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THE PROPERTIES, INEQUALITIES AND NUMERICAL APPROXIMATION OF MODIFIED BESSEL FUNCTIONS*

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Dedicated to Ed Saff on the occasion of his 60th birthday

Abstract. Some new properties of kernels of modified Kontorovitch–Lebedev integral transforms — modified Bessel functions of the second kind with complex order $K_{\frac{1}{2}+i\beta}(x)$ are presented. Inequalities giving estimations for these functions with argument x and parameter β are obtained. The polynomial approximations of these functions as a solutions of linear differential equations with polynomial coefficients and their systems are proposed.

Key words. Chebyshev polynomials, modified Bessel functions, Lanczos Tau method, Kontorovich-Lebedev integral transforms

AMS subject classifications. 33C10, 33F05, 65D20

1. Some properties of the functions $ReK_{\frac{1}{2}+i\beta}(x)$ and $ImK_{\frac{1}{2}+i\beta}(x)$.

In this section new properties of the kernels of modified Kontorovitch–Lebedev integral transforms are deduced, and some of their known properties are collected, which are necessary later on.

It is possible to write the kernels of these transforms in the form

$$ReK_{\frac{1}{2}+i\beta}(x) = \frac{K_{\frac{1}{2}+i\beta}(x) + K_{\frac{1}{2}-i\beta}(x)}{2} \quad \text{and} \quad ImK_{\frac{1}{2}+i\beta}(x) = \frac{K_{\frac{1}{2}+i\beta}(x) - K_{\frac{1}{2}-i\beta}(x)}{2i},$$

where $K_\nu(x)$ is the modified Bessel function of the second kind (also called MacDonald function).

The functions $ReK_{\frac{1}{2}+i\beta}(x)$ and $ImK_{\frac{1}{2}+i\beta}(x)$ have integral representations [8]

$$ReK_{\frac{1}{2}+i\beta}(x) = \int_0^\infty e^{-x\cosh t} \cosh\frac{t}{2}\cos(\beta t)dt, \tag{1.1}$$

$$ImK_{\frac{1}{2}+i\beta}(x) = \int_0^\infty e^{-x\cosh t} \sinh\frac{t}{2}\sin(\beta t)dt. \tag{1.2}$$

The vector-function $(y_1(x), y_2(x))$ with the components $y_1(x) = ReK_{\frac{1}{2}+i\beta}(x)$, $y_2(x) = ImK_{\frac{1}{2}+i\beta}(x)$ is the solution of the system of differential equations

$$\begin{aligned}
&\frac{d^2y_1}{dx^2} + \frac{1}{x}\frac{dy_1}{dx} - \left(1 + \frac{\frac{1}{4}-\beta^2}{x^2}\right)y_1 + \frac{\beta}{x^2}y_2 = 0,\\
&\frac{d^2y_2}{dx^2} + \frac{1}{x}\frac{dy_2}{dx} - \frac{\beta}{x^2}y_1 - \left(1 + \frac{\frac{1}{4}-\beta^2}{x^2}\right)y_2 = 0.
\end{aligned}$$

The functions $ReK_{\frac{1}{2}+i\beta}(x)$ and $ImK_{\frac{1}{2}+i\beta}(x)$ are even and odd functions, respectively of the variable β,

$$ReK_{\frac{1}{2}+i\beta}(x) = ReK_{\frac{1}{2}-i\beta}(x),$$

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$$ImK_{\frac{1}{2}+i\beta}(x) = -ImK_{\frac{1}{2}-i\beta}(x).$$

The functions $ReK_{\frac{1}{2}+i\beta}(x)$ and $ImK_{\frac{1}{2}+i\beta}(x)$ are related to the modified Bessel functions of the first kind $I_\nu(x)$ as follows,

$$ReK_{\frac{1}{2}+i\beta}(x) = \frac{\pi}{\cosh(\pi\beta)} \frac{ReI_{-\frac{1}{2}-i\beta}(x) - ReI_{\frac{1}{2}+i\beta}(x)}{2}, \tag{1.3}$$

$$ImK_{\frac{1}{2}+i\beta}(x) = \frac{\pi}{\cosh(\pi\beta)} \frac{ImI_{-\frac{1}{2}-i\beta}(x) - ImI_{\frac{1}{2}+i\beta}(x)}{2}. \tag{1.4}$$

