APPROXIMATION OF SEMIGROUPS AND RELATED OPERATOR FUNCTIONS BY RESOLVENT SERIES

VOLKER GRIMM* AND MARTIN GUGAT†

Abstract. We consider the approximation of semigroups $e^{\tau A}$ and of the functions $\varphi_j(\tau A)$ that appear in exponential integrators by resolvent series. The interesting fact is that the resolvent series expresses the operator functions $e^{\tau A}$ and $\varphi_j(\tau A)$, respectively, in efficiently computable terms. This is important for semigroups, where the new approximation is different from well-known approximations by rational functions, as well as for the application of exponential integrators, which are currently of high interest and which are usually studied in a semigroup setting on Banach spaces. The approximation of the operator functions $\varphi_j(\tau A)$ in a general strongly continuous semigroup setting has not been discussed in the literature so far, while this is crucial for an application of these integrators with unbounded operators or bounded operators (like discretization matrices) with large norm and eigenvalues somewhere in the left half plane.

Key words. Semigroup, rational approximation, resolvent series, exponential integrator.

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1. Introduction and main results. In this note we will discuss approximations to semigroups and to the operator functions that appear in exponential Runge–Kutta methods by resolvent series. Let A be the infinitesimal generator of a strongly continuous bounded semigroup on a Banach space X. (Without loss of generality, we will only discuss bounded semigroups. The results for a general semigroup can be obtained via the common rescaling procedure, e.g. page 60 in [4].) The resolvent series

$$e^{\tau A}v = v + \sum_{k=1}^{\infty} a_k (\tau A)^k (\gamma - \tau A)^{-k} v, \qquad a_k = (-1)^k L_k^{(-1)}(\gamma), \qquad \gamma > 0 \tag{1.1}$$

can be used to represent the semigroup for $v \in \mathcal{D}(A)$, where $L_k^{(-1)}$ are generalized Laguerre polynomials and can be expressed in terms of standard Laguerre polynomials $L_k^{(1)}$ via

$$L_k^{(-1)}(x) = -\frac{x}{k} L_{k-1}^{(1)}(x), \qquad k \geq 1. \tag{1.2}$$

One can use the $m-$th partial sum of the series, $s_m(\tau)$, in order to approximate the semigroup. For $v \in \mathcal{D}(A^q)$, we have

$$\left\| e^{\tau A}v - s_m(\tau)v \right\| \leq C \frac{\tau^q}{m^{\frac{q}{2}-\frac{1}{4}}} \|A^q v\|, \tag{1.3}$$

where C only depends on γ. Here and in the following, C denotes a generic constant. The approximation $s_m(\tau)$ of the semigroup is interesting. There are several results on the approximation of semigroups by rational functions that are based on the A-acceptability of these rational functions (e.g. [1, 3, 7, 14]). The result above is obtained by different means and believed to be new. The series approximation possesses a computational advantage which is illustrated with a well-known rational approximation of a semigroup, the implicit Euler method,

$$e^{\tau A}v = \lim_{n\to\infty} (1 - \tfrac{\tau}{n} A)^{-n} v, \tag{1.4}$$

which can also be considered as an application of the Post-Widder inversion formula to the Laplace transform (cf. [20]). For this method, as well as for the rational approximations in the references mentioned above, one has to start all over again and compute $m > n$ resolvents $(1 - \frac{\tau}{m}A)^{-m}v$

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in order to improve the approximation $(1-\frac{\tau}{n}A)^{-n}v$. With the series approximation, it suffices to compute $a_{n+1}\tau A(\gamma-\tau A)^{-1}h$, where $h = A^n(\gamma-\tau A)^{-n}v$ has already been computed in the previous step, and to add it to the current approximation. This computational advantage comes at the cost of a slightly slower convergence rate (1.3) compared to $m^{-1/2}\log(m+1)$ of (1.4) that has been proved in [1] for $v \in \mathcal{D}(A)$. However, for smoother data, that is for $v \in \mathcal{D}(A^q)$ with $q \geq 3$, the implicit Euler method converges with the rate m^{-1}, whereas the series converges faster and faster the smoother the data is. All previously mentioned rational approximations possess an upper bound of the attainable convergence rate and one has to choose the rational approximation carefully according to the smoothness of the data. The series converges faster for smoother data without the need of adapting the approximation. One can use series (1.1) as it is and does not need to know the smoothness of the initial data v. Whenever the operator A is bounded, $s_m(\tau)$ converges linearly (also called geometrically) in the operator norm. γ can be adjusted to obtain any desired rate in this case.

The operator functions under consideration for use in exponential integrators are given by

$$\varphi_j(\tau A) = \int_0^1 e^{(1-s)(\tau A)}\frac{s^{j-1}}{(j-1)!}\,ds = \frac{1}{\tau^j}\int_0^\tau e^{(\tau-s)A}\frac{s^{j-1}}{(j-1)!}\,ds, \qquad j \geq 1. \tag{1.5}$$

With $\varphi_0(z) = e^z$, we note for later use the functions

$$\varphi_{k+1}(z) = \frac{\varphi_k(z) - 1/k!}{z}, \qquad \varphi_k(0) = \frac{1}{k!}, \qquad k \geq 0. \tag{1.6}$$

Several of these functions appear in exponential Runge–Kutta methods. We refer the reader to the review [13] for an introduction to exponential integrators. Exponential integrators are currently of great interest since they allow for a time integration where the step size is not affected by the unboundedness of the operator A. For discretizations of Partial Differential Equations (PDEs), this means that the time integrator is independent of the norm of the discretization matrix. For the application of these integrators, it is important to know how to approximate the φ-functions while preserving this independence. Here an approximation $s_m(\tau)$ is proposed as the $m-th$ partial sum of the series

$$\varphi_q(\tau A) = \sum_{k=1}^{\infty} a_k(\tau A)^{k-1}(\gamma-\tau A)^{-k}, \qquad \gamma > 0.$$

A sublinear convergence is obtained

$$\|\varphi_q(\tau A) - s_m(\tau)\| \leq C\frac{1}{m^{\frac{q}{2}-\frac{1}{4}}},$$

where the constant C only depends on γ and is independent of time τ. This is the statement of Theorem 4.1. Thus this convergence is again independent of the norm of the discretization matrix in the PDE case. Neither local refinement nor global refinement of the discretization can change the estimate above provided that the discretization satisfies appropriate resolvent bounds. This property, that is illustrated in Section 2, makes the series approximation interesting for exponential integrators.

For the use in exponential integrators, the φ-functions are applied with scaled time-steps. For example, the second-order family of explicit exponential Runge–Kutta methods given by the tableau

$$\begin{array}{c|cc} 0 & & \\ c_2 & c_2\varphi_1(c_2\tau A) & \\ \hline & \varphi_1(\tau A) - \frac{1}{c_2}\varphi_2(\tau A) & \frac{1}{c_2}\varphi_2(\tau A) \end{array}$$

proposed in [15], requires the evaluation of φ_1 at time τ and $c_2\tau$, and of φ_2 at time τ. Usually, the computation of the resolvent times a vector is the most expensive part, when one is using the exponential Runge–Kutta method and partial sums of the series for the $\varphi-$functions to solve discretized PDEs. Therefore, it is interesting that one can use just m such operations to compute all appearing φ-functions at all time steps by adjusting γ correspondingly. In the example above, one could first choose a fixed γ and the resolvent $(\gamma - \tau A)^{-1}$. With this, the computation of $\varphi_1(\tau A)$ and $\varphi_2(\tau A)$ can be done by using the same resolvent. In order to use the same resolvent for $\varphi_1(c_2\tau A)$, one can choose $\tilde{\gamma} = c_2\gamma$ and one obtains

$$\varphi_1(c_2\tau A) = \sum_{k=1}^{\infty} \tilde{a}_k (c_2\tau A)^{k-1} (\tilde{\gamma} - c_2\tau A)^{-k} = \frac{1}{c_2} \sum_{k=1}^{\infty} \tilde{a}_k (\tau A)^{k-1} (\gamma - \tau A)^{-k},$$

with $\tilde{a}_k = (-1)^k L_k^{(-1)}(\tilde{\gamma})$. That is, another combination of the same resolvent. Therefore, all $\varphi-$functions at different time-steps can be approximated by series using the same resolvent.

The partial sums converge faster than the operator bound indicates for smoother initial data. Results analogous to the approximation of the semigroup can be obtained with the methods presented in this paper. The proofs in this paper are generally applicable. One can derive resolvent series for all operator functions that fit into the functional calculus in Section 3.

