

HIGHER ORDER GRÜNWARD APPROXIMATIONS OF FRACTIONAL DERIVATIVES AND FRACTIONAL POWERS OF OPERATORS

BORIS BAEUMER, MIHÁLY KOVÁCS, AND HARISH SANKARANARAYANAN

ABSTRACT. We give stability and consistency results for higher order Grünwald-type formulae used in the approximation of solutions to fractional-in-space partial differential equations. We use a new Carlson-type inequality for periodic Fourier multipliers to gain regularity and stability results. We then generalise the theory to the case where the first derivative operator is replaced by the generator of a bounded group on an arbitrary Banach space.

1. INTRODUCTION

In a series of articles Meerschaert, Scheffler and Tadjeran [16, 17, 18, 19, 20] explored consistency and stability for numerical schemes for fractional-in-space partial differential equations using a shifted Grünwald formula to approximate the fractional derivative. In particular, in [20] they showed consistency if the order of the spatial derivative is less or equal to 2. They obtained a specific error term expansion for $f \in C^{4+n}(\mathbb{R})$, where n is the number of error terms, as well as stability for the Crank-Nicolson scheme using Gershgorin’s theorem to determine the spectrum of the Grünwald matrix. Richardson extrapolation then gave second order convergence in space and time of the numerical scheme.

In this article we explore convergence with error estimates for higher order Grünwald-type approximations of semigroups generated first by a fractional derivative operator on $L^1(\mathbb{R})$ and then, using a transference principle, by fractional powers of group or semigroup generators on arbitrary Banach spaces.

It was already shown in [2, Proposition 4.9] that for all

$$f \in X_\alpha(\mathbb{R}) := \{f \in L_1(\mathbb{R}) : \exists g \in L_1(\mathbb{R}) \text{ with } \hat{g}(k) = (-ik)^\alpha \hat{f}(k), k \in \mathbb{R}\}$$

the first order Grünwald scheme

$$(1) \quad A_{h,p}^\alpha f(x) = \frac{1}{\Gamma(-\alpha)} \frac{1}{h^\alpha} \sum_{m=0}^{\infty} \frac{\Gamma(m-\alpha)}{\Gamma(m+1)} f(x - (m-p)h)$$

converges in $L_1(\mathbb{R})$ to $f^{(\alpha)}$ as $h \rightarrow 0+$ and any shift $p \in \mathbb{R}$. Here $\hat{g}(k) = \int_{-\infty}^{\infty} e^{ikx} g(x) dx$ denotes the Fourier transform of g and for $f \in X_\alpha(\mathbb{R})$, $f^{(\alpha)} = g$ iff $(-ik)^\alpha \hat{f} = \hat{g}$. In Section 3 we develop higher order Grünwald-type approximations

Received by the editors June 3, 2012.

Key words and phrases. Fractional Derivatives, Grünwald Formula, Fourier Multipliers, Carlson’s Inequality, Fractional Differential Equations, Fractional Powers of Operators.

\tilde{A}_h^α . In Corollary 3.5 we can then give the consistency error estimate

$$(2) \quad \left\| \tilde{A}_h^\alpha f - f^{(\alpha)} \right\|_{L_1(\mathbb{R})} \leq Ch^n \|f^{(\alpha+n)}\|_{L_1(\mathbb{R})}$$

for an n -th order scheme.

Using a new Carlson-type inequality for periodic multipliers developed in Section 2 (Theorem 2.4) we investigate the stability and smoothing of certain approximation schemes \tilde{A}_h^α in Section 4. The main tool is Theorem 4.1 which gives a sufficient condition for multipliers associated with difference schemes approximating the fractional derivative to lead to stable schemes with desirable smoothing. In particular, we show in Proposition 4.2 that stability for a numerical scheme using (1) to solve the Cauchy problem

$$(3) \quad \frac{\partial}{\partial t} u(t, x) = (-1)^{q+1} \frac{\partial^\alpha}{\partial x^\alpha} u(t, x); u(0, x) = f(x)$$

with $2q - 1 < \alpha < 2q + 1, q \in \mathbb{N}$ can only be achieved for a unique shift p ; i.e. it is necessary that $p = q$ for $(-1)^{q+1} A_{h,p}^\alpha$ to generate bounded semigroups on $L_1(\mathbb{R})$ where the bound is uniform in h . Furthermore, in Theorem 4.5 we prove stability and smoothing of a second order scheme.

Developing the theory in L_1 allows in Section 5 the transference of the theory to fractional powers of the generator $-A$ of a strongly continuous (semi-)group G on a Banach space $(X, \|\cdot\|)$, noting that $f(x - (m - p)h)$ in (1) will read as $G((m - p)h)f$ [2]. The abstract Grünwald approximations with the optimal shifts generate analytic semigroups, uniformly in h , as shown in Theorem 5.1. This is the main property needed in Corollary 5.3 to show that the error between the solution $S_\alpha(t)f = e^{t(-1)^{q+1}A^\alpha} f$ and a fully discrete solution u_n obtained via a Runge-Kutta method with stage order s , order $r \geq s + 1$ and an $N + 1$ order Grünwald approximation is bounded by

$$\|S_\alpha(t)f - u_n\| \leq C \left(n^{-r} \|f\| + h^{N+1} \left| \log \frac{t}{h^\alpha} \right| \|A^{N+1} f\| \right), \quad h > 0, \quad t = n\tau.$$

Note that this yields error estimates of our numerical approximation schemes applied to (3) in spaces where the translation semigroup is strongly continuous, such as $L_p(\mathbb{R}), 1 \leq p < \infty, BUC(\mathbb{R}), C_0(\mathbb{R})$, etc. Using the abstract setting we can also conclude that the consistency error estimate (2) holds in those spaces, with the L_1 norm replaced by the appropriate norm.

Finally, in Section 6, we give results of some numerical experiments, including a third order scheme, highlighting the efficiency of the higher order schemes and the dependence of the convergence order on the smoothness of the initial data.

2. PRELIMINARIES

A measurable function $\psi : \mathbb{R} \rightarrow \mathbb{C}$ is called an L_1 -multiplier, if for all $f \in L_1 = L_1(\mathbb{R})$ there exists a $v \in L_1$ such that $\psi \hat{f} = \hat{v}$ where $\hat{f}(k) = \int_{-\infty}^{\infty} e^{ikx} f(x) dx$ denotes the Fourier transform of f . Define an operator, using the uniqueness of Fourier transforms, $T_\psi : L_1 \rightarrow L_1$ by $T_\psi f := v$ where v is defined as above. It is well known that T_ψ is a closed operator and since it is everywhere defined, by the closed graph theorem, it is bounded. Moreover, if ψ is an L_1 -multiplier then $\psi(k) = \hat{\mu}(k) = \int_{-\infty}^{\infty} e^{ikx} d\mu(x)$ for some bounded Borel measure μ and $\|T_\psi\|_{\mathcal{B}(L_1)} = \|\mu\|_{\text{TV}}$

where TV refers to the total variation of the measure and $\|\cdot\|_{\mathcal{B}(L_1)}$ is the operator norm on L_1 . Furthermore, if the measure μ has a density distribution g then

$$(4) \quad \|T_\psi\|_{\mathcal{B}(L_1)} = \|g\|_{L_1} = \|\check{\psi}\|_{L_1},$$

where $\check{\psi}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} g(k) dk$ denotes the inverse Fourier transform of ψ . In the sequel we will also make use of the following scaling property. If $a \in \mathbb{R}$, $h > 0$, and $\psi^a(k) = \psi(k+a)$ and $\psi_h(k) = \psi(hk)$, then

$$(5) \quad \|T_\psi\|_{\mathcal{B}(L_1)} = \|T_{\psi_h}\|_{\mathcal{B}(L_1)} = \|T_{\psi^a}\|_{\mathcal{B}(L_1)}.$$

The following inequality is of crucial importance in our error analysis. It is a special case of a more general Carlson type inequality, see [13, Theorem 5.10, p.107]. We give an elementary proof here to keep the presentation self contained. The case $r = 2$ is referred to as Carlson-Beurling Inequality, and for a proof see [1, p.429] and [7].

The space $W_r^1(\mathbb{R})$, $r \geq 1$, denotes the Sobolev space of $L_r(\mathbb{R})$ -functions with generalised first derivative in $L_r(\mathbb{R})$; that is, $f \in W_r^1(\mathbb{R})$ if $f \in L_r(\mathbb{R})$, f is locally absolutely continuous, and $f' \in L_r(\mathbb{R})$.

Proposition 2.1 (Carlson-type inequality). *If $g \in W_r^1(\mathbb{R})$, $1 < r \leq 2$, then there exists $f \in L_1$ and a constant $C(r) > 0$, independent of f and g , such that $\hat{f} = g$ a.e. and*

$$(6) \quad \|f\|_{L_1} \leq C(r) \|g\|_{L_r}^{\frac{1}{s}} \|g'\|_{L_r}^{\frac{1}{r}},$$

where $\frac{1}{r} + \frac{1}{s} = 1$.

Proof. First, since $g \in L_r(\mathbb{R})$, $f := \check{g} \in L_s(\mathbb{R})$. Also recall the Hausdorff-Young-Titchmarsh inequality [6, p.211]

$$(7) \quad \|\hat{u}\|_{L_s} \leq \sqrt{2\pi} \|u\|_{L_r}, u \in L_r, 1 \leq r \leq 2, \frac{1}{r} + \frac{1}{s} = 1.$$

Note that $\|f\|_{L_1} = \|\check{g}\|_{L_1} = \frac{1}{2\pi} \|\hat{g}\|_{L_1}$ and $\hat{g}'(x) = (-ix)\hat{g}(x)$. If $g \equiv 0$ there is nothing to prove. Otherwise, using Hölder's inequality, (7), and setting $v =$

$\frac{\|g'\|_{L_r}}{(r-1)^{1/r} \|g\|_{L_r}}$ we get

$$\begin{aligned} \|f\|_{L_1} &= \frac{1}{2\pi} \|\hat{g}\|_{L_1} = \frac{1}{2\pi} \left(\int_{|x| \leq v} |\hat{g}(x)| dx + \int_{|x| > v} \left| \frac{1}{x} (x\hat{g}(x)) \right| dx \right) \\ &\leq \frac{2^{1/r}}{2\pi} \left(v^{\frac{1}{r}} \|\hat{g}\|_{L_s} + v^{-\frac{1}{s}} \|(\cdot)\hat{g}(\cdot)\|_{L_s} (r-1)^{-1/r} \right) \\ &\leq \frac{2^{1/r}}{\sqrt{2\pi}} \left(v^{\frac{1}{r}} \|g\|_{L_r} + v^{-\frac{1}{s}} \|g'\|_{L_r} (r-1)^{-1/r} \right) \\ &= \sqrt{\frac{2}{\pi}} \frac{2^{1/r}}{(r-1)^{1/r^2}} \|g\|_{L_r}^{\frac{1}{s}} \|g'\|_{L_r}^{\frac{1}{r}}. \end{aligned}$$

Thus $f \in L_1$, \hat{f} exists and $g = \hat{g} = \hat{f}$ a.e. □

Remark 2.2. Inequality (6) can be rewritten in multiplier notation as

$$\|T_g\|_{\mathcal{B}(L_1)} \leq C(r) \|g\|_{L_r}^{\frac{1}{s}} \|g'\|_{L_r}^{\frac{1}{r}}.$$

