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APPROXIMATIONS OF THE MITTAG-LEFFLER OPERATOR FUNCTION WITH EXPONENTIAL ACCURACY AND THEIR APPLICATION TO SOLVING EVOLUTION EQUATIONS WITH FRACTIONAL DERIVATIVE IN TIME

НАБЛИЖЕННЯ ОПЕРАТОРНОЇ ФУНКЦІЇ МІТТАГ-ЛЕФФЛЕРА З ЕКСПОНЕНЦІАЛЬНОЮ ТОЧНІСТЮ ТА ЇХ ЗАСТОСУВАННЯ ДО РОЗВ'ЯЗУВАННЯ ЕВОЛЮЦІЙНИХ РІВНЯНЬ З ДРОБОВОЮ ПОХІДНОЮ ЗА ЧАСОМ

In the present paper, we propose and analyse an efficient discretization of the Mittag-Leffler operator function $E_{1+\alpha}(-At^{1+\alpha}) = \sum_{k=0}^{\infty} \dfrac{(-At^{1+\alpha})^k}{\Gamma(1+k(1+\alpha))}$, where A is a self-adjoint positive definite operator. This function possesses a broad field of applications; for example, it presents a solution operator to the evolution problem $\partial_t u + \partial_t^{-\alpha} Au = 0,\ t > 0,$ $u(0) = u_0,$ that includes a spatial operator A and its fractional time-derivative of the order α (in the Riemann – Liouville sense), i.e., $u(t) = E_{1+\alpha}(-At^{1+\alpha})u_0$. We apply the Cayley transform method that allows us to recursively separate the variables and represent the Mittag-Leffler function in the form of an infinite series of products of the Laguerre – Cayley functions in time variable (i.e., polynomials in $t^{1+\alpha}$) and of powers of the Cayley transform of the spatial operator. The approximate representation is the truncated series with N terms. We estimate the precision of the N-term approximation scheme depending on α and N.

Запропоновано та проаналізовано ефективну дискретизацію операторної функції Міттаг-Леффлера $E_{1+\alpha}(-At^{1+\alpha}) = \sum_{k=0}^{\infty} \dfrac{(-At^{1+\alpha})^k}{\Gamma(1+k(1+\alpha))}$, де A — самоспряжений додатно визначений оператор. Ця функція має багато застосувань. Наприклад, вона дає операторний розв'язок еволюційної задачі $\partial_t u + \partial_t^{-\alpha} Au = 0,\ t > 0,$ $u(0) = u_0,$ з просторовим оператором A та його дробовими похідними порядку α за часом (у сенсі Рімана – Ліувілля), тобто $u(t) = E_{1+\alpha}\left(-At^{1+\alpha}\right)u_0$. Використано метод перетворень Келі, який дозволяє рекурсивно відокремити змінні та подати функцію Міттаг-Леффлера у вигляді нескінченного ряду добутків функцій Лагерра – Келі щодо змінної часу (тобто поліномів від $t^{1+\alpha}$) та степенів перетворень Келі просторового оператора. Наближення задається скінченним відрізком ряду, що складається з N доданків. Вивчено точність цього наближення в залежності від α та N.

1. Introduction. During the last two decades the Mittag-Lefler function has come into prominence after about nine decades of its discovery in 1902 by the Swedish Mathematician Gösta Mittag-Leffler, due to its success in many areas of science and engineering (see, e.g., [8, 18, 20] and the literature therein). The (classical) Mittag-Leffler function has been introduced as a power series to give an answer to a classical question of complex analysis, namely, to describe the procedure of analytic continuation of power series outside the disc of their convergence.

The importance of the Mittag-Leffler function was re-discovered when its connection to fractional calculus was fully understood. This function has its applications amongst other things in solving the problems of physical, biological, engineering, earth and other sciences. Novadays there exist many modifications of the Mittag-Leffler function in the literature but the literature about methods to compute the Mittag-Leffler function is rather rare. We mention [23], where the algorithms using the Taylor series, the exponentially improved asymptotic series, and integral representations to obtain optimal stability are discussed. Articles about the Mittag-Leffler functions that depend on an operator are unknown to us.

One of the important and prominent applications of the Mittag-Leffler function is the representation of the solutions of the fractional differential equations. Diffusion is one of the most prominent transport mechanisms found in nature. The classical diffusion model $\partial_t u - Au = f$, which employs a first-order derivative $\partial_t u$ in time and the Laplace operator $Au = -\Delta u$ in space, is based on the assumption that the particle motion is Brownian. One of the distinct features of Brownian motion is a linear growth of the mean squared particle displacement with the time t. Over the last few decades, a long list of experimental studies indicates that the Brownian motion assumption may not be adequate for accurately describing some physical processes, and the mean squared displacement can grow either sublinearly or superlinearly with time t, which are known as subdiffusion and superdiffusion, respectively, in the literature (see, e.g., [22]). These experimental studies cover an extremely broad and diverse range of important practical applications in engineering, physics, biology and finance, including electron transport in Xerox photocopier, visco-elastic materials, thermal diffusion in fractal domains, column experiments and protein transport in cell membrane etc. The original equation connects the fractional derivative of the unknown function in time with a spatial operator A. The input data of a problem and the output ones (the solution) are connected through the so called solution operator $E_{1+\alpha}\left(-At^{1+\alpha}\right)$ which maps the input into output. The connection between a fractional derivative and fractional powers of operators was studied, e.g., in [3]. An algorithmical representation of fractional powers of a positive operator A was proposed in [11].