The expansion of $I_{\frac{1}{2}+i\beta}(x)$ in ascending powers of x has the form

$$\begin{aligned} I_{\frac{1}{2}+i\beta}(x) = \left(\frac{x}{2}\right)^{\frac{1}{2}} \left(\cos\left(\beta\ln\frac{x}{2}\right) + i\sin\left(\beta\ln\frac{x}{2}\right)\right) \\ \times \sum_{k=0}^{\infty} \frac{\left(\frac{x^2}{4}\right)^k}{k!\Gamma\left(k+\frac{3}{2}+i\beta\right)} = \sum_{k=0}^{\infty}(a_k + ib_k), \end{aligned} \tag{1.5}$$

where a_k and b_k satisfy the following recurrence relations:

$$a_0 + ib_0 = \left(\frac{x}{2}\right)^{\frac{1}{2}} \frac{\cos\left(\beta\ln\frac{x}{2}\right) + i\sin\left(\beta\ln\frac{x}{2}\right)}{\Gamma\left(\frac{3}{2}+i\beta\right)},$$

$$m_k = x^2\frac{k+\frac{1}{2}}{4k\left(\left(k+\frac{1}{2}\right)^2+\beta^2\right)}, \qquad n_k = x^2\frac{\beta}{4k\left(\left(k+\frac{1}{2}\right)^2+\beta^2\right)},$$

$$a_k = a_{k-1}m_k + b_{k-1}n_k, \qquad b_k = b_{k-1}m_k - a_{k-1}n_k.$$

The expansion of $I_{-\frac{1}{2}-i\beta}(x)$ in ascending powers of x has the form

$$\begin{aligned} I_{-\frac{1}{2}-i\beta}(x) = \left(\frac{x}{2}\right)^{-\frac{1}{2}} \left(\cos\left(\beta\ln\frac{x}{2}\right) - i\sin\left(\beta\ln\frac{x}{2}\right)\right) \\ \times \sum_{k=0}^{\infty} \frac{\left(\frac{x^2}{4}\right)^k}{k!\Gamma\left(k+\frac{1}{2}-i\beta\right)} = \sum_{k=0}^{\infty}(c_k + id_k), \end{aligned} \tag{1.6}$$

where c_k and d_k satisfy the following recurrence relations:

$$c_0 + id_0 = \left(\frac{x}{2}\right)^{-1/2} \frac{\cos\left(\beta\ln\frac{x}{2}\right) - i\sin\left(\beta\ln\frac{x}{2}\right)}{\Gamma\left(\frac{1}{2}-i\beta\right)},$$

$$p_k = x^2\frac{k-\frac{1}{2}}{4k\left(\left(k-\frac{1}{2}\right)^2+\beta^2\right)}, \qquad q_k = x^2\frac{\beta}{4k\left(\left(k-\frac{1}{2}\right)^2+\beta^2\right)},$$

$$c_k = c_{k-1}p_k - d_{k-1}q_k, \qquad d_k = d_{k-1}p_k + c_{k-1}q_k.$$

The expansions (1.5) and (1.6) converge for all $0 < x < \infty$ and $0 \leq \beta < \infty$.

It follows from (1.1)–(1.2) that it is possible to write $ReK_{\frac{1}{2}+i\beta}(x)$ in the form of the Fourier cosinus-transform

$$ReK_{\frac{1}{2}+i\beta}(x) = \left(\frac{\pi}{2}\right)^{\frac{1}{2}} F_C\left[e^{-x\cosh t}\cosh\frac{t}{2}; t \to \beta\right], \tag{1.7}$$

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and $ImK_{\frac{1}{2}+i\beta}(x)$ in the form of the Fourier sinus-transform

$$ImK_{\frac{1}{2}+i\beta}(x) = \left(\frac{\pi}{2}\right)^{\frac{1}{2}} F_S\left[e^{-x\cosh t}\sinh\frac{t}{2}; t\to\beta\right]. \tag{1.8}$$

