$ we have $BT(t)x \geqslant 0$ for $t > 0$.

If $\mathcal{D}(A)_+$ is dense in X_+, where the subscript $+$ denotes the positive cone of $\mathcal{D}(A)$ and X, respectively, and if $B = I$ in Definition 20, then the semigroup preserves positivity; if $X = L^p[a,b]$ and $(Bf)(x) := \frac{\partial^2 f(x)}{\partial x^2}$, then the semigroup preserves convexity and if $(Bf)(x) := \chi_{(c,d)} \frac{\partial f(x)}{\partial x}$, $a < c < d < b$, then the semigroup preserves monotonicity on (c,d).

Proposition 21. *If in addition to the assumptions on B in Definition* 20 *we also have that $\mathcal{D}(A) = \mathcal{D}(B)$ and B is invertible, then $T(\cdot)$ generated by A preserves B-shape if and only if the semigroup $S(t) := BT(\cdot)B^{-1}$ generated by BAB^{-1} with domain $\mathcal{D}(BAB^{-1}) = \{y \in Y\colon\ AB^{-1}y \in \mathcal{D}(B)\}$ is positive. Moreover, if $T(\cdot)$ is of type (M,ω), then $S(\cdot)$ is of type $(\tilde{M},\omega)$.*

Proof. To see that $S(\cdot)$ is a C_0-semigroup on Y, let $y \in Y$ and $x := B^{-1}y$. Since $x \in \mathcal{D}(B) = \mathcal{D}(A)$ it follows that $x = (\lambda_0 I - A)^{-1}z$ for some $z \in X$, $\lambda_0 > 0$, and

$$S(t)y = BT(t)(\lambda_0 I - A)^{-1}z = B(\lambda_0 I - A)^{-1}T(t)z.$$

Since $B(\lambda_0 I - A)^{-1}$ and $(\lambda_0 I - A)B^{-1}$ are bounded, $S(\cdot)$ is a C_0-semigroup and

$$\big\|S(t)y\big\| \leqslant \big\|B(\lambda_0 I - A)^{-1}\big\| \cdot \big\|T(t)\big\| \cdot \big\|(\lambda_0 I - A)B^{-1}\big\| \cdot \|y\|.$$

Thus, $S(\cdot)$ is of type $(\tilde{M},\omega)$ for some $\tilde{M} \geqslant 1$. Let C be the generator of $S(\cdot)$. For $y \in Y$ we have

$$S(t)y = B(\lambda_0 I - A)^{-1}T(t)(\lambda_0 I - A)B^{-1}y.$$

Thus,

$$\mathcal{D}(C) = \big\{y \in Y\colon\ (\lambda_0 I - A)B^{-1}y \in \mathcal{D}(A)\big\} = \big\{y \in Y\colon\ AB^{-1}y \in \mathcal{D}(A) = \mathcal{D}(B)\big\}$$

and $C = BAB^{-1}$. For the equivalence assume first that $T(\cdot)$ preserves B-shape. If $y \in Y_+$, then $x := B^{-1}y \in \mathcal{D}(A) = \mathcal{D}(B)$ and $Bx \geqslant 0$. Thus $S(t)y = BT(t)B^{-1}y = BT(t)x \geqslant 0$. Conversely, if $S(\cdot)$ is positive and $x \in \mathcal{D}(A)$ with $Bx \geqslant 0$, then there is a $y \in Y$ with $x = B^{-1}y$ and $Bx = y \geqslant 0$. Thus $BT(t)x = BT(t)B^{-1}y = S(t)y \geqslant 0$. □

Corollary 22. *Let X be a Banach space, Y be Banach lattice, $A \in \mathcal{B}(X)$ and $B \in \mathcal{B}(X,Y)$. Assume that B is invertible. Then, the following statements are equivalent*:

(i) *The semigroup $T(\cdot)$ generated by A is preserves B-shape.*
(ii) *The semigroup $BT(\cdot)B^{-1}$ is positive.*
(iii) $BAB^{-1} + \|BAB^{-1}\|I \geqslant 0$.

Proof. The statement follows from Proposition 21 and Lemma 15. □

We remark that if in addition to the assumptions of Corollary 22 we have that $X = Y$ and $AB = BA$, then $T(\cdot)$ is B-shape preserving if and only if $T(\cdot)$ is positive. In the following we discuss conditions which guarantee that $r(\tau A)$ *preserves* B*-shape*, that is, $Br(\tau A)x \geqslant 0$ for $x \in \mathcal{D}(A)$ with $Bx \geqslant 0$. The first theorem is on unconditional B-shape preservation.

