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Hierarchical Tensor-Product Approximation to the Inverse and Related Operators for High-Dimensional Elliptic Problems

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Abstract

The class of $\mathscr{H}$-matrices allows an approximate matrix arithmetic with almost linear complexity. In the present paper, we apply the $\mathscr{H}$-matrix technique combined with the Kronecker tensor-product approximation (cf. [2, 20]) to represent the inverse of a discrete elliptic operator in a hypercube $(0,1)^d \in \mathbb{R}^d$ in the case of a high spatial dimension d. In this data-sparse format, we also represent the operator exponential, the fractional power of an elliptic operator as well as the solution operator of the matrix Lyapunov-Sylvester equation. The complexity of our approximations can be estimated by $\mathcal{O}(dn \log^q n)$, where $N = n^d$ is the discrete problem size.

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1. Introduction

There are several sparse $N \times N$-matrix approximations which allow to construct optimal solution methods for elliptic/parabolic boundary value problems with $\mathcal{O}(N)$ arithmetic operations. In many applications, one has to deal with full matrices arising from boundary element discretisations (BEM) or FEM methods. In the latter case the inverse of a sparse FEM matrix is a full matrix.

A class of hierarchical ($\mathscr{H}$) matrices has been introduced and developed in [15]-[19], [11]. These structured matrices allow an approximate matrix arithmetic (including the computation of the inverse) of almost linear complexity and can be considered as data-sparse. Given an elliptic operator $\mathscr{A}$, it is of important theoretical and practical interest to find $\mathscr{H}$-matrix approximations of the operator exponential $\exp(t\mathscr{A})$, of $\sinh(t\sqrt{\mathscr{A}})$ and of $\cos(t\sqrt{\mathscr{A}})$, which represent the solution operators for evolution differential equations of parabolic, elliptic and hyperbolic types, respectively. Another interesting example of an operator-valued function is given by sign ($\mathscr{A}$) that arises in many-particle simulations, control theory and linear algebra. Data-sparse ($\mathscr{H}$)-matrix approximations of almost linear complexity in N based on the efficient *Sinc*-quadrature for the Dunford-

Cauchy integral representation to the above mentioned operator-valued functions have been developed in [7]-[9]. Note that generalised Gaussian quadratures for certain improper integrals were described in [27]. The basic approximation theory by exponential sums is presented in [3].

There are important applications requiring computations in higher spatial dimensions, where the problem size may grow exponentially in d, i.e., $N = \mathcal{O}(n^d)$. In particular, we mention the many-particle Schrödinger equation in quantum chemistry and material sciences, the Black-Scholes equation describing option pricing problems in financial models as well as multi-dimensional data mining problems. We stress that due to the "curse of dimensionality", in the case of higher dimensions linear complexity $\mathcal{O}(N)$ is not satisfactory, hence we are looking for efficient methods with a cost $\mathcal{O}(dn^p \log^q n)$, with p, q independent of d. A desirable cost would be a clearly sublinear cost like $\mathcal{O}(dn \log^q n)$ (i.e., $p = 1$).

The approximability of integral operators in higher dimensions using the so-called *hierarchical Kronecker tensor-product format* (abbreviation: **HKT** format) is proven in [20]. Therein, also numerical experiments indicating exponential convergence of the HKT approximation to the inverse of an elliptic operator were presented. Moreover, the efficiency of the corresponding matrix algebra involving tensor-product vector representation was also addressed (see also [26] for tensor representation of function generated matrices). In paper [2], the idea was described on how the inverse to the multi-dimensional Laplace operator Δ can be approximated in the Kronecker tensor-product format using an integral representation to $(-\Delta)^{-1}$ that includes the operator exponential $\exp(t\Delta)$ (cf. (37)). However, both the theoretical analysis and numerical tests are missing there. Computational aspects of a low Kronecker-rank approximation to the solution of a tensor system with tensor right-hand side were considered in [10]. The HKT approximation to the matrix-valued functions A^{-1} and sign (A) for indefinite matrices A representing the discrete elliptic operators is addressed in [18].

In the present paper, we construct and analyse an HKT approximation to $\mathcal{A}^{-1}$ and to $\exp(-t\mathcal{A})$ in higher dimensions d for the general class of strongly positive operators $\mathcal{A}$ in $\mathbb{R}^d$, defined as a sum of low-dimensional commutative operators. Combining the tensor-product representation that includes one-dimensional operators and then approximating the latter in the $\mathcal{H}$-format, we arrive at the complexity $\mathcal{O}(dN^{1/d} \log^q N^{1/d}) = \mathcal{O}(dn \log^q n)$. Finally, we develop the data-sparse HKT approximation to fractional powers $\mathcal{A}^{-\sigma}$ ($\sigma > 0$) of an elliptic operator as well as to the solution operator of the matrix Lyapunov-Sylvester equation. In the case of discrete elliptic operators we provide a unified construction of the approximate inverse to a family of matrices provided that the spectrum of the corresponding matrix family lies in a fixed sector in the right half-plane.

Note that our approach represents the (approximate) inverse of the finite difference or finite element approximations to $\mathcal{A}^{-1}$ on a hypercube and, hence, it can be interpreted as an extension of the widely used Fast Fourier Transform (FFT). In fact, contrary to the FFT, the presented method applies to nonuniform tensor-product grids and to variable equation coefficients.

2. Preliminaries

In the following, we use the notation $\mathscr{A}, \mathscr{B}, \ldots$ for operators and $A, B, \ldots$ for matrices.

2.1. Excursus to the Approximation Theory

Practically relevant methods approximating functions in higher dimensions are usually based on some kind of separation of variables. One may try to approximate a multi-variate function $F : \mathbb{R}^d \to \mathbb{R}$, $d \geq 2$, in the form

$$F_r(x_1, \ldots, x_d) := \sum_{k=1}^{r} \Phi_k^1(x_1) \cdots \Phi_k^d(x_d) \approx F, \tag{2.1}$$

where the set of functions $\{\Phi_k^l(x_l)\}$ can be fixed or chosen adaptively (cf. discussion in [2]). Here the key quantity is r, which is usually called the *separation rank* and which should be reasonably small. One expects the approximation error to tend to zero as $r \to \infty$, but the crucial question is how r depends on the required approximation accuracy.

Let $\varepsilon > 0$ be the required approximation accuracy. In the case of globally analytic data, the classical polynomial approximation by interpolation at tensor-product Chebyshev nodes implies

$$r = \mathcal{O}\Big((\log|\log \varepsilon|)^{d-1} |\log \varepsilon|^{d-1}\Big), \tag{2.2}$$

where the low-order factor $\mathcal{O}((\log|\log \varepsilon|)^{d-1})$ appears because of the bound $\mathcal{O}(\log|\log \varepsilon|)$ on the Lebesque constant due to the tensor-product interpolation (cf. [17], [21, Theorem 4.1]). The above mentioned estimates are based on the standard results for the best polynomial approximation of analytic functions. Let $I_0 := [-1, 1]^d$ and let $E_r^1 \subset \mathbb{C}$ be the interior of the ellipse with focal points ± 1 such that the sum of semi-axes equals $r > 1$. We set $E_{\mathbf{r}} := E_{r_1}^1 \times \ldots \times E_{r_d}^1$. Let $A(E_{\mathbf{r}}, I_0; M)$ be the subset of those continuous functions on I_0 which can be extended analytically into $E_{\mathbf{r}}$ and are bounded there by the positive constant M. In opposite to the one-dimensional construction in the multi-dimensional case there are various possibilities to choose the polynomial space $\pi_{\mathbf{m}}$. One can use, for example,

$$P(\mathbf{x}) = \sum_{\mathbf{0} \leq \mathbf{k} \leq \mathbf{m}-\mathbf{1}} a_{\mathbf{k}} \mathbf{x}^{\mathbf{k}} \in \pi_{\mathbf{m}}, \quad \mathbf{x} \in I_0 \subset \mathbb{R}^d,$$

with the multi-index notation $\mathbf{k} = (k_1, \ldots, k_d)$, $\mathbf{m} = (m_1, \ldots, m_d)$, $\mathbf{m} - \mathbf{1} = (m_1 - 1, \ldots, m_d - 1)$, $\mathbf{x}^{\mathbf{k}} = x_1^{k_1} \cdots x_d^{k_d}$, where $\mathbf{0} \leq \mathbf{k} \leq \mathbf{m} - \mathbf{1}$ means the componentwise inequalities $0 \leq k_j \leq m_j - 1$ $(j = 1, \ldots, d)$. The dimension of $\pi_{\mathbf{m}}$ is $N = \dim \pi_{\mathbf{m}} = \prod_{j=1}^{d} m_j$. Given a function $f(\mathbf{x}) \in A(E_{\mathbf{r}}, I_0; M)$, choosing N points $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N)}$ lying on a $m_1 \times \ldots \times m_d$ tensor-product grid in I_0, we want to determine a polynomial $P(\mathbf{x}^{(j)}) = P(\mathbf{x}^{(j)}, f)$ – the interpolation polynomial – satisfying

$$P(\mathbf{x}^{(j)}, f) = f(\mathbf{x}^{(j)}), \qquad j = 1, ..., N.$$

These conditions define the projector $\mathbf{P} : C(I_0) \to \mathscr{L}$, $\mathbf{P} : f \to P(\cdot, f)$. It is known (see, e.g., [17]) that for $m_1 = \cdots = m_d = m$ there exists a constant C independent of n such that

$$\|f(\mathbf{x}) - P(\mathbf{x}^{(j)})\|_\infty \leq C(\log m)^d r^{-m}$$

for some $r > 1$. Thus, in order to arrive at a given tolerance ε, we require $m = \mathcal{O}((\log|\log\varepsilon|)|\log\varepsilon|)$, i.e., one needs at least

$$N_\varepsilon = \mathcal{O}\Big((\log|\log\varepsilon|)^d |\log\varepsilon|^d\Big)$$

parameters. Obviously, one can apply interpolation algorithms to achieve these optimal characteristics for the separable approximation (2.1). The constructions of such algorithms for analytic data that represent certain operator-valued functions is one of the aims of this paper.