The reach of Carlson's inequality can be greatly improved by the use of a partition of unity:

Corollary 2.3. *Let ϕ_j be such that $\sum_j \phi_j(x) = 1$ for almost all x . If $g\phi_j \in W_r^1(\mathbb{R})$, $1 < r \leq 2$, for all j and $\sum_j \|g\phi_j\|_{L_r}^{\frac{1}{s}} \|(g\phi_j)'\|_{L_r}^{\frac{1}{r}} < \infty$, where $\frac{1}{r} + \frac{1}{s} = 1$, then there exists $f \in L_1(\mathbb{R})$ and a constant $C(r)$ independent of f and g , such that $\hat{f} = g$ a.e. and*

$$\|f\|_{L_1} = C(r) \sum_j \|g\phi_j\|_{L_r}^{\frac{1}{s}} \|(g\phi_j)'\|_{L_r}^{\frac{1}{r}}.$$

Proof. By design, $g = \sum_j g\phi_j$. Let $f_j \in L_1(\mathbb{R})$ be such that $\hat{f}_j = g\phi_j$ by Proposition 2.1. By assumption

$$\left\| \sum_{j=1}^n f_j \right\|_{L_1} \leq \sum_{j=1}^n \|f_j\|_{L_1} \leq C(r) \sum_j \|g\phi_j\|_{L_r}^{\frac{1}{s}} \|(g\phi_j)'\|_{L_r}^{\frac{1}{r}} < \infty.$$

So $\sum_{j=1}^{\infty} f_j$ converges to some $f \in L_1$, $\|f\|_{L_1} \leq C(r) \sum_j \|g\phi_j\|_{L_r}^{\frac{1}{s}} \|(g\phi_j)'\|_{L_r}^{\frac{1}{r}}$ and $\hat{f} = \sum_j \hat{f}_j = g$ a.e., as $\lim_{n \rightarrow \infty} \left\| \hat{f} - \sum_{j=1}^n \hat{f}_j \right\|_{L_1} \leq \lim_{n \rightarrow \infty} \left\| f - \sum_{j=1}^n f_j \right\|_{L_1} = 0$. \square

2.1. Periodic multipliers. For periodic multipliers a Carlson type inequality is not directly applicable as these are not Fourier transforms of L_1 -functions. We mention that in [5] a suitable smooth cut-off function η was used where $\eta = 1$ in a neighborhood of $[-\pi, \pi]$ and η has compact support to estimate the multiplier norm of a periodic multiplier ψ by the non-periodic one $\eta\psi$. For the multiplier norm of $\eta\psi$ the above Carlson's type inequality can be then used. However, we prove a result similar to Proposition 2.1 for periodic multipliers which makes the introduction of a cut-off function superfluous and hence simplifies the technicalities in later estimates.

The space $W_{r,per}^1[-\pi, \pi]$ below denotes the Sobolev space of 2π -periodic functions g on \mathbb{R} where both g and its generalized derivative g' belong to $L_r[-\pi, \pi]$.

Theorem 2.4. *Let $g \in W_{r,per}^1[-\pi, \pi]$, $1 < r \leq 2$, then g is an L_1 -multiplier and there is $C > 0$, independent of g , such that*

$$\|T_g\|_{\mathcal{B}(L_1)} \leq |a_0| + C \|g\|_{L_r[-\pi, \pi]}^{\frac{1}{s}} \|g'\|_{L_r[-\pi, \pi]}^{\frac{1}{r}},$$

where $\frac{1}{r} + \frac{1}{s} = 1$ and $a_0 = \frac{1}{2\pi} \int_{-\pi}^{\pi} g(x) dx$, denotes the 0^{th} Fourier coefficient of g .

Proof. Since $g \in L_r[-\pi, \pi]$ and is 2π -periodic it can be written as a Fourier series $g(x) = \sum_{k=-\infty}^{\infty} a_k e^{ikx}$, where $a_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-ikx} g(x) dx$, denotes the k^{th} Fourier coefficient of g . If $\mu := \sum_{k=-\infty}^{\infty} a_k \delta_k$, where δ_k is the Dirac measure at k , then $g = \hat{\mu}$ and hence g is an L_1 -multiplier if and only if $\|T_g\|_{\mathcal{B}(L_1)} = \|\mu\|_{\text{TV}} = \sum_{k=-\infty}^{\infty} |a_k| < \infty$. First, note that $|a_0| \leq \frac{1}{2\pi} \int_{-\pi}^{\pi} |g(x)| dx < \infty$ and that ika_k are the Fourier coefficients of g' . Using Bellman's inequality [4] with $\alpha = \beta = s$, and Hausdorff-Young inequality, (see [10, 23]), we have

$$\sum_{k=1}^{\infty} |a_k| \leq C \left(\sum_{k=1}^{\infty} |a_k|^s \right)^{\frac{1}{s^2}} \left(\sum_{k=1}^{\infty} |(ika_k)|^s \right)^{\frac{1}{s} \left(\frac{s-1}{s} \right)} \leq C \|g\|_{L_r[-\pi, \pi]}^{\frac{1}{s}} \|g'\|_{L_r[-\pi, \pi]}^{\frac{1}{r}}.$$

Clearly, the same inequality holds for $\sum_{k=-\infty}^{-1} |a_k|$. Thus

$$\sum_{k=-\infty}^{\infty} |a_k| \leq |a_0| + C \|g\|_{L_r[-\pi, \pi]}^{\frac{1}{s}} \|g'\|_{L_r[-\pi, \pi]}^{\frac{1}{r}} < \infty$$

and the proof is complete. \square

Remark 2.5. The term $|a_0|$ cannot be removed from the above estimate in general as the specific example $g \equiv 1$ shows.

3. CONSISTENCY: HIGHER ORDER GRÜNWARD-TYPE FORMULAE

Let $\alpha \in \mathbb{R}_+$ and let

$$X_\alpha(\mathbb{R}) := \{f \in L_1 = L_1(\mathbb{R}) : \exists g \in L_1 \text{ with } \hat{g}(k) = (-ik)^\alpha \hat{f}(k), k \in \mathbb{R}\}.$$

For $f \in X_\alpha(\mathbb{R})$ define $f^{(\alpha)} = g$ if $g \in L_1$ and $(-ik)^\alpha \hat{f}(k) = \hat{g}(k)$ for $k \in \mathbb{R}$. The function $f^{(\alpha)}$, defined uniquely by the uniqueness of the Fourier transform, is called the *Riemann-Liouville fractional derivative* of f . Set $\|f\|_\alpha := \|f^{(\alpha)}\|_{L_1(\mathbb{R})}$ for $f \in X_\alpha(\mathbb{R})$. Similarly, we define

$$X_\alpha(\mathbb{R}_+) := \{f \in L_1(\mathbb{R}_+) : \exists g \in L_1(\mathbb{R}_+) \text{ with } \hat{g}(z) = (-z)^\alpha \hat{f}(z), \operatorname{Re} z \leq 0\},$$

where $\hat{f}(z) = \int_0^\infty e^{zt} f(t) dt$ denotes the Laplace transform of f . For $f \in X_\alpha(\mathbb{R}_+)$ define $f^{(\alpha)} = g$ if $g \in L_1(\mathbb{R}_+)$ and $(-z)^\alpha \hat{f}(z) = \hat{g}(z)$ for $\operatorname{Re} z \leq 0$. Set $\|f\|_\alpha := \|f^{(\alpha)}\|_{L_1(\mathbb{R}_+)}$ for $f \in X_\alpha(\mathbb{R}_+)$.

In order to calculate the fractional derivative of f , a shifted Grünwald formula was introduced in [18] given by

$$(8) \quad A_{h,p}^\alpha f(x) = \frac{1}{\Gamma(-\alpha)} \frac{1}{h^\alpha} \sum_{m=0}^{\infty} \frac{\Gamma(m-\alpha)}{\Gamma(m+1)} f(x - (m-p)h),$$

where p is an integer.

Remark 3.1. When (8) is applied to a function $f \in L_1(\mathbb{R}_+)$, we extend f to $L_1(\mathbb{R})$ by setting $f(x) = 0$ for $x < 0$. Hence, if $p \leq 0$, then with this convention, $A_{h,p}^\alpha f$ is supported on \mathbb{R}_+ and hence $A_{h,p}^\alpha$ can be regarded as an operator on $L_1(\mathbb{R}_+)$.

In [2, Proposition 4.9] it is shown that for all $f \in X_\alpha(\mathbb{R})$ we have $A_{h,p}^\alpha f \rightarrow f^{(\alpha)}$ in $L_1(\mathbb{R})$ as $h \rightarrow 0+$. For $p = 0$, $\alpha > 0$ and $f \in X_\alpha(\mathbb{R}_+)$, see [21, Theorem 13] for the same result. Theorem 3.3 shows that for $f \in X_{\alpha+\beta}(\mathbb{R})$ the convergence rate in $L_1(\mathbb{R})$ is of order h^β , $0 < \beta \leq 1$ as $h \rightarrow 0+$, and if $p \leq 0$, then the same holds for $f \in X_{\alpha+\beta}(\mathbb{R}_+)$ in $L_1(\mathbb{R}_+)$.

Furthermore, a detailed error analysis allows for higher order approximations by combining Grünwald formulas with different shifts p and accuracy h , cancelling out higher order terms. This will be shown in Corollary 3.5.

In the error analysis of Theorem 3.3 below, the function

$$(9) \quad \omega_{p,\alpha}(z) = \left(\frac{1 - e^{-z}}{z} \right)^\alpha e^{zp},$$

where $\alpha \in \mathbb{R}_+$ and $p \in \mathbb{R}$, plays a crucial role. As we take the negative real axis as the branch cut for the fractional power, $\omega_{p,\alpha}$ is analytic, except where $(1 - e^{-z})/z$

is on the negative real axis and at $z = 0$. As $\lim_{z \rightarrow 0} \omega_{p,\alpha}(z) = 1$, the singularity at zero is removable and hence there exists $R > 0, a_j \in \mathbb{R}$ such that

$$(10) \quad \omega_{p,\alpha}(z) = \sum_{j=0}^{\infty} a_j z^j \text{ for all } |z| < 2R.$$

In particular, $a_0 = 1$ and $a_1 = (p - \alpha/2)$. Furthermore, this implies that there exists $C > 0$ such that

$$(11) \quad |\omega_{p,\alpha}(z) - 1| \leq \begin{cases} C|z| & \text{for } |z| < R, \\ C & \text{for } z \in i\mathbb{R}, \\ C & \text{for } \operatorname{Re} z \geq 0 \text{ \& } p \leq 0. \end{cases}$$

It was shown in [21, Lemma 2] that

$$(12) \quad \left(\frac{1 - e^{-z}}{z} \right)^\alpha = \int_0^\infty e^{-zt} q_\alpha(t) dt, \quad \operatorname{Re} z \geq 0, \quad q_\alpha \in L_1(\mathbb{R}_+),$$

and $\int_0^\infty q_\alpha(t) dt = 1$.