After Section 2 with motivating examples, the remainder of this paper is devoted to the proof of the series representations and to the convergence rates for their partial sums. For this purpose, a functional calculus is introduced in Section 3. With the help of this calculus, the main theorems are stated and proved in Sections 4 and 5.

2. Numerical examples. In this section, we illustrate the advantage of the grid-independent error bounds of the resolvent series. Let B be a positive selfadjoint operator with compact resolvent on a Hilbert space H, so that B has an orthonormal basis of eigenvectors $e_i \in H$ with eigenvalues $\lambda_i > 0$, $i = 1, 2, \ldots$. In this case, the domains can be written as

$$\mathcal{D}(B^q) := \left\{ x = \sum_{i=1}^{\infty} b_i e_i \in H \mid \sum_{i=1}^{\infty} |\lambda_i|^{2q} |b_i|^2 < \infty \right\} = \{x \mid \|B^q x\| < \infty\}$$

and the definition is valid for arbitrary real $q > 0$. Let $X = \mathcal{D}(B^{\frac{1}{2}}) \times H$, with norm $\|(y, \dot{y})\|^2 = \|B^{\frac{1}{2}} y\|^2 + \|\dot{y}\|^2$, and define $A : \mathcal{D}(A) \to X$ by

$$A = \begin{bmatrix} 0 & I_H \\ -B & 0 \end{bmatrix},$$

where the domain is given by $\mathcal{D}(A) = \mathcal{D}(B) \times \mathcal{D}(B^{\frac{1}{2}})$. Then A has a compact resolvent and generates a C_0-group. A typical example is the wave equation with $B = -\triangle$, homogeneous Dirichlet boundary conditions on the unit square $\Omega = [0, 1]^2$ (or a more general bounded domain), and $H = L^2(\Omega)$. For the wave equation, the operator A has a point spectrum on the imaginary axis that extends to infinity. We are interested in solving the wave equation efficiently. After a discretization in space, the operator A turns into a large matrix. The most highly cited paper in exponential integrators [11] suggests to approximate $\exp(\tau A)v$ in the Krylov subspace

$$\mathcal{K}_m(A, v) = \operatorname{span}\left\{v, Av, A^2 v, \cdots, A^{m-1} v\right\},$$

which reduces the large matrix to a small matrix H_m, and to compute $\exp(\tau H_m)e_1$ by efficient methods (cf. [9]). The main contribution in [11] was to show that the convergence to $\exp(\tau A)v$ is faster than that to the solution of the linear system $(I - \tau A)x = v$. More precisely, it was shown that the Krylov method starts to converge superlinearly after $m \geq \|\tau A^{\frac{1}{2}}\|$ steps for a spectrum on the imaginary axis. A direct application of the Krylov method to the abstract equation would require the initial data to be in $\mathcal{D}(A^{m-1})$ which is much smoother than the natural requirements for the initial data. Therefore, in general, an application to the abstract equation is impossible. In contrast to this, the resolvent method can be directly applied to the abstract equation as well as to the discretized equation and the error bound has no dependence on the norm of the matrix after discretization. This is again completely different from the situation for the standard Krylov method where the start of the superlinear convergence depends on the norm of the discretization matrix. In the following examples in Sections 2.1 and 2.2 we show how this leads to a superior convergence of the resolvent series for a pseudospectral discretization and a finite element discretization of wave equations.

2.1. Pseudospectral discretization. We consider the operator $Bu = -u_{xx}$ on the interval $\Omega = [0,1]$ for the Hilbert space $H = L^2(0,1)$. We then have the Sobolev spaces $\mathcal{D}(B^{\frac{1}{2}}) = H_0^1(0,1)$ and $\mathcal{D}(B) = H_0^1(0,1) \cap H^2(0,1)$. The eigenpairs (e_k, λ_k) of the operator B are

$$e_k = \sqrt{2}\sin(k\pi x), \qquad \lambda_k = (k\pi)^2, \qquad k = 1, 2, \cdots .$$

We now approximate

$$\begin{bmatrix} y(\tau) \\ \dot{y}(\tau) \end{bmatrix} = \exp(\tau A) \begin{bmatrix} y_0 \\ \dot{y}_0 \end{bmatrix}, \tag{2.1}$$

where

$$A = \begin{bmatrix} 0 & I \\ \partial_{xx} & 0 \end{bmatrix}, \qquad y_0 = 0, \qquad \dot{y}_0 = \begin{cases} x & \text{for} \quad 0 \le x \le \frac{1}{2} \\ 1 - x & \text{for} \quad \frac{1}{2} < x < 1 \end{cases} .$$

Galerkin discretization with respect to the subspace $V_N = \{e_1, \cdots, e_N\}$ leads to the matrix

$$A_N = \begin{bmatrix} 0 & I \\ -B_N & 0 \end{bmatrix}, \qquad B_N = \operatorname{diag}(\pi^2, (2\pi)^2, \cdots, (N\pi)^2),$$

and the initial condition

$$v_N = \begin{bmatrix} y_{0,N} \\ \dot{y}_{0,N} \end{bmatrix}, \qquad y_{0,N} = 0, \qquad \dot{y}_{0,N} = \left\{ \frac{2\sqrt{2}}{(k\pi)^2} \sin\left(\frac{k\pi}{2}\right) \right\}_{k=1,\cdots,N} .$$

For this example, it is possible to determine the exact solution which allows to compare it to the approximations. In Figure 2.1, the exact solution (solid), the approximations to $\dot{y}(0.3)$ and $y(0.3)$ via the Krylov subspace method and the resolvent series approximation with parameter $\gamma = 3$ are given after 10 and 30 steps for $N = 63$. We just count steps, since the work per step for both methods is comparable. In timings, the resolvent series approximation is faster because the Krylov method needs to evaluate the matrix exponential for smaller matrices from time to time. It can be seen that the resolvent series first approximates the low frequencies in the solution whereas the Krylov subspace method first approximates the high frequencies which can be seen in the smoothening of the kink.

In Figure 2.2, the analogous results are shown for $N = 1023$. The approximation of the Krylov subspace method deteriorates. One might say that the approximation gets lost in the smoothening of the kink since there are now much more high frequencies to approximate. The resolvent series method does not seem to be affected by the finer space discretization. This can be explained by the following proposition that states that the bound for the resolvent series approximation for the abstract equation is a uniform bound for all pseudospectral discretizations.

Proposition 2.1. *For the discretization described above, we have for the resolvent approximation*

$$\|\exp(\tau A_N)v_N - s_m(\tau)v_N\| \le \frac{\tau}{m^{\frac{1}{4}}} C\|Av\|, \qquad \textit{for} \qquad v = (y_0, \dot{y}_0) \in \mathcal{D}(A), \tag{2.2}$$

where C is independent of N.

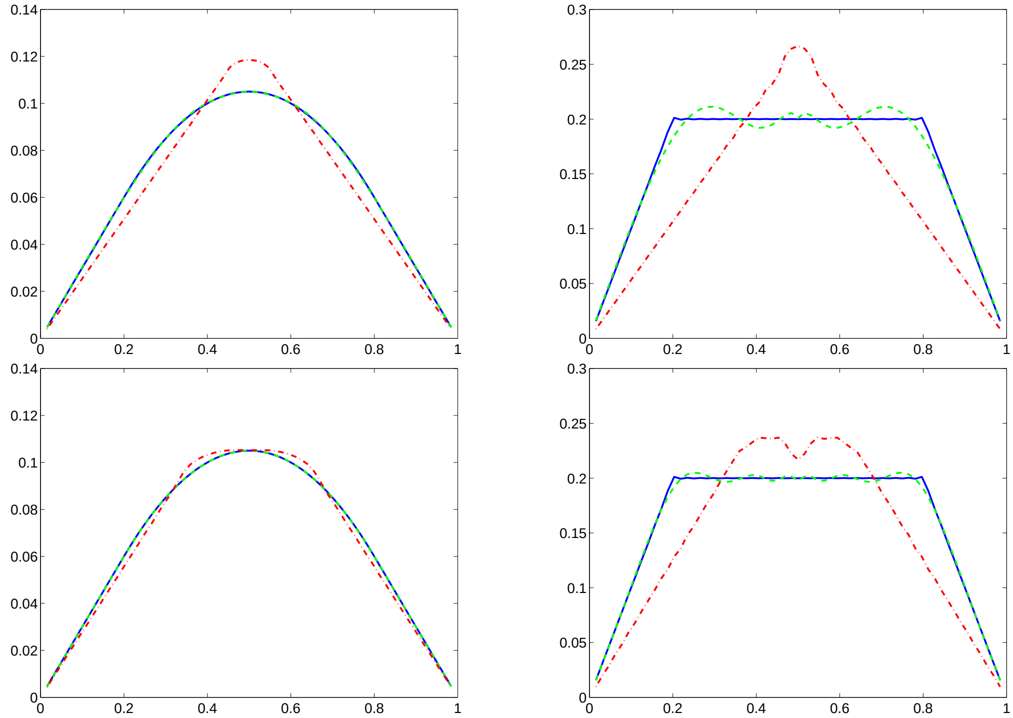

FIG. 2.1. *Plot of* $y_N(0.3)$ *for* $N = 63$ *(solid) in the left column and of* $\dot{y}_N(0.3)$ *(solid) in the right column together with the approximations by the Krylov subspace method (dash-dot) and the resolvent series approximation (dashed) after* 10 *steps (top) and* 30 *steps (bottom).*