In the present paper we consider a Mittag-Leffler function depending on a self-adjoint positive definite operator and construct an efficient approximation for it.

The extensive literature is dedicated to various discretization methods for mathematical models using the Mittag-Leffler functions explicitely or implicitely (see, e.g., [19]). The drawback of some discretizations, e.g., from [19], is that the constants in accuracy estimates depend exponentially on t. In [9, 10, 15] the solution operator, which is the operator exponential and the exact solution of the heat conduction equation in abstract setting was represented by a series using the Laguerre orthogonal polynomials of t and the Cayley transform of the spatial operator A (the separation of variables). It was shown that the truncated series with N terms converges exponentially in N in the case of analytical input data and polynomially in N in the case of input data which belong to the domain of a power of A. Exponential convergence of approximations to operator valued functions and the differential equations with unbounded operator coefficients plays a crucial role to obtain algorithms of optimal or near optimal complexity [12, 13]. Note, that the Cayley transform can be used as a time discretization scheme (see, e.g., [17] and the literature therein).

The present paper continues the series of works mentioned above. We propose a discretization of the operator Mittag-Leffler function which is interesting in itself and, besides, represents the solution operator of the PDE like to the heat conduction equation with the fractional time derivative and with an abstract operator coefficient A in the "spatial part" of the equation. We propose a representation of the Mittag-Leffler function as a series with products of the Laguerre – Cayley functions of t and of powers of the Cayley transform of A. A similar technique for the operator exponential with the Laguerre polynomials in t was used in [2, 4]. That is the motivation to call these functions as the Laguerre – Cayley functionss. Some formal results are inspired by experimentation, conjectures suggested by experiments and data supporting.

2. The operator-valued functions as the solution operators of differential problems. The solution operator of a differential problem maps the input data on the problem solution. For example, in the case of the initial value problem

$$u'(t) + Au = 0, \qquad u(0) = u_0 \tag{2.1}$$

with an operator coefficient A in a Hilbert space and the input data u_0 the solution operator is the operator exponential $S = S(t, A) = e^{-At}$, so that $u(t) = S(t, A)u_0$.

The next example deals with the problem

$$\begin{gathered} {}_tD^{\alpha+1}_{\infty} u(t) + Au(t) = 0, \qquad t \in (0, \infty), \quad \alpha \in (-1, 1), \\ u(0) = u_0, \end{gathered} \tag{2.2}$$

where ${}_tD^{1+\alpha}_{\infty}$ is the (right) Riemann – Liouville derivative given by

$${}_tD^{\nu}_{\infty} f(t) = \begin{cases} \dfrac{1}{\Gamma(-\nu)} \displaystyle\int_t^{\infty} (s - t)^{-\nu-1} f(s) ds, & \nu < 0, \\ \dfrac{1}{\Gamma\big(1 - \{\nu\}\big)} \left(-\dfrac{d}{dt}\right)^{[\nu]+1} \displaystyle\int_t^{\infty} \dfrac{f(s)}{(s - t)^{\{\nu\}}} ds, & \nu \geq 0, \end{cases} \tag{2.3}$$

A is a strongly positive operator with a dense domain $D(A)$ in a Banach space X. Its spectrum lies in the sector $\Sigma(A)$

$$\Sigma(A) = \left\{ z = a_0 + re^{i\theta} : a_0 > 0,\, r \in [0, \infty),\, |\theta| < \varphi < \frac{\pi}{2} \right\}$$

and on its boundary Γ_{Σ} and outside of it the estimate

$$\big\| (zI - A)^{-1} \big\| \leq \frac{M}{1 + |z|}$$

is valid with some constant M. It was shown in [16] that under the assumptions

$$\begin{gathered} \lim_{s \to \infty} \big[(s - t)^{\alpha+1} {}_sD^{\alpha}_{\infty} u(s) \big] = 0, \\ \lim_{s \to \infty} \big[(s - t)^{\alpha} {}_sD^{\alpha-1}_{\infty} u(s) \big] = 0, \end{gathered} \tag{2.4}$$

the solution is presented by

$$u(t) = \exp\big(- A^{1/(1+\alpha)} t \big) u(0), \tag{2.5}$$

i.e., the solution operator is given by

$$S(t, A) = \exp\big(- A^{1/(1+\alpha)} t \big). \tag{2.6}$$

This formula is obtained by applying of the operator (2.3) to the equation (2.2) with taking into account (2.4). As consequence we obtain the equation

$$-u(t) + A\, {}_tD_{\infty}^{-(\alpha+1)}u(t) = 0, \qquad t \in (0,\infty), \quad \alpha \in (-1,1),$$

which coindcides with the Hardy – Titchmarsh integral equation [21] (with change α to $\alpha+1$). Thus, its solution can be represented by (2.5).

Further, we consider the example of the following abstract initial value problem [19]:

$$\partial_t u + \partial_t^{-\alpha} A u = f(t), \quad t > 0,$$

$$u(0) = u_0,$$

where $\partial_t = \dfrac{\partial}{\partial t}$,

$$\partial_t^{-\alpha} u = \begin{cases} \partial_t \displaystyle\int_0^t \frac{(t-s)^{\alpha}}{\Gamma(1+\alpha)} u(s)ds, & -1 < \alpha \le 0, \\ \displaystyle\int_0^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)} u(s)ds, & 0 < \alpha < 1, \end{cases}$$

is the fractional order time-derivative $(\alpha < 0)$ or integral $(\alpha > 0)$ in the Riemann – Liouville sense.