Moreover, for $\alpha > 1$ and $k \in \mathbb{R}$, or for $0 < \alpha < 1$ and $-\pi < k < \pi$, it is easily verified that

$$(13) \quad \left| \frac{d}{dk} (\omega_{p,\alpha}(-ik)) \right| \leq C.$$

Lemma 3.2. *Let*

$$\hat{g}_{\beta,N,p}(k) = \frac{\omega_{p,\alpha}(-ik) - \sum_{j=0}^N a_j (-ik)^j}{(-ik)^{N+\beta}},$$

where $\omega_{p,\alpha}(z)$ is given by (9), a_j by (10) and $0 < \beta \leq 1, N \in \mathbb{N}$. Then $\hat{g}_{\beta,N,p}$ is the Fourier transform of some $g_{\beta,N,p} \in L_1$. Furthermore, $\operatorname{supp}(g_{\beta,N,p}) \subset [-p, \infty) \cup \mathbb{R}_+$.

Proof. Note that for $N, p = 0, \beta < 1$, this was shown in [21, Lemma 5]. Let $N = 0, \beta < 1$ and $p \neq 0$. Then

$$\hat{g}_{\beta,0,p}(k) = \frac{\omega_{p,\alpha}(-ik) - 1}{(-ik)^\beta} = e^{-ikp} g_{\beta,0,0}(k) + \frac{e^{-ikp} - 1}{(-ik)^\beta}.$$

The inverse of the first term is given by $t \mapsto g_{\beta,0,0}(t+p)$; the second term inverts to $t \mapsto ((t+p)^{\beta-1} H(t+p) - t^{\beta-1} H(t))/\Gamma(\beta)$, where H is the unit step function. Clearly, both functions are in L_1 and their support is contained in $[-p, \infty) \cup \mathbb{R}_+$. Assume $N = 0$ and $\beta = 1$, or $N \geq 1$.

Case 1: $\alpha \geq 1$ in equation (9). Clearly, each term of \hat{g} is the Fourier transform of a tempered distribution satisfying the support condition and hence all that remains to show is that $\hat{g}_{\beta,N,p}$ is the Fourier transform of an L_1 function. Note that $\hat{g}_{\beta,N,p} \notin L_2$ for $\beta < 1/2$. Hence we use Corollary 2.3, choosing a particular partition of unity $(\phi_j)_{j \in \mathbb{Z}}$. If in (10) $R > 1$, set $R = 1$ and define $\phi_0(x) = 1$ for $|x| < R/2, 2(R-|x|)/R$ for $R/2 \leq |x| \leq R, 0$ else. Then $\operatorname{supp}(\phi_0) \subset [-R, R]$. Define $\phi_1(x) = 2(x - R/2)/R$ for $R/2 \leq |x| \leq R, \phi_1(x) = 1$ for $R \leq x \leq 1$ and $\phi_1(x) = 2 - x$ for $1 < x < 2$ and $\operatorname{supp}(\phi_1) \subset [R/2, 2]$. For $j > 1$, let

$$\phi_j(x) = \begin{cases} (x - 2^{j-2})/2^{j-2} & \text{for } 2^{j-2} < x < 2^{j-1}, \\ (2^j - x)/2^{j-1} & \text{for } 2^{j-1} < x < 2^j, \\ 0 & \text{else.} \end{cases}$$

Then $\text{supp}(\phi_j) \subset [2^{j-2}, 2^j]$. For $j < 0$, define $\phi_j(x) = \phi_{-j}(-x)$. Hence there exists C such that $\|\phi'_j(x)\|_\infty \leq C2^{-|j|+2}$ for all $j \in \mathbb{Z}$. By Corollary 2.3, we are done if we can show that $\sum_j \|\hat{g}\phi_j\|_{L_2}^{\frac{1}{2}} \|(\hat{g}\phi_j)'\|_{L_2}^{\frac{1}{2}} < \infty$.

As \hat{g} is analytic in $(-2R, 2R)$, $\hat{g}\phi_0 \in W_2^1(\mathbb{R})$. For $j \neq 0$,

$$\begin{aligned} \hat{g}_{\beta, N, p}(k)\phi_j(k) &= \frac{\omega_{p, \alpha}(-ik) - \sum_{m=0}^{N-1} a_m(-ik)^m}{(-ik)^{N+\beta}} \phi_j(k) - \frac{a_N}{(-ik)^\beta} \phi_j(k) \\ &= T_1(k) - T_2(k). \end{aligned}$$

By (11) and (13), $\omega_{p, \alpha}$ and $\omega'_{p, \alpha}$ are bounded. Recall that either $N = 0$ and $\beta = 1$, or $N \geq 1$. In either case, the exponent in the denominator of T_1 is at least one. Hence there exists C independent of j such that $|T_1(k)| \leq C2^{2-|j|}$, and $|T'_1(k)| \leq C2^{2-|j|}$. The length of the support of T_1 is less than $2^{|j|}$. Hence

$$\|T_1\|_{L_2}^{\frac{1}{2}} \leq C^{1/2}(2^{4-2|j|}2^{|j|})^{1/4} \leq C2^{-|j|/4}.$$

Same for $\|T'_1\|_{L_2}^{\frac{1}{2}}$. To estimate T'_2 recall that $\|\phi'_j\|_\infty \leq 2^{-|j|+2}$. Thus there exists C independent of j such that $|T'_2(k)| \leq C2^{(|j|-2)(-\beta-1)} + C2^{(|j|-2)(-\beta)}2^{-|j|+2} = C2^{3+\beta}2^{-(\beta+1)|j|}$, and hence

$$\|T'_2\|_{L_2}^{\frac{1}{2}} \leq C(2^{-2(\beta+1)|j|}2^{|j|})^{1/4} = C2^{-|j|(2\beta+1)/4}.$$

The norm of T_2 is bounded by

$$\|T_2\|_{L_2}^{\frac{1}{2}} \leq C(2^{-2|j|\beta}2^{|j|})^{1/4} \leq C2^{|j|(1-2\beta)/4}.$$

This implies that $\|\hat{g}_{\beta, N, p}\phi_j\|_{L_2} \|(\hat{g}_{\beta, N, p}\phi_j)'\|_{L_2} \leq C2^{|j|(1-2\beta)/4}2^{-|j|/4} = C2^{-|j|\beta/2}$, and hence $\sum_j \|\hat{g}_{\beta, N, p}\phi_j\|_{L_2} \|(\hat{g}_{\beta, N, p}\phi_j)'\|_{L_2} < \infty$ and therefore $g_{\beta, N, p} \in L_1(\mathbb{R})$.

Case 2: $\alpha < 1$ in equation (9). For $\alpha < 1$, $\omega'_{p, \alpha}$ is not bounded; if $\alpha \leq 1/2$ it is not even locally in L_2 , making the above method unfeasible. Instead we use induction on N . We already established that the assertion holds for $N = 0$, $\beta < 1$, so assume it holds for some N ; i.e. assume $\hat{g}_{\beta, N, p}$ is the Fourier transform of an L_1 function satisfying the support condition. Then using the fact that the convolution of L_1 functions is an L_1 function and the fact that we established the assertion for $\alpha = 1$, we obtain that $k \mapsto \hat{g}_{\beta, N, p}(k) \frac{1 - e^{ik} - ik}{-ik}$ is also the Fourier of an L_1 function satisfying the support condition as the support of the inverse of the second factor

is in \mathbb{R}_+ . Furthermore,

$$\begin{aligned}
\hat{g}_{\beta, N, p}(k) \frac{\frac{1-e^{ik}}{-ik} - 1}{-ik} &= \frac{\left(\frac{1-e^{ik}}{-ik}\right)^{\alpha+1} e^{-ikp} - \left(\frac{1-e^{ik}}{-ik}\right) \sum_{j=0}^N a_j (-ik)^j}{(-ik)^{N+1+\beta}} \\
&\quad - \frac{\left(\frac{1-e^{ik}}{-ik}\right)^{\alpha} e^{-ikp} - \sum_{j=0}^N a_j (-ik)^j}{(-ik)^{N+1+\beta}} \\
&= \frac{\left(\frac{1-e^{ik}}{-ik}\right)^{\alpha+1} e^{-ikp} - \sum_{j=0}^{N+1} b_j (-ik)^j}{(-ik)^{N+1+\beta}} \\
&\quad - \sum_{j=0}^N a_j \frac{\left(\frac{1-e^{ik}}{-ik}\right) - \sum_{m=0}^{N+1-j} c_m (-ik)^m}{(-ik)^{N+1-j+\beta}} \\
&\quad - \frac{\left(\frac{1-e^{ik}}{-ik}\right)^{\alpha} e^{-ikp} - \sum_{j=0}^{N+1} d_j (-ik)^j}{(-ik)^{N+1+\beta}} \\
&= I_1 - I_2 - I_3,
\end{aligned}$$

where the b_j are Taylor coefficients of $\omega_{p, \alpha+1}$, the c_m are the Taylor coefficients of $\frac{1-e^{-z}}{z}$ and d_j are such that equality holds. As by case 1, I_1 and I_2 are Fourier transforms of L_1 functions, so is I_3 . Hence I_3 at $k = 0$ has to be bounded and therefore $d_j = a_j$ and hence $\hat{g}_{\beta, N+1, p} = I_3$.

The same argument about the convolution of L_1 -functions applies to the remaining case of $N = 0, \beta = 1$, using (12) and the fact that

$$\omega_{p, \alpha}(-ik) \frac{\frac{1-e^{ik}}{-ik} - 1}{-ik} = \frac{\omega_{p, \alpha+1}(-ik) - 1}{-ik} - \frac{\omega_{p, \alpha}(-ik) - 1}{-ik}.$$

□

Theorem 3.3. *Let $0 \leq \beta \leq 1$. Then there exists $C > 0$ such that $f \in X_{\alpha+\beta}(\mathbb{R})$ implies that*

$$\left\| A_{h, p}^{\alpha} f - f^{(\alpha)} \right\|_{L_1(\mathbb{R})} \leq Ch^{\beta} \|f\|_{\alpha+\beta}$$

as $h \rightarrow 0+$. If $p \leq 0$ and $f \in X_{\alpha+\beta}(\mathbb{R}_+)$, then $\left\| A_{h, p}^{\alpha} f - f^{(\alpha)} \right\|_{L_1(\mathbb{R}_+)} \leq Ch^{\beta} \|f\|_{\alpha+\beta}$.

In case of $\beta = 0$, $f \in X_{\alpha}$, $\left\| A_{h, p}^{\alpha} f - f^{(\alpha)} \right\|_{L_1(\mathbb{R})} \rightarrow 0$.

Proof. The case $\beta = 0$ was already shown in [2, Proposition 4.9] and is only included in the statement of the theorem for completeness.