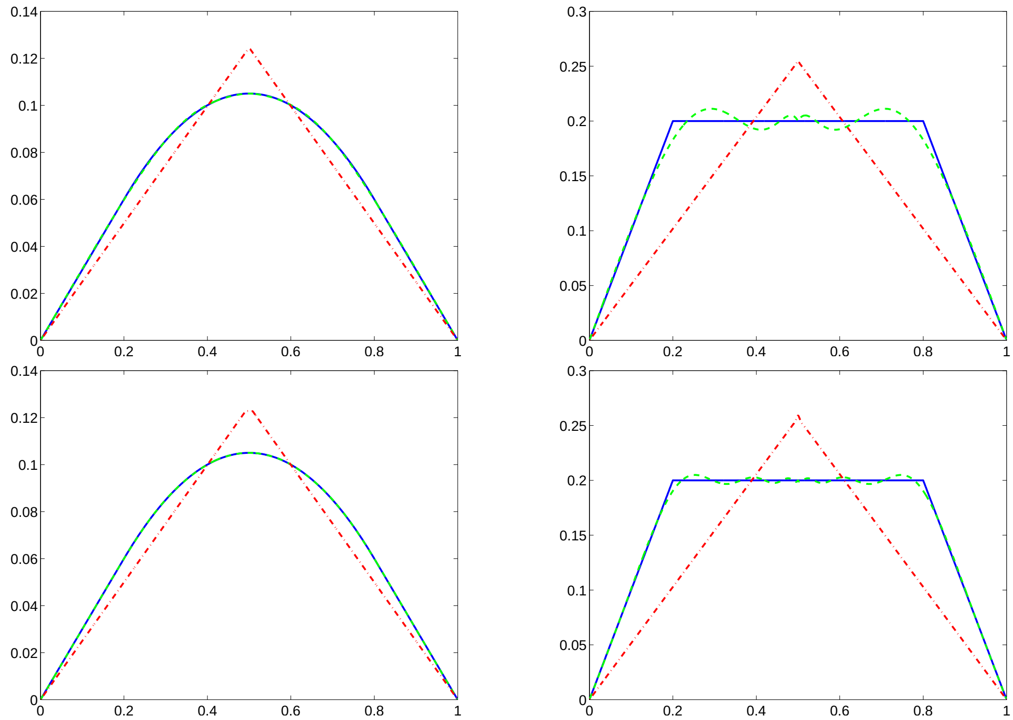

FIG. 2.2. *Plot of* $y_N(0.3)$ *for* $N = 1023$ *(solid) in the left column and of* $\dot{y}_N(0.3)$ *(solid) in the right column together with the approximations by the Krylov subspace method (dash-dot) and the resolvent series approximation (dashed) after* 10 *steps (top) and* 30 *steps (bottom).*

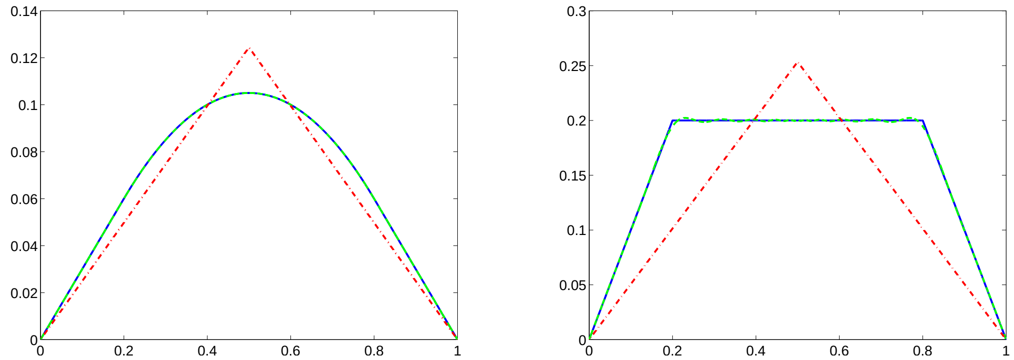

FIG. 2.3. *Plot of* $y_N(0.3)$ *for* $N = 1048575$ *(solid) in the left column and of* $\dot{y}_N(0.3)$ *(solid) in the right column together with the approximations by the Krylov subspace method (dash-dot) and the resolvent series approximation (dashed) after* 100 *steps.*

The proof of the proposition is an immediate consequence of the general proof for the resolvent series. To numerically further illustrate the proposition, we also computed the approximations for $N = 1048575$, that is for about one million Fourier modes. The picture for 10 and 30 steps is comparable to Figure 2.2, therefore we show the approximations for 100 steps in Figure 2.3.

We repeated the experiments above for several $\gamma \in [1, 10]$ and the results are comparable.

We also compare the `exp4` exponential integrator proposed in [12] to the resolvent series for $N = 4095$. After 54.11 seconds and 5852 internal Krylov steps, the `exp4` integrator gives a clearly visible worse approximation than the resolvent series after 0.63 seconds and 1000 steps in Figure 2.4. The `exp4` integrator internally uses the Krylov subspace method proposed in [11] for the approximation of the φ-functions. Since this approximation is not efficient for our test problem, the `exp4` integrator is not efficient. This suggests that for fine discretizations of PDEs with non-smooth initial data alternative methods (as the proposed resolvent series) should be used in the `exp4` integrator to approximate the φ-functions.

2.2. Finite element discretization. We consider the operator $B = -\triangle$ on the bounded domain Ω shown in Figure 2.5, which is a subset of the unit square, for the Hilbert space $H = L^2(\Omega)$. We obtain the Sobolev spaces $\mathcal{D}(B^{\frac{1}{2}}) = H_0^1(\Omega)$ and $\mathcal{D}(B) = H_0^1(\Omega) \cap H^2(\Omega)$. We have in (2.1)

$$A = \begin{bmatrix} 0 & I \\ \triangle & 0 \end{bmatrix}, \qquad \dot{y}_0 = 0, \qquad y_0 = \begin{cases} \left(x - \frac{1}{4}\right)\left(\frac{3}{4} - x\right)\left(y - \frac{1}{4}\right)\left(\frac{3}{4} - y\right) & \text{for} \quad \frac{1}{4} \le x, y \le \frac{3}{4} \\ 0 & \text{elsewhere} \end{cases}.$$

Galerkin discretization with respect to the nodal basis $V_N = \{\varphi_1, \cdots, \varphi_N\}$ leads to the matrix

$$A_N = D_N^{-1} E_N, \qquad D_N = \begin{bmatrix} I & 0 \\ 0 & M_N \end{bmatrix}, \qquad E_N = \begin{bmatrix} 0 & I \\ -S_N & 0 \end{bmatrix}$$

where M_N is the mass matrix and S_N is the stiffness matrix. The norm of the discretized problem, which corresponds to the L_2-norm, is given by the M_N-norm of the coefficients, that is $\|\cdot\|_{M_N} = \|M_N^{\frac{1}{2}} \cdot\|$, where $\|\cdot\|$ denotes the Euclidean norm. We use the orthogonal projection of the continuous initial values as initial values for the discrete system.