The solution operator $S(t, A)$ of this problem can be represented through the operator Mittag-Leffler function as [19]

$$S(t,A) = E_{1+\alpha}(-At^{1+\alpha}) = \sum_{k=0}^{\infty} \frac{(-At^{1+\alpha})^k}{\Gamma\big(1 + k(1+\alpha)\big)}$$

and its solution in the form

$$u(t) = E_{1+\alpha}(-At^{1+\alpha})u_0 + \int\limits_0^t E_{1+\alpha}(-As^{1+\alpha}) f(t-s)ds.$$

For particular values of α one can obtain the closed explicit representations of the Mittag-Leffler function. For example, for $\alpha = 0$ we have

$$E_1(-At) = e^{-At}.$$

In the case $\alpha = -0.5$ this function can be expressed in terms of the complementary error function

$$E_{1/2}(-A\sqrt{t}) = e^{A^2 t}\operatorname{erfc}(A\sqrt{t}).$$

The substitution $s = ty^2$ in the formula above yields then the representation [19]

$$u(t) = E_{1/2}(-A\sqrt{t}) + \int\limits_0^1 E_{1/2}(-A\sqrt{ty}) f(t - ty^2) 2ty dy.$$

3. The solution operator and the Cayley transform. The Cayley transform of unbounded operators allows one to switch from the study of solution operator as a function of an unbounded operator coefficient to a function (series) of some bounded operators and then to use an appropriate approximation (e.g., an interpolation formula, a quadrature rule etc.) with a high accuracy.

This idea can be also used to “separate the variables” and in this way to obtain algorithms of low complexity. In the case when the “spatial” operator involved is of the form $B = B_1 + B_2 + \ldots + B_d$ one can separate the „spatial” operators $B_1, B_2, \ldots, B_d$ via the tensor product and so arrive at a fully separated approximation with a linear dependence on the problem dimension d [12]. Concerning the time-dependent problems the Cayley transform allows to switch from “continuous time” to the discrete one [2] as well as to separate the time variable from the spatial ones [2, 4].

In the theory of operators in Hilbert space the Cayley transform $T_{\gamma,\delta}^{\alpha,\beta} = (\alpha I + \beta A)(\gamma I - \delta A)^{-1}$, $\alpha, \beta, \gamma, \delta \in \mathbb{C}$ is frequently used to switch from the study of closed but in general unbounded linear operator A with the dense domain $D(A)(\overline{D}(A) = H)$ to that of the bounded operators $T_{\gamma,\delta}^{\alpha,\beta}$ (see, e.g., [1], where the transform $T_\gamma = (\gamma I + A)(\gamma I - A)^{-1}$, $\gamma = -i$ converts a self-adjoint (symmetric, dissipative) operator A into unitary (respectively, isometric, contractive) operator T_γ).

In [2, 4] the Cayley transform has been used to obtain explicit and constructive representations of the solution operator and of solutions of various evolution differential equations with operator coefficients where, in fact, the solution with continuous time parameter where represented through the ones with discrete time. In [11, 14] the Cayley transform has been used to obtain explicit representation of some important operator equations, e.g., the Lyapunov equation, the equation defining fractional powers of an operator etc. A further important feature of these representation is the fact that they serve as the basis for algorithms without accuracy saturation, i.e., their accuracy increases automatically and unboundedly together with the smoothness of the input data. In the case of analytical input data the convergence rate becomes exponential.

In [10] the idea was applied to the Schrödinger differential equation in abstract setting with a strongly positive “spatial” operator coefficient B in some Banach space (the spectral set of such operator coefficient lies in some angle in the right half-plane and the resolvent possesses a prescribed behavior at the infinity). On the basis of an exact representation of the solution with use of the Cayley transform, an approximation was proposed with the accuracy depending on the smoothness of this solution. It was shown that for the analytical initial vectors this approximation possesses a super exponential convergence rate. These ideas together with special tensor-product representation were developed in [12] for multidimensional (d-dimensional) abstract differential equations in order to obtain algorithms with linear in d complexity.

In the case when A is a self-adjoint positive definite unbounded operator with the spectrum $\Sigma = \Sigma(A) \in [\lambda_0, \infty)$, $\lambda_0 > 0$, in a Hilbert space H the solution operator for (2.1) can be represented by the Stieltjes integral

$$S(t; A) = \int_{\lambda_0}^{\infty} e^{-t\lambda} dE_\lambda,$$

where E_λ is the resolution of the identity for A.

We say that the solution operator is generated by the function $F(t, \lambda) = e^{-t\lambda}$ and by the operator A. Analogously one can define the so called Schrödinger operator exponential $S(t) = e^{iBt}$ as the solution operator for the Schrödinger equation which can be represented by the corresponding Stieltjes integral too.

In the case when B is a self-adjoint positive definite operator with the spectrum $\Sigma = \Sigma(B) \in \in [\lambda_0, \infty)$, $\lambda_0 > 0$, in a Hilbert space H an arbitrary solution operator generated by B and by a function $F(t,\lambda)$ can be represented by the Stieltjes integral

$$F(t,B) = \int_{\lambda_0}^{\infty} F(t,\lambda) dE_\lambda,$$

where E_λ is the resolution of the identity for B.