For more general classes of multi-variate functions one obtains much worse complexity estimates. Let $X = W_p^r(M; I)$ with $M = (M_1, ..., M_d)$ and $r = (r_1, ..., r_d)$ be the class of anisotropic Sobolev spaces defined on the d-dimensional interval $I = \prod_{j=1}^d [a_j, b_j]$ possessing generalised x_j-derivatives of order r_j which are bounded by the constants M_j with respect to the Chebyshev norm $\|\cdot\|_\infty$. The important characteristics of this function class are the effective *class smoothness* $\rho = 1/(\sum_{j=1}^d r_j^{-1})$ and the *class constant* $\mu = \prod_{j=1}^d M_j^{\rho/r_j}$ (cf. [1, p. 81]). It is known (cf. [1, p. 232]) that for this class we need

$$N_\varepsilon^{(opt)} \asymp const(\mu) \cdot \varepsilon^{-1/(\rho - 1/p)}$$

parameters in order to approximate an arbitrary function of this class with a given tolerance ε. Note that $N_\varepsilon^{(opt)}$ grows exponentially as $d \to \infty$. This phenomenon is known as the "curse of dimensionality".

The familiar hyperbolic-cross approximation (cf. [25], [13]) allows to get rid of this phenomenon. It applies to the class of functions with higher mixed derivatives and leads to a complexity $r = \mathcal{O}(n \log^{d-1} n)$.

On the level of operators (matrices) we distinguish the following structure. Given a matrix $A \in \mathbb{C}^{N \times N}$ of order $N = n^d$, we try to approximate A by a matrix A_r of the form

$$A_r = \sum_{k=1}^r V_k^1 \otimes \cdots \otimes V_k^d \approx A, \tag{2.3}$$

where the V_k^ℓ are $n \times n$-matrices and $\otimes$ denotes the Kronecker product operation. Now the crucial parameter is r, called the *Kronecker rank* (cf. [20]). Very little is known about the approximability of nonlocal operators (e.g., integral and pseudo-differential operators, operator-valued functions) by the Kronecker tensor-product ansatz (2.3). The HKT approximation to the integral operators with asymptotically smooth kernel was introduced in [20], tensor approximations of some function-related matrices have been addressed in [26].

The main result of the present paper is a proof for the existence of tensor product approximations to $\exp(-t\mathscr{A})$, $\mathscr{A}^{-\sigma}$ ($\sigma > 0$) and the Lyapunov-Sylvester solution operator, in the form (2.3) with a Kronecker rank $r = \mathcal{O}(|\log \varepsilon|^2)$ independent of d (cf. (2.2)). Furthermore, we provide a constructive algorithm producing A_r in the HKT form (cf. [20]), where each Kronecker factor V_k^ℓ is given in the $\mathscr{H}$-matrix format with complexity $\mathcal{O}(n \log^4 n)$. This leads to an overall cost $\mathcal{O}(dn \log^4 n |\log \varepsilon|^2)$ to compute the discrete elliptic inverse $\mathscr{A}^{-1}$. Note that the dimension d appears as a factor but not in the exponent.

2.2. Strongly Positive Operators

The following notation is commonly used in operator theory. A densely defined closed linear operator $\mathscr{A}$ with the domain $D(\mathscr{A})$ in a Banach space X, with the spectral set $\sigma(\mathscr{A})$, the resolvent set $\rho(\mathscr{A})$ and the numerical range $v(\mathscr{A})$ is said *to be of type* (θ, M) for $\theta \in (0, \pi/2)$ and $M \geq 1$, if $\mathbb{C} \backslash \Sigma_\theta \subset \rho(\mathscr{A})$,

$$\|(zI - \mathscr{A})^{-1}\| \leq \frac{M}{|z|} \qquad \text{for } \Re e\, z < 0,$$

$$\|(zI - \mathscr{A})^{-1}\| \leq \frac{M_\epsilon}{|z|} \qquad \text{for } \theta + \epsilon \leq |\arg z| \leq \pi \text{ with } \epsilon > 0,$$

where $\Sigma_\theta = \{z \in \mathbb{C} : 0 \leq |\arg z| \leq \theta\}$ for $\theta \in (0, \pi/2)$ (cf. [5, p. 6]). In what follows, we suppose that zero belongs to the resolvent set of $\mathscr{A}$. By $\mathscr{L}(X)$, we denote the space of bounded linear operators in a Banach space X.

Let $a_{ij}(x) = a_{ji}(x)$, $b_j(x)$, $c(x)$ be real valued smooth functions on $\overline{\Omega} \in \mathbb{R}^d$ and suppose uniform ellipticity,

$$\Re e \sum_{i,j=1}^{d} a_{ij}(x)\xi_i\xi_j \geq \sigma|\xi|^2 \qquad \text{for } \xi = (\xi_1, \ldots, \xi_d) \in \mathbb{R}^d \text{ and } x \in \overline{\Omega}$$

with a constant $\sigma > 0$. Given

$$\mathscr{A} = -\sum_{i,j=1}^{d} \frac{\partial}{\partial x_i} a_{ij}(x) \frac{\partial}{\partial x_j} + \sum_{j=1}^{d} b_j(x) \frac{\partial}{\partial x_j} + c(x)$$

with $X = L^2(\Omega)$ the associated bilinear form reads

$$a(u, v) = \int_\Omega \left\{ \sum_{i,j=1}^{d} a_{ij}(x) \frac{\partial u}{\partial x_j} \frac{\partial \overline{v}}{\partial x_i} + \sum_{j=1}^{d} b_j(x) \frac{\partial u}{\partial x_j} \overline{v} + c(x) u \overline{v} \right\} dx$$

with $V = H_0^1(\Omega)$. The bilinear form $a : V \times V \to \mathbb{R}$ is continuous and it is assumed to be V-elliptic:

$$|a(u,v)| \le C\|u\|_V \|v\|_V, \qquad \Re e\, a(v,v) \ge \delta_0 \|v\|_V^2, \quad \delta_0 > 0,$$

and the corresponding elliptic operator $\mathscr{A}$ satisfies

$$\|(zI - \mathscr{A})^{-1}\|_{X \leftarrow X} \le \frac{1}{|z| \sin(\theta_1 - \theta)} \qquad \text{for all } z \in \mathbb{C} \text{ with } \theta_1 \le |\arg z| \le \pi, \tag{2.4}$$

for any $\theta_1 \in (\theta, \pi)$, where $\cos\theta = \delta_0 / C$.

Note that operators of type (θ, M) are also called strongly positive with the spectral angle $\theta \in (0, \pi/2)$ (see, e.g., [6] and the references therein).

In the case of discrete elliptic operators (say, $\mathscr{A}$ is the FEM stiffness matrix corresponding to a) the bound (2.4) on the matrix resolvent is valid uniformly in the mesh-size h (cf. Example 4.3).

3. Exponentially Convergent Quadrature Rules

In the following, our low Kronecker rank tensor-product approximations are based on efficient quadratures for the arising improper integrals on $\mathbb{R} := (-\infty, \infty)$. Quadrature rules with an exponentially convergent rate can be based on the so-called *Sinc-quadrature* formulae from [24]. We consider the integral

$$I(\mathscr{F}) = \int_\omega \mathscr{F}(x)dx \qquad (\omega = \mathbb{R} \ \text{ or } \omega = \mathbb{R}_+), \tag{3.1}$$

under different assumptions on the integrand $\mathscr{F} : \omega \to \mathscr{L}(X)$. The quadratures discussed below can be applied, in particular, to operator- or matrix-valued functions of a strongly positive elliptic operator $\mathscr{A}$.

Let $\omega = \mathbb{R}$. We introduce the family $\mathbf{H}^1(D_\delta)$ of all operator-valued functions of strongly positive operators, which are analytic in $D_\delta := \{z \in \mathbb{C} : |\Im m z| \le \delta\}$, $0 < \delta < \pi$, such that for each $\mathscr{F} \in \mathbf{H}^1(D_\delta)$ there holds $\|\mathscr{F}\|_{\mathbf{H}^1(D_\delta)} < \infty$ with

$$\|\mathscr{F}\|_{\mathbf{H}^1(D_\delta)} := \int_{\partial D_\delta} \|\mathscr{F}(z)\| |dz|.$$

3.1. *Standard* Sinc *Quadrature*

Given $\mathscr{F} \in \mathbf{H}^1(D_\delta)$, $h > 0$, and $M \in \mathbb{N}$, we use the notations

$$\begin{aligned} T(\mathscr{F}, h) &= h \sum_{k=-\infty}^{\infty} \mathscr{F}(kh), \qquad & T_M(F, h) &= h \sum_{k=-M}^{M} \mathscr{F}(kh), \\ \eta(\mathscr{F}, h) &= I(\mathscr{F}) - T(\mathscr{F}, h), \qquad & \eta_M(\mathscr{F}, h) &= I(\mathscr{F}) - T_M(\mathscr{F}, h). \end{aligned} \tag{3.2}$$

In the case $\omega = \mathbb{R}$, the error estimate of η_M is as follows (cf. [24]). If

$$\|\mathscr{F}(\xi)\| \le C \exp(-b|\xi|) \qquad \text{for all } \xi \in \mathbb{R} \text{ with } b, C > 0, \tag{3.3}$$

then the error η_M from (3.2) satisfies

$$\|\eta_M(\mathscr{F},h)\| \le C\left[\frac{e^{-2\pi\delta/h}}{1-e^{-2\pi\delta/h}}\|\mathscr{F}\|_{\mathbf{H}^1(D_\delta)} + \frac{1}{b}\exp(-bhM)\right]. \tag{3.4}$$

The choice $h = \sqrt{2\pi\delta/M}$ leads to the exponential convergence rate

$$\|\eta_M(\mathscr{F},h)\| \le Ce^{-\sqrt{2\pi\delta M}} \tag{3.5}$$

with a positive constant C independent of M (cf. [24], [8], [9]). Note that $2M+1$ is the number of quadrature points. If $\mathscr{F}$ is even function, the number of quadrature points reduces to $M+1$.