To prove the first statement, first note that $(1+z)^{\alpha} = \sum_{m=0}^{\infty} \binom{\alpha}{m} z^m$ for $z \in \mathbb{C}$, $|z| < 1$ and $\alpha \in \mathbb{R}_+$. Moreover, the binomial coefficients are related to the Gamma function by the following equation $\binom{\alpha}{m} = \frac{(-1)^m \Gamma(m-\alpha)}{\Gamma(-\alpha) \Gamma(m+1)}$. Taking Fourier transforms in (8) we get

$$\begin{aligned}
\widehat{(A_h^{\alpha} f)}(k) &= h^{-\alpha} \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} e^{ik(m-p)h} \hat{f}(k) = h^{-\alpha} e^{-ikh p} (1 - e^{ikh})^{\alpha} \hat{f}(k) \\
&= (-ik)^{\alpha} \omega_{p, \alpha}(-ikh) \hat{f}(k) = \widehat{f^{(\alpha)}}(k) + \hat{\zeta}_h(k),
\end{aligned}$$

where $\omega_{p,\alpha}(z)$ is given by (9) and $\hat{\zeta}_h(k) = (-ik)^\alpha(\omega_{p,\alpha}(-ikh) - 1)\hat{f}(k)$. We rewrite the error term $\hat{\zeta}_h(k)$ as a product of Fourier transforms of L_1 -functions:

$$(14) \quad \hat{\zeta}_h(k) = (-ik)^\alpha(\omega_{p,\alpha}(-ikh) - 1)\hat{f}(k) = h^\beta \hat{g}_{\beta,0,p}(kh) \widehat{f^{(\alpha+\beta)}}(k),$$

where, by Lemma 3.2, $\hat{g}_{\beta,0,p}(k) = \left(\frac{\omega_{p,\alpha}(-ik)-1}{(-ik)^\beta}\right)$ is the Fourier transform of an L_1 function $g_{\beta,0,p}$ and $f^{(\alpha+\beta)} \in L_1$ by assumption. Thus $\hat{\zeta}_h$ is indeed the Fourier transform of an L_1 -function ζ_h and, by (4), (5) and Lemma 3.2,

$$\begin{aligned} \|\zeta_h\|_{L_1(\mathbb{R})} &\leq h^\beta \|T_{\hat{g}_{\beta,0,p}(h\cdot)}\|_{\mathcal{B}(L_1(\mathbb{R}))} \|f^{(\alpha+\beta)}\|_{L_1(\mathbb{R})} = h^\beta \|g_{\beta,0,p}\|_{L_1(\mathbb{R})} \|f^{(\alpha+\beta)}\|_{L_1(\mathbb{R})} \\ &\leq Ch^\beta \|f\|_{\alpha+\beta}. \end{aligned}$$

Finally, the second statement follows the same way, taking Remark 3.1 into account and noting that if $p \leq 0$, then $\text{supp}(\zeta_h) \subset \mathbb{R}_+$ and using Lemma 3.2 in (14). \square

Remark 3.4. Let $\alpha \in \mathbb{R}_+$, $2q - 1 < \alpha < 2q + 1$, $q \in \mathbb{N}$, and

$$(15) \quad \psi_{\alpha,h,p}(z) = (-1)^{q+1} h^{-\alpha} e^{-h pz} (1 - e^{hz})^\alpha.$$

Then the proof of Theorem 3.3 shows that the Grünwald formula (8) can be expressed in the multiplier notation of Section 2 as $A_{h,p}^\alpha = T_{(-1)^{q+1}\psi_h^p}$ where

$$(16) \quad \psi_h^p(k) = \psi_{\alpha,h,p}(ik) = (-1)^{q+1} h^{-\alpha} e^{-ikh p} (1 - e^{ikh})^\alpha.$$

Analyzing the error term $\hat{\zeta}_h$ in (14) further allows for higher order approximations by combining Grünwald formulae with different shifts p and accuracy h , cancelling out lower order error terms. Consider the Taylor expansion of $\omega_{p,\alpha}$ in (10) and let $N \geq 0$ and for $0 \leq j \leq N$ let $b_j, p_j \in \mathbb{R}$ and $c_j > 0$ be such that there exist d_j with

$$\sum_{j=0}^N b_j \omega_{p_j,\alpha}(c_j z) - 1 = \sum_{j=N+1}^{\infty} d_j z^j$$

for $|z| < 2R$; i.e. consider a linear combinations of $\omega_{p_j,\alpha}$'s cancelling out the lower order terms. Define

$$(17) \quad \tilde{A}_h^\alpha f := \sum_{j=0}^N b_j A_{c_j h, p_j}^\alpha f = T_{(-1)^{n+1} \sum_{j=0}^N b_j \psi_{c_j h}^{p_j}}$$

to be an $N + 1$ order Grünwald approximation. This is justified according to the following Corollary.

Corollary 3.5. *Let $0 < \beta \leq 1$, $N \in \mathbb{N}$ and \tilde{A}_h^α be an $N + 1$ order Grünwald approximation. Then there exists $C > 0$ such that $f \in X_{\alpha+N+\beta}(\mathbb{R})$ implies that*

$$\left\| \tilde{A}_h^\alpha f - f^{(\alpha)} \right\|_{L_1(\mathbb{R})} \leq Ch^{N+\beta} \|f\|_{\alpha+N+\beta}.$$

as $h \rightarrow 0^+$. If $p_j \leq 0$ for all $0 \leq j \leq N$ and $f \in X_{\alpha+N+\beta}(\mathbb{R}_+)$ then

$$\left\| \tilde{A}_h^\alpha f - f^{(\alpha)} \right\|_{L_1(\mathbb{R}_+)} \leq Ch^{N+\beta} \|f\|_{\alpha+N+\beta}.$$

Proof. Note that $\sum_{j=0}^N b_j = 1$ and for $n > 0$, we have that $\sum_{j=0}^N b_j a_{j,n} = 0$. Following the same argument that led to (14), we obtain that the error term can be expressed as

$$\begin{aligned}\hat{\zeta}_h(k) &= \widehat{\left(\tilde{A}_h^\alpha f - f^{(\alpha)}\right)}(k) = \sum_{j=0}^N b_j \left(\omega_{p_j, \alpha}(-ikc_j h) - 1\right) (-ik)^\alpha \hat{f}(k) \\ &= \sum_{j=0}^N b_j \left(\omega_{p_j, \alpha}(-ikc_j h) - \sum_{n=0}^N a_{j,n} (-ikc_j h)^n\right) (-ik)^\alpha \hat{f}(k) \\ &= h^{N+\beta} \sum_{j=0}^N b_j c_j^{N+\beta} \frac{\omega_{p_j, \alpha}(-ikc_j h) - \sum_{n=0}^N a_{j,n} (-ikc_j h)^n}{(-ikc_j h)^{N+\beta}} (-ik)^{\alpha+N+\beta} \hat{f}(k),\end{aligned}$$

where $a_{j,n}$ are the Taylor coefficients of $\omega_{p_j, \alpha}$. By Lemma 3.2,

$$\hat{g}(k) = \sum_{j=0}^N b_j c_j^{N+\beta} \frac{\omega_{p_j, \alpha}(-ikc_j) - \sum_{n=0}^N a_{j,n} (-ikc_j)^n}{(-ikc_j)^{N+\beta}}$$

is the finite sum of Fourier transforms of L_1 functions and hence $\hat{\zeta}_h$ is the Fourier transform of an L_1 function with

$$\|\zeta_h\|_{L_1(\mathbb{R})} \leq Ch^{N+\beta} \|f\|_{\alpha+N+\beta}.$$

The second statement follows along the same lines. \square

4. STABILITY AND SMOOTHING: SEMIGROUPS GENERATED BY PERIODIC MULTIPLIERS APPROXIMATING THE FRACTIONAL DERIVATIVE

The next result is the main technical tool of the paper. It gives a sufficient condition for multipliers associated with difference schemes approximating the fractional derivative to lead to stable schemes with desirable smoothing. In error estimates later, the smoothing of the schemes will be used in an essential way to reduce the regularity requirements on the initial data to obtain optimal convergence rates when considering space-time discretizations of Cauchy problems with fractional derivatives or, more generally, fractional powers of operators.

Theorem 4.1. *Let $\alpha \in \mathbb{R}_+$ and ψ be an absolutely continuous 2π -periodic function that satisfies the following:*

- (i) $|\psi(k)| \leq C |k|^\alpha$ for some $C > 0$,
- (ii) $|\psi'(k)| \leq C' |k|^{\alpha-1}$ for some $C' > 0$,
- (iii) $\operatorname{Re}(\psi(k)) \leq -c |k|^\alpha$ for some $c > 0$.

Then $\psi \in W_{r, \text{per}}^1[-\pi, \pi]$, where $r = 2$ if $\alpha > \frac{1}{2}$ and $r < \frac{1}{1-\alpha}$ if $\alpha \leq \frac{1}{2}$. Moreover,

- (a) $\|T_{e^{t\psi}}\|_{\mathcal{B}(L_1)} \leq K$ for $t \geq 0$,
- (b) $\|T_{\psi e^{t\psi}}\|_{\mathcal{B}(L_1)} \leq \frac{M}{t}$ for $t > 0$,

where K and M depend on c, C and C' above.

Proof. Set $r = 2$ if $\alpha > \frac{1}{2}$ and $r < \frac{1}{1-\alpha}$ if $\alpha \leq \frac{1}{2}$, where

$$(18) \quad 1 < r \leq 2 \quad \text{and} \quad \frac{1}{r} + \frac{1}{s} = 1.$$

Note that $r(\alpha - 1) > -1$, then from the assumptions we have $\psi \in W_{r,per}^1[-\pi, \pi]$, and for $t \geq 0$, we also have $e^{t\psi} \in W_{r,per}^1[-\pi, \pi]$. By Theorem 2.4,

$$(19) \quad \|T_{e^{t\psi}}\|_{\mathcal{B}(L_1)} \leq |a_0| + C \|e^{t\psi}\|_{L_r}^{\frac{1}{s}} \|(e^{t\psi})'\|_{L_r}^{\frac{1}{r}}.$$

Firstly $|a_0| = \left| \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{t\psi(k)} dk \right| \leq \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{t \operatorname{Re}(\psi(k))} dk \leq \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-ct|k|^\alpha} dk \leq 1$, where we have used Assumption (iii). Now, using Assumption (iii) again together with the substitution $\tau = t^{\frac{1}{\alpha}}|k|$,

$$(20) \quad \begin{aligned} \|e^{t\psi}\|_{L_r[-\pi, \pi]}^{\frac{1}{s}} &= \left(\int_{-\pi}^{\pi} |e^{t\psi(k)}|^r dk \right)^{\frac{1}{rs}} \leq C \left(\int_{-\pi}^{\pi} e^{rt \operatorname{Re}(\psi(k))} dk \right)^{\frac{1}{rs}} \\ &\leq C \left(\int_{-\pi}^{\pi} e^{-rct|k|^\alpha} dk \right)^{\frac{1}{rs}} \leq C \left(\frac{1}{t^{\frac{1}{\alpha}}} \int_{\mathbb{R}} e^{-rc|\tau|^\alpha} d\tau \right)^{\frac{1}{rs}} \leq Ct^{-\frac{1}{\alpha rs}}. \end{aligned}$$

Making use of Assumptions (ii) and (iii), we have

$$\left| \frac{d}{dk} (e^{t\psi(k)}) \right|^r = \left| t \frac{d\psi(k)}{dk} e^{t\psi(k)} \right|^r \leq C (t^r |k|^{r(\alpha-1)}) e^{-rct|k|^\alpha},$$

Since $r(\alpha - 1) > -1$, an application of (18) and the substitution $\tau = t^{\frac{1}{\alpha}}|k|$, yields

$$(21) \quad \left\| (e^{t\psi})' \right\|_{L_r[-\pi, \pi]}^{\frac{1}{r}} \leq C \left(t^{\frac{r-1}{\alpha}} \int_{\mathbb{R}} \tau^{r(\alpha-1)} e^{-rc\tau^\alpha} d\tau \right)^{\frac{1}{r^2}} \leq Ct^{\frac{1}{\alpha rs}}.$$

The proof of (a) is complete in view of (19), (20) and (21).