One can separate the variable t from the operator B by the separation of the variables t and λ in the function $F(t,\lambda)$.

If B is an unbounded operator, then the more general idea to switch to the study of bounded operators is the following.

We can use some rational transform $\eta = C(w) = \dfrac{\lambda\alpha - \beta w}{-\lambda + w}$, $w = \lambda\dfrac{\alpha+\eta}{\beta+\eta} = \dfrac{a+b\eta}{c+d\eta}$, $a/c \neq \neq b/d$, $\lambda = b/d$, $\alpha = a/b$, $\beta = c/d$, $\alpha \neq \beta$, where the variable w can remain in some bounded domain. The function $F(t,\eta) = F(t, C(w)) = F\Big(t, \dfrac{\lambda\alpha - \beta w}{-\lambda + w}\Big)$ can be represented as a power series in w or approximated by a polynomial of w and we obtain a function of the bounded variable w.

If $F(t,z)$ is analytical with respect to z in the unit disc $|z| < 1$, then the Taylor expansion

$$F(t,z) = \sum_{n=0}^{\infty} c_n(t) z^n, \quad |z| < 1,$$

separates the both variables. The Taylor coefficients are given by

$$c_n(t) = \frac{1}{n!} F_z^{(n)}(t,z)\big|_{t=0} = \frac{1}{2\pi i} \int_{|\xi|=\rho} \frac{F(t,z)}{\xi^{n+1}} d\xi.$$

The next example shows the use of the Cayley transform for the representation of the operator exponential (the solution operator for the heat and the Schrödinger equations).

***Example* 3.1.** Let $F(t,z) = F(t,z;\alpha) = (1-z)^{-\alpha-1} e^{\frac{tz}{z-1}}$, where for not integer parameter α we mean the principal value [24]. This is the generating function for the Laguerre polynomials $L_n^{(\alpha)}(t)$. For each fixed t the function $F(t,z)$ is analytic in the disc $|z| < 1$. We have for its Taylor coefficients

$$c_n(t) = c_n(t;\alpha) = \frac{1}{2\pi i} \int_{|\xi|=\rho} (1-\xi)^{-\alpha-1} e^{\frac{t\xi}{\xi-1}} \xi^{-n-1} d\xi, \quad 0 < \rho < 1.$$

We change the variables by

$$u = \frac{t}{1-\xi}, \qquad \xi = 1 - \frac{t}{u}, \qquad d\xi = \frac{t}{u^2} du,$$

where the linear-fractional mapping $u = \dfrac{t}{1-\xi}$ translates the circle $|\xi| = \rho < 1$ into a circle Γ which includes the point $t > 0$ but does not include the point 0. Then we get

$$c_n(t) = c_n(t;\alpha) = \frac{1}{2\pi i}\int\limits_\Gamma \left(\frac{u}{t}\right)^{\alpha+1} e^{t-u}\left(\frac{u-t}{u}\right)^{-n-1}\frac{t}{u^2}du =$$

$$= t^{-\alpha}e^t\frac{1}{2\pi i}\int\limits_\Gamma \frac{u^{\alpha+n}e^{-u}}{(u-t)^{n+1}}du = t^{-\alpha}e^t\frac{1}{n!}\big(t^{\alpha+n}e^{-t}\big)^{(n)}.$$

Comparing this equality with the Rodrigue's formula for the Laguerre polynomials we see that $c_n(t) = c_n(t;\alpha) = L_n^{(\alpha)}(t)$, i.e., we have the expansion (see also [5], Ch. 10.12)

$$(1-z)^{-\alpha-1}e^{\frac{tz}{z-1}} = \sum_{n=0}^{\infty} L_n^{(\alpha)}(t)z^n.$$

Replacing formally $\dfrac{z}{z-1}$ by A we obtain the following representation for the operator exponential e^{-At}, generated by the unbounded operator A:

$$e^{-At} = (E-A)^{-\alpha-1}\sum_{n=0}^{\infty} L_n^{(\alpha)}(t)\big[A(A+E)^{-1}\big]^n.$$

Analogously after the substitution $z \to iB(iB-I)^{-1}$ we have formally for the solution operator

$$e^{iBt} = -(iB-I)^{-1}\sum_{n=0}^{\infty} L_n^{(0)}(t)T^n,$$

of the abstract Schrödinger equation

$$u'(t) - iBu = 0, \qquad u(0) = u_0,$$

where $T = T(B) = iB(iB-I)^{-1}$ is the Cayley transform of the operator B. It was shown in [10] that truncated series with N summands converge exponentially in N provided that they are applied to an analytical vector and, thus, represent exponentially convergent algorithms for the corresponding problems.

An another option for constructing a fractional rational representation of operators is to interpolate the function $\tilde{F}(t,z) = F(t,w) = F\left(t, \dfrac{a+bz}{c+dz}\right)$ by a polynomial $\mathcal{I}_N\tilde{F}(t,z)$ on the Chebyshev, Chebyshev – Radou or Chebyshev – Gauss – Lobatto nodes (see, e.g., [13]), i.e., $F(t,w) = F\left(t, \dfrac{a+bz}{c+dz}\right) = \mathcal{I}_N(t,z) + R_N(t,z)$, $z \in (-1,1)$, with the reminder $R_N(t,z)$. Then the operator $F(t,B)$ can be represented by

$$F(t,B) = \mathcal{I}_N\big(t, C(B)\big) + R_N\big(t, C(B)\big),$$

where $C(B) = (\lambda\alpha - \beta B)(-\lambda + B)^{-1}$ is the Cayley transform of B. The corresponding exponentially accurate approximations of such solution operators, e.g., of the operator exponential or the Schrödinger operator exponential were proposed and justified in [10].