The resolvent series approximation is computed as the partial sum of the series

$$e^{\tau A_N} v = v + \sum_{k=1}^{\infty} a_k (\gamma D_N - \tau E_N)^{-k} E_N^k v.$$

Hence in every step a linear system has to be solved. The Krylov subspace approximation can be computed similarly by preconditioning techniques (cf. [5]), and also requires the solution of a

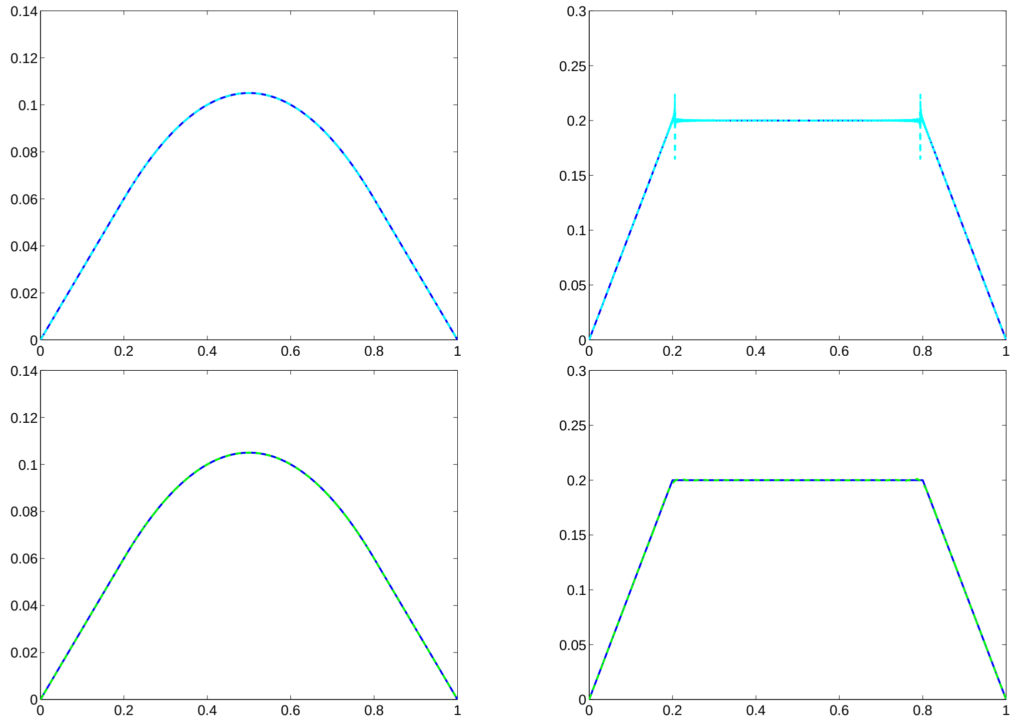

FIG. 2.4. *Plot of* $y_N(0.3)$ *for* $N = 4095$ *(solid) in the left column and of* $\dot{y}_N(0.3)$ *(solid) in the right column together with the approximations by the exponential integrator (dashed) after* 5852 *Krylov steps and* 54.11 *seconds at the top and the resolvent series approximation (dashed) after* 1000 *steps and* 0.63 *seconds for* $\gamma = 1$ *at the bottom.*

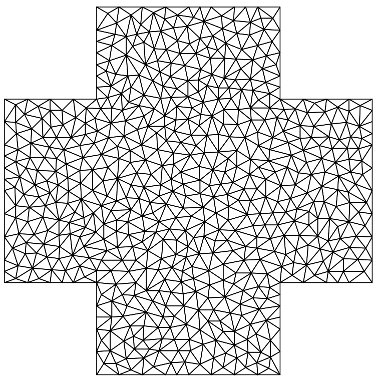

FIG. 2.5. *Mesh and domain for the second experiment.*

linear system. Again both methods require about the same amount of numerical work per step and we therefore use again the number of advanced steps as a measure for this work.

For our second experiment, we use the mesh with 546 nodes, shown in Figure 2.5, a coarser mesh with 43 nodes and a finer mesh with 5723 nodes. A comparison of the methods is shown in Figure 2.6, where the L_2-error is plotted versus the advanced number of steps for $\tau = 0.3$ and $\gamma = 3$. The standard Krylov subspace method is faster for the coarsest grid, but for the finer grids with 546 nodes and 5723 nodes, the resolvent series approximation is clearly more efficient than the Krylov subspace method. One can see how the superlinear convergence starts later for the finer discretizations. The convergence of the resolvent series is not affected by the refinement of the grid. Proposition 2.1 also applies to this example if the norm $\|\cdot\|$ on the left-hand side of inequality (2.2) is replaced by the M_N-norm $\|\cdot\|_{M_N}$. Again, this result is an immediate

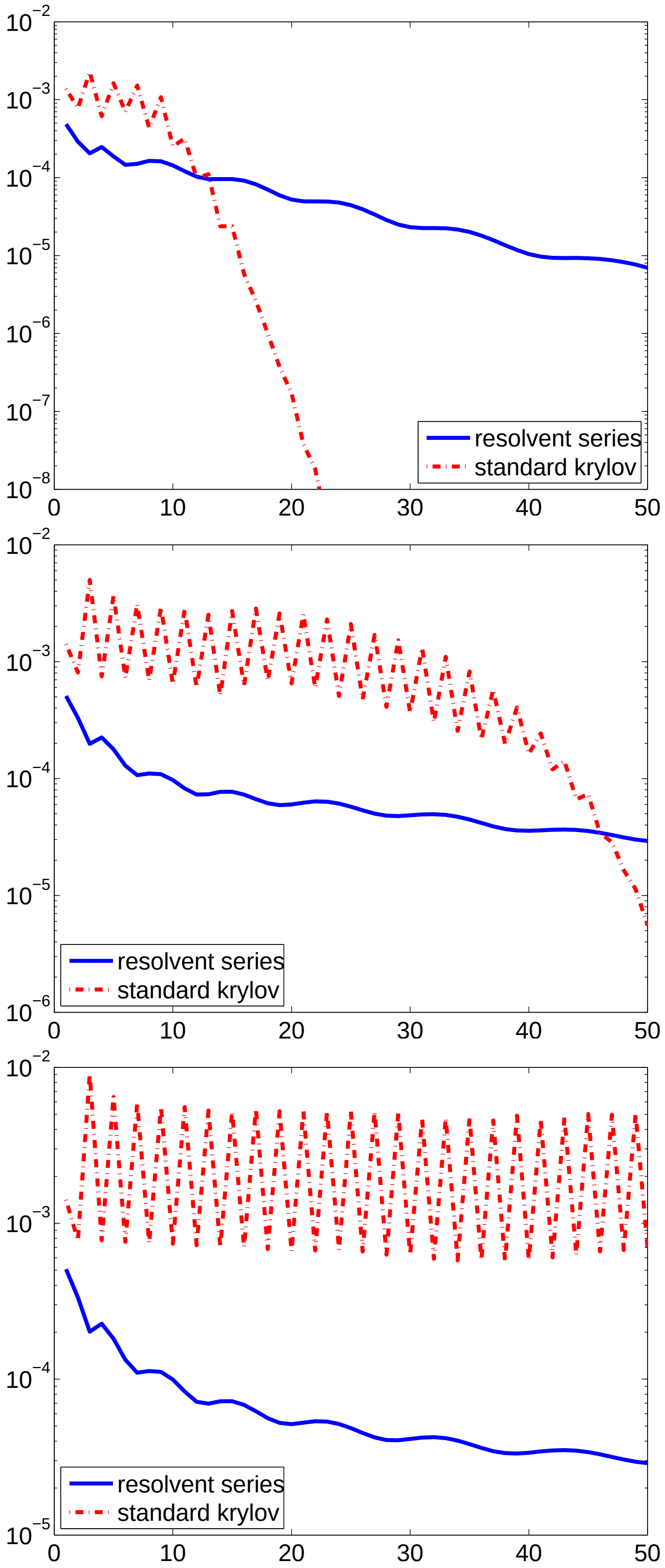

FIG. 2.6. *Comparison of the resolvent series approximation and the Krylov method by the L_2-error for the grids with 43, 546 and 5723 nodes (top to bottom) and steps $m = 1, \dots, 50$.*

consequence of the general theory, that we present in the following sections. Experiments with the φ_1-function showed nearly identical results for the examples given above, which is no surprise, since the approximation of the semigroup with $v \in \mathcal{D}(A)$ can be seen as an approximation to the φ_1-function for a $v \in X$. For $\varphi-$functions with a higher index, the Krylov method as well as the resolvent series converge faster, where the resolvent series is again more efficient for larger systems.

3. A functional calculus. We use a functional calculus that might be seen as a slightly simpler version of the functional calculus of Hille and Phillips in [10]. The notation of the calculus and its introduction are based on recent presentations (cf. [3, 6]).