The inversion formulas have the respective forms

$$F_C\left[ReK_{\frac{1}{2}+i\beta}(x);\beta\to t\right] = \left(\frac{\pi}{2}\right)^{\frac{1}{2}} e^{-x\cosh t}\cosh\frac{t}{2},$$
$$F_S\left[ImK_{\frac{1}{2}+i\beta}(x);\beta\to t\right] = \left(\frac{\pi}{2}\right)^{\frac{1}{2}} e^{-x\cosh t}\sinh\frac{t}{2}$$

or, in integral form,

$$\int_0^\infty ReK_{\frac{1}{2}+i\beta}(x)\cos(t\beta)d\beta = \frac{\pi}{2}e^{-x\cosh t}\cosh\frac{t}{2}, \tag{1.9}$$
$$\int_0^\infty ImK_{\frac{1}{2}+i\beta}(x)\sin(t\beta)d\beta = \frac{\pi}{2}e^{-x\cosh t}\sinh\frac{t}{2}. \tag{1.10}$$

Differentiating equations (1.9) and (1.10) with respect to t, we obtain

$$\int_0^\infty \beta ReK_{\frac{1}{2}+i\beta}(x)\sin(t\beta)d\beta = \frac{\pi}{2}\left(x\sinh t\cosh\frac{t}{2} - \sinh\frac{t}{2}\right)e^{-x\cosh t},$$
$$\int_0^\infty \beta ImK_{\frac{1}{2}+i\beta}(x)\cos(t\beta)d\beta = \frac{\pi}{2}\left(\cosh\frac{t}{2} - x\sinh t\sinh\frac{t}{2}\right)e^{-x\cosh t}. \tag{1.11}$$

It follows from (1.9) that

$$\int_0^\infty ReK_{\frac{1}{2}+i\beta}(x)d\beta = \frac{\pi}{2}e^{-x},$$

and from (1.11) that

$$\int_0^\infty \beta ImK_{\frac{1}{2}+i\beta}(x)d\beta = \frac{\pi}{2}e^{-x}.$$

Differentiating (1.9) and (1.10) $2n$ times with respect to t, we obtain

$$\int_0^\infty \beta^{2n} ReK_{\frac{1}{2}+i\beta}(x)\cos(t\beta)d\beta = \frac{\pi}{2}(-1)^n D_t^{2n}\left(e^{-x\cosh t}\cosh\frac{t}{2}\right),$$
$$\int_0^\infty \beta^{2n} ImK_{\frac{1}{2}+i\beta}(x)\sin(t\beta)d\beta = \frac{\pi}{2}(-1)^n D_t^{2n}\left(e^{-x\cosh t}\sinh\frac{t}{2}\right),$$

from which there follows, for $t=0$,

$$\int_0^\infty \beta^{2n} ReK_{\frac{1}{2}+i\beta}(x)d\beta = \frac{\pi}{2}(-1)^n D_t^{2n}\left(e^{-x\cosh t}\cosh\frac{t}{2}\right)_{t=0}.$$

Differentiating (1.9) and (1.10) $2n+1$ times with respect to t, we obtain

$$\int_0^\infty \beta^{2n+1} ReK_{1/2+i\beta}(x)\sin(t\beta)d\beta = \frac{\pi}{2}(-1)^{n+1} D_t^{2n+1}\left(e^{-x\cosh t}\cosh\frac{t}{2}\right),$$
$$\int_0^\infty \beta^{2n+1} ImK_{1/2+i\beta}(x)\cos(t\beta)d\beta = \frac{\pi}{2}(-1)^{n} D_t^{2n+1}\left(e^{-x\cosh t}\sinh\frac{t}{2}\right).$$

whence, for $t = 0$,

$$\int_0^\infty \beta^{2n+1} ImK_{1/2+i\beta}(x)d\beta = \frac{\pi}{2}(-1)^n D_t^{2n+1}\left(e^{-x\cosh t}\sinh\frac{t}{2}\right)_{t=0}.$$

For the computation of certain integrals of the functions $ReK_{\frac{1}{2}+i\beta}(x)$ and $ImK_{\frac{1}{2}+i\beta}(x)$, integral identities are useful. They reduce this problem to the computation of some other integrals of elementary functions.