In the case of integrals defined on $\mathbb{R}_+$ one has to substitute the corresponding integral by $\xi = \varphi(z)$ with a bijection $\varphi : \mathbb{R} \to \mathbb{R}_+$. This changes $\mathscr{F}$ into the integrand $\mathscr{F}_1 := \varphi' \cdot (\mathscr{F} \circ \varphi)$ over $\mathbb{R}$. Assuming $\mathscr{F}_1 \in \mathbf{H}^1(D_\delta)$, one can apply (7)–(9) to the transformed function. For the respective families of operator-valued functions on $\mathbb{R}_+$, the domain of analyticity D_δ will be substituted by $D_\delta^{(1)}$ or $D_\delta^{(2)}$, specified in the examples below.

3.1.1. Example 1: Polynomial Decay

Let us set $\omega = \mathbb{R}_+$ and assume the following two conditions (cf. [24, p. 193]):

(i) the integrand $\mathscr{F}$ can be analytically extended from the real half-axis into the sector

$$D_\delta^{(1)} = \{z \in \mathbb{C} : |\arg(z)| < \delta\} \qquad \text{for some } 0 < \delta < \pi;$$

(ii) $\mathscr{F}$ satisfies the inequality

$$\|\mathscr{F}(z)\| \le c|z|^{\alpha-1}(1+|z|)^{-\alpha-\beta} \qquad \text{for some } 0 < \alpha, \beta \le 1 \text{ and all } z \in D_\delta^{(1)}. \tag{3.7}$$

For the ease of exposition we consider only the case $\alpha = 1$. Choosing $m \in \mathbb{N}$ and taking

$$h^{(1)} = \sqrt{2\pi\delta/(\beta m)}, \tag{3.8}$$

we define the corresponding quadrature rule

$$I_M^{(1)}(\mathscr{F}) = h^{(1)} \sum_{k=-\beta M}^{M} \kappa_k^{(1)} \mathscr{F}(z_k^{(1)}), \qquad z_k^{(1)} = e^{kh^{(1)}}, \quad \kappa_k^{(1)} = e^{kh^{(1)}}, \tag{3.9}$$

possessing the exponential convergence rate

$$\left\| I(\mathscr{F}) - I_M^{(1)}(\mathscr{F}) \right\| \le Ce^{-\sqrt{2\pi\delta\beta M}} \tag{3.10}$$

with a positive constant C independent of M. Note that in the case $\beta = 1$, the bound (3.10) coincides with the standard estimate (3.5).

3.1.2. Example 2: Exponential Decay

Let us set $\omega = \mathbb{R}_+$ and assume that the integrand $\mathscr{F}$ in (3.1) can be analytically extended into the "bullet-shaped" domain $D^{(2)}_\delta = \{z \in \mathbb{C} : |\arg(\sinh z)| < \delta\}$ for some $\delta \in (0, \pi)$, and that $\mathscr{F}$ satisfies

$$\|\mathscr{F}(z)\| \le C\left(\frac{|z|}{1+|z|}\right)^{\alpha-1} e^{-\beta \Re e z} \qquad \text{in } D^{(2)}_\delta \text{ with } \alpha, \beta \in (0, 1].$$

Again we set $\alpha = 1$. Then choosing $h^{(2)} = h^{(1)}$, we obtain the quadrature rule

$$I^{(2)}_m(\mathscr{F}) = h^{(2)} \sum_{k=-\beta M}^{M} \kappa^{(2)}_k \mathscr{F}(z^{(2)}_k), \;\; z^{(2)}_k = \log[e^{kh^{(2)}} + \sqrt{1+e^{2kh^{(2)}}}], \;\; \kappa^{(2)}_k = 1 + e^{-2kh^{(2)}} \tag{3.11}$$

possessing again the exponential convergence rate (3.10).

3.2. Improved Quadratures in the Case of Hyper-Exponential Decay

In this section, we construct a new Sinc-quadrature rule for the integral (3.1) defined on $\mathbb{R}$ with the operator-valued function $\mathscr{F}$ of a strongly positive operator. This quadrature is similar to that one in [9] and converges faster than (3.5).

Adapting the ideas of [24], [9], one can prove the following approximation results for functions from $\mathbf{H}^1(D_\delta)$, describing the accuracy of $T(\mathscr{F}, h)$ and $T_M(\mathscr{F}, h)$ (cf. Lemma 2.4 in [9]).

Lemma 3.1: *For any operator valued function $\mathscr{F} \in \mathbf{H}^1(D_\delta)$, there holds*

$$\|\eta(\mathscr{F}, h)\| \le \frac{e^{-\pi\delta/h}}{2\sinh(\pi\delta/h)} \|\mathscr{F}\|_{\mathbf{H}^1(D_\delta)}. \tag{3.12}$$

If, in addition, f satisfies the condition

$$\|\mathscr{F}(\xi)\| \le C \exp(-be^{a|\xi|}) \qquad \text{for all } \xi \in \mathbb{R} \text{ with } a, b, C > 0, \tag{3.13}$$

then the error η_M of the quadrature $T_M(\mathscr{F}, h)$ satisfies

$$\|\eta_M(\mathscr{F}, h)\| \le C\left[\frac{e^{-2\pi\delta/h}}{1 - e^{-2\pi\delta/h}} \|\mathscr{F}\|_{\mathbf{H}^1(D_\delta)} + \frac{1}{ab} \exp(-be^{ahM})\right] \tag{3.14}$$

with the parameter δ from $\mathbf{H}^1(D_\delta)$.

Proof: The bound (3.12) is proven in [8]. Assumption (3.13) now implies

$$\|\eta_M(\mathscr{F},h)\| \leq \|\eta(\mathscr{F},h)\| + h\sum_{|k|>M}\|\mathscr{F}(kh)\|$$
$$\leq \frac{\exp(-\pi\delta/h)}{2\sinh(\pi\delta/h)}\|\mathscr{F}\|_{\mathbf{H}^1(D_\delta)} + ch\sum_{k:|k|>M}\exp(-be^{a|kh|}). \qquad (3.15)$$

For the last sum we use the simple estimate to obtain

$$\sum_{k:|k|>M}\exp(-be^{a|kh|}) = 2\sum_{k=M+1}^{\infty}\exp(-be^{a|kh|})$$
$$\leq 2\int_M^\infty \exp(-be^{a|xh|})dx \; = \frac{2}{abh}\exp(-be^{ahM}). \qquad (3.16)$$

Now (3.15) and (3.16) imply (3.14) completing the proof. □

Due to Lemma 3.1, we can improve the asymptotical convergence of the above quadratures for the integral (5) in the case $\omega = \mathbb{R}$. Let $D_\delta^{(3)}$ be the domain

$$D_\delta^{(3)} := \left\{ z = u + iv : \frac{v^2}{\sin^2\delta} - \frac{u^2}{\cos^2\delta} \leq 1 \right\},$$

where $0 < \delta < \pi/2$ (see Fig. 3.1). Returning to the integral (3.1), we can change the variables by $z = \sinh w$ and obtain the integral

$$I(\mathscr{F}) = \int_{\mathbb{R}} \mathscr{F}(z)dz = \int_{\mathbb{R}} \tilde{\mathscr{F}}(w)dw$$

with the integrand $\tilde{\mathscr{F}}(w) = \cosh w \mathscr{F}(\sinh w)$. Under the assumption that $\mathscr{F}(z)$ satisfies (3.3), and that it can be analytically extended into the domain $D_\delta^{(3)}$, we conclude that the new integrand $\tilde{\mathscr{F}}(w)$ possesses a hyper-exponential decay (3.13)

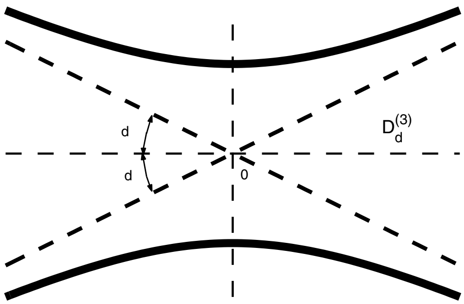

Fig. 3.1. The analyticity domain $D_\delta^{(3)}$

and can be analytically extended into the domain D_δ. Now assuming that $\tilde{\mathscr{F}} \in \mathbf{H}^1(D_\delta)$, we arrive at the situation of Lemma 3.1 and get the following quadrature rule for (3.1):

$$I_M^{(3)}(\mathscr{F}) = h^{(3)} \sum_{k=-M}^{M} \kappa^{(3)} \mathscr{F}(z_k^{(3)}), \tag{3.17}$$

where, with some fixed constant $C_{int} > 0$,

$$h^{(3)} = C_{int} \frac{\log M}{M}, \quad \kappa^{(3)} = \cosh(w_k), \quad w_k = kh^{(3)}, \quad z_k^{(3)} = \sinh w_k^{(3)}.$$

Due to Lemma 3.1 (cf. (3.4)), there are some positive constants C, s such that

$$\left\| I(\mathscr{F}) - I_M^{(3)}(\mathscr{F}) \right\| \leq Ce^{-sM/(\log M)}. \tag{3.18}$$

3.3. Numerics I

To complete this section, we present numerical results characterising the exponential convergence of the quadrature rules (3.9) and (3.11). We compute the integral

$$\frac{1}{r} = \int_0^\infty e^{-rt} dt, \qquad r > 0. \tag{3.19}$$

The table below represents the error of $I_m^{(2)}(\mathscr{F})$ from (3.11), where m is the parameter from (3.8).

Quadrature (3.11), $r = 1.0$

m	4	9	16	25	36	49	64
ε	2.6_{10}-3	6.0_{10}-5	1.3_{10}-6	1.8_{10}-8	3.9_{10}-10	5.4_{10}-11	3.6_{10}-12

The next table shows the error of quadrature $I_m^{(1)}(\mathscr{F})$ from (3.19) applied to the above integral.