Theorem 23. *Assume that the C_0 semigroup $T(\cdot)$ of type (M,ω) generated by A preserves B-shape. If r is a.m. on $(-\infty,\tau\omega]$ for $\tau > 0$, then $r(\tau A)$ preserves B-shape.*

Proof. By Corollary 9, $r \in \mathcal{F}_{\tau\omega}$ and $r(u) = \int_0^\infty e^{ut}\,d\beta(t)$ $(u \in (-\infty,\tau\omega])$ where $\beta \in NBV_{\tau\omega}$ is nondecreasing. If $x \in D(A)$ then $x = (\lambda_0 I - A)^{-1}z$ for some $\lambda_0 > 0$ and $z \in X$. Since $BR(\lambda_0 I - A)^{-1}$ is bounded, the map $t \to BT(t)x = B(\lambda_0 I - A)^{-1}T(t)z$ is continuous for $x \in \mathcal{D}(\mathcal{A})$ and $\|BT(t)x\| \leqslant \tilde{M}e^{\omega t}\|z\|$. Therefore, by the H–P functional calculus,

$$Br(\tau A)x = B\int_0^\infty T(\tau t)x\,d\beta(t) = \int_0^\infty BT(\tau t)x\,d\beta(t) \geqslant 0$$

for all $x \in \mathcal{D}(A)$ with $Bx \geqslant 0$. □

Theorem 24. *Let X be a Banach space and Y a Banach lattice. Assume that the semigroup $T(\cdot)$ of type (M,ω) generated by $A \in \mathcal{B}(X)$ preserves B-shape, $B \in \mathcal{B}(X,Y)$ is invertible and $BAB^{-1} + cI \geqslant 0$ for some $c \geqslant \max\{0,-\omega\}$. If $r \in \mathcal{F}_{\tau\omega}$ is a.m. at $-\tau c$ for some $\tau > 0$, then $r(\tau A)$ preserves B-shape.*

Proof. By Corollary 22, $T(\cdot)$ preserves B-shape if and only if the semigroup $S(\cdot)$ generated by BAB^{-1} is positive. By Proposition 21, $S(\cdot)$ is of type $(\tilde{M},\omega)$. Thus, by Theorem 16, $r(\tau BAB^{-1})y \geqslant 0$ for $y \geqslant 0$. Using the H–P functional calculus, we see that $r(\tau BAB^{-1}) = Br(\tau A)B^{-1}$. Hence, if $x \in \mathcal{D}(A)$ with $Bx := y \geqslant 0$, then $Br(\tau A)x = Br(\tau A)B^{-1}y \geqslant 0$. □

We remark that we can obtain results for variable step-sizes and multi-step schemes with obvious modification of the corollaries in Section 3. Next, we show two simple applications of Theorems 23 and 24. Let us consider the heat equation

$$\begin{aligned}&\frac{\partial u(s,t)}{\partial t} = \frac{\partial}{\partial s}D(s)\frac{\partial}{\partial s}u(s,t) \quad \text{for } t \geqslant 0,\ s \in (0,1),\\ &u(t,0) = u(t,1) = 0 \quad \text{and} \quad u(0,s) = u_0(s) \quad \text{for } t \geqslant 0,\ s \in [0,1],\end{aligned}$$

and the corresponding abstract Cauchy problem with $X := L^2[0,1]$, $(Af)(s) := (D(s)f'(s))'$ with $\mathcal{D}(A) := H^2[0,1] \cap H_0^1[0,1]$ and $x := u_0$. We would like to investigate concavity preservation; i.e., if the initial function is concave, do the solution and a suitable approximation preserve this property? The initial function is concave if $\frac{\partial^2 u_0(s)}{\partial s^2} \leqslant 0$, or, equivalently, if $x'' \leqslant 0$. Therefore, we can look at B-shape preservation with $Bf := -f''$, $\mathcal{D}(B) := \mathcal{D}(A)$ and $Y := X$. By Proposition 21, it is enough to show that BAB^{-1} generates a positive semigroup $S(\cdot)$. Assume that D is sufficiently smooth and $\inf_{s\in(0,1)} D(s) > 0$.