PROPOSITION 1.1. *If f is absolutely integrable on $[0,\infty)$, then the following identities hold,*

$$\int_0^\infty ReK_{\frac{1}{2}+i\beta}(x)f(\beta)d\beta = \left(\frac{\pi}{2}\right)^{\frac{1}{2}}\int_0^\infty e^{-x\cosh t}\cosh\frac{t}{2}F_C(t)dt, \tag{1.12}$$

$$\int_0^\infty ImK_{\frac{1}{2}+i\beta}(x)f(\beta)d\beta = \left(\frac{\pi}{2}\right)^{\frac{1}{2}}\int_0^\infty e^{-x\cosh t}\sinh\frac{t}{2}F_S(t)dt, \tag{1.13}$$

where $F_C(t)$ is the Fourier cosinus-transform of $f(\beta)$, and $F_S(t)$ the Fourier sinus-transform of $f(\beta)$.

Proof. Multiplying both sides of the equalities (1.7) and (1.8) by $f(\beta)$, integrating with respect to β from 0 to ∞, and applying Fubini's theorem for singular integrals with parameter [22], we obtain (1.12) and (1.13). □

PROPOSITION 1.2. *If f is absolutely integrable on $[0,\infty)$, then the following identities hold*

$$\int_0^\infty ReK_{\frac{1}{2}+i\beta}(x)F_C(\beta)d\beta = \left(\frac{\pi}{2}\right)^{\frac{1}{2}}\int_0^\infty e^{-x\cosh t}\cosh\frac{t}{2}f(t)dt, \tag{1.14}$$

$$\int_0^\infty ImK_{\frac{1}{2}+i\beta}(x)F_S(\beta)d\beta = \left(\frac{\pi}{2}\right)^{\frac{1}{2}}\int_0^\infty e^{-x\cosh t}\sinh\frac{t}{2}f(t)dt. \tag{1.15}$$

Proof. This follows from (1.9)–(1.10) and from Fubini's theorem [22]. □

The equations (1.12)–(1.15) are useful for the simplification and the calculation of different integrals containing $ReK_{1/2+i\beta}(x)$ and $ImK_{1/2+i\beta}(x)$.

For example, let $f(\beta) = e^{-\alpha\beta}$, then $F_C(t) = \sqrt{\frac{2}{\pi}}\frac{\alpha}{\alpha^2+t^2}$, $F_S(t) = \sqrt{\frac{2}{\pi}}\frac{t}{\alpha^2+t^2}$ and

$$\int_0^\infty ReK_{\frac{1}{2}+i\beta}(x)e^{-\alpha\beta}d\beta = \alpha\int_0^\infty(\alpha^2+t^2)^{-1}e^{-x\cosh t}\cosh\frac{t}{2}dt,$$

$$\int_0^\infty ReK_{\frac{1}{2}+i\beta}(x)\frac{1}{\alpha^2+\beta^2}d\beta = \frac{\pi}{2\alpha}\int_0^\infty e^{-\alpha t - x\cosh t}\cosh\frac{t}{2}dt,$$

$$\int_0^\infty ImK_{\frac{1}{2}+i\beta}(x)e^{-\alpha\beta}d\beta = \int_0^\infty t(\alpha^2+t^2)^{-1}e^{-x\cosh t}\sinh\frac{t}{2}dt,$$

$$\int_0^\infty ImK_{\frac{1}{2}+i\beta}(x)\frac{\beta}{\alpha^2+\beta^2}d\beta = \frac{\pi}{2}\int_0^\infty e^{-\alpha t - x\cosh t}\sinh\frac{t}{2}dt.$$

If $f(\beta) = \Gamma(\frac{1}{4}+\frac{i\beta}{2})\Gamma(\frac{1}{4}-\frac{i\beta}{2})$, then $F_C(t) = \frac{2\pi}{\sqrt{\cosh t}}$ and

$$\int_0^\infty ReK_{\frac{1}{2}+i\beta}(x)\Gamma(\frac{1}{4}+\frac{i\beta}{2})\Gamma(\frac{1}{4}-\frac{i\beta}{2})d\beta =$$

$$= \sqrt{2\pi}\pi\int_0^\infty e^{-x\cosh t}\frac{\cosh\frac{t}{2}}{\sqrt{\cosh t}}dt = \pi\sqrt{\pi}e^{-\frac{x}{2}}K_0(\frac{x}{2}).$$