Quadrature (3.9), $r = 1.0$

m	4	9	16	25	36	49	64
ε	1.3_{10}-2	6.7_{10}-4	5.1_{10}-5	6.7_{10}-7	1.0_{10}-7	6.4_{10}-10	1.8_{10}-10

The last table shows the dependence of m (necessary to achieve the accuracy $\varepsilon \leq 4.0_{10} - 7$) with respect to the parameter β from 10 in the case of quadrature (12). Here a small $\beta > 0$ corresponds to a small parameter r in the exponent in the right-hand side of (3.19).

Quadrature (3.9), accuracy $\varepsilon \leq 4.0 \cdot 10^{-7}$

r	1.0	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}
m	36	81	121	169	200	280	440

3.4. Numerics II

We present numerical results for the quadrature rule (3.17) applied to $F(u) = e^{-r^2u^2}$. We confirm exponential convergence of the quadrature (3.20), namely

$$h \sum_{k=-M}^{M} \cosh(kh) F(\sinh(kh)) \approx \int_{\mathbb{R}} F(u)du = \int_{\mathbb{R}} \cosh(w) F(\sinh(w))dw, \tag{3.20}$$

approximating the Gauss integral

$$\frac{1}{r} = \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} e^{-r^2t^2} dt. \tag{3.21}$$

This integral is commonly used in quantum chemistry calculations as well for representation of certain matrix valued functions. Clearly, in a certain range $[R_1, R_2]$ of r ($R_1 < 1 < R_2$), the function $\cosh(w)F(\sinh(w))$ satisfies all conditions of Lemma 3.1. Thus, we choose $h = C_{\text{int}} \frac{\log M}{M}$ and obtain fast exponential convergence $\mathcal{O}(e^{-cM/\log M})$ for $r \in [R_1, R_2]$.

Quadrature (3.20) for (3.21), $r = 1.0$

M	4	9	16	25	36
ε	1.1_{10}-4	1.5_{10}-6	2.3_{10}-9	2.0_{10}-12	$< 1.0_{10}$-15

Figure 3.2 represents the convergence history for (3.20) corresponding to the choice $r = 1$ and $C_{\text{int}} = 1.0$. This quadrature shows a similar convergence in the interval $r \in [0.2, 10]$, i.e., in this case $R_2/R_1 \approx Q = 50$. An application of this quadrature for a larger range $[R_{min}, R_{max}]$ requires piecewise quadrature using a rescaling of r in each subinterval., thus, in general, we need about pM quadrature points, where $Q^p \approx R_{max}/R_{min}$ (cf. [18] for a quadrature, which is robust with respect to the condition number R_{max}/R_{min}).

The following table shows the quadrature error of (3.9) applied to the integral (3.21) with $r = 0.1$.

Quadrature (3.9), $r = 0.1$

M	4	9	16	25	36	49	64
ε	6.2_{10}-2	1.8_{10}-3	2.8_{10}-4	1.5_{10}-5	3.7_{10}-7	2.0_{10}-9	1.3_{10}-10

In the second example, we set $F(u) := e^{u-re^u}$ in (23), which applies to the integral

$$\frac{1}{r} = \int_{\mathbb{R}} e^{u-re^u} du, \tag{3.22}$$

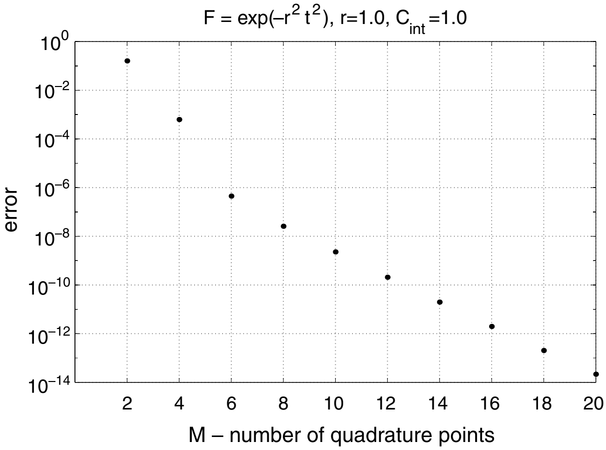

Fig. 3.2. Approximation to the integral (3.21)

obtained from (3.19) by the substitution $t = e^u$, $u \in \mathbb{R}$. Here we choose $h = C_{\text{int}} \frac{\log M}{M}$ with $C_{\text{int}} = 1.35$.

Quadrature (3.20) for (3.22), $r = 1.0$

M	4	9	16	25	36	49	64
ε	1.6_{10}-2	1.0_{10}-5	2.6_{8}-6	4.1_{10}-9	2.7_{10}-11	2.1_{10}-12	5.2_{10}-14

Figure 3.3 illustrates exponential convergence (we use a semi-logarithmic scale), though the theoretical analysis does not imply the desired estimate. The above quadrature converges faster than (3.11), however, the convergence rate strongly deteriorates if R_{max}/R_{min} increases. The robust quadrature for the integral (3.19) is presented in [18].

4. Tensor-Product Approximation to $\exp(-t\mathscr{A})$

4.1. Approximation to $\exp(-t\mathscr{A})$ *by a Sum of Few Resolvents*

It was shown in [22, p. 30] that each operator exponential $e^{-t\mathscr{A}}$ with $t \in [0, \infty)$ (belonging to the semi-group $\{e^{-t\mathscr{A}}\}_{t\geq 0}$ generated by a strongly positive operator $\mathscr{A}$) can be represented by the Dunford-Cauchy integral

$$\begin{aligned} T(t;\mathscr{A}) := e^{-t\mathscr{A}} &= \frac{1}{2\pi i}\int_{\Gamma} e^{-tz}(zI - \mathscr{A})^{-1}dz \\ &= \frac{1}{2\pi i}\int_{\Gamma_+} e^{-tz}(zI - \mathscr{A})^{-1}dz + \frac{1}{2\pi i}\int_{\Gamma_-} e^{-tz}(zI - \mathscr{A})^{-1}dz, \end{aligned}$$

where $\Gamma = \Gamma_+ + \Gamma_-$ is a curve in the resolvent set with the ray $\Gamma_+ = \{z : z = \rho e^{i\theta_1}, \rho \in (0,\infty)\}$ running from ∞e^{θ_1} to 0 and the ray $\Gamma_- = \{z : z = \rho e^{-i\theta_1}, \rho \in (0,\infty)\}$ running from 0 to $\infty e^{-\theta_1}$. This leads to the representation

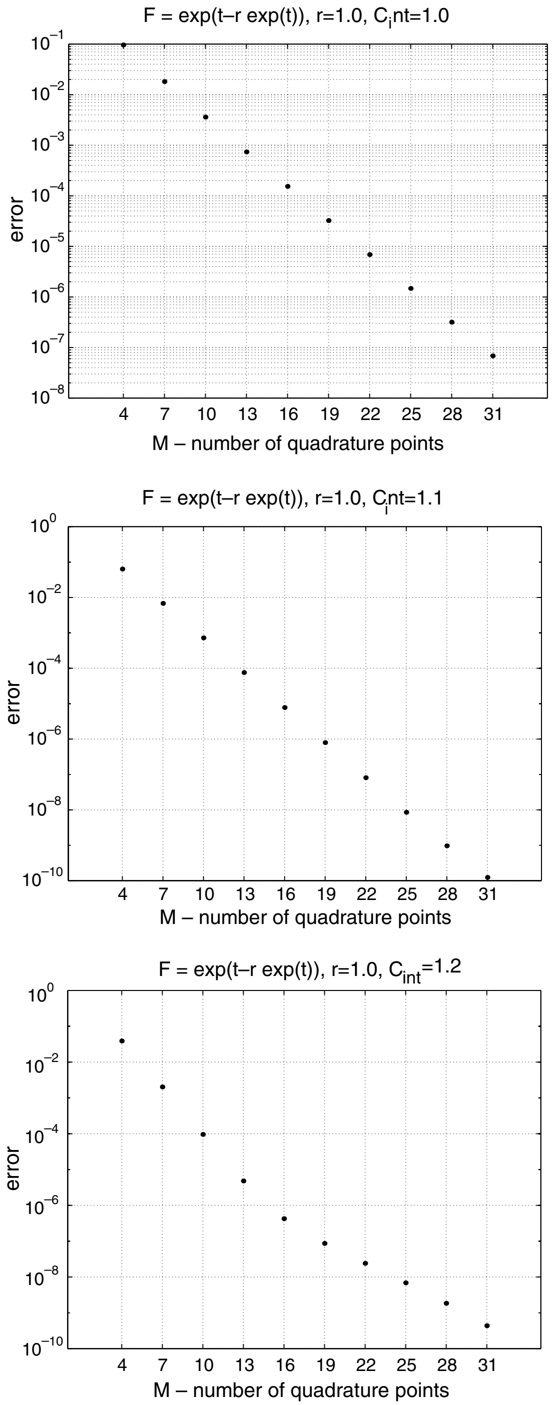

Fig. 3.3. Quadrature (3.20) for the integral (3.22), $r = 1.0$, with different C_{int}

$$T(t;\mathscr{A}) = \frac{1}{2\pi i}\int_0^\infty F(t,\rho)d\rho, \tag{4.1}$$

where $F = -e^{i\theta_1}F_1 + e^{-i\theta_1}F_2$ with

$$F_1(t,\rho) = e^{-t\rho(\cos\theta_1 + i\sin\theta_1)}(\rho e^{i\theta_1}I - \mathscr{A})^{-1},$$
$$F_2(t,\rho) = e^{-t\rho(\cos\theta_1 - i\sin\theta_1)}(\rho e^{-i\theta_1}I - \mathscr{A})^{-1}.$$