4. The Mittag-Leffler operator valued function and the Laguerre–Cayley functions. We consider the Mittag-Leffler operator function, generating by an operator A:

$$E_{1+\alpha}\left(-At^{1+\alpha}\right) = \sum_{j=0}^{\infty}\left(-At^{1+\alpha}\right)^j \frac{1}{\Gamma\big(1+j(\alpha+1)\big)}.$$

We replace here $A = q(I-q)^{-1}$ with the identity operator I and some operator q and then develop the Mittag-Leffler operator function into a McLaurin series

$$E_{1+\alpha}\big(-q(I-q)^{-1}t^{1+\alpha}\big) = \sum_{j=0}^{\infty}\big(-q(I-q)^{-1}t^{1+\alpha}\big)^j \frac{1}{\Gamma\big(1+j(\alpha+1)\big)} = \sum_{j=0}^{\infty} q^j p_j^{\alpha}(t^{1+\alpha}), \tag{4.1}$$

$$p_j^{\alpha}(t^{1+\alpha}) = \frac{1}{j!}\frac{\partial^j}{\partial q^j}\, E_{1+\alpha}\big(-q(I-q)^{-1}t^{1+\alpha}\big)\big|_{q=0},$$

and call the functions

$$p_j^{\alpha}(t^{1+\alpha}) = \frac{1}{j!}\frac{\partial^j}{\partial x^j}\, E_{1+\alpha}\big(-x(1-x)^{-1}t^{1+\alpha}\big)\big|_{x=0}$$

the Laguerre–Cayley functions. From this definition we obtain the following explicit representation of these functions:

$$p_k^{\alpha}(t^{1+\alpha}) = p^{-,\alpha}_{k}(t^{1+\alpha}) + p^{+,\alpha}_{k}(t^{1+\alpha}) = \sum_{s=0}^{k-1} C_{k-1}^{s}\frac{(-1)^{s+1}t^{(s+1)(1+\alpha)}}{\Gamma\big(1+(\alpha+1)(s+1)\big)},$$

$$p^{-,\alpha}_{k}(t^{1+\alpha}) = -\sum_{s=1}^{\left[\frac{k+1}{2}\right]} C_{k-1}^{2s-2}\frac{t^{(2s-1)(1+\alpha)}}{\Gamma\big(2s+(2s-1)\alpha\big)}, \tag{4.2}$$

$$p^{+,\alpha}_{k}(t^{1+\alpha}) = \sum_{s=1}^{\left[\frac{k}{2}\right]} C_{k-1}^{2s-1}\frac{t^{2s(1+\alpha)}}{\Gamma(2s+1+2s\alpha)}.$$

Lemma 4.1. *For the Laguerre–Cayley functions the formula* (4.2) *is valid iff*

$$p_{k+1}^{\alpha}(t^{1+\alpha}) = p_k^{\alpha}(t^{1+\alpha}) - \frac{1}{\Gamma(\alpha+1)}\int_0^t (t-s)^{\alpha}p_k^{\alpha}(s^{1+\alpha})ds, \qquad \alpha\in(-1,1), \quad k=1,2,\ldots, \tag{4.3}$$

$$p_k^{\alpha}(t^{1+\alpha}) = -\frac{t^{1+\alpha}}{\Gamma(\alpha+2)}.$$

Proof. Let (4.2) holds true, then using the relation

$$\frac{1}{\Gamma(\alpha+1)}\int_0^t (t-s)^{\alpha}s^{k(1+\alpha)}ds = \frac{t^{k(1+\alpha)+\alpha+1}}{\Gamma(\alpha+1)}\int_0^1 (1-s)^{\alpha}s^{k(1+\alpha)}ds =$$

$$= \frac{t^{(k+1)(1+\alpha)}\Gamma(k\alpha+k+1)}{\Gamma\big((k+1)\alpha+k+2\big)}$$

one can see that the both parts of (4.3) are equal.

The sufficiency of (4.3) can be proven by induction.

Lemma is proved.

Let us introduce the generating function

$$f^{\alpha}(q,t)=\sum_{k=0}^{\infty} q^k p_k^{\alpha}(t^{1+\alpha}), \qquad p_0^{\alpha}(t^{1+\alpha})=1.$$

Multiplying the both parts of (4.3) by z^k and summing over k from 0 to ∞, we come to the integral equation

$$(1-q)f^{(\alpha)}(q,t)+\frac{z}{\Gamma(1+\alpha)}\int\limits_0^t (t-s)^{\alpha} f^{(\alpha)}(q,s)ds=1.$$