Then A generates an analytic C_0-semigroup on X (see [23, p. 112]). From Proposition 21 it follows that $S(\cdot)$ is also C_0. Thus, if BAB^{-1} is dispersive, then $S(\cdot)$ is a positive contraction on X; see [20, C-II, Theorem 1.2]. A straightforward computation shows that

$$\big(B^{-1}f\big)(s) = -\int_0^s rf(r)\,dr - s\int_s^1 f(r)\,dr + s\int_0^1 rf(r)\,dr$$

and that

$$\big(BAB^{-1}f\big)(s) = D'''(s)\left(-\int_s^1 f(r)\,dr + \int_0^1 rf(r)\,dr\right) + 3D''(s)f(s) + 2D'(s)f'(s) + D(s)f''(s).$$

Also observe that $\mathcal{D}(BAB^{-1}) = \mathcal{D}(A)$. Let $D(s) = as^2 + bs + c$ with $D(s) > 0$ on $[0,1]$ and $a \leqslant 0$. We show that in this case BAB^{-1} is dispersive, that is, $\langle BAB^{-1}f, \phi\rangle \leqslant 0$ for every $f \in \mathcal{D}(BAB^{-1})$ and for some

$$\phi \in dN^+(f) := \big\{\phi \in X_+^*\colon\ \|\phi\| \leqslant 1,\ \langle f,\phi\rangle = \|f^+\|\big\},$$

where f^+ denotes the positive part of f. If $f^+ \neq 0$, then $dN^+(f)$ consists of one element of the form $\phi(s) = c_0 f(s)$ if $f(s) > 0$ and $\phi(s) = 0$ if $f(s) \leqslant 0$ with $c_0 > 0$ suitably chosen. If $f^+ = 0$, then we can choose $c_0 = 0$. For $f \in \mathcal{D}(BAB^{-1})$ the set $M := \{s \in (0,1)\colon\ f(s) > 0\}$ is open and therefore $M = \bigcup_{n\in\mathbb{N}}(a_n, b_n)$. Then,

$$\begin{aligned}\big\langle BAB^{-1}f, \phi\big\rangle &= c_0\sum_{n\in N}\int_{a_n}^{b_n}\big(BAB^{-1}f\big)(s)f(s)\,ds\\ &= c_0\sum_{n\in N}\int_{a_n}^{b_n}\big[6af(s) + (4as+2b)f'(s)\\ &\quad + \big(as^2+bs+c\big)f''(s)\big]f(s)\,ds.\end{aligned}$$

Integration by parts yields

$$\big\langle BAB^{-1}f, \phi\big\rangle = c_0\sum_{n\in N}\int_{a_n}^{b_n}\big[5af^2(s) - \big(as^2+bs+c\big)\big(f'(s)\big)^2\big] \leqslant 0.$$

Thus, BAB^{-1} is dispersive, and hence $T(\cdot)$ preserves B-shape. Therefore, if r is a.m. on $(-\infty,0]$, then $r(\tau A)$ preserves B-shape too without any restriction on the time step. We remark that convexity preservation can be considered in $\mathbb{R}^2$ (and in $\mathbb{R}^n$) as well. There we have to define $B : X \supset \mathcal{D}(B) \to X^{\mathbb{R}^2\times\mathbb{R}^2} := Y$ with $P_{x,y}(Bf)(s_1,s_2) := \langle D^2f(s_1,s_2)x, y\rangle$, where $x, y \in \mathbb{R}^2$, $D^2f(s_1,s_2)$ denotes the second derivative matrix of f, $\langle\cdot,\cdot\rangle$ denotes the standard scalar product in $\mathbb{R}^2$ and $P_{x,y}$ denotes the canonical projection $P_{x,y} : X^{\mathbb{R}^2\times\mathbb{R}^2} \to X$, $P_{x,y}(\{z_{\alpha,\beta}\}) = z_{x,y}$.

In the next example we consider the heat equation after a centered spatial finite difference discretization with $D = 1$ for simplicity. Let $y_i(t)$ $(i = 0, 1, \dots, N)$ denote the approximation of $u(t, ih)$, where $h := 1/N$ and N is the dimension of the space discretization, let $y(t) := (y_0(t), \dots, y_N(t))^\top$ and let $X := (\mathbb{R}^{N+1}, \|\cdot\|_\infty)$. Then, the semidiscrete solution satisfies the equation $y'(t) = A_h y(t)$ for $t \geqslant 0$, $y(0) = y^0$, where $A_h : X \to X$ is defined as

$$\bigl(A_h y(t)\bigr)_i = \frac{1}{h^2}\bigl(y_{i+1}(t) - 2y_i(t) + y_{i-1}(t)\bigr) \quad (i = 1, \dots, N-1);$$

$(A_h y(t))_0 := (A_h y(t))_N = 0$, and $(y^0)_i = u_0(ih)$ $(i = 0, 1, \dots, N)$. It is easy to see that A_h generates a semigroup of type $(1, \omega)$ with $\omega < 0$. Let us consider B-shape preservation with $B := A_h$ and $Y := X$. This means convexity preservation in $\mathbb{R}^{N+1}$ (see, for example, [11]). The semigroup generated by A_h preserves A_h-shape by Corollary 22. For $B := A_h$ the conditions of Theorem 24 are satisfied with $c \geqslant 2/h^2$. Therefore, if $r \in \mathcal{F}_0$ is a.m. at τc for some $\tau > 0$, then $r(\tau A_h)$ preserves A_h-shape.