We choose $\theta_2 > 0$ such that $\theta_1 + \theta_2 < \pi/2$ and $\theta_1 - \theta_2 > \theta$. Considering $\rho = |\rho|e^{i\phi}$, $|\phi| < \theta_2$, as a complex variable, one can easily see that the integral can be extended analytically into the sector

$$\Sigma_{\theta_2} = \{\rho = |\rho|e^{i\phi} : |\rho| \in (0,\infty), \phi \in (-\theta_2, \theta_2)\},$$

and the following estimates hold in Σ_{θ_2}:

$$\begin{aligned}\|F_1(t,\rho)\| &= \|e^{-t|\rho|e^{i(\phi+\theta_1)}}(|\rho|e^{i(\phi+\theta_1)}I - \mathscr{A})^{-1}\| \\ &\leq e^{-t|\rho|\cos(\phi+\theta_1)}(1+|\rho|)^{-1} \leq e^{-t|\rho|\cos(\theta_2+\theta_1)}(1+|\rho|)^{-1}, \\ \|F_2(t,\rho)\| &= \|e^{-t|\rho|e^{i(\phi-\theta_1)}}(|\rho|e^{i(\phi-\theta_1}I - \mathscr{A})^{-1}\| \leq e^{-t|\rho|\cos(\theta_2+\theta_1)}(1+|\rho|)^{-1}.\end{aligned}$$

Thus, the integrand in (4.1) can be analytically extended into the sector $D_\delta^{(1)}$ from [24, p. 68] (see also (3.6)) with $\delta = \theta_2$ and in this region the estimate (3.7) holds with $\alpha = \beta = 1$. This means that we can apply the quadrature rule (3.9) with $h^{(1)} = \sqrt{2\pi\delta/M}$ to derive

$$I(t) \approx I_M^{(1)}(t) = \frac{h^{(1)}}{2\pi i}\sum_{k=-M}^{M}\kappa_k^{(1)}F(t, z_k^{(1)}), \qquad \kappa_k^{(1)} = e^{kh^{(1)}}, \quad z_k^{(1)} = e^{kh^{(1)}}, \tag{4.2}$$

which possesses the accuracy $\mathcal{O}(e^{-\sqrt{2\pi\delta M}})$. The formulae

$$T(t;\mathscr{A}) \approx T_M^{(1)}(t;\mathscr{A}) = I_M^{(1)}(t) \equiv \sum_{k=-M}^{M}\left[\kappa_{k,1}^{(1)}(t)(\zeta_{k,1}^{(1)}I - \mathscr{A})^{-1} + \kappa_{k,2}^{(1)}(t)(\zeta_{k,2}^{(1)}I - \mathscr{A})^{-1}\right] \tag{4.3}$$

with

$$\kappa_{k,1}^{(1)}(t) = -\frac{e^{i\theta_1}h^{(1)}}{2\pi i}e^{-te^{kh^{(1)}}(\cos\theta_1 + i\sin\theta_1)}e^{kh^{(1)}},$$
$$\kappa_{k,2}^{(1)}(t) = \frac{e^{-i\theta_1}h}{2\pi i}e^{-te^{kh^{(1)}}(\cos\theta_1 - i\sin\theta_1)}e^{kh^{(1)}},$$
$$\zeta_{k,1}^{(1)} = e^{kh^{(1)}}e^{i\theta_1},\ \zeta_{k,2}^{(1)} = e^{kh^{(1)}}e^{-i\theta_1},$$

and $I_M^{(1)}(t)$ computed according to (4.2) represents new exponentially convergent algorithms for the operator exponential of a strongly positive operator with the accuracy $e^{-s\sqrt{M}}$, where the constant s depends on the spectral characteristics of $\mathscr{A}$.

Due to Lemma 3.1, we can improve the asymptotical convergence of the above quadratures to the better estimate (21). Let us defines the so-called spectral curve

$$\Gamma_S = \{z = \xi + i\eta : \xi = a_p\eta^2 + b_p\}, \tag{4.4}$$

containing the spectrum $sp(\mathscr{A})$ of the operator $\mathscr{A}$.

Lemma 4.1 [9]: *Let the spectral curve for $\mathscr{A}$ be Γ_S defined by (4.4). Choose the (integration) curve $\Gamma_I = \{z = \xi + i\eta : \xi = a_e\cosh(s), \eta = b_e\sinh s\}$ with a_e, b_e such that Γ_I envelops Γ_S. Then the operator exponential $T(t;\mathscr{A}) = e^{-t\mathscr{A}}$ can be represented by the Dunford-Cauchy integral*

$$T(t;\mathscr{A}) = \frac{1}{2\pi i}\int_{\Gamma_I} e^{-zt}(zI - \mathscr{A})^{-1}dz = \int_{\mathbb{R}} F_1(s,t)ds,$$

where the integrand

$$\begin{gathered} F_1(s,t) = -\tfrac{1}{2\pi i}e^{-zt}z'(s)(zI - \mathscr{A})^{-1}, \\ z = a_e\cosh(s) + ib_e\sinh(s),\ z'(s) = a_e\sinh(s) + ib_e\cosh(s),\ s \in \mathbb{R}, \end{gathered} \tag{4.5}$$

can be estimated on the real axis by

$$\|F_1(\eta,t)\| \le M_1 e^{-t\sqrt{a_e^2+b_e^2}|\sinh s|} \qquad \text{for } s \in \mathbb{R}$$

with some positive constant M_1. Moreover, $F_1(\cdot,t)$ can be analytically extended into the strip D_δ of the width $\delta > 0$ and belongs to the class $\mathbf{H}^1(D_\delta)$ (even to the suitably defined spaces $\mathbf{H}^p(D_\delta)$ for all $p \in [1,\infty]$).

The operator exponential $T(t;\mathscr{A})$ is represented as integral according to Lemma 4.1. Applying the quadrature rule T_M (cf. (3.2)) to the operator valued function $F_1(\eta,t)$ given by (4.5), we obtain for the operator family $\{I(t) \equiv T(t;\mathscr{A}) : t > 0\}$ (cf. (3.1)) that

$$I(t) \approx T_M(F_1,h) = h\sum_{k=-M}^{M} F_1(kh,t). \tag{4.6}$$

The error analysis is due to Lemma 4.1: Set $h = \frac{\log M}{M}$, then (cf. Theorem 2.5 in [9])

$$\|T(t,\mathscr{A}) - T_M(t,\mathscr{A})\| \lesssim \frac{1}{t\sqrt{a_e^2+b_e^2}}\left(e^{-2\pi\delta M/\log M} + e^{-t\sqrt{a_e^2+b_e^2}M}\right).$$

We see that for fixed $t > 0$, the error of this quadrature becomes $\mathcal{O}(e^{-cM/\log M})$.

4.2. Tensor-Product Representation of $\exp(-t\mathscr{A})$ *in* $\mathbb{R}^d$

Let $\mathscr{A} = \sum_{j=1}^{d} \mathscr{A}_j$ be a strongly positive operator, where $\mathscr{A}_j$ are mutually commutative, strongly positive operators with the respective spectral sectors S_j. Then we introduce the tensor-product approximant

$$T(t;\mathscr{A}) = \prod_{j=1}^{d} T(t;\mathscr{A}_j) = \prod_{j=1}^{d} e^{-t\mathscr{A}_j} \approx T_{\mathbf{m}}(t) = T_{\mathbf{m}}(t;\mathscr{A}) = \prod_{j=1}^{d} T_{m_j}(t;\mathscr{A}_j), \quad (4.7)$$

where each of the operator exponentials $T_{m_j}(t;\mathscr{A}_j)$ can be computed by Algorithm (4.3) or (4.6). Here we use the notations $\mathbf{m} = (m_1, \ldots, m_d)$. We denote by m_j the quadrature parameter in the quadratures above. For simplicity, we consider only the case $\mathbf{m} = (m, \ldots, m)$ with fixed $m_j = m$.

Lemma 4.2: *For any fixed* $t > 0$, *the approximation error by (4.7) satisfies*

$$\|e^{-t\mathscr{A}} - T_{\mathbf{m}}(t;\mathscr{A})\| \le Cde^{-sM}, \quad (4.8)$$

where $M = \sqrt{m}$ *in the case of (4.3) and* $M = m/\log m$ *in the case of (4.6), and where* C *and* s *depend neither on* d *nor on* $\mathbf{m}$.

Proof: Representing the error by a chain sum, we arrive at the estimate (say in the case (4.3))

$$\begin{aligned}\|e^{-t\mathscr{A}} - T_{\mathbf{m}}(t;\mathscr{A})\| &= \|[e^{-t\mathscr{A}_1} - T_m]e^{-t\mathscr{A}_2}\cdots e^{-t\mathscr{A}_d} + T_m(t)[e^{-t\mathscr{A}_2} - T_m(t)]e^{-t\mathscr{A}_3}\cdots e^{-t\mathscr{A}_d} \\ &\quad + \ldots + T_m(t)\cdots T_m(t)[e^{-t\mathscr{A}_d} - T_m(t)]\| \\ &\le Cde^{-s\sqrt{m}}\end{aligned}$$

providing an error bound (4.8) with C, s being independent of d, $\mathbf{m}$.

To represent the operator exponential with small $t > 0$, in the following proposition we use an approximation to the weighted exponential $T_\sigma(t) = T_\sigma(t;\mathscr{A}) := \mathscr{A}^{-\sigma}e^{-t\mathscr{A}}$, $t \ge 0$, $\sigma > 1$, which guarantees an exponential convergence rate for all $t \ge 0$.