The Lebesgue spaces of complex-valued functions defined on $\mathbb{R}$ are denoted by $L^q(\mathbb{R})$ with norm $\|\cdot\|_q$. Besides

$$W^{1,2}(\mathbb{R}) = \left\{ f : \mathbb{R} \to \mathbb{C} \,|\, f \,\text{and}\, f' \in L^2(\mathbb{R}) \right\}$$
$$C(\mathbb{R}) = \left\{ f : \mathbb{R} \to \mathbb{C} \,|\, f \,\text{is continuous on}\, \mathbb{R} \right\},$$

let

$$\mathcal{M}_+ = \left\{ f \in C(\mathbb{R}) \,|\, \mathcal{F}f \in L^1(\mathbb{R}) \,\text{and}\, \mathcal{F}f \,\text{is supported in}\, [0,\infty) \right\}, \tag{3.1}$$

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

$$\mathcal{F}f(s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ixs} f(x)\, dx.$$

For each function holomorphic in some left half plane, we denote by $f_{(c)} : \mathbb{R} \to \mathbb{C}$ the restriction of f to $\operatorname{Re} z = c$ so that $f_{(c)}(\xi) = f(c + i\xi)$ and define the algebra

$$\widetilde{\mathcal{M}} := \left\{ f \,\text{holomorphic and bounded in}\, \operatorname{Re} z \le 0 \mid f_{(0)} \in \mathcal{M}_+ \right\}.$$

Let now A generate a bounded strongly continuous semigroup on some Banach space X, that is $\|e^{\tau A}\| \le N$. For functions $f \in \widetilde{\mathcal{M}}$, we define a functional calculus via

$$f(A) = \int_0^{\infty} e^{sA}\, \mathcal{F}f_{(0)}(s)\, ds.$$

This defines a bounded linear operator $f(A)$ satisfying

$$\|f(A)\| \le N \|\mathcal{F}f_{(0)}\|_1,$$

and the following lemma is a standard conclusion.

LEMMA 3.1. *The mapping $f \to f(A)$ defined by the functional calculus is a homomorphism of $\widetilde{\mathcal{M}}$ into the algebra of bounded linear operators on X.*

The following lemma ensures that the functions $\varphi_j(z)$, $j = 1, 2, \cdots$ used with the functional calculus defined above coincide with the definition (1.5) of the bounded operators $\varphi_j(\tau A)$ given in the literature about exponential integrators.

LEMMA 3.2. *The functions defined in the recursion (1.6) are analytic in the left half plane, belong to $\widetilde{\mathcal{M}}$, and with the functional calculus we have*

$$\varphi_k(\tau A) = \int_0^{\infty} e^{s\tau A}\, \mathcal{F}\varphi_{k,(0)}(s)\, ds = \frac{1}{\tau^k} \int_0^{\tau} e^{(\tau - s)A} \frac{s^{k-1}}{(k-1)!}\, ds.$$

Proof. We have

$$\mathcal{F}\varphi_{k,(0)}(s) = \mathbf{1}_{[0,1]}(s)\, \frac{(1-s)^{k-1}}{(k-1)!},$$

where $\mathbf{1}_{[0,\tau]}$ denotes the indicator function for the interval $[0,\tau]$. The right-hand side is integrable and has support $[0,1]$. Hence the functions $\varphi_{k,(0)}$ are in $\mathcal{M}_+$, and, since the functions φ_k are holomorphic and bounded in the left half plane, we therefore have $\varphi_k \in \widetilde{\mathcal{M}}$. A simple integral transform now shows

$$\varphi_k(\tau A) = \int_0^\infty e^{s\tau A}\,\mathbf{1}_{[0,1]}(s)\,\frac{(1-s)^{k-1}}{(k-1)!}\,ds = \frac{1}{\tau^k}\int_0^\tau e^{(\tau-s)A}\frac{s^{k-1}}{(k-1)!}\,ds$$

and the statement follows. □

Analogously, for $f(z) = (z_0 - z)^{-1}$ with $\operatorname{Re} z_0 > 0$, we have, by elementary semigroup theory,

$$\left(\frac{1}{z_0 - z}\right)(A) = \int_0^\infty e^{sA}e^{-sz_0}\,ds = (z_0 - A)^{-1},$$

that is, the definition coincides with the definition in terms of the resolvent. It follows from the homomorphy of the mapping in Lemma 3.1, that the definition of $r(A)$ via the functional calculus for any rational function

$$r(z) = \frac{p(z)}{q(z)}, \qquad \operatorname{degree} p < \operatorname{degree} q$$

analytic in the left half plane coincides with the definition of $r(A)$ in terms of resolvents. We also note for later use:

Lemma 3.3. *If $f \in \widetilde{\mathcal{M}}$, then $f(h\xi) \in \widetilde{\mathcal{M}}$ for $h > 0$ and*

$$\left\|\mathcal{F}\left(f_{(0)}(h\xi)\right)\right\|_1 = \left\|\mathcal{F}\left(f_{(0)}(\xi)\right)\right\|_1.$$

In order to bound $\|\mathcal{F}f\|$ for $f \in \mathcal{M}_+ \cap W^{1,2}(\mathbb{R})$ we will use Carlson's inequality (cf. [2])

$$\|\mathcal{F}f\|_1 \le \sqrt{2}\|f\|_2^{\frac{1}{2}}\|f'\|_2^{\frac{1}{2}}.$$

For our functions, whose Fourier transforms are zero on the negative line, the square root of two could actually be dropped. But, in order to avoid confusion and since it is not important for our further analysis, we keep the constant. The functional calculus so far is suitable to treat the φ-functions. We will need another extension in order to include the semigroup. Let

$$\mathcal{M}_0 := \{f \text{ holomorphic for } \operatorname{Re} z \le 0 \,|\, \exists n \in N : \frac{f(z)}{(1-z)^n} \in \widetilde{M}\}.$$

For $f \in \mathcal{M}_0$, we now define

$$f(A) := (1-A)^n\left(\frac{f(z)}{(1-z)^n}\right)(A),$$

where n is such that $\frac{f(z)}{(1-z)^n} \in \widetilde{M}$. Note that, due to Lemma 3.1, the definition does not depend on the choice of n. The definition results in a closed operator on X. Finally, we define

$$\mathcal{M} := \{f \in \mathcal{M}_0 \,|\, f(A) : X \to X \text{ is bounded}\}.$$

We have again

Lemma 3.4. *The mapping $f \to f(A)$ is a homomorphism of $\mathcal{M}$ into the algebra of bounded linear operators on X.* The result can be found as Proposition 1.12 in [6]. Now the semigroup is within reach of our functional calculus.

Lemma 3.5. *We have ($\tau \ge 0$)*

$$\left(e^{\tau z}\right)(A) = e^{\tau A}.$$

Proof. With $n = 1$, we obtain

$$\left(\frac{e^{\tau z}}{1-z}\right)(A) = \int_\tau^\infty e^{sA} e^{\tau - s}\, ds = \int_0^\infty e^{(s+\tau)A}\, e^{-s}\, ds$$
$$= e^{\tau A} \cdot \int_0^\infty e^{sA}\, e^{-s}\, ds = e^{\tau A}(1-A)^{-1},$$

where we have used semigroup theory. Hence we have

$$\left(e^{\tau z}\right)(A) = (1-A)e^{\tau A}(1-A)^{-1} = e^{\tau A},$$

and the statement follows. □

Analogously, one can show that for rational functions $p(z)/q(z)$ with all its poles in the right half plane and bounded for $\operatorname{Re} z \le 0$, we have

$$\left(\frac{p(z)}{q(z)}\right)(A) = p(A)(q(A))^{-1}.$$

Since for all functions relevant to our discussion, the functional calculus coincides with the known definition in semigroup theory, we will no longer use different notation.

4. Main theorem on $\varphi-$functions. We first consider the approximation of $\varphi_k(\tau A)$, $k = 1, 2, \cdots$, where A is the infinitesimal generator A of a bounded strongly continuous semigroup in a Banach space X.