5. Norm-bound preserving schemes

Next we prove two theorems on norm-bound preserving schemes. The first one is on unconditional norm-bound preservation which is slightly more general then a corresponding statement in [22, Theorem 2.4] where quasi-contraction semigroups and constant step-sizes were considered. Moreover, using the H–P functional calculus instead of the Dunford–Taylor functional calculus, our proof becomes significantly simpler. We note that the idea of using Bernstein's theorem for unconditional contractivity in the case $X = \mathbb{R}^n$ also appears is [13, Theorem 11.15, p. 189]. The following two results are stated for one-step schemes and variable step-size; however, similar results hold for multi-step schemes with obvious modifications in the statements and proofs.

Theorem 25. *Let A generate a C_0-semigroup $T(\cdot)$ of type (M, ω) on a Banach space X. Let $\tau_i > 0$, $i = 1, \dots, n$, be positive numbers. If r is a.m. on $(-\infty, \tau_i\omega]$, $i = 1, \dots, n$, then $\|\prod_{i=1}^n r(\tau_i A)\| \leqslant M \prod_{i=1}^n r(\tau_i\omega)$.*

Proof. By Corollary 9, $r \in \mathcal{F}_{\tau_i\omega}$ and $r(u) = \int_0^\infty e^{ut}\,d\beta(t)$ $(u \in (-\infty, \tau_i\omega])$, where $\beta \in NBV_{\tau_i\omega}$ is nondecreasing. Then,

$$r(\tau_i A)x = \int_0^\infty T(\tau_i t)x\,d\beta(t) = \int_0^\infty T(t)x\,d\beta\left(\frac{t}{\tau_i}\right) := \int_0^\infty T(t)x\,d\beta_i(t).$$

We see from the proof of Theorem 6 that

$$\prod_{i=1}^n r(\tau_i A)x = \int_0^\infty T(t)x\,d\beta^{n*}(t),$$

where $\beta^{n*} := \beta_1 * \beta_2 * \cdots * \beta_n$. Since β is nondecreasing, the same holds for β_i and β^{n*}. Therefore,

$$\left\| \prod_{i=1}^{n} r(\tau_i A)x \right\| \leqslant \int_0^\infty \|T(t)x\| \, d\beta^{n*}(t) \leqslant M \prod_{i=1}^{n} r(\tau_i \omega)\|x\|$$

for all $x \in X$. □

Theorem 25 has the following important corollary (cf. [22, Theorem 1.2]).

Corollary 26. *Assume that $T(\cdot)$ is of type $(M, 0)$. If r approximates the exponential function and is a.m. on $(-\infty, 0]$, then $\|\prod_{i=1}^{n} r(\tau_i A)\| \leqslant M$ for all $\tau_i > 0$ $(i = 1, \ldots, n)$.*

Proof. Note that since r approximates the exponential function it follows that $r(0) = 1$. Then, the statement follows immediately from Theorem 25. □

In [22], Spijker considered $A \in \mathcal{B}(X)$ which satisfy a "circle condition" of the form $\|A + cI\| \leqslant \omega + c$ for some fixed $\omega \in \mathbb{R}$, $c \geqslant 0$. Let us denote this class by $\mathcal{B}(X, c, \omega)$. Clearly, if $A \in \mathcal{B}(X)$, then $A \in \mathcal{B}(X, c, \|A\|)$. If $A \in \mathcal{B}(X, c, \omega)$, then $T(t) = e^{tA}$ is of type $(1, \omega)$ since

$$\|T(t)\| = \|e^{ct}T(t)e^{-ct}\| = \|e^{ct}T(t)\|e^{-ct} \leqslant e^{(\omega+c)t}e^{-ct} = e^{\omega t}.$$

The assumptions on the time-step in Theorem 27 will depend on c and ω. In [22] a similar theorem is stated for rational functions [22, Theorem 3.3] and, as in the case of conditional positivity, absolute monotonicity was required in an interval. Here, as in the previous section, we can consider nonrational functions. Although we only require absolute monotonicity at a single point we showed at the end of Section 3 that this is equivalent to require absolute monotonicity on an appropriate interval if $r \in \mathcal{F}_{\tau\omega}$. We would like to emphasize that the use of the H–P functional calculus allows us to treat both unconditional and conditional norm-bound preservation within the same framework.