We have that $\psi e^{t\psi} \in W_{r,per}^1[-\pi, \pi]$ and once again by Theorem 2.4,

$$(22) \quad \|T_{\psi e^{t\psi}}\|_{\mathcal{B}(L_1)} \leq |a_0| + C \|\psi e^{t\psi}\|_{L_r[-\pi, \pi]}^{\frac{1}{s}} \|(\psi e^{t\psi})'\|_{L_r[-\pi, \pi]}^{\frac{1}{r}}.$$

Note that $|a_0| \leq \frac{1}{2\pi} \int_{-\pi}^{\pi} |\psi(k)| e^{t \operatorname{Re}(\psi(k))} dk \leq C \int_{-\pi}^{\pi} |k|^\alpha e^{-ct|k|^\alpha} dk \leq C/t$, where we have used Assumptions (i) and (iii). The use of the substitution $\tau = t^{\frac{1}{\alpha}}|k|$ and the Assumptions (i) and (iii), yield

$$(23) \quad \|\psi e^{t\psi}\|_{L_r[-\pi, \pi]}^{\frac{1}{s}} \leq C \left(\int_{\mathbb{R}} |k|^{r\alpha} e^{-rct|k|^\alpha} dk \right)^{\frac{1}{rs}} \leq Ct^{-\frac{1}{s} - \frac{1}{\alpha rs}}.$$

We also have by virtue of (21) and the three assumptions,

$$\begin{aligned} \left| \frac{d}{dk} (\psi e^{t\psi})(k) \right|^r &= \left| \psi(k) \frac{d}{dk} (e^{t\psi(k)}) + \frac{d\psi(k)}{dk} e^{t\psi(k)} \right|^r \\ &\leq 2^{r-1} (t^r |\psi(k)|^r + 1) |(\psi(k))'|^r |e^{t\psi(k)}|^r \\ &\leq C(|k|^{r(\alpha-1)} + t^r |k|^{r(2\alpha-1)}) e^{-rct|k|^\alpha}. \end{aligned}$$

Thus, using (18) and the substitution $\tau = t^{\frac{1}{\alpha}}|k|$, and noting that $r(2\alpha - 1) > r(\alpha - 1) > -1$,

$$(24) \quad \begin{aligned} \left\| \frac{d}{dk} (\psi e^{t\psi}) \right\|_{L_r[-\pi, \pi]}^{\frac{1}{r}} &\leq Ct^{-\frac{1}{r} + \frac{1}{\alpha rs}} \left(\int_{\mathbb{R}} (|\tau|^{r(\alpha-1)} + |\tau|^{r(2\alpha-1)}) e^{-rc\tau^\alpha} d\tau \right)^{\frac{1}{r^2}} \\ &\leq Ct^{-\frac{1}{r} + \frac{1}{\alpha rs}}, \end{aligned}$$

and the proof of (b) is complete in view of (18), (22), (23) and (24). \square

4.1. The shifted Grünwald formula of order 1. First, we make the following two observations about the multiplier associated with the shifted Grünwald formula given by (16). Note that for $p, k \in \mathbb{R}$ and $h, \alpha \in \mathbb{R}_+$, such that $2q - 1 < \alpha < 2q + 1$, $q \in \mathbb{N}$,

$$(25) \quad \psi_h^p(k) = (-1)^{q+1} h^{-\alpha} e^{-ikh} (1 - e^{ikh})^\alpha = (-1)^{q+1} h^{-\alpha} (-ikh)^\alpha \omega_{p,\alpha}(-ikh),$$

where $\omega_{p,\alpha}(z)$ is given by (9). Note also that

$$(26) \quad \psi_h^p(k) = h^{-\alpha} \psi_1^p(hk).$$

We now show that the range of the symbol associated with the shifted Grünwald formula is completely contained in a half-plane if and only if the shift is optimal.

Proposition 4.2. *Let $\psi_h^p(k) = (-1)^{q+1} h^{-\alpha} e^{-iphk} (1 - e^{ikh})^\alpha$, where the shift $p \in \mathbb{N}$, $k \in \mathbb{R}$, $h > 0$, $\alpha \in \mathbb{R}_+$ and $q \in \mathbb{N}$ such that $2q - 1 < \alpha < 2q + 1$. Then*

- (a) ψ_h^p satisfies Assumptions (i) and (ii) of Theorem 4.1 with C, C' independent of h .
- (b) $\operatorname{Re}(\psi_h^p)$ does not change sign if and only if $|p - \frac{\alpha}{2}| < \frac{1}{2}$ if and only if ψ_h^p satisfies the Assumption (iii) of Theorem 4.1 with c independent of h .

Proof. Proof of (a):

Recall that by (11) and (13), $|\omega_{p,\alpha}(-ikh)| \leq C$ and $|\omega'_{p,\alpha}(-ikh)| \leq C$, for $k \in [-\pi, \pi]$, respectively. Thus using (25), for $k \in [-\pi, \pi]$,

$$(27) \quad |\psi_h^p(k)| \leq C |k|^\alpha, \text{ and}$$

$$(28) \quad \left| \frac{d\psi_h^p(k)}{dk} \right| = h^{-\alpha} |-\alpha ih (-ikh)^{\alpha-1} \omega_{p,\alpha}(-ikh) + (-ikh)^\alpha \omega'_{p,\alpha}(-ikh)| \leq C |k|^{\alpha-1},$$

for some $C > 0$.

Proof of (b): It is enough to consider the case $h = 1$ in view of (26), so let $\psi := \psi_1^p$. Since ψ is 2π -periodic and $\psi(k) = \overline{\psi(-k)}$, it is sufficient to consider $k \in [0, \pi]$. Now

$$\psi(k) = (-1)^{q+1} e^{-ipk} \left(e^{\frac{ik}{2}} (e^{-\frac{ik}{2}} - e^{\frac{ik}{2}}) \right)^\alpha = (-1)^{q+1} e^{i(\frac{\alpha}{2}-p)k} \left(-2i \sin\left(\frac{k}{2}\right) \right)^\alpha.$$

Using the fact that for $x \geq 0$, $(-ix)^\alpha = x^\alpha e^{-i\alpha\frac{\pi}{2}}$, we obtain

$$\psi(k) = (-1)^{q+1} 2^\alpha \sin^\alpha\left(\frac{k}{2}\right) e^{i(\frac{\alpha}{2}-p)k - \frac{i\alpha\pi}{2}}; \quad 0 \leq k \leq \pi,$$

and therefore

$$(29) \quad \begin{aligned} \operatorname{Re}(\psi(k)) &= (-1)^{q+1} 2^\alpha \sin^\alpha\left(\frac{k}{2}\right) \cos\left(\left(\frac{\alpha}{2} - p\right)k - \frac{\alpha\pi}{2}\right) \\ &= (-1)^{q+1-p} 2^\alpha \sin^\alpha\left(\frac{k}{2}\right) \cos\left(\left(\frac{\alpha}{2} - p\right)(k - \pi)\right). \end{aligned}$$

Clearly, as $0 \leq k \leq \pi$, (29) changes sign if and only if $|\frac{\alpha}{2} - p| > \frac{1}{2}$. Note that by assumption $|\frac{\alpha}{2} - p| \neq \frac{1}{2}$. Furthermore, Assumption (iii) of Theorem 4.1 implies that there is no sign change. Hence all that remains to show is that $|p - \frac{\alpha}{2}| < \frac{1}{2}$ implies Assumption (iii) of Theorem 4.1. The fact that c is independent of h follows from (26).

Note that $|p - \frac{\alpha}{2}| < \frac{1}{2}$ implies that $p = q$ and hence, using that for $0 \leq x \leq \pi$, $\sin(x/2) \geq x/\pi$ and $\cos((\frac{\alpha}{2} - p)(x - \pi)) \geq \cos(-(\frac{\alpha}{2} - p)\pi)$,

$$(30) \quad \begin{aligned} \operatorname{Re}(\psi(k)) &= -2^\alpha \sin^\alpha\left(\frac{k}{2}\right) \cos\left(\left(\frac{\alpha}{2} - p\right)(k - \pi)\right) \\ &\leq -2^\alpha \left(\frac{k}{\pi}\right)^\alpha \cos\left(\left(\frac{\alpha}{2} - p\right)\pi\right) = -k^\alpha 2^\alpha \cos\left(\left(\frac{\alpha}{2} - p\right)\pi\right) / \pi^\alpha. \end{aligned}$$

□

Next, we show that with the optimal shift; i.e., $p = q$, the operators T_{ψ_h} generate strongly continuous semigroups on $L_1(\mathbb{R})$, and in the case when $p = 0$; i.e., $0 < \alpha < 1$, on $L_1(\mathbb{R}_+)$, that are bounded uniformly in h . Since the range of ψ_h is always contained in the spectrum of T_{ψ_h} , the semigroups generated by T_{ψ_h} will not be uniformly bounded if the shift is not optimal as shown by Proposition 4.2. In fact we show more: if the shift is optimal then the semigroups are uniformly analytic in h ; i.e., there is $M > 0$ such that the uniform estimate $\|T_{\psi_h, e^{t\psi_h}}\|_{\mathcal{B}(L_1)} \leq Mt^{-1}$ holds for $t, h > 0$. This fact will have significance when proving error estimates for numerical schemes for fractional differential equations.

Theorem 4.3. *Let $\alpha \in \mathbb{R}_+$, $2p - 1 < \alpha < 2p + 1$, $p \in \mathbb{N}$, and*

$$\psi_h(k) = (-1)^{p+1} h^{-\alpha} e^{-ipkh} (1 - e^{ikh})^\alpha.$$

Then the following hold.

- (a) $\{T_{e^{t\psi_h}}\}_{t \geq 0}$ are strongly continuous semigroups on $L_1(\mathbb{R})$ that are bounded uniformly in $h > 0$ and $t \geq 0$. In particular, if $1 < \alpha < 2$, then $\{T_{e^{t\psi_h}}\}_{t \geq 0}$ is a positive contraction semigroup on $L_1(\mathbb{R})$ and for $0 < \alpha < 1$, on $L_1(\mathbb{R}_+)$.
- (b) The semigroups $\{T_{e^{t\psi_h}}\}_{t \geq 0}$ are uniformly analytic in $h > 0$; i.e. there is $M > 0$ such that the uniform estimate $\|T_{\psi_h, e^{t\psi_h}}\|_{\mathcal{B}(L_1)} \leq Mt^{-1}$ holds for $t, h > 0$.