Proposition 4.3 *[9]: (a) Let* $\varepsilon > 0$ *be given. In order to obtain* $\|T_\sigma(t) - T_{\sigma,M}(t)\| \lesssim \varepsilon$ *uniformly with respect to* $t \ge 0$, *choose*

$$\begin{aligned} M &= O(|\log\varepsilon|^2), \quad h = \sqrt{\pi\delta/[\sigma M]}, \\ z_k &= z(kh) = \xi(kh) + i\psi(kh) \ \ (k = -M, \ldots, M), \\ \xi(s) &= a_e \cosh s, \ \psi(s) = b_e \sinh s, \\ \gamma_{\sigma,k}(t) &= z_k^{-\sigma} e^{-z_k t} \frac{h}{2\pi i} z'(kh). \end{aligned}$$

Then $T_{\sigma,M}(t)$ *is a linear combination of* $2M + 1$ *resolvents with scalar weights depending on* t:

$$T_{\sigma,M}(t) = \sum_{k=-M}^{M} \gamma_{\sigma,k}(t)(z_k I - \mathscr{A})^{-1},$$

so that the computation of $T_{\sigma,M}(t)$ *requires* $2M + 1 = O(|\log \varepsilon|^2)$ *evaluations of the resolvents* $(z_k I - \mathscr{A})^{-1}$, $k = -M, \ldots, M$.

(b) The evaluations (or approximations) of the resolvents can be performed in parallel. Note that the shifts z_k *are independent of* t.

(c) Having evaluated the resolvents, $T_{\sigma,M}(t)$ *can be determined in parallel for different* t-values $t_1, t_2, \ldots$.

In practical computations one can choose $\sigma = 2$. Hence, the operator exponential $T_{m_j}(t; \mathscr{A}_j)$ in (33) can be approximated by

$$T_{m_j}(t; \mathscr{A}_j) \approx A_j^2 T_{2,m_j}(t; \mathscr{A}_j). \tag{4.9}$$

4.3. Some Examples

Example 4.4: *As a basic example we consider the elliptic operator* $\mathscr{A} = \sum_{j=1}^{d} \mathscr{A}_j$ *in the* d*-dimensional unit hypercube* $(0,1)^d$, *subject to zero Dirichlet boundary conditions, where*

$$\mathscr{A}_j = \sum_{k=0}^{2m} a_k(x_j) \frac{\partial^k}{\partial x_j^k}, \qquad (-1)^m a_{2m}(x_j) \geq \mu > 0,$$

is a one-dimensional, strongly elliptic operator. It is known (cf. [7], [22]) *that* $\mathscr{A}$ *and each* $\mathscr{A}_j$ *are strongly positive (m-sectorial). Furthermore, it is easy to see that the operators* $\mathscr{A}_j : H^{-m}(0,1) \to H_0^m(0,1)$ *are commutative.*

Example 4.5: *Consider the elliptic operator of divergent type,*

$$\mathscr{A} := -\sum_{j=1}^{d} \partial_j a_j(x_j) \partial_j, \qquad x \in \Omega := (0,1)^d,$$

defined on the Sobolev space $H_0^1(\Omega)$. *We assume that* $a_j \geq a_0 > 0$. *Introduce a uniform grid with step size* h *and* $N = n^d$ *interior nodes. Using the* $(2d+1)$*-point stencil, we obtain the finite difference discretization*

$$A_h z := -\sum_{j=1}^{d} \frac{2a_{i_j}^j z_{i_1 \ldots i_d} - b_{i_j-1}^j z_{i_1 \ldots (i_j-1) \ldots i_d} - c_{i_j+1}^j z_{i_1 \ldots (i_j+1) \ldots i_d}}{h^2}, \qquad 1 \leq i_j \leq n, \tag{4.10}$$

where z *denotes the vector corresponding to* $[z_{i_1 \ldots i_d}]_{i_j=1}^n \in \mathbb{R}^N$ *given in the tensor-product numbering. In fact, we can regard* d*-dimensional* $n \times \ldots \times n$ *arrays* *(tensors) also as one-dimensional ones (vectors) with n^d components. Then the matrix A_h in (4.10) takes the form*

$$A_h = \sum_{j=1}^{d} A_j,$$

where

$$A_1 = V^1 \times I \times \ldots \times I, \quad A_2 = I \times V^2 \times \ldots \times I, \ \ldots, \ A_d = I \times \ldots \times I \times V^d$$

with

$$V^j = \frac{1}{h^2} \begin{bmatrix} 2a_1^j & -c_1^j & & & \\ -b_2^j & 2a_2^j & -c_2^j & & \\ & \ddots & \ddots & \ddots & \\ & & -b_{n-1}^j & 2a_{n-1}^j & -c_{n-1}^j \\ & & & -b_n^j & 2a_n^j \end{bmatrix}_{n \times n}, \quad I = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix}_{n \times n}.$$

It is easy to see that $A_j > 0$ for all $j = 1, \ldots, d$, and that they commute pairwise, i.e., $A_j A_m = A_m A_j$. Finally, (4.7) implies the following tensor-product representation

$$e^{-tA} \approx \bigotimes_{j=1}^{d} T_{m_j}(t; V^j).$$

Example 4.6: *In the situation of Example 4.5, we consider an application to parabolic problems in $\mathbb{R}^d$ posed in the semi-discrete form. Using the semigroup theory (see [22] for more details), the solution of the first-order evolution equation*

$$\frac{du}{dt} + A_h u = f, \quad u(0) = u_0 \in \mathbb{R}^N,$$

with a given initial vector u_0 and with a given right-hand side $f \in L^2(Q_T)$, $Q_T := (0, T) \times \mathbb{R}^N$, can be represented as

$$u(t) = \exp(-tA_h)u_0 + \int_0^t \exp(-(t-s)A_h) f(s) ds, \qquad t \in (0, T].$$

Assume that our input data can be represented in the tensor-product form

$$u_0 \approx \sum_{k=1}^{r} u_1^k(x_1) \otimes \ldots \otimes u_d^k(x_d), \qquad f \approx \sum_{k=1}^{r} f_1^k(s; x_1) \otimes \ldots \otimes f_d^k(s; x_d)$$

with $u_i^k, f_i^k \in \mathbb{R}^n$, $i = 1, ..., d$, and with $r = \mathcal{O}(|\log \varepsilon|^q)$. Then we obtain the tensor-product approximation

$$\widetilde{u}(t) = \sum_{k=1}^{r} \left\{ \bigotimes_{j=1}^{d} T_{n_j}(t; V^j) u_j^k(x_j) + \int_0^t \bigotimes_{j=1}^{d} T_{n_j}(t-s; V^j) f_j^k(s; x_j) ds \right\} \approx u(t)$$

which can be implemented with the complexity $\mathcal{O}(rdn \log^p n)$.

5. A Separable Representation to $\mathcal{A}^{-1}$ and Further Applications

5.1. Inverse of a Strongly Positive Operator

Lemma 5.1: *Let* $\mathcal{A}$ *be a densely defined, strongly positive operator with the spectral set* $\sigma(\mathcal{A})$. *Then the following integral representation holds:*

$$\mathcal{A}^{-1} = \int_0^\infty e^{-t\mathcal{A}} dt. \tag{5.1}$$

Proof: For $\mathcal{A}$ being strongly positive, the semigroup $\{e^{-t\mathcal{A}}\}_{t\geq 0}$ can be extended to an analytic semigroup in the sector

$$\Delta_\delta = \{w : |\arg(w)| < \delta\}$$

of the complex w-plane and $\|e^{-w\mathcal{A}}\|$ is uniformly bounded in every closed subsector $\overline{\Delta}_{\delta'}$, $\delta' < \delta$, of Δ_δ (see [22, p. 61]).

Let $\Gamma = \partial\Omega_\Gamma$ be a closed path in the complex z-plane consisting of the two rays

$$S(\pm\phi) = \left\{\rho e^{\pm i\phi} : \gamma \leq \rho < \infty\right\}$$

and the circular arc $C = \left\{z : |z| = \gamma, |\arg z| \leq \phi\right\}$ (see Fig. 4) with ϕ such that

$$\Sigma(\mathcal{A}) \subset \Omega_\Gamma.$$

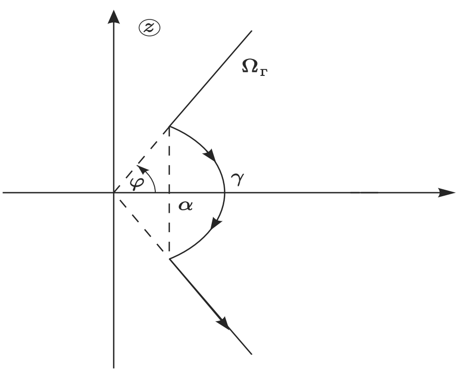

Fig. 5.1. The integration path for an unbounded operator $\mathcal{A}$

Let $w = |w|e^{i\psi} \in \overline{\Delta}_{\delta'}$ and $|\psi| \leq \delta'$. For any $\phi < \pi/2$, there exists a positive number $\delta'' = \delta''(\phi)$ such that $\delta'' < \phi$ and $\phi + \delta'' < \pi/2$. Using the representation of $e^{-w\mathscr{A}}$ by the Dunford-Cauchy integral along the path Γ, we conclude for $w \in \overline{\Delta}_{\delta''}$ that

$$\begin{aligned}
\|e^{-w\mathscr{A}}\| = \Bigg\| \frac{1}{2\pi i}\Bigg[&-\int_\gamma^\infty e^{-w\rho\exp(i\phi)}(\rho\exp(i\phi)-\mathscr{A})^{-1}d\rho \\
&-i\gamma\int_{-\phi}^{\phi} e^{-w\exp(i\gamma\theta)}e^{i\gamma\theta}(\gamma e^{i\gamma\theta}-\mathscr{A})^{-1}d\theta \\
&+\int_\gamma^\infty e^{-w\rho\exp(-i\phi)}(\rho e^{-i\phi}-\mathscr{A})^{-1}d\rho\Bigg]\Bigg\| \\
= \Bigg\| \frac{1}{2\pi i}\Bigg[&-\int_\gamma^\infty e^{-|w|\rho\exp(i(\phi+\psi))}(\rho\exp(i\phi)-\mathscr{A})^{-1}d\rho \\
&-i\gamma\int_{-\phi}^{\phi} e^{-|w|\exp(i\gamma(\theta+\psi))}e^{i\gamma\theta}(\gamma e^{i\gamma\theta}-\mathscr{A})^{-1}d\theta \\
&+\int_\gamma^\infty e^{-|w|\rho\exp(-i(\phi-\psi))}(\rho\exp(-i\phi)-\mathscr{A})^{-1}d\rho\Bigg]\Bigg\| \\
\leq c\Bigg[&\int_\gamma^\infty e^{-|w|\rho\cos(\phi+\delta'')}\frac{d\rho}{\rho}+\gamma\int_{-\phi}^{\phi} e^{-|w|\gamma\cos(\theta+\delta'')}\frac{d\theta}{\gamma}+\int_\gamma^\infty e^{-|w|\rho\cos\phi}\frac{d\rho}{\rho}\Bigg].
\end{aligned} \tag{5.2}$$