THEOREM 4.1. *Let $q \ge 1$ and $\gamma > 0$ be arbitrarily chosen. Then the series representation*

$$\varphi_q(\tau A) = \sum_{k=1}^\infty a_k^{(-q)} \frac{(\tau A)^{k-1}}{(\gamma - \tau A)^k}$$

holds true with the coefficients $a_k^{(-q)} = \frac{(-1)^{k+q-1}}{(\gamma)^{q-1}} L_{k+q-1}^{(-q)}(\gamma)$, where $L_k^{(-q)}$ are generalized Laguerre polynomials. If $s_m(\tau)$ denotes the $m-th$ partial sum of the series, then we have

$$\|\varphi_q(\tau A) - s_m(\tau)\| \le C \frac{1}{m^{\frac{q}{2}-\frac{1}{4}}}, \tag{4.1}$$

where C only depends on γ and q.

More details about generalized Laguerre polynomials

$$L_n^{(-q)}(x) = (-x)^q \frac{(n-q)!}{n!} \sum_{\nu=0}^{n-q} \binom{n}{n-q-\nu} \frac{(-x)^\nu}{\nu!} = (-x)^q \frac{(n-q)!}{n!} L_{n-q}^{(q)}(x), \tag{4.2}$$

where $n \ge q$ are positive integers, can be found in [16]. With the help of (4.2), the series can be rescaled to have time-dependent coefficients instead of time-dependent resolvents. The rescaled series reads

$$\varphi_q(\tau A) = \sum_{k=1}^\infty b_k^{(-q)}(\tau) \frac{A^{k-1}}{(\gamma - A)^k}$$

with the coefficients $b_k^{(-q)}(\tau) = \gamma(-1)^{k-1} \frac{(k-1)!}{(k+q-1)!} L_{k-1}^{(q)}(\gamma\tau)$. This representation is more efficient when the functions need to be evaluated for different τ and when the computation of the resolvent is costly as in exponential integrators for the solution of PDEs. The coefficients are now dependent on τ and the convergence bound for the rescaled series is no longer uniform in τ.

In the proof of Theorem 4.1, it becomes apparent that the coefficients of the series are Fourier coefficients of a well-known rational basis of $L^2(\mathbb{R})$ and as such can be computed efficiently with the Fast Fourier Transform (FFT). Analogously to the results for semigroups in Section 5, the series converges faster for smoother data.

PROPOSITION 4.1. *For smooth data v, the term $s_m(\tau)v$ converges faster to $\varphi_q(\tau A)v$ than in (4.1) in Theorem 4.1. More precisely, we have*

$$\|\varphi_q(\tau A)v - s_m(\tau)v\| \leq C\frac{1}{m^{\frac{q+l}{2}-\frac{1}{4}}}\tau^l\|A^l v\| \qquad \text{for } v \in \mathcal{D}(A^l).$$

A main ingredient in the proof of Theorem 4.1 is a bound for the operator function $f(A)$ in terms of the Fourier transform along the imaginary axis $\|\mathcal{F}f_{(0)}\|_1$. This norm is usually known as a Fourier multiplier norm in Fourier analysis. The functions we need to bound are holomorphic in $\operatorname{Re} z < \gamma$ with $\gamma > 0$ and this allows an intriguing method to bound the Fourier multiplier norm by the L^2-norm of the shifted function. This method is well-known as damping in the theory of Laplace transforms with respect to the L^2-norm. But the use of this technique to bound Fourier multipliers in L^1 is new to the knowledge of the authors and is interesting on its own. The main difficulty is that after applying Carlson's inequality, one obtains the L^2-norm of the function and its derivative. However, since the functions are holomorphic, the derivative can also be bounded by the L^2-norm of the shifted function. Lemma 4.2 elaborates the bounds according to this idea. The first inequality is the standard damping result and the proof is only given for the convenience of the reader. The more interesting part of our lemma is the fact that the same idea can be used to bound the derivative.

LEMMA 4.2. *For functions holomorphic and bounded in $\operatorname{Re} z \leq \sigma$, ($\sigma > 0$), with $f_{(\sigma)} \in \mathcal{M}_+ \cap W^{1,2}$, we have $f \in \widetilde{\mathcal{M}}$ with*

$$\|f_{(0)}\|_2 \leq \|f_{(\sigma)}\|_2 \qquad \text{and} \qquad \|f'_{(0)}\|_2 \leq \frac{1}{\sigma e}\|f_{(\sigma)}\|_2.$$

Proof. With the help of the Cauchy integral formula and the dominated convergence theorem one obtains for $\operatorname{Re} z < \sigma$

$$f(z) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{f(\sigma+iy)}{\sigma+iy-z}\,dy, \qquad f'(z) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{f(\sigma+iy)}{(\sigma+iy-z)^2}\,dy.$$

Hence we have

$$f_{(0)}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{f(\sigma+iy)}{\sigma+iy-ix}\,dy = \frac{1}{2\pi}\left(f_{(\sigma)} \star \frac{1}{-i\cdot+\sigma}\right)(x).$$

Since $\mathcal{F}f_{(\sigma)} \in L_2(\mathbb{R})$ and

$$\mathcal{F}\left(\frac{1}{\sigma - i\cdot}\right)(x) = \begin{cases} e^{-\sigma x}, & \text{for } x > 0 \\ \frac{1}{2}, & \text{for } x = 0 \\ 0, & \text{for } x < 0 \end{cases}$$

we have

$$\mathcal{F}\left(\frac{1}{\sigma - i\cdot}\right)\cdot\mathcal{F}f_{(\sigma)} \in L_2(\mathbb{R}) \cap L_1(\mathbb{R})$$

and $f \in \widetilde{M}$ is an immediate consequence of

$$f_{(0)} = \frac{1}{2\pi}\left(f_{(\sigma)} \star \frac{1}{-i\cdot+\sigma}\right) = \mathcal{F}^{-1}\left(\mathcal{F}\left(\frac{1}{\sigma-i\cdot}\right)\cdot\mathcal{F}f_{(\sigma)}\right) \in L_2(\mathbb{R}).$$

And therefore with

$$|\mathcal{F}f_{(0)}(x)|^2 \leq |\mathcal{F}f_{(\sigma)}(x)|^2$$

we find

$$\|f_{(0)}\|_2^2 = 2\pi\|\mathcal{F}f_{(0)}\|_2^2 \le 2\pi\|\mathcal{F}f_{(\sigma)}\|_2^2 = \|f_{(\sigma)}\|_2^2.$$

Hence we have proved the first inequality. The second inequality is proved along the same lines. We start with

$$f'_{(0)}(x) = \frac{i}{2\pi}\int_{-\infty}^{\infty} \frac{f(\sigma+iy)}{(\sigma+iy-ix)^2}\,dy = \frac{i}{2\pi}\left(f_{(\sigma)} \star \frac{1}{(-i\cdot+\sigma)^2}\right)(x).$$

Since $\mathcal{F}f_{(\sigma)} \in L_2(\mathbb{R})$ and

$$\mathcal{F}\left(\frac{1}{(\sigma - i\cdot)^2}\right)(x) = \begin{cases} xe^{-\sigma x}, & \text{for } x \ge 0 \\ 0, & \text{for } x < 0 \end{cases}$$

we have

$$i\,\mathcal{F}\left(\frac{1}{(\sigma - i\cdot)^2}\right)\cdot \mathcal{F}f_{(\sigma)} \in L_2(\mathbb{R}) \cap L_1(\mathbb{R})$$

and

$$f'_{(0)} = \frac{i}{2\pi}\left(f_{(\sigma)} \star \frac{1}{(-i\cdot+\sigma)^2}\right) = \mathcal{F}^{-1}\left(i\,\mathcal{F}\left(\frac{1}{(\sigma - i\cdot)^2}\right)\cdot\mathcal{F}f_{(\sigma)}\right) \in L_2(\mathbb{R}).$$

And therefore with

$$|\mathcal{F}f'_{(0)}(x)|^2 \le \max_{\omega\ge 0}|\omega^2 e^{-2\sigma\omega}|\cdot|\mathcal{F}f_{(\sigma)}(x)|^2 \le \frac{1}{\sigma^2}e^{-2}\cdot|\mathcal{F}f_{(\sigma)}(x)|^2$$

we find

$$\|f'_{(0)}\|_2^2 = 2\pi\|\mathcal{F}f'_{(0)}\|_2^2 \le \frac{2\pi}{(e\sigma)^2}\|\mathcal{F}f_{(\sigma)}\|_2^2 = \frac{1}{(e\sigma)^2}\|f_{(\sigma)}\|_2^2.$$

Hence our lemma is proved. ☐

With the help of Carlson's inequality and Lemma 4.2, one can bound the Fourier multiplier norm by the L^2- norm of the shifted function. The idea is to choose the shift in such a way that our rational function is transformed in a well-known orthogonal rational basis of L^2. For example, the basis has been used by Weeks to invert the Laplace transformation in [18], by Weber to compute the Fourier transform in [17], and by Weidemann to compute the Hilbert transform in [19]. The Fourier coefficients for the best L^2-approximation and the resulting bound are given in Lemma 4.3.