Using the Laplace transform one can obtain the explicite solutions of this integral equation. In particular, for $\alpha=-1/2,\ 0,\ 1/2,\ 1,$ we obtain

$$f^{(-1/2)}(q,t)=e^{q^2t/(1-q)^2}\left[\operatorname{erf}\left(-\frac{q\sqrt{t}}{1-q}\right)+1\right], \qquad f^{(0)}(q,t)=e^{\frac{qt}{q-1}},$$

$$f^{(1)}(q,t)=\cos\left(t\sqrt{\frac{q}{1-q}}\right),$$

$$f^{(1/2)}(q,t)=\frac{1}{3\sqrt{\pi}(-1+q)}\left[4q\,t^{3/2}\text{hypergeom}\left([1],\left[\frac{5}{6},\frac{7}{6},\frac{9}{6}\right],\frac{q^2t^3}{27(-1+q)^2}\right)+\right.$$

$$\left.+\sqrt{\pi}(-1+q)2\exp\left(-\frac{q^{2/3}t}{2(-1+q)^{2/3}}\right)\cos\left(\frac{\sqrt{3}q^{2/3}t}{2(-1+q)^{2/3}}\right)-\sqrt{\pi}\exp\left(\frac{q^{2/3}t}{(-1+q)^{2/3}}\right)\right].$$

More simple way to obtain solutions for different α is the use of the left part of formula (4.1).

The following proposition holds true.

Proposition 4.1. *It holds*

$$\frac{1}{k!}\sum_{s=k}^{\infty} p_s^{\alpha}(1)\frac{k!}{(k-s)!}=(-1)^k\sum_{s=0}^{k-1}\frac{(-1)^s C_{k-1}^s}{\Gamma\big(-\alpha-s(1+\alpha)\big)}=$$

$$=\lim_{x\to 1-0}\frac{1}{k!}\frac{\partial^k}{\partial x^k}f^{(\alpha)}(x,1). \tag{4.4}$$

Proof performed by using the Abel theorem with the support of computer algebra programm Maple.

In cases when for concrete α the use of formula (4.4) causes difficulties it is resonable to go an other way.

One can choosethe Taylor series

$$E_{1+\alpha}\big(-q(I-q)^{-1}t^{1+\alpha}\big)=$$

$$=\sum_{j=0}^{\infty}\big(-q(I-q)^{-1}t^{1+\alpha}\big)^j\frac{1}{\Gamma(1+j(\alpha+1))}=\sum_{j=0}^{\infty}(q+I)^j S_j^{\alpha}(t^{1+\alpha}),$$

where

$$S_j^{\alpha}(t^{1+\alpha}) = \frac{1}{j!}\frac{\partial^j}{\partial x^j}\, E_{1+\alpha}\left(-\frac{x}{1-x}t^{1+\alpha}\right)\Big|_{q=-1} = \frac{1}{j!}\sum_{s=j}^{\infty}(-1)^s p_s^{\alpha}(t^{1+\alpha})\frac{s!}{(s-j)!}. \tag{4.5}$$

Proposition 4.2. *Let* $\alpha \in (-1, 0)$, *then for each natural* j *the formula* (4.5) *is valid.*

The calculation of the left-hand side of formula (4.5) is technically much more simple then the calculation of the right-hand side of formula (4.4), since the function $E_{1+\alpha}\big(-x(1-x)^{-1}t^{1+\alpha}\big)$ and all its partial derivatives with respect to x do not have singularities at $x - 1$.

The propositions above imply that for all $\alpha \in (-1, 0)$ and for each non negative j the limit value holds true

$$\lim_{s\to\infty} p_s^{\alpha}(t^{1+\alpha})\frac{s!}{(s-j)!} = 0$$

provided the series (4.5) is convergent. This equality means that there exists a constant c independent of s such that

$$\left|p_s^{\alpha}(t^{1+\alpha})\right| \le c\frac{(s-j)!}{s!} = \frac{1}{(s-j+1)(s-j+2)\ldots s} \le s^{-s}.$$

In the case $\alpha = 0$ it follows from the generating function $f^{(0)}(q,t)$ that the Laguerre–Cayley functions can be represented through the Laguerre polynomials

$$p_k^0(t) = L_k(t) - L_{k-1}(t),$$

for which the inequality

$$\left|p_k^0(t)\right| \le 2e^{\frac{t}{2}}$$

holds true.

For $\alpha \in (0, 1)$ with assistance of Maple it can be shown that there exist such natural $\mu(\alpha)$, that the series

$$\sum_{k=1}^{\infty} p_k^{\alpha}(1)\, k^{-\mu(\alpha)}$$

are convergent (Maple provides the exact sums). Thus, the estimate

$$\left|p_k^{\alpha}(1)\right| \le Ck^{\mu(\alpha)}, \quad \alpha \in (0,1),$$

is valid. In particular, $\mu(\alpha) = 6$ for $\alpha = \dfrac{1}{m}$, $m = 4, \ldots, 13$, $\mu(\alpha) = 7$ for $\alpha = \dfrac{m}{m+1}$, $m = 2, 3, 4$, and $\mu\left(\dfrac{1}{2}\right) = 8$. Further analogously one can get that

$$\sum_{k=1}^{\infty}\left|p_k^1(1)\right| k^{-4} = 0.53631821\ldots,$$

i.e., the estimate

$$\left|p_k^1(1)\right| \le C\, k^4$$

holds true.

Let us summarize the estimates for $p_k^{\alpha}(t^{1+\alpha})$ in the following lemma.