Theorem 27. *Let X be a Banach space and $A \in \mathcal{B}(X, c, \omega)$. Let τ_i, $i = 1, \ldots, n$, be positive numbers. If $r \in \mathcal{F}_{\tau_i\omega}$ a.m. at $-\tau_i c$, $i = 1, \ldots, n$, then $\|\prod_{i=1}^{n} r(\tau_i A)\| \leqslant \prod_{i=1}^{n} r(\tau_i \omega)$.*

Proof. Since $r \in \mathcal{F}_{\tau_i\omega}$ as in the proof of Theorem 25, we have $\prod_{i=1}^{n} r(\tau_i A)x = \int_0^\infty T(t)x \, d\alpha^{n*}(t)$. Using the fact that $A \in \mathcal{B}(X)$ and that r is absolutely monotonic at $-\tau_i c$ $(i = 1, \ldots, n)$, we obtain

$$\begin{aligned}
\left\| \prod_{i=1}^{n} r(\tau_i A) \right\| &= \left\| \int_0^\infty T(t) \, d\alpha^{n*}(t) \right\| = \left\| \int_0^\infty e^{ct}T(t)e^{-ct} \, d\alpha^{n*}(t) \right\| \\
&= \left\| \int_0^\infty \sum_{k=0}^{\infty} \frac{(t(A + cI))^k}{k!} e^{-ct} \, d\alpha^{n*}(t) \right\|
\end{aligned}$$

$$
\begin{aligned}
&= \left\| \sum_{k=0}^{\infty} \frac{(A+cI)^k}{k!} \int_0^{\infty} t^k e^{-ct}\, d\alpha^{n*}(t) \right\| \\
&= \left\| \sum_{k=0}^{\infty} \frac{(A+cI)^k}{k!} \frac{d^k}{dz^k} \left[\int_0^{\infty} e^{zt}\, d\alpha^{n*}(t) \right]\Big|_{z=-c} \right\| \\
&= \left\| \sum_{k=0}^{\infty} \frac{(A+cI)^k}{k!} \frac{d^k}{dz^k} \left[\prod_{i=1}^{n} r(\tau_i z) \right]\Big|_{z=-c} \right\| \\
&\leqslant \sum_{k=0}^{\infty} \frac{\|A+cI\|^k}{k!} \frac{d^k}{dz^k} \left(\prod_{i=1}^{n} r(\tau_i z) \right)\Big|_{z=-c} \\
&= \sum_{k=0}^{\infty} \frac{\|A+cI\|^k}{k!} \int_0^{\infty} t^k e^{-ct}\, d\alpha^{n*}(t) \\
&\leqslant \sum_{k=0}^{\infty} \frac{(\omega+c)^k}{k!} \int_0^{\infty} t^k e^{-ct}\, d\alpha^{n*}(t) = \int_0^{\infty} \sum_{k=0}^{\infty} \frac{(t(\omega+c))^k}{k!} e^{-ct}\, d\alpha^{n*}(t) \\
&= \int_0^{\infty} e^{t(\omega+c)-ct}\, d\alpha^{n*}(t) = \prod_{i=1}^{n} r(\tau_i \omega),
\end{aligned}
$$

provided that we can interchange sums and integrals. Since $A \in \mathcal{B}(X, c, \omega)$, we can replace the estimate in (19) by

$$
\begin{aligned}
&\left\| \sum_{n=N+1}^{\infty} \frac{(t(A+cI))^n}{n!} e^{-ct} \right\| \\
&\quad \leqslant \sum_{n=N+1}^{\infty} \frac{(t\|A+cI\|)^n}{n!} e^{-ct} \sum_{n=0}^{\infty} \frac{(t(\omega+c))^n}{n!} e^{-ct} = e^{\omega t}.
\end{aligned}
$$

Now the proof can be completed as the proof of Theorem 16. □

Corollary 28. *Let $A \in \mathcal{B}(X, c, 0)$. If $r \in \mathcal{F}_0$ approximates the exponential function and is a.m. at $-\tau_i c$, $\tau_i > 0$ for $i = 1, \ldots, n$, then $\|\prod_{i=1}^{n} r(\tau_i A)\| \leqslant 1$.*

Proof. Since r approximates the exponential function, we have that $r(0) = 1$. Now the statement follows from Theorem 27. □

We remark that the converse of Theorems 25 and 27 is also true in the same sense as for positivity preserving schemes in Remarks 11 and 19 (see also [18]).

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