LEMMA 4.3. *For $\sigma = \frac{\gamma}{2}$ and fixed q, there exists a sequence of functions $b_{q,m}(z)$, holomorphic in $\operatorname{Re} z < \gamma$, of the form*

$$b_{q,m}(z) = \varphi_q(z) - \sum_{k=1}^{m} a_k^{(-q)}\frac{z^{k-1}}{(\gamma - z)^k}, \qquad a_k^{(-q)} = \frac{(-1)^{k+q-1}}{(\gamma)^{q-1}}L_{k+q-1}^{(-q)}(\gamma),$$

such that for all m

$$\|b_{q,m,(\sigma)}\|_2 \le \frac{C}{m^{\frac{q}{2}-\frac{1}{4}}},$$

where C only depends on q and γ.

Proof. With $\sigma = \frac{\gamma}{2}$, we have

$$\|b_{q,m,(\sigma)}\|_2^2 = \int_{-\infty}^{\infty}\left|\varphi_q(\sigma+i\omega) - \sum_{k=1}^{m} a_k^{(-q)}\frac{(\sigma+i\omega)^{k-1}}{(\sigma-i\omega)^k}\right|^2 d\omega.$$

Hence with

$$\tilde{a}_k^{(-q)} := \sqrt{\frac{\pi}{\sigma}} a_k^{(-q)},$$

we have

$$\|b_{q,m,(\sigma)}\|_2^2 = \int_{-\infty}^{\infty} \left| \varphi_q(\sigma + i\omega) - \sum_{k=1}^{m} \tilde{a}_k^{(-q)} \sqrt{\frac{\sigma}{\pi}} \frac{(\sigma + i\omega)^{k-1}}{(\sigma - i\omega)^k} \right|^2 d\omega.$$

The set

$$\left\{ \sqrt{\frac{\sigma}{\pi}} \frac{(\sigma + i\omega)^{k-1}}{(\sigma - i\omega)^k}, \qquad k = 0, \pm 1, \pm 2, \dots \right\}$$

forms a complete orthonormal basis in $L^2(\mathbb{R})$ (cf. [8], page 64). The Fourier coefficients of the functions $\varphi_{q,(\sigma)}$ with respect to this basis are computed to

$$\begin{cases} \tilde{a}_k^{(-q)} & = & 0 & \text{for } k \leq 0 \\ \tilde{a}_k^{(-q)} & = & 2\sqrt{\sigma\pi}\, \frac{(-1)^{k+q-1}}{(2\sigma)^q} L_{k+q-1}^{(-q)}(2\sigma) & \text{for } k \geq 1, \end{cases} \tag{4.3}$$

where $L_k^{(-q)}(x)$ are the generalized Laguerre polynomials (4.2). Hence we have chosen the coefficients in $b_{q,m,(\sigma)}$ to be the best approximation in the subspace of the basis above with indices of absolute value smaller and equal to m. From [16], it is known that we have

$$|L_{k+q-1}^{(-q)}(2\sigma)| \leq \frac{C}{k^{\frac{q}{2}+\frac{1}{4}}}, \qquad \text{for} \quad k \geq 1, \tag{4.4}$$

and therefore the same estimate can be given for the $\tilde{a}_k^{(-q)}$, where the constant only depends on q and γ. Using (4.3) and (4.4), we have for the remainder of the series

$$\sum_{k=m+1}^{\infty} |\tilde{a}_k^{(-q)}|^2 \leq \tilde{C}^2 \sum_{k=m+1}^{\infty} \frac{1}{k^{q+\frac{1}{2}}} \leq \tilde{C}^2 \int_{m+1}^{\infty} \frac{1}{x^{q+\frac{1}{2}}}\, dx = \frac{\tilde{C}^2}{q - \frac{1}{2}} \frac{1}{(m+1)^{q-\frac{1}{2}}} \leq \frac{C^2}{m^{q-\frac{1}{2}}}.$$

Hence, by using the remainder of the series to estimate the error of the best approximation, we arrive at

$$\|b_{q,m,(\sigma)}\| \leq \sqrt{\sum_{k=m+1}^{\infty} |\tilde{a}_k^{(-q)}|^2} \leq \frac{C}{m^{\frac{q}{2}-\frac{1}{4}}}.$$

□

After the presentation of the main idea of the proof and the auxiliary results above, we can prove our main Theorem 4.1.

Proof. [*of Theorem 4.1*] For fixed q, we consider any linear combination

$$f_{q,m}(z) = \sum_{k=1}^{m} a_k^{(-q)} \frac{z^{k-1}}{(\gamma - z)^k}$$

and, with $\tau > 0$,

$$\tilde{b}_{q,m}(z) = \varphi_q(\tau z) - f_{q,m}(\tau z).$$

Due to Lemma 3.2 and subsequent remarks, we have $\tilde{b}_{q,m} \in \widetilde{\mathcal{M}}$ and

$$\|\varphi_q(\tau A) - \tilde{f}(\tau A)\| \leq N \|\mathcal{F}\tilde{b}_{q,m,(0)}\|_1.$$

Lemma 3.3 implies the equations

$$\|\mathcal{F}\tilde{b}_{q,m,(0)}\|_1 = \|\mathcal{F}b_{q,m,(0)}\|_1, \qquad b_{q,m}(z) = \varphi_q(z) - f_{q,m}(z).$$

By Carlson's inequality (cf. [2]), $\|\mathcal{F}b_{q,m,(0)}\|_1$ can be estimated by

$$\|\mathcal{F}b_{q,m,(0)}\|_1 \le \sqrt{2}\|b_{q,m,(0)}\|_2^{\frac{1}{2}} \|b'_{q,m,(0)}\|_2^{\frac{1}{2}}.$$

Our problem is now to estimate $\|b_{q,m,(0)}\|_2$ and $\|b'_{q,m,(0)}\|_2$ simultaneously. Or to put it another way, to estimate the Sobolev 1−norm. Since $b_{q,m}(z)$ is holomorphic in $\operatorname{Re} z < \gamma$, this is possible as Lemma 4.2 shows and we obtain the bound

$$\|\mathcal{F}b_{q,m,(0)}\|_1 \le \frac{\sqrt{2}}{e\sigma}\|b_{q,m,(\sigma)}\|_2,$$

with $\sigma = \frac{\gamma}{2}$. Now, we have to face the much simpler problem of estimating the 2−norm alone. Here orthogonal rational functions come to help. Lemma 4.3 shows that with the $a_k^{(-q)}$ chosen as in the theorem, we have

$$\|b_{q,m,(\sigma)}\|_2 \le \frac{C}{m^{\frac{q}{2}-\frac{1}{4}}},$$

where C only depends on q and γ, and the theorem is proved. □

5. Main theorem on semigroups. In this section we consider the approximation of a bounded strongly continuous semigroup in a Banach space X by resolvent series.

THEOREM 5.1. *Choose $\gamma > 0$. Then the series representation*

$$e^{\tau A}v = v + \sum_{k=1}^{\infty} a_k \frac{(\tau A)^k}{(\gamma - \tau A)^k} v \tag{5.1}$$

with coefficients $a_k = (-1)^k L_k^{(-1)}(\gamma)$ holds true for $v \in \mathcal{D}(A)$. For the $m-th$ partial sum $s_m(\tau)$ of the series, we have

$$\|e^{\tau A}v - s_m(\tau)v\| \le C\frac{\tau^q}{m^{\frac{q}{2}-\frac{1}{4}}}\|A^q v\|, \qquad \textit{for } v \in \mathcal{D}(A^q),$$

where C only depends on γ and q. The series can be rescaled to time-dependence in the coefficients instead of the resolvent to give

$$e^{\tau A}v = v + \sum_{k=1}^{\infty} b_k(\tau)\frac{A^k}{(\gamma - A)^k}v,$$

with $b_k(\tau) = (-1)^k L_k^{(-1)}(\gamma\tau)$. This rescaling immediately shows an interesting corollary of Theorem 5.1. In [4], it is mentioned that a remarkable consequence of the Phragmén inversion formula were "that the values of the resolvent in $m_0 + \mathbb{N}$, i.e. $R(m, A)$ for $m \ge m_0$, already determine uniquely the associated semigroup". The rescaled resolvent series shows that actually the resolvent at a single real value is enough to determine the semigroup uniquely. Therefore the rescaled version of our theorem answers an interesting question in semigroup theory and leads to the corollary:

COROLLARY 5.2. *A semigroup is uniquely determined by its resolvent at a single real value.*

In order to prepare the proof of Theorem 5.1, we need the following lemma which is a corollary of Theorem 4.1.