If $f(\beta) = \frac{\sinh(2\pi\beta)}{\cosh(2\pi\beta)+\cos(2\pi\alpha)}$, $|Re\alpha| < \frac{1}{2}$, then $F_S(t) = \frac{\cosh(\alpha t)}{\sqrt{2\pi}\sinh\frac{t}{2}}$ and

$$\int_0^\infty \frac{ImK_{\frac{1}{2}+i\beta}(x)\sinh(2\pi\beta)}{\cosh(2\pi\beta)+\cos(2\pi\alpha)}d\beta = \frac{1}{2}\int_0^\infty e^{-x\cosh t}\cosh(\alpha t)dt = \frac{1}{2}K_\alpha(x).$$

REMARK 1.3. *All formulas of the present paragraph remain valid if x is changed to z lying in the right-hand half-plane.*

1.1. The Laplace transform of $ReK_{\frac{1}{2}+i\beta}(x)$ and $ImK_{\frac{1}{2}+i\beta}(x)$.
The Laplace transform of $K_{i\beta}(x)$ is computed in [21]. We use the representation (1.1) for the evaluation of the Laplace transformation of $ReK_{\frac{1}{2}+i\beta}(x)$. We have

$$\begin{aligned} L\left[ReK_{\frac{1}{2}+i\beta}(x);\beta\right] &= \int_0^\infty \cos(\beta t)\cosh\frac{t}{2}\int_0^\infty e^{-(p+\cosh t)x}\,dx\,dt \\ &= \int_0^\infty \frac{\cos(\beta t)\cosh\frac{t}{2}}{\cosh t+\cosh\alpha}dt\ (p=\cosh\alpha) \\ &= \sqrt{\frac{\pi}{2}}F_C\left(\frac{\cosh\frac{t}{2}}{\cosh t+\cosh\alpha}\right) = \frac{\pi}{2}\frac{\cos(\alpha\beta)}{\cosh\frac{\alpha}{2}\cosh(\pi\beta)}. \end{aligned}$$

Equivalently, we can write

$$L^{-1}\left[\frac{\cos(\beta\cosh^{-1}p)}{\sqrt{\frac{p+1}{2}}}\right] = \left(\frac{\pi}{2}\right)^{-1}\cosh(\pi\beta)ReK_{\frac{1}{2}+i\beta}(x).$$

For the evaluation of the Laplace transform of $ImK_{\frac{1}{2}+i\beta}(x)$ we utilize the representation (1.2). We have

$$L\left[ImK_{\frac{1}{2}+i\beta}(x);p\right] = \sqrt{\frac{\pi}{2}}F_S\left(\frac{\sinh\frac{t}{2}}{\cosh t+\cosh\alpha}\right) = \frac{\pi}{2}\frac{\sin(\alpha\beta)}{\cosh(\pi\beta)\sinh\frac{\alpha}{2}},$$

or, equivalently,

$$L^{-1}\left[\frac{\sin(\beta\cosh^{-1}p)}{\sqrt{\frac{p-1}{2}}}\right] = \sqrt{\frac{\pi}{2}}\cosh(\pi\beta)ImK_{\frac{1}{2}+i\beta}(x).$$

We note that these equations can also be obtained directly from the formula for the Laplace transforms of $K_\nu(x)$ by separating real and imaginary parts.

1.2. The asymptotic behavior of $ReK_{\frac{1}{2}+i\beta}(x)$ and $ImK_{\frac{1}{2}+i\beta}(x)$ for $x\to 0, x\to\infty$ and $\beta\to\infty$. For $ReK_{\frac{1}{2}+i\beta}(x)$ and $ImK_{\frac{1}{2}+i\beta}(x)$ the following asymptotic formulas for $\beta\to\infty$ are valid [8],

$$\begin{aligned} ReK_{\frac{1}{2}+i\beta}(x) &\sim \left(\frac{\pi}{x}\right)^{\frac{1}{2}} e^{-\frac{\pi\beta}{2}}\cos\left(\beta\ln\beta-\beta-\beta\ln\frac{x}{2}\right), \\ ImK_{\frac{1}{2}+i\beta}(x) &\sim \left(\frac{\pi}{x}\right)^{\frac{1}{2}} e^{-\frac{\pi\beta}{2}}\sin\left(\beta\ln\beta-\beta-\beta\ln\frac{x}{2}\right), \end{aligned}$$

where x is a fixed positive number.