Table 4.1

N	$\overset{N}{\delta}(2)$
20	$7.72 \cdot 10^{-11}$
40	$3.42 \cdot 10^{-19}$
80	$6.49 \cdot 10^{-34}$
160	$5.02 \cdot 10^{-64}$

Lemma 4.2. *The following estimates hold true*:

$$\left|p_k^{\alpha}(t^{1+\alpha})\right| \le c \begin{cases} k^{-k}, & \textit{if} \quad \alpha \in (-1,0), \\ 1, & \textit{if} \quad \alpha = 0, \\ k^{\mu(\alpha)}, & \textit{if} \quad \alpha \in (0,1). \end{cases} \tag{4.6}$$

Besides we have

$$\left|p_k^{1}(1)\right| \le c_1 k^4, \tag{4.7}$$

where constants c, c_1 do not depend on k.

Remark **4.1.** Such technique demands to proof simultaniously whether the general summand of the series tends to zero or whether the series is absolutely convergent.

Example **4.1.** Let us consider the example (2.2) with $\alpha = -1/2,\ A = 1,\ t = 2$ which was considered also in [19] and with the exact solution

$$u(2) = e^2 \operatorname{erfc}(\sqrt{2}).$$

Note that in the case of the differential operator $A = -\dfrac{\partial^2}{\partial x^2}$ this example deals with a parabolic problem in the language of PDEs.

The Cayley transform method leads to the approximate N-terms representation

$$\overset{N}{u}(2) = 1 + \sum_{k=1}^{N} 2^{-k} p_k^{-1/2}(\sqrt{2}), \qquad q = A(1+A)^{-1} = \frac{1}{2}.$$

The numerical values of the absolute error $\delta^N(2) = \left|u(2) - \overset{N}{u}(2)\right|$ for Example 4.1 are given in Table 4.1.

Example **4.2.** Now let us consider problem (4.1) with $u_0 = 1,\ \alpha = 1/2,\ A = 1, q = 1/2$. The solution is the Mittag-Leffler function

$$u(t) = E_{3/2}\big(-t^{3/2}\big) = \sum_{j=0}^{\infty} \big(-t^{3/2}\big)^j \frac{1}{\Gamma(1+3j/2)}. \tag{4.8}$$

For $t = 1$ we have

Table 4.2

N	$\overset{N}{\delta}(1)$
8	$1.22 \cdot 10^{-9}$
16	$8.460928 \cdot 10^{-6}$
32	$3.814396 \cdot 10^{-11}$
64	$1.856974 \cdot 10^{-20}$

Table 4.3

N	$\overset{N}{\delta}(1)$
8	0.7683484749
16	0.2696535165
32	$0.930343601 \cdot 10^{-1}$
64	$0.84225987 \cdot 10^{-4}$

$$u(1) = E_{3/2}(-1) = \frac{e}{3} + \frac{2e^{-1/2}}{3}\cos\left(\frac{\sqrt{3}}{2}\right) - \frac{4}{3\sqrt{\pi}} \quad \text{hypergeom} \quad \left([1], \left[\frac{5}{6}, \frac{7}{6}, \frac{9}{6}\right], \frac{1}{27}\right) =$$

$$= .39662936531808808449161 4\ldots .$$

The exact representation due to the Cayley transform method (the power series in q) is

$$u(1) = E_{3/2}(-1) = \sum_{k=0}^{\infty} \left(\frac{1}{2}\right)^k p_k^{1/2}(1)$$

and the N-term approximation is

$$\overset{N}{u}(1) = \sum_{k=0}^{N} \left(\frac{1}{2}\right)^k p_k^{1/2}(1).$$

The numerical values of the absolute error

$$\overset{N}{\delta}(1) = \left|u(1) - \overset{N}{u}(1)\right|$$

are given by Table 4.2.

***Example* 4.3.** Now let us consider the two-dimensional problem (4.1) with the unbounded operator $A = -\dfrac{d^2}{dx^2}$ and $t = 1,\ \alpha = 1/2,\ u_0 = \sin(\pi x),\ x = \dfrac{1}{2}$ and the homogeneous Dirichlet boundary conditions. In this case formula (4.8) takes the form

$$E_{3/2}\left(\frac{d^2}{dx^2}\right)\sin(\pi x)\bigg|_{x=1/2} =$$

$$= \frac{e^{\pi^{4/3}}}{3} + \frac{2e^{-\pi^{4/3}/2}}{3}\cos\left(\frac{\sqrt{3}\pi^{4/3}}{2}\right) - \frac{4\pi^{3/2}}{3} \quad \text{hypergeom} \quad \left([1], \left[\frac{5}{6}, \frac{7}{6}, \frac{9}{6}\right], \frac{\pi^4}{27}\right) =$$

$$= -.11527434844270767536 30\ldots.$$

Our algorithm for $t = 1, x = 1/2$ provides numerical results given by Table 4.3.

5. Accuracy estimates of the Cayley transform method. We consider the case of the Hilbert space and of the positive definite operator A and let us estimate the accuracy of the application of the Cayley transform approximation of the Mittag-Leffler function to an vector u_0 from the domain of an operator A^σ.