Proof. Proof of (a): To begin, note that $\psi_h(k) = \psi_h^p(k)$ with $p = q$. We only have to show that $\|T_{e^{t\psi_h}}\|_{\mathcal{B}(L_1)} \leq K$, for all $t \geq 0$ and $h > 0$, for some $K \geq 1$ and strong continuity follows by [1, Proposition 8.1.3]. Furthermore, it is enough to consider $h = 1$ in view of (5) and (26), so let $\psi := \psi_1$. First, let $0 < \alpha < 1$ or $1 < \alpha < 2$ and hence $p = 0$ or 1, respectively. We have, taking Remark 3.4 into account, that

$$\begin{aligned} (T_\psi f)(x) &= (-1)^{p+1} \left(\sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} f(x - (m - p)) \right) \\ &= -\binom{\alpha}{p} f(x) + (-1)^{p+1} \sum_{m=0, m \neq p}^{\infty} (-1)^m \binom{\alpha}{m} f(x - (m - p)) \\ &= -\binom{\alpha}{p} I f(x) + (T_{\tilde{\psi}} f)(x). \end{aligned}$$

Since $(-1)^{p+1} (-1)^m \binom{\alpha}{m} \geq 0$, for $m \neq p$, it follows that $T_{\tilde{\psi}}$ is a positive operator on $L_1(\mathbb{R})$ (or, $L_1(\mathbb{R}_+)$ for $0 < \alpha < 1$ by recalling Remark 3.1) and so is $e^{tT_{\tilde{\psi}}} = T_{e^{t\tilde{\psi}}}$. Therefore, noting the fact that $\sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} = 0$,

$$T_{e^{t\psi_1}} = e^{tT_\psi} = e^{t(-\binom{\alpha}{p}I + T_{\tilde{\psi}})} = e^{-\binom{\alpha}{p}t} e^{tT_{\tilde{\psi}}} \geq 0,$$

and

$$\|T_{e^{t\psi}}\|_{L_1} \leq e^{-\binom{\alpha}{p}t} e^{t\|T_{\psi}\|_{L_1}} = e^{-\binom{\alpha}{p}t} e^{(-1)^{p+1} \sum_{m=0, m \neq p}^{\infty} (-1)^m \binom{\alpha}{m} t} = 1.$$

Let now $\alpha > 2$, then by Proposition 4.2, ψ_h satisfies the hypothesis of Theorem 4.1 and the proof of (a) is complete.

Proof of (b): Let $\alpha > 0$, then the statement follows from Theorem 4.1 in view of Proposition 4.2. \square

4.2. Examples of second order stable Grünwald-type formulae. Let $\alpha \in \mathbb{R}_+$, $2q - 1 < \alpha < 2q + 1$, and $q \in \mathbb{N}$. Consider the mixture of symbols of Grünwald formulae yielding a second order approximation of the form

$$\phi_h(k) := a\psi_h^{p_1}(k) + (1-a)\psi_{2h}^{p_2}(k),$$

where $\psi_h^p(k) = (-1)^{q+1} h^{-\alpha} e^{-ipkh} (1 - e^{ikh})^\alpha$, the symbol of the p -shifted Grünwald formula and thus $\hat{A}_h^\alpha = (-1)^{q+1} T_{\phi_h}$. There are of course many combinations of α, a, p_1 , and p_2 that yield a second order approximation; however only some are stable. It is straight-forward to show that if $0 < \alpha < 1$, then $a = 2, p_1 = p_2 = 0$ give a second order approximation and similarly for $1 < \alpha < 2$, $a = 2 - \frac{2}{\alpha}, p_1 = 1, p_2 = \frac{1}{2}$. So we only show stability.

Proposition 4.4. *Let $\phi_h(k)$ be as above, where $a = 2, p_1 = p_2 = 0$, if $0 < \alpha < 1$ and $a = 2 - \frac{2}{\alpha}, p_1 = 1, p_2 = \frac{1}{2}$, if $1 < \alpha < 2$. Then ϕ_h satisfies the assumptions of Theorem 4.1 with constants c, C and C' independent of h .*

Proof. Assumptions (i) and (ii) of Theorem 4.1 are clearly satisfied in view of (27) and (28).

Proof of (iii): As

$$\phi_h(k) = h^{-\alpha} \phi_1(hk),$$

it is sufficient to consider the case $h = 1$, so let $\phi := \phi_1$. That is,

$$\phi(k) = \phi_1(k) = (-1)^{q+1} (ae^{-ip_1k} (1 - e^{ik})^\alpha + (1-a)2^{-\alpha} e^{-i2p_2k} (1 - e^{i2k})^\alpha)$$

and note that ϕ is 2π -periodic. By symmetry, we only need to consider the real part for $0 \leq k \leq \pi$, and so using (29) and the double angle formula we have

$$\operatorname{Re}(\phi(k)) = (-1)^{q+1} 2^\alpha \sin^\alpha \left(\frac{k}{2} \right) \left(a \cos A + (1-a) \cos^\alpha \left(\frac{k}{2} \right) \cos B \right),$$

where $A = (\frac{\alpha}{2} - p_1)k - \frac{\alpha\pi}{2}$ and $B = (\alpha - 2p_2)k - \frac{\alpha\pi}{2}$.

We consider for $0 \leq k \leq \pi$, the function

$$F(k) = (-1)^{q+1} (a \cos A + (1-a) \cos B)$$

and show that $F(k) \leq F(\pi) < 0$. Then, since $a > 0$ and p_1 is the optimal shift, if $\operatorname{Re}((1-a)\psi_h^{p_2}(k)) < 0$, by (30), $\operatorname{Re}(\phi(k)) \leq -ak^\alpha 2^\alpha \cos((\frac{\alpha}{2} - p)\pi) / \pi^\alpha$. If $\operatorname{Re}((1-a)\psi_h^{p_2}(k)) > 0$, we will have the estimate

$$\operatorname{Re}(\phi(k)) \leq F(\pi) 2^\alpha \sin^\alpha \left(\frac{k}{2} \right) \leq k^\alpha F(\pi) 2^\alpha / \pi^\alpha.$$

An easy check shows that $F(\pi) < 0$. It remains to show that $F'(k) > 0$. Now, as in both cases $2p_1 = p_2$ and $(1-a)(\alpha - 2p_2) = -a\left(\frac{\alpha}{2} - p_1\right)$,

$$\begin{aligned} F'(k) &= (-1)^{q+1} \left(-a \left(\frac{\alpha}{2} - p_1 \right) \sin(A) - (1-a)(\alpha - 2p_2) \sin(B) \right) \\ &= C(\alpha) (\sin(A) - \sin(B)) = 2C(\alpha) \cos\left(\frac{A+B}{2}\right) \sin\left(\frac{A-B}{2}\right) \end{aligned}$$

where $C(\alpha) = -a\left(\frac{\alpha}{2} - p_1\right)$, $\frac{A+B}{2} = \left(\frac{3\alpha}{4} - p_1\right)k - \frac{\alpha\pi}{2}$, and $\frac{A-B}{2} = \frac{-\alpha k}{4}$. Checking the range of the arguments, the cosine factor is negative if $\alpha > 1$ and positive if $\alpha < 1$, the sine factor is always negative, and hence $F'(k) > 0$. \square

Theorem 4.5. *Let $\phi_h(k)$ and a be as in Proposition 4.4. If $0 < \alpha < 1$ and $a = 2$, or if $1 < \alpha < 2$ and $a = 2 - \frac{2}{\alpha}$, then $\{T_{e^{t\phi_h}}\}_{t \geq 0}$ are semigroups on $L_1(\mathbb{R}_+)$, or $L_1(\mathbb{R})$, respectively, that are uniformly bounded in h and t , strongly continuous, and uniformly analytic in h .*

Proof. The statement follows from Theorem 4.1 in view of Proposition 4.4. \square

5. APPLICATION TO FRACTIONAL POWERS OF OPERATORS

Let X be a Banach space and $-A$ be the generator of a strongly continuous group of bounded linear operators $\{G(t)\}_{t \in \mathbb{R}}$ on X with $\|G(t)\|_{\mathcal{B}(X)} \leq M$ for all $t \in \mathbb{R}$ for some $M \geq 1$. If μ is a bounded Borel measure on \mathbb{R} and if we set $\psi(z) := \hat{\mu}(z) = \int_{-\infty}^{\infty} e^{zs} d\mu(s)$, ($z = ik$), we may define the bounded linear operator

$$(31) \quad \psi(-A)x := \int_{\mathbb{R}} G(s)x d\mu(s), \quad x \in X.$$

It is well known that the map $\psi \rightarrow \psi(-A)$ is an algebra homomorphism and is called the Hille-Phillips functional calculus, see for example, [11]. That is, if $\psi = \hat{\mu}$ and $\phi = \hat{\nu}$, for some bounded Borel measures μ and ν , then $(\phi + \psi)(-A) = \phi(-A) + \psi(-A)$, $(\phi \cdot \psi)(-A) = \phi(-A)\psi(-A)$ and $(c\phi)(-A) = c\phi(-A)$, $c \in \mathbb{C}$. A simple transference principle shows, see e.g. [2, Theorem 3.1], that,

$$(32) \quad \|\psi(-A)\|_{\mathcal{B}(X)} \leq M \|T_{k \mapsto \psi(ik)}\|_{\mathcal{B}(L_1(\mathbb{R}))}.$$

Note that if $\text{supp } \mu \subset \mathbb{R}_+$, then we may take $-A$ to be the generator of a strongly continuous semigroup and the properties of the Hille-Phillips functional calculus (31) and the transference principle (32) still holds.

Let $2p - 1 < \alpha < 2p + 1$, $\alpha \in \mathbb{R}^+$, $p \in \mathbb{N}$ and $\{\mu_t\}_{t \geq 0}$ be the family of Borel measures on \mathbb{R} such that $\hat{\mu}_t(z) = e^{t(-1)^{p+1}(-z)^\alpha}$, ($z = ik$). Then the operator family given by

$$S_\alpha(t)x := \int_{\mathbb{R}} G(s)x d\mu_t(s), \quad x \in X, t \geq 0,$$

is a uniformly bounded (analytic) semigroup of bounded linear operators on X , see [2, Theorems 4.1 and 4.6] for the group case. In case $0 < \alpha < 1$, we have $\text{supp } \mu_t \subset \mathbb{R}^+$ and hence $-A$ is allowed to be a semigroup generator and G to be a strongly continuous semigroup and the analyticity of S_α holds, see [3] and [22]. The fractional power A^α of A is then defined to be the generator of S_α multiplied by $(-1)^{p+1}$. We note that the fractional power of A may be defined via an unbounded functional calculus for group generators (or, semigroup generators), formally given by $f_\alpha(-A)$, where $f_\alpha(z) = (-z)^\alpha$. This coincides with the definition given here for groups and, in case $0 < \alpha < 1$, for semigroups, see [2] and [3] for more details.

Thus, for the additional case of $-A$ being a semigroup generator and $\alpha > 1$, we just set $A^\alpha = f_\alpha(-A)$ as in [3].

The following theorem shows the rate of convergence for the Grünwald formula approximating fractional powers of operators in this general setting. For the sake of notational simplicity we only give the first order version; the higher order version follows exactly along the same lines and is discussed in Corollary 5.3.

Theorem 5.1. *Let X be a Banach space and $p \in \mathbb{N}$. Assume that $-A$ is the generator of a strongly continuous group, in case $p = 0$, semigroup, of uniformly bounded linear operators $\{G(t)\}_{t \in \mathbb{R}}$ on X . Define*

$$\Phi_{\alpha,h}^p x = h^{-\alpha} \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} G((m-p)h)x = (-1)^{q+1} \psi_{\alpha,h,p}(-A)x, \quad x \in X,$$

where $\psi_{\alpha,h,p}(z)$ is given by (15) and $\alpha \in \mathbb{R}^+$ such that $2q-1 < \alpha < 2q+1$, $q \in \mathbb{N}$.

Then, as $h > 0$, we have

$$(33) \quad \|\Phi_{\alpha,h}^p x - A^\alpha x\| \leq Ch \|A^{\alpha+1} x\|, \quad x \in \mathcal{D}(A^{\alpha+1}).$$

Furthermore, if $p = q$, then $(-1)^{p+1} \Phi_{\alpha,h}^p$ generate $\{S_{\alpha,h}^p(t)\}_{t \geq 0}$, strongly continuous semigroups of linear operators on X that are uniformly bounded in $h > 0$ and $t \geq 0$ and uniformly analytic in $h > 0$; i.e., there is $M > 0$ such that $\|S_{\alpha,h}^p(t)\|_{\mathcal{B}(X)} \leq M$ and $\|\Phi_{\alpha,h}^p S_{\alpha,h}^p(t)\|_{\mathcal{B}(X)} \leq Mt^{-1}$ for all $t, h > 0$.