The function $f(\tau) = \tau e^{-\tau}$ is bounded on $[0, \infty)$ by a constant c yielding the estimate

$$\|e^{-w\mathscr{A}}\| \leq c\left[\frac{1}{|w|\cos(\phi+\delta'')}\int_\gamma^\infty \rho^{-2}d\rho + \frac{2\phi}{|w|\cos(\phi+\delta'')} + \frac{1}{|w|\cos\phi}\int_\gamma^\infty \rho^{-2}d\rho\right], \tag{5.3}$$

which we use for $|w|$ small enough. For $|w|$ large enough and for some positive $\epsilon_1 < \gamma$, we get

$$\begin{aligned}
\|e^{-w\mathscr{A}}\| &\leq c\left[\int_\gamma^\infty e^{-|w|(\rho-\epsilon_1+\epsilon_1)\cos(\phi+\delta'')}\frac{d\rho}{\rho}+\frac{2\phi}{|w|\cos(\phi+\delta'')}+\int_\gamma^\infty e^{-|w|(\rho-\epsilon_1+\epsilon_1)\cos\phi}\frac{d\rho}{\rho}\right] \\
&\leq c\Bigg[e^{-|w|\epsilon_1\cos(\phi+\delta'')}\int_\gamma^\infty e^{-|w|(\rho-\epsilon_1)\cos(\phi+\delta'')}\frac{d\rho}{\rho} \\
&\quad+\frac{2\phi}{|w|\cos(\phi+\delta'')}+e^{-|w|\epsilon_1\cos\phi}\int_\gamma^\infty e^{-|w|(\rho-\epsilon_1)\cos\phi}\frac{d\rho}{\rho}\Bigg] \\
&\leq ce^{-|w|\epsilon_1\cos(\phi+\delta'')}.
\end{aligned} \tag{5.4}$$

The estimates (5.3), (5.4) imply that there exists a constant c_0 independent of γ, ϕ and constants $c = c(\gamma, \phi) \leq \frac{c_0}{\gamma\cos(\phi+\delta'')}$, $\beta = \beta(\gamma, \phi) \leq \gamma\cos(\phi + \delta'')$ such that (5.3) holds for all $w \in \Delta_{\delta''}$. The condition $w \in \Delta_{\delta''}$ now implies

$$\|e^{-w\mathscr{A}}\| \leq c\frac{1}{1+|w|}e^{-\beta \Re e\, w}, \tag{5.5}$$

where $c \to \infty$, $\beta \to 0$ as $\gamma \to 0$ or $\phi \to \pi/2$.

The asymptotics in (5.5) ensure the existence of the integral in (5.1). Finally, the assertion follows from

$$\mathscr{A}\left(\int_0^\infty \exp(-t\mathscr{A})dt\right) = -\int_0^\infty \frac{\partial}{\partial t}\exp(-t\mathscr{A})dt = \exp(0) = I,$$

due to the main property of the continuous semigroup $\{e^{-t\mathscr{A}}\}_{t\geq 0}$. □

Remark 5.2: *In the case of a bounded operator $\mathscr{A}$, one can integrate in (5.2), e.g., along the closed path as in Fig. 5.2, and gets the estimate (5.5) with constants depending on γ, and the angle ϕ.*

Let $\mathscr{A} = \sum \mathscr{A}_j$ with commutative matrices (operators) $\mathscr{A}_j$ as above. Now, given M, we get $\alpha = 1$, $\beta = \max(1, \gamma\cos(\phi + \delta''))$ and h (cf. (3.8)) which define the following quadrature rule:

$$\mathscr{A}^{-1} = \int_0^\infty e^{-t\mathscr{A}}dt \approx h^{(2)} \sum_{k=-\beta M}^{M} \kappa_k^{(2)} e^{-z_k^{(2)}\mathscr{A}} = h^{(2)} \sum_{k=-\beta M}^{M} \kappa_k^{(2)} \prod_{j=1}^{d} e^{-z_k^{(2)}\mathscr{A}_j}$$

$$\approx h^{(2)} \sum_{k=-\beta M}^{M} \kappa_k^{(2)} \prod_{j=1}^{d} T_m^{(\ell(k))}(z_k^{(2)}; \mathscr{A}_j) := \mathscr{A}_r,$$

where, first, the quadrature (3.11) with $h^{(2)} = h^{(1)}$ given by (3.8) can be used in order to approximate the integral $\int_0^\infty e^{-t\mathscr{A}}dt$ and then $T_m^{(\ell(k))}(z_k^{(2)}; \mathscr{A}_j)$ represents each exponent $e^{-z_k^{(2)}\mathscr{A}_j}$ by Algorithm (4.9) for $\ell(k) = 3$ or by (35) for $\ell(k) = 2$, where $\ell(k)$ is defined by

$$\ell(k) = \begin{cases} 3 & \text{if } |z_k^{(2)}| \geq t_0 \\ 2 & \text{if } |z_k^{(2)}| < t_0 \end{cases} \qquad \text{for some } t_0 > 0\,, \tag{5.6}$$

and so we arrive at the desired product representation.

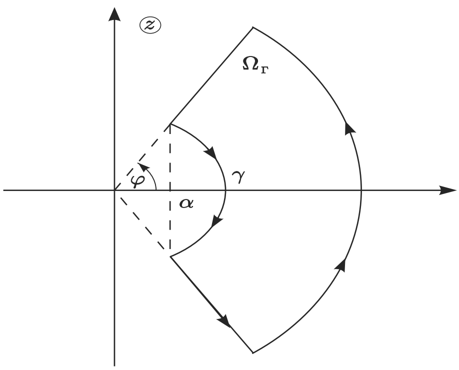

Fig. 5.2. The integration path for a bounded operator $\mathscr{A}$

Let $\beta = 1$, then the quadrature error to approximate the Laplace transform is $\mathcal{O}(e^{-s_1\sqrt{M}})$. Furthermore, the quadrature error of our representations to each individual exponential is $\mathcal{O}(e^{-s_2\sqrt{m}})$ for $\ell = 2$ and $\mathcal{O}(e^{-s_3 m/\log m})$ for $\ell = 3$ in the operator norm. Hence, with $r = 2M + 1$, we obtain

$$\|\mathcal{A}^{-1} - \mathcal{A}_r\| \leq C_1 e^{-s_1\sqrt{M}} + C_2 e^{-s_2\sqrt{m}} + C_3 e^{-s_3 m/\log m}.$$

Remark 5.3: *For the matrix arising in Example 4.5, $\mathcal{A} = A_h$, we obtain the following low Kronecker rank tensor-product approximation*

$$A_h^{-1} \approx h^{(2)} \sum_{k=-\beta M}^{M} \kappa_k^{(2)} \bigotimes_{j=1}^{d} T_m^{(\ell(k))}(z_k^{(2)}; V^j) := A_r \tag{5.7}$$

with $\ell(k)$ defined in (5.6). Here each low-dimensional component $T_m^{(\ell(k))}(z_k^{(2)}; V^j) \in \mathbb{R}^{n\times n}$ is a sum of $2m+1$ rank-1 $\mathcal{H}$-matrices via the weak admissible partitioning. Hence $T_m^{(\ell(k))}(z_k^{(2)}; V^j)$ is at most the rank-$(2m+1)$ $\mathcal{H}$-matrix and (5.7) is the desired HKT approximation to A_h^{-1}.

5.2. Numerics III

We give numerical examples that illustrate the accuracy of our quadrature rule for the integral (5.1) in the case of the Laplace operator in $\mathbb{R}^d$. We show the spectral norm of the matrix (see Example 4.5) that represents the approximation error for the quadrature $I_m^{(2)}$,

$$\delta := \left\| A_h^{-1} - h \sum_{k=-m}^{m} (1 + e^{-2kh}) \bigotimes_{j=1}^{d} e^{-z_k V^j} \right\|_2,$$

where the sum of Kronecker tensor-product terms is calculated with linear complexity $\mathcal{O}(dmW(n))$ with $W(n)$ being the cost to compute a matrix exponential in $\mathbb{R}^{n\times n}$. The main observation is that the rate of exponential convergence does not depend on the spatial dimension d and also the rate turns out to be nearly the same as that for the quadrature rules from above applied to the integrals of analytic functions (compare the tables in Sect. 4).

Approximation to $A_h^{-1} = \Delta_h^{-1}$ in $[0,1]^d$, with $N = n^d$, $n = 4$

m	4	9	16	25	36
$d = 1$	4.9_{10}-3	1.6_{10}-4	6.7_{10}-6	2.8_{10}-7	1.1_{10}-8
$d = 2$	6.2_{10}-3	2.9_{10}-4	1.2_{10}-5	4.3_{10}-7	2.4_{10}-8
$d = 3$	4.4_{10}-3	1.9_{10}-4	7.4_{10}-6	2.9_{10}-7	1.3_{10}-8
$d = 4$	4.2_{10}-3	1.8_{10}-4	7.9_{10}-6	3.3_{10}-7	1.4_{10}-8

Our calculations also show that the approximation error practically does not depend on the "one-dimensional" problem size n, which is also confirmed by our theory. The next table shows that with a fixed number of terms in the quadrature rule (we choose $m = 4$), we obtain the same accuracy δ for different values of the problem size n.