It means that we assume the initial vector u_0 to be such that

$$\big\|A^\sigma u_0\big\| < \infty.$$

Then we obtain: 1) in the case $\alpha \in (-1, 0)$

$$\Big\|E_{1+\alpha}\big(-At^{1+\alpha}\big) - \overset{N}{E}_{1+\alpha}\big(-At^{1+\alpha}\big)\Big\| = \left\|\sum_{k=N+1}^{\infty} q^k p_k^\alpha(t^{1+\alpha})u_0\right\| =$$

$$= \left\|\sum_{k=N+1}^{\infty} \int\limits_{\gamma}^{\infty} F(\lambda)p_k^\alpha(t^{1+\alpha})dE_\lambda A^\sigma u_0\right\|,$$

where $F(\lambda) = \lambda^{-\sigma}\left(\frac{\lambda}{1+\lambda}\right)^k$. The function $F(\lambda)$ arrives its maximum $F_{\max} = \mathcal{O}(k^{-\sigma})$ at the point $\lambda_{\max} = \frac{k-\sigma}{\sigma}$:

$$F'(\lambda) = -\sigma\lambda^{-\sigma-1}\left(\frac{\lambda}{1+\lambda}\right)^k + k\lambda^{-\sigma}\left(\frac{\lambda}{1+\lambda}\right)^{k-1}\frac{1}{(1+\lambda)^2},$$

$$\lambda^{-\sigma-1}\left(\frac{\lambda}{1+\lambda}\right)^{k-1}\left(-\sigma\frac{\lambda}{1+\lambda} + \lambda k\frac{1}{(1+\lambda)^2}\right) = 0.$$

Taking into account Lemma 4.2, we obtain

$$\Big\|E_{1+\alpha}(-At^{1+\alpha})u_0 - \overset{N}{E}_{1+\alpha}(-At^{1+\alpha})u_0\Big\| = \left\|\sum_{k=N+1}^{\infty} q^k p_k^\alpha(t^{1+\alpha})u_0\right\| =$$

$$= \left\|\sum_{k=N+1}^{\infty} \int\limits_{\gamma}^{\infty} \lambda^{-\sigma}\left(\frac{\lambda}{1+\lambda}\right)^k p_k^\alpha(t^{1+\alpha})dE_\lambda A^\sigma u_0\right\| \le$$

$$\le c\sum_{k=N+1}^{\infty} k^{-k-\sigma+\varepsilon+1}k^{-1-\varepsilon}\|A^\sigma u_0\| \le cN^{-N-\sigma+\varepsilon}\|A^\sigma u_0\|, \tag{5.1}$$

where c is a constant independent of N and ε is an arbitrarily small positive number.

2) Analogously for $\alpha = 0$ we have

$$\left\| E_1(-At)u_0 - \overset{N}{E}_1(-At)u_0 \right\| = \left\| \sum_{k=N+1}^{\infty} q^k p_k^{\alpha}(t)u_0 \right\| =$$

$$= \left\| \sum_{k=N+1}^{\infty} \int_{\gamma}^{\infty} \lambda^{-\sigma} \left(\frac{\lambda}{1+\lambda} \right)^k p_k^0(t) dE_\lambda A^\sigma u_0 \right\| \leq$$

$$\leq c \sum_{k=N+1}^{\infty} k^{-\sigma+\varepsilon+1} k^{-1-\varepsilon} \| A^\sigma u_0 \| \leq c N^{-\sigma+1+\varepsilon} \| A^\sigma u_0 \|. \tag{5.2}$$

3) If $\alpha \in (0,1)$, then using estimate (4.6) we get

$$\left\| E_{1+\alpha}(-At^{1+\alpha})u_0 - \overset{N}{E}_{1+\alpha}(-At^{1+\alpha})u_0 \right\| = \left\| \sum_{k=N+1}^{\infty} q^k p_k^{\alpha}(t^{1+\alpha})u_0 \right\| =$$

$$= \left\| \sum_{k=N+1}^{\infty} \int_{\gamma}^{\infty} \lambda^{-\sigma} \left(\frac{\lambda}{1+\lambda} \right)^k p_k^{\alpha}(t^{1+\alpha}) dE_\lambda A^\sigma u_0 \right\| \leq$$

$$\leq c \sum_{k=N+1}^{\infty} k^{-\sigma+\mu(\alpha)+\varepsilon+1} k^{-1-\varepsilon} \| A^\sigma u_0 \| \leq c N^{-\sigma+\mu(\alpha)+\varepsilon} \| A^\sigma u_0 \|. \tag{5.3}$$

By using the estimate (4.7), we obtain analogously the following accuracy estimate for $\alpha = 1$ at $t = 1$:

$$\left\| E_2(-At^2)u_0 - \overset{N}{E}_2(-At^2) \right\| = \left\| \sum_{k=N+1}^{\infty} q^k p_k^1(t^2)u_0 \right\| \leq$$

$$\leq c \sum_{k=N+1}^{\infty} k^{-\sigma+4+\varepsilon+1} k^{-1-\varepsilon} \| A^\sigma u_0 \| \leq c N^{-\sigma+5+\varepsilon} \| A^\sigma u_0 \|. \tag{5.4}$$

Thus, we have proven the following assertion.

Theorem 5.1. *Let A be a self-adjoint positive definite operator in a Hilbert space H and $q = A(I+A)^{-1}$. Then for the accuracy of the Cayley transform method on a vector $u_0 \in D(A^\sigma)$ the estimates* (5.1)–(5.3) *or* (5.4) *hold true provided the corresponding assumptions from above are fulfilled and σ is such that the powers of N are negative.*

***Remark* 5.1.** With $\alpha = 1$ and with the additional initial condition $\dfrac{du(0)}{dt} = 0$ one can see that the Cayley transform method (without accuracy saturation) improves our algorithm from [7, 9] for the corresponding initial value problem for an abstract hyperbolic equation with the exact solution $u(t) = \cos(t\sqrt{A})u_0$.

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