Proof. If \hat{g} is defined by $\hat{g}(z) = \frac{\omega_{p,\alpha}(-z)^{-1}}{-z}$, $\operatorname{Re} z \leq 0$, then by Lemma 3.2 with $N = 0$ and $\beta = 1$ and (5) we have that $\|T_{k \rightarrow h\hat{g}(ikh)}\|_{\mathcal{B}(L_1(\mathbb{R}))} \leq Ch$. In case $p = 0$, we have that $\operatorname{supp}(g) \subset \mathbb{R}_+$ and hence $\|T_{k \rightarrow h\hat{g}(ikh)}\|_{\mathcal{B}(L_1(\mathbb{R}_+))} \leq Ch$. Therefore, by the transference estimate (32), $\|h\hat{g}(-hA)\|_{\mathcal{B}(X)} \leq Ch$ for some $C > 0$. Thus, if $x \in \mathcal{D}(A^{\alpha+1})$, then $\|h\hat{g}(-hA)A^{\alpha+1}x\| \leq Ch \|A^{\alpha+1}x\|$. Using the unbounded functional calculus developed in [2] (in case $p = 0$ see [3]), we have, for $x \in \mathcal{D}(A^{\alpha+1})$,

$$\begin{aligned} h\hat{g}(-hA)A^{\alpha+1}x &= \left[h\hat{g}(hz)(-z)^{\alpha+1} \Big|_{z=-A} \right] x \\ &= \left[\left(h^{-\alpha} \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} e^{(m-p)h(z)} - (-z)^\alpha \right) \Big|_{z=-A} \right] x \\ &= \Phi_{\alpha,h}^p x - A^\alpha x \end{aligned}$$

and the proof of (33) is complete.

The strong continuity of $S_{\alpha,h}^p$ follow from Theorem 4.3 and [2, Theorem 4.1], where the latter theorem establishes the transference of strong continuity, from $L_1(\mathbb{R})$ to a general Banach space X (see, [3, Theorem 5.1] for the same result in the unilateral case). Finally, the operator norm estimates follow from the L_1 -norm estimates in Theorem 4.3 and the transference estimate (32), noting that by the functional calculus of [2] and [3] it follows that $(\psi_{\alpha,h,p} e^{t\psi_{\alpha,h,p}})(-A) = (-1)^{p+1} \Phi_{\alpha,h}^p S_{\alpha,h}^p(t)$ for $t > 0$ where $\psi_{\alpha,h,p}$ is given by (15) and $p = q$. \square

The stability and consistency estimates of Theorem 5.1 allow us to obtain unconditionally convergent numerical schemes for the associated Cauchy problem in the abstract setting together with error estimates. To demonstrate this, we use the optimally shifted first order Grünwald scheme as ‘‘spatial’’ approximation together with a first order scheme for time stepping, the Backward (Implicit) Euler scheme, to match the spatial order. Let $2p-1 < \alpha < 2p+1$, $\alpha \in \mathbb{R}^+$, $p \in \mathbb{N}$, let X be a

Banach space and $-A$ be the generator of a uniformly bounded strongly continuous group (semigroup if $p = 0$) of operators on X and set $A_\alpha := (-1)^{p+1}A^\alpha$. Consider the abstract Cauchy problem

$$\dot{u}(t) = A_\alpha u(t); \quad u(0) = x,$$

with solution operator $\{S_\alpha(t)\}_{t \geq 0}$, where, as we already mentioned, S_α is a uniformly bounded analytic semigroup as shown in [2, Theorem 4.6] and in [22] for $0 < \alpha < 1$; that is when $-A$ is a semigroup generator. For its numerical approximation set

$$\frac{u_{n+1} - u_n}{\tau} = (-1)^{p+1} \Phi_{\alpha,h}^p u_{n+1}; \quad u_0 = x, n = 0, 1, 2, \dots;$$

that is, with $A_{\alpha,h} := (-1)^{p+1} \Phi_{\alpha,h}^p$,

$$u_n = (I - \tau A_{\alpha,h})^{-n} x, n = 1, 2, \dots$$

We have the following smooth data error estimate.

Theorem 5.2. *Let $2p - 1 < \alpha < 2p + 1$, $\alpha \in \mathbb{R}^+$, $p \in \mathbb{N}$, $n \in \mathbb{N}$, and $0 < \varepsilon \leq 1$. Let X be a Banach space and $-A$ be the generator of a uniformly bounded strongly continuous group (semigroup if $p = 0$) of operators on X and set $t = n\tau$. If $x \in \mathcal{D}(A^{1+\varepsilon})$, then*

$$(34) \quad \|S_\alpha(t)x - u_n\| \leq C(n^{-1}\|x\| + h \frac{\alpha t^{\frac{\varepsilon}{\alpha}}}{\varepsilon} \|A^{1+\varepsilon}x\|), \quad n = 1, 2, \dots; t > 0,$$

and, if $x \in \mathcal{D}(A)$, then

$$(35) \quad \|S_\alpha(t)x - u_n\| \leq C(n^{-1}\|x\| + (1 + \alpha)h \left| \log \frac{t}{h^\alpha} \right| \|Ax\|), \quad n = 1, 2, \dots; t > 0.$$

Proof. To show (34), we split the error as

$$S_\alpha(t)x - u_n = S_\alpha(t)x - S_{\alpha,h}(t)x + S_{\alpha,h}^p(t)x - u_n := e_1 + e_2.$$

It was shown in Theorem 5.1 that $S_{\alpha,h}^p$ are bounded analytic semigroups on X , uniformly in h . Therefore, $\|e_2\| \leq Cn^{-1}\|x\|$, $n \in \mathbb{N}$, as shown in [8], with C independent of h and t . To bound e_1 we use the fact that all operators appearing commute being functions of A , to write

$$(36) \quad e_1 = S_\alpha(t)x - S_{\alpha,h}^p(t)x = \int_0^t (A_\alpha - A_{\alpha,h})S_\alpha(r)S_{\alpha,h}^p(t-r)x \, dr$$

Note that the analyticity of the semigroup S_α implies that there is a constant M such that for $0 \leq \varepsilon \leq 1$, the estimate $\|A_\alpha^{1-\varepsilon}S_\alpha(t)\| \leq Mt^{\varepsilon-1}$ holds for all $t > 0$. Then, by Theorem 5.1,

$$\begin{aligned} \|e_1\| &\leq Ch \int_0^t \|A^{\alpha+1}S_\alpha(r)S_{\alpha,h}^p(t-r)x\| \, dr \\ &= Ch \int_0^t \|A_\alpha^{1-\frac{\varepsilon}{\alpha}}S_\alpha(r)S_{\alpha,h}^p(t-r)A^{1+\varepsilon}x\| \, dr \leq Ch \frac{\alpha t^{\frac{\varepsilon}{\alpha}}}{\varepsilon} \|A^{1+\varepsilon}x\|, \end{aligned}$$

which completes the proof of (34).

To show (35), write e_1 in (36) as

$$e_1 = \int_0^{h^\alpha} (A_\alpha - A_{\alpha,h})S_\alpha(r)S_{\alpha,h}^p(t-r)x \, dr + \int_{h^\alpha}^t (A_\alpha - A_{\alpha,h})S_\alpha(r)S_{\alpha,h}^p(t-r)x \, dr$$

It is already known that $A_{\alpha,h}x \rightarrow A_\alpha x$ as $h \rightarrow 0+$ for all $x \in \mathcal{D}(A_\alpha)$, see [2, Proposition 4.9] and [21], and hence we have stability $\|A_{\alpha,h}x - A_\alpha x\| \leq C\|A_\alpha x\|$ for all $x \in \mathcal{D}(A_\alpha)$. Therefore,

$$\begin{aligned} \|e_1\| &\leq C \int_0^{h^\alpha} \|A_\alpha^{1-\frac{1}{\alpha}} S_\alpha(r)Ax\| dr + Ch \left| \int_{h^\alpha}^t \|A_\alpha S_\alpha(r)Ax\| dr \right| \\ &\leq C(h\alpha + h \left| \log \frac{t}{h^\alpha} \right|) \|Ax\|. \end{aligned}$$

□

Note that the condition $x \in \mathcal{D}(A^{1+\varepsilon})$ in (34) might be hard to check for $\varepsilon \neq 1$, depending on A and the Banach space X . However, one can always use $\varepsilon = 1$ as $\mathcal{D}(A^2)$ is usually quite explicit. We also obtain convergence and error estimates of stable higher order schemes (such as the second order Grünwald formulae introduced in Section 4.2).

Corollary 5.3. *Let $\alpha \in \mathbb{R}_+$ with $2q - 1 < \alpha < 2q + 1$, $q \in \mathbb{N}$ and let*

$$\Psi_{\alpha,h} := (-1)^{q+1} \sum_{j=0}^N b_j \Phi_{\alpha,c_j h}^{p_j} = \sum_{j=0}^N b_j \psi_{\alpha,c_j h,p_j}(-A)$$

be an $N + 1$ -order Grünwald approximation, where $\psi_{\alpha,h,p}(z)$ is given by (15) and b_j, c_j, p_j are as defined in (17). Assume the multiplier $\sum_{j=0}^N b_j \psi_{c_j h}^{p_j}(k)$, where $\psi_h^p(k)$ is given by (16), satisfies (i)-(iii) of Theorem 3.3 with constants independent of h . If one solves the Cauchy problem

$$\dot{u}(t) = \Psi_{\alpha,h} u(t); \quad u(0) = x,$$

with a strongly A -stable Runge-Kutta method of with stage order s and order $r \geq s + 1$, then, denoting the discrete solution by u_n at time level $t = n\tau$,

$$\|S_\alpha(t)x - u_n\| \leq C \left(n^{-r} \|x\| + h^{N+1} \left| \log \frac{t}{h^\alpha} \right| \|A^{N+1}x\| \right), \quad h > 0, \quad t = n\tau,$$

for all $x \in \mathcal{D}(A^{N+1})$.

Proof. It is straight forward to see that Theorem 5.1 holds for $\Psi_{\alpha,h}$; i.e.,

$$\|\Psi_{\alpha,h}x - A^\alpha x\| \leq Ch^{N+1} \|A^{\alpha+N+1}x\|, \quad x \in \mathcal{D}(A^{\alpha+N+1}),$$

$\|e^{t\Psi_{\alpha,h}}\|_{\mathcal{B}(X)} \leq M$ and $\|\Psi_{\alpha,h}e^{t\Psi_{\alpha,h}}\|_{\mathcal{B}(X)} \leq M/t$. Following the proof of Theorem 5.2 we obtain the “spatial” error estimate

$$(37) \quad \|S_\alpha(t)x - e^{t\Psi_{\alpha,h}}x\| \leq Ch^{N+1} \left| \log \frac{t}{h^\alpha} \right| \|A^{N+1}x\|.$$

Since the analyticity of the semigroups $e^{t\Psi_{\alpha,h}}$ is uniform in h (the constant M does not depend on h), the statement follows from [15, Theorem 3.2] (see also [14]). □

Remark 5.4. The error estimates (34) and (35) are almost optimal in terms of the regularity of the data. We conjecture that one could remove the slight growth in t from (34) or the logarithmic factor in (35) by considering the L_1 -case again and using the theory of Fourier multipliers on Besov spaces. Then use the transference principle to derive the abstract result. We do not pursue this issue here any further.