LEMMA 5.3. *For data $v \in \mathcal{D}(A^q)$ and $\gamma > 0$, we have*

$$e^{\tau A}v = \sum_{k=0}^{q-1}\frac{1}{k!}(\tau A)^k v + \tau^q \sum_{k=1}^{\infty} a_k^{(-q)}\frac{(\tau A)^{k-1}}{(\gamma - \tau A)^k} A^q v,$$

with the coefficients as in Theorem 4.1. Let $y_m(\tau) = s_m(\tau)v$, where s_m denotes the $m-th$ partial sum of the series, then we have

$$\left\|e^{\tau A}v - y_m(\tau)\right\| \le C\frac{\tau^q}{m^{\frac{q}{2}-\frac{1}{4}}}\|A^q v\|, \qquad \forall m \ge q,$$

where C only depends on γ and q.

Proof. We prove for $v \in \mathcal{D}(A^q)$

$$e^{\tau A}v - \sum_{k=0}^{q-1}\frac{1}{k!}(\tau A)^k v - \tau^q \sum_{k=1}^{\infty} a_k^{(-q)}\frac{(\tau A)^{k-1}}{(\gamma-\tau A)^k}\, A^q v = \left[\varphi_q(\tau A) - \sum_{k=1}^{\infty} a_k^{(-q)}\frac{(\tau A)^{k-1}}{(\gamma-\tau A)^k}\right](\tau A)^q v,$$

and the statement is seen to be a consequence of Theorem 4.1. By Lemma 3.4, since

$$f(z) = \frac{e^z - \sum_{k=0}^{q-1}\frac{1}{k!}z^k}{(1-\epsilon z)^q}, \qquad g(z) = \frac{f(z)}{z^q} \qquad \text{and} \qquad \frac{z^q}{(1-\epsilon z)^q} \qquad (\text{with } \epsilon > 0)$$

belong to $\mathcal{M}$, we have

$$\left(e^{\tau A} - \sum_{k=0}^{q-1}\frac{1}{k!}(\tau A)^k\right)(1-\epsilon\tau A)^{-q}v = \varphi_q(\tau A)(\tau A)^q(1-\epsilon\tau A)^{-q}v.$$

Standard semigroup theory shows for $v \in \mathcal{D}(A^q)$

$$\left(e^{\tau A} - \sum_{k=0}^{q-1}\frac{1}{k!}(\tau A)^k\right)(1-\epsilon\tau A)^{-q}v = (1-\epsilon\tau A)^{-q}\left(e^{\tau A} - \sum_{k=0}^{q-1}\frac{1}{k!}(\tau A)^k\right)v$$

and

$$(\tau A)^q(1-\epsilon\tau A)^{-q}v = (1-\epsilon\tau A)^{-q}(\tau A)^q v.$$

Since for $w \in X$

$$\|(1-\epsilon\tau A)^{-q}w - w\| \to 0 \qquad \text{as} \qquad \epsilon \to 0,$$

it now follows for $v \in \mathcal{D}(A^q)$ that

$$\left(e^{\tau A} - \sum_{k=0}^{q-1}\frac{1}{k!}(\tau A)^k\right)v = \varphi_q(\tau A)(\tau A)^q v.$$

□

Proof. [*of Theorem 5.1*] With the help of the relation

$$L_{k+1}^{(-q)}(x) - L_k^{(-q)}(x) = L_{k+1}^{(-q-1)}(x), \qquad (k \ge q),$$

which follows from (4.2) by elementary calculations, and the definition of $a_k^{(-q)}$, we can show the relation

$$\frac{1}{\gamma}\left(a_{k+1}^{(-q)} + a_k^{(-q)}\right) = a_k^{(-(q+1))}, \qquad (k \ge 1).$$

With the help of this relation, we can show

$$e^{\tau A}v = v + \sum_{\nu=1}^{q-1}\frac{1}{\gamma}a_1^{(-\nu)}(\tau A)^\nu v + \left(\sum_{k=1}^{m-(q-1)} a_k^{(-q)}\frac{(\tau A)^{k-1}}{(\gamma-\tau A)^k}\right)(\tau A)^q v \tag{5.2}$$

$$+\left(\sum_{k=1}^{q-1}\frac{1}{\gamma}a_{m-k+1}^{(-k)}\frac{(\tau A)^{m-q+1}}{(\gamma-\tau A)^{m-k+1}}\right)(\tau A)^q v \tag{5.3}$$

for $v \in \mathcal{D}(A^q)$ by induction. To get from q to $q+1$, one can use

$$\frac{1}{\gamma - \tau A} = \frac{1}{\gamma} + \frac{1}{\gamma}\,\frac{\tau A}{\gamma - \tau A}$$

in the second sum on the right-hand side and rearrange the terms.

Now the relation

$$\frac{1}{\gamma} a_1^{(-\nu)} = \frac{(-1)^\nu}{\gamma^\nu} L_\nu^{(-\nu)}(\gamma) = \frac{(-1)^\nu}{\gamma^\nu}(-\gamma)^\nu\,\frac{1}{\nu!} = \frac{1}{\nu!}$$

shows that the first line in the equation, (5.2), corresponds to $e^{\tau A}v = y_{m-(q-1)}(\tau)$ in Lemma 5.3 and the difference of these terms is therefore bounded as stated in our theorem. It remains to bound (5.3). The bound on the Laguerre polynomials (4.4), and direct verification of

$$\left\| \frac{(\tau A)^{m-q+1}}{(\gamma - \tau A)^{m-k+1}} \right\| \le C \frac{1}{m^{\frac{q-k}{2} - \frac{1}{4}}} \qquad \text{(for } q > k\text{)} \tag{5.4}$$

via the functional calculus show the bound

$$\left\| \sum_{k=1}^{q-1} \frac{1}{\gamma} a_{m-k+1}^{(-k)} \frac{(\tau A)^{m-q+1}}{(\gamma - \tau A)^{m-k+1}} \right\| \le C \sum_{k=1}^{q-1} \frac{1}{(m-k+1)^{\frac{k}{2}+\frac{1}{4}}}\,\frac{1}{m^{\frac{q-k}{2}-\frac{1}{4}}} \le \frac{qC}{m^{\frac{q}{2}}},$$

and our theorem is proved. For the convenience of the reader, we add a sketch of how to show (5.4). For $q > k$, the function f below is in $\widetilde{M}$ and we have

$$\left\| \frac{(\tau A)^{m-q+1}}{(\gamma - \tau A)^{m-k+1}} \right\| \le C \|\mathcal{F} f_{(0)}\|_1, \qquad \text{with} \qquad f(z) = \frac{z^{m-q+1}}{(\gamma - z)^{m-k+1}}.$$

Since $f_{(0)} \in W^{1,2}(\mathbb{R})$, we can apply Carlson's inequality to obtain

$$\left\| \frac{(\tau A)^{m-q+1}}{(\gamma - \tau A)^{m-k+1}} \right\| \le C \|f_{(0)}\|_2^{\frac{1}{2}} \|f'_{(0)}\|_2^{\frac{1}{2}},$$

and bound the right-hand side by standard methods for complex functions. □

6. Conclusion. We have discussed rational approximations to semigroups and to operator functions that appear in exponential Runge–Kutta methods. The new rational approximations can be updated at the cost of the computation of a single resolvent whereas the computational cost for an update of a standard rational approximation based on A-acceptability is in general much higher. The speed of the convergence of the series increases with the regularity of the initial data. This is in contrast to the standard rational approximations that have a fixed maximal rate of convergence. The proved error bounds for the semigroup and the φ-functions applied to an infinitesimal generator turn into uniform error bounds for the matrix exponential and the matrix φ-functions for matrices stemming from discretizations of PDEs. This is particularly important in the context of the numerical solution of finite element discretizations of partial differential equations by exponential integrators. The proposed rational approximations perform particularly well for problems where the solutions have low regularity. This advantage has been illustrated by comparing the resolvent series approximation and the mostly used standard Krylov subspace method for a finite element discretization of a wave equation on a Greek cross.

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