Approximation for Δ_h^{-1} in $[0,1]^d$, with $m = 4$, $d = 2$

n	4	8	16	32	64
δ	6.2 $_{10}$-3	7.3$_{10}$-3	7.4 $_{10}$-3	7.4 $_{10}$-3	7.6$_{10}$-3

5.3. Negative Fractional Powers of $\mathscr{A}$

Similar to the previous section, we can prove the following result.

Theorem 5.4: *Let $\mathscr{A}$ be a densely defined, strongly positive operator, then the following integral representation holds*

$$\mathscr{A}^{-\sigma-1} = \frac{1}{\Gamma(\sigma+1)} \int_0^\infty t^\sigma e^{-t\mathscr{A}} dt, \quad \sigma > -1.$$

Moreover, let $A_h = \sum A_j$ with commutative matrices A_j as in Example 4.5. Define $\ell(k)$ as in (5.6), then the following Kronecker tensor-product approximation obtained by combining the three quadrature algorithms from above,

$$A_h^{-\sigma-1} \approx h^{(2)} \sum_{k=-M}^{M} \kappa_k^{(2)} (z_k^{(2)})^\sigma \bigotimes\nolimits_{j=1}^d T_m^{(\ell(k))}(z_k^{(2)}; V^j) := A_r \qquad (r = 2M+1),$$

has an error estimate

$$\|A_h^{-\sigma-1} - A_r\| \le C_1 e^{-s_1\sqrt{M}} + C_2 e^{-s_2\sqrt{m}} + C_3 e^{-s_3 m/\log m}.$$

Proof: Analogously to the previous section, the integrand $I_\sigma(t) = t^\sigma e^{-t\mathscr{A}}$ can be analytically extended into the sector $\Delta_\delta = \{z : |\arg(z)| < \delta\}$ and $\|I_\sigma(z)\|$ is uniformly bounded in every closed subsector $\overline{\Delta}_{\delta'}$, $\delta' < \delta$, of Δ_δ. Thus, given M, we get $\alpha = 1$, $\beta = \max(1, \gamma \cos(\phi + \delta''))$ and h (see (3.8)) and obtain the representation

$$A_h^{-\sigma-1} = \int_0^\infty t^\sigma e^{-tA_h} dt \approx h^{(2)} \sum_{k=-\beta M}^{M} \kappa_k^{(2)} (z_k^{(2)})^\sigma e^{-z_k^{(2)} A_h} = h^{(2)} \sum_{k=-\beta M}^{M} \kappa_k^{(2)} (z_k^{(2)})^\sigma \bigotimes\nolimits_{j=1}^d e^{-z_k V^j}$$

$$\approx h^{(2)} \sum_{k=-\beta M}^{M} \kappa_k^{(2)} (z_k^{(2)})^\sigma \bigotimes\nolimits_{j=1}^d T_m^{(\ell(k))}(z_k^{(2)}; V^j)$$

(see (3.11)) with an error $\mathcal{O}(e^{-s_1\sqrt{M}})$ for the external quadrature. Now, we can represent each $e^{-z_k V^j}$ by the algorithms (4.9) or (4.6) with an error $\mathcal{O}(e^{-s_2\sqrt{m}})$ for $\ell = 2$ and $\mathcal{O}(e^{-s_3 m/\log m})$ for $\ell = 3$ in the operator norm, which leads to the desired HKT (tensor) representation of $A_h^{-\sigma-1}$. $\square$

We note that the case $A_h^{-1/2}$ plays the important role for the interface preconditioning in FEM and BEM applications.

5.4. A HKT Representation to the Lyapunov-Sylvester Solution Operator

As an example we consider the matrix Sylvester equation

$$AX + XB = G$$

with the solution given by the integral

$$\mathscr{F}(G; A, B) = \int_0^\infty e^{-tA} G e^{-tB} dt, \tag{5.8}$$

(see, e.g. [8]), where we suppose that A, B provide the existence of this integral (for example, that A, B are strongly positive and G is bounded). A particular case is the Lyapunov equation

$$AX + XA = G$$

with the solution

$$\mathscr{F}(G; A) = \int_0^\infty e^{-tA^\top} G e^{-tA} dt$$

generated by a discrete elliptic operator A.

Analogously as above for A being strongly positive, the semigroup $\{e^{-tA}\}_{t\geq 0}$ can be extended to an analytic semigroup in the sector

$$\Delta_{\delta_A} = \{w : |\arg(w)| < \delta_A\}$$

of the complex w-plane and $\|e^{-wA}\|$ is uniformly bounded in every closed subsector $\overline{\Delta}_{\delta'_A}$, $\delta'_A < \delta_A$, of Δ_{δ_A}. Let $\Gamma_A = \partial\Omega_\Gamma$ be a closed path in the complex z-plane consisting of the two rays

$$S_A(\pm\varphi_A) = \left\{\varrho e^{\pm i\varphi_A} : \gamma_A \leq \varrho < \infty\right\}$$

and the circular arc $C = \left\{z : |z| = \gamma_A, |\arg z| \leq \varphi_A\right\}$ with φ_A such that

$$\sigma(A) \subset \Omega_{\Gamma_A}.$$

Let $w = |w|e^{i\psi} \in \overline{\Delta}_{\delta'_A}$ and $|\psi| \leq \delta'_A$. Since $\phi_A < \pi/2$, there exists a positive number $\delta''_A = \delta''_A(\phi_A)$ such that $\delta''_A < \phi_A$ and $\phi_A + \delta''_A < \pi/2$. Using the representation of e^{-wA} by the Dunford-Cauchy integral along the path Γ_A, analogously as above we get the estimate

$$\|e^{-wA}\| \leq c_A \frac{1}{1+|w|} e^{-\beta_A \Re e\, w}$$

for all $w \in \Delta_{\delta''}$, where $c_A = c_A(\gamma_A, \phi_A) \leq \frac{c_{0,A}}{\gamma_A \cos(\phi_A + \delta''_A)}$, $\beta_A = \beta_A(\gamma_A, \phi_A) \leq \gamma_A \cos(\phi_A + \delta''_A)$, the constant c_0 is independent of γ_A, ϕ_A and $c_A \to \infty$, $\beta_A \to 0$ as $\gamma_A \to 0$ or $\phi_A \to \pi/2$.

Similarly, one defines the constants $\delta_B, \delta'_B, \delta''_B, \gamma_B, \phi_B, c_B, \beta_B$ and gets the estimate

$$\|e^{-wB}\| \le c_B \frac{1}{1+|w|} e^{-\beta_B \Re e\, w}$$

for all $w \in \Delta_{\delta''_B}$. Thus, in the smallest of the two sectors $\Delta_{\delta''_A}, \Delta_{\delta''_B}$ we have

$$\|e^{-wA} G e^{-wB}\| \le c_A c_B \frac{1}{1+|w|} e^{-(\beta_A+\beta_B)\Re e\, w},$$

which provides the representation (5.8). Moreover we can use the quadrature (3.11) in order to approximate the integral $\int_0^\infty e^{-tA} G e^{-tB} dt$ and then again one of the quadratures (3.11) or (3.17) in order to approximate the split operator exponentials:

$$\begin{aligned} \mathscr{F}(G; A, B) &= \int_0^\infty e^{-tA} G e^{-tB} dt \approx h^{(2)} \sum_{k=-M}^{M} \kappa_k^{(2)} e^{-z_k^{(2)} A} G e^{-z_k^{(2)} B} \\ &= h^{(2)} \sum_{k=-M}^{M} \kappa_k^{(2)} \left(\prod_{j=1}^{d} e^{-z_k^{(2)} A_j} \right) G \left(\prod_{j=1}^{d} e^{-z_k^{(2)} B_j} \right) \\ &\approx h^{(2)} \sum_{k=-M}^{M} \kappa_k^{(2)} \left(\prod_{j=1}^{d} T_m^{(\ell(k))}(z_k^{(2)}; A_j) \right) G \left(\prod_{j=1}^{d} T_m^{(\ell(k))}(z_k^{(2)}; B_j) \right), \end{aligned} \tag{5.9}$$

where $T_m^{(\ell(k))}(z_k^{(2)}; A_j)$, $T_m^{(\ell(k))}(z_k^{(2)}; B_j)$, for various $\ell(k) = 2, 3$ denote one of the algorithms (4.9), (4.6). The accuracy of the product approximation (5.9) is bounded by the error $\mathcal{O}(e^{-s\sqrt{M}})$ for external integral, while for internal quadratures we have the error $\mathcal{O}(e^{-s_2\sqrt{m}})$ for $\ell = 2$ and $\mathcal{O}(e^{-s_3 m/\log m})$ for $\ell = 3$, respectively, in the operator norm. Now, we can summarize our considerations in the following assertion.

Theorem 5.5: *Let A and B be strongly positive matrices, then the following integral representation*

$$\mathscr{F}(G; A, B) = \int_0^\infty e^{-tA} G e^{-tB} dt$$

holds. Moreover, let $A = A_1 + \ldots + A_d, B = B_1 + \ldots + B_d$ and let $\{A_j\}, \{B_j\}$ be commutative sets of matrices (but A_j must not necessarily commute with B_l), then the tensor-product approximation

$$\mathscr{F}(G; A, B) \approx h^{(2)} \sum_{k=-M}^{M} \kappa_k^{(2)} \left(\prod_{j=1}^{d} T_m^{(\ell(k))}(z_k^{(2)}; A_j) \right) G \left(\prod_{j=1}^{d} T_m^{(\ell(k))}(z_k^{(2)}; B_j) \right) := A_r$$

with $\ell(k)$ defined by (5.6) allows an error bound

$$\|\mathscr{F}(G;A,B)-A_r\|\leq C_1e^{-s_1\sqrt{M}}+C_2e^{-s_2\sqrt{m}}+C_3e^{-s_3m/\log m}$$

in the operator norm.

The statement similar to Remark 5.3 remains true.

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