Remark 5.5. The convergence rate given in Corollary 5.3 can be extended using the stability estimate

$$\|S_\alpha(t)x - e^{t\Psi_{\alpha,h}}x\| \leq C\|x\|$$

and (37) to certain real interpolation spaces as in [12, Corollary 4.4]. We note that while the spaces $\mathcal{D}(A^s)$ endowed with the graph norm are, in general, not interpolation spaces, they are embedded within appropriate interpolation spaces (see, for example, [9, Corollary 6.6.3]) and therefore we obtain

$$\|S_\alpha(t)x - u_n\| \leq C \left(n^{-r}\|x\| + h^s \left| \log \frac{t}{h^\alpha} \right|^{\frac{s}{N+1}} (\|A^s x\| + \|x\|) \right), \quad h > 0, \quad t = n\tau,$$

for all $x \in \mathcal{D}(A^s)$, $s \in [0, N+1]$. Also note that we indeed have convergence of u_n to $S_\alpha(t)x$ for all $x \in X$ as $\tau \rightarrow 0$ and $h \rightarrow 0$ by Lax's Equivalence Theorem as a consequence of stability and consistency. The order of convergence, however, might be very low depending on x .

6. NUMERICAL EXPERIMENTS

In this section we give the results of two numerical experiments. The first is to explore the effect of the regularity of the initial distribution on the rate of convergence as needed for Corollary 5.3, the other is to see how well a second and third order scheme fare in the numerical experiment done by Tadjeran et. al [20].

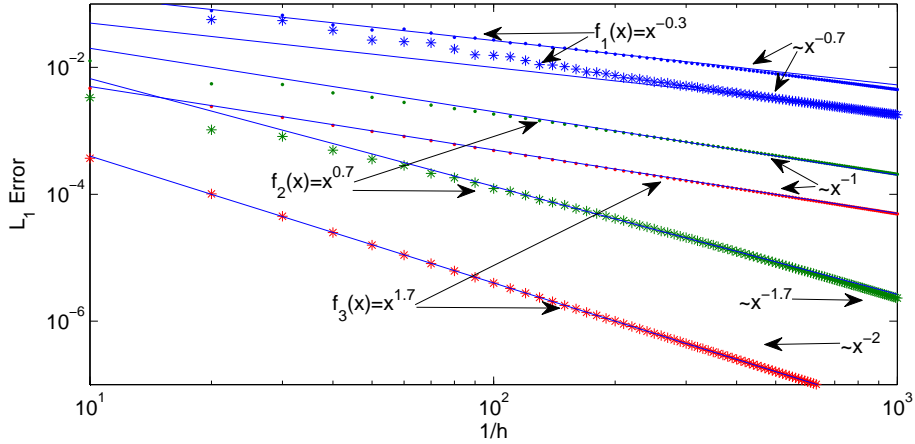


FIGURE 1. L_1 -error for different initial conditions f_i and a first (\cdot) and second order ($*$) scheme. Note the less than first order convergence for a “bad” initial condition; i.e. one that is not in the domain of A . Also note the less than second order convergence for a second order scheme but first order convergence for the first order scheme for an initial condition that is in the domain of A but not in the domain of A^2 .

Example 6.1. We consider $X = L_1[0, 1]$ and $A = (d/dx)$ with

$$D(A) = \{f : f' \in L_1, f(0) = 0\}$$

and $\alpha = 0.8$. We approximate the solution to the Cauchy problems

$$u'(t) = -A^\alpha u(t); u(0) = f_i, \quad i = 1, 2, 3$$

at $t = 1$ with

$$f_1(x) = x^{-0.3}, \quad f_2(x) = x^{0.7}, \quad f_3(x) = x^{1.7},$$

with first and second order Grünwald schemes (as in Proposition 4.4) as well as via a convolution of f_i with an α -stable density, which gives the exact solution but both the convolution and the density are computed numerically on a very fine grid. Note that $f_1 \notin D(A)$, $f_2 \in D(A)$ but $f_2 \notin D(A^2)$ and $f_3 \in D(A^2)$. However, $f_1 \in D(A^{\beta_1})$ for $\beta_1 < 0.7$ and $f_2 \in D(A^{\beta_2})$ for $\beta_2 < 1.7$. By Remark 5.5 we expect about 0.7-order convergence for both schemes in case of $u_0 = f_1$, and first order convergence for the first order scheme for the other initial conditions. We expect about 1.7-order convergence for the second order scheme in case of $u_0 = f_2$ and second order convergence in case of $u_0 = f_3$. For the temporal discretization we use MATLAB's ode45, a fourth-order Runge-Kutta method with a forced high degree of accuracy in order to investigate the pure spatial discretization error. We see in Figure 1 that we obtain the expected convergence in all cases.

Example 6.2. Even though our theoretical framework is not directly applicable, because the fractional differential operator appearing in (38) is defined on a finite domain with boundary conditions and has a multiplicative perturbation and hence it is not a fractional power of an auxiliary operator, we apply the second and third order approximations to the problem investigated by Tadjeran et al. [20], namely approximating the solution to

$$(38) \quad \frac{\partial u(x, t)}{\partial t} = \frac{\Gamma(2.2)}{3!} x^{2.8} \frac{\partial^{1.8} u(x, t)}{\partial x^{1.8}} - (1+x)e^{-t} x^3; u(x, 0) = x^3$$

on the interval $[0, 1]$ with boundary conditions $u(0, t) = 0, u(1, t) = e^{-t}$. The exact solution is given by $e^{-t} x^3$, which can be verified directly.

A second order approximation of the fractional derivative is given by Proposition 4.4. In order to obtain a third order approximation we consider

$$\phi_h(k) = a\psi_h^1 + b\psi_{2h}^{\frac{1}{2}} + c\psi_h^0$$

with the coefficients a, b and c such that ϕ_h is a third order approximation; i.e.

$$a = \frac{7 - 8\alpha + 3\alpha^2}{3(\alpha - 1)}, b = \frac{-7 + 3\alpha}{3(\alpha - 1)}, c = 1 - a - b.$$

A quick plot of $\phi_h(k)$ for $k \in \mathbb{R}$ strengthens the conjecture that the spectrum is in a sector in the left half plane and hence we expect stability and smoothing.

We use again a fourth order Runge-Kutta method to solve the systems to $t = 1$. Table 1 suggests that we indeed have second and third order convergence with respect to the spatial discretization parameter Δx .

REFERENCES

1. W. Arendt, C. J. K. Batty, M. Hieber, and F. Neubrander, *Vector-valued Laplace transforms and Cauchy problems*, Birkhäuser Verlag, 2000.
2. B. Baeumer, M. Haase and M. Kovács, *Unbounded functional calculus for bounded groups with applications*, Journal of Evolution Equations **9** (2009), no. 1, 171–195.
3. A. V. Balakrishnan, *An operational calculus for infinitesimal generators of semigroups.*, Trans. Amer. Math. Soc. **91** (1959), 330–353.

TABLE 1. Maximum error behaviour for second and third order Grünwald approximations.

Δx	Error 2 nd	Error rate	Error 3 rd	Error rate
1/10	6.825×10^{-5}	-	9.180×10^{-6}	-
1/15	3.048×10^{-5}	$2.24 \approx (15/10)^2$	1.933×10^{-6}	$4.75 > (15/10)^3$
1/20	1.708×10^{-5}	$1.78 \approx (20/15)^2$	7.825×10^{-7}	$2.47 \approx (20/15)^3$
1/25	1.088×10^{-5}	$1.57 \approx (25/20)^2$	3.922×10^{-7}	$2 \approx (25/20)^3$

4. R. Bellman. *An integral inequality*. Duke Math. J. **10**(1943) ,547-550.
5. P. Brenner, V. Thomée, and L. B. Wahlbin, *Besov spaces and applications to difference methods for initial value problems*, Springer-Verlag, Berlin Heidelberg New York, 1975.
6. P. L. Butzer and R. J. Nessel, *Fourier analysis and approximation*, Academic Press, New York and London, 1971
7. F. Carlson, *Une inégalité*, Ark. Mat. **25B** (1935), 1–5.
8. M. Crouzeix, S. Larsson, S. Piskarëv, and V. Thomée, *The stability of rational approximations of analytic semigroups*, BIT **33** (1993), no. 1, 74–84.
9. M. Haase, *The functional calculus for sectorial operators*, Birkhäuser Verlag, Basel-Boston-Berlin, 2006.
10. F. Hausdorff, *Eine ausdehnung des Parsevalschen Satzes über Fourierreihen*, Springer, Berlin-Heidelberg, **16** 1923, 163–169.
11. S. Kantorovitz, *On the operational calculus for groups of operators*, Proc. Amer. Math. Soc. **26** (1970), 603–608.
12. M. Kovács, *On the convergence of rational approximations of semigroups on intermediate spaces*, Math. Comp. **76**(257) (2007), 273–286.
13. L. Larsson, L. Maligranda, J. Pečarić, and L. Persson, *Multiplicative inequalities of Carlson type and interpolation*, World Scientific Publishing Co. Pte. Ltd., 2006.
14. M. N. Le Roux, *Semidiscretization in time for parabolic problems*. Math. Comp. **33** (1979), 919–931.
15. Ch. Lubich and A. Ostermann, *Runge-Kutta methods for parabolic equations and convolution quadrature*. Math. Comp. **60** (1993), 105–131
16. M. M. Meerschaert, H. P. Scheffler, and C. Tadjeran, *Finite difference methods for two-dimensional fractional dispersion equation*, Journal Of Computational Physics **211** (2006), no. 1, 249–261.
17. ———, *A second-order accurate numerical method for the two-dimensional fractional diffusion equation*, Journal of Computational Physics **220** (2007), no. 2, 813.
18. M. M. Meerschaert and C. Tadjeran, *Finite difference approximations for fractional advection-dispersion flow equations*, Journal of Computational and Applied Mathematics **172** (2004), no. 1, 65–77.
19. ———, *Finite difference approximations for two-sided space-fractional partial differential equations*, Applied Numerical Mathematics **56** (2006), no. 1, 80–90.
20. C. Tadjeran, M. M. Meerschaert, and H. P. Scheffler, *A second-order accurate numerical approximation for the fractional diffusion equation*, Journal Of Computational Physics **213** (2006), no. 1, 205–213.
21. U. Westphal, *An approach to fractional powers of operators via fractional differences*, Proceedings of the London Mathematical Society **s3-29** (1974), no. 3, 557–576.
22. K. Yosida, *Fractional powers of infinitesimal generators and the analyticity of the semi-groups generated by them*, Proc. Japan Acad. **36** (1960), 86–89.
23. W. H. Young, *Sur la généralisation du théorème de Parseval, Sur la sommabilité d'une fonction dont la série de Fourier est donnée*, Comptes rendus155, (1912, 1. Juli u. 26. August), **S. 30-33**, 472-475]; *On the multiplication of successions of Fourier constants*, Lond. Roy. Soc. Proc., **87** (1912), S. 331-339, *On the determination of the summability of a function by means of its Fourier constants*, Lond. Math. Soc. Proc. (**2**)**12** (1912), S. 71-88.