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It follows immediately from (1.3)–(1.6) that for $x \to 0$ we have

$$K_{\frac{1}{2}+i\beta}(x) \sim \frac{1}{2}\left(\frac{x}{2}\right)^{-\frac{1}{2}} \frac{\cos\left(\beta \ln \frac{x}{2}\right) - i \sin\left(\beta \ln \frac{x}{2}\right)}{\Gamma\left(\frac{1}{2} - i\beta\right)},$$

whence

$$\begin{aligned} ReK_{\frac{1}{2}+i\beta}(x) \sim \frac{1}{2}\left(\frac{x}{2}\right)^{-\frac{1}{2}} \Bigg(& Re\Gamma\left(\frac{1}{2}+i\beta\right)\cos\left(\beta\ln\frac{x}{2}\right) \\ & + Im\Gamma\left(\frac{1}{2}+i\beta\right)\sin\left(\beta\ln\frac{x}{2}\right)\Bigg), \\ ImK_{\frac{1}{2}+i\beta}(x) \sim \frac{1}{2}\left(\frac{x}{2}\right)^{-\frac{1}{2}} \Bigg(& Im\Gamma\left(\frac{1}{2}+i\beta\right)\cos\left(\beta\ln\frac{x}{2}\right) \\ & - Re\Gamma\left(\frac{1}{2}+i\beta\right)\sin\left(\beta\ln\frac{x}{2}\right)\Bigg), \end{aligned}$$

For large values x the following asymptotic expansion is valid [9]

$$K_{\frac{1}{2}+i\beta}(x) \sim \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} e^{-x} \sum_{k=0}^{\infty} \left(\frac{1}{2}+i\beta, k\right)(2x)^{-k},$$

where

$$(\nu, k) = \frac{(4\nu^2-1^2)(4\nu^2-3^2)\cdots(4\nu^2-(2k-1)^2)}{2^{2k}k!}.$$

In particular, therefore,

$$\begin{aligned} ReK_{\frac{1}{2}+i\beta}(x) &\sim \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} e^{-x}\left(1 - \frac{\beta^2}{2x} + \cdots\right), \\ ImK_{\frac{1}{2}+i\beta}(x) &\sim \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} e^{-x}\left(\frac{\beta}{2x} + \cdots\right) = \frac{\beta}{2x}\left(\frac{\pi}{2x}\right)^{\frac{1}{2}} e^{-x}(1+\cdots). \end{aligned}$$

1.3. The series expansions in powers of β. The solutions of problems in mathematical physics connected with the use of the Kontorovitch–Lebedev integral transforms are often expressed as integrals with respect to β of the functions $K_{i\beta}(x)$, $ReK_{\frac{1}{2}+i\beta}(x)$ and $ImK_{\frac{1}{2}+i\beta}(x)$. Both the asymptotic expansions of these integrals for large values β, and the expansions of these functions in powers of β, are of interest for the analysis of the behavior of these integrals.

The expansions of these functions in powers of β are deduced from their integral representations (1.1)–(1.2). Substituting in them $\cos(\beta t)$ and $\sin(\beta t)$ by their series expansions and interchanging the order of the summation and integration, we obtain

$$\begin{aligned} K_{i\beta}(x) &= \sum_{k=0}^{\infty} \frac{\beta^{2k}}{(2k)!} \int_0^{\infty} t^{2k} e^{-x\cosh t} dt = \\ &= K_0(x) - \frac{\beta^2}{2!}\int_0^{\infty} t^2 e^{-x\cosh t} dt + \frac{\beta^4}{4!}\int_0^{\infty} t^4 e^{-x\cosh t} dt + \cdots, \end{aligned} \tag{1.16}$$

$$ReK_{\frac{1}{2}+i\beta}(x) = \sum_{k=0}^{\infty} \frac{\beta^{2k}}{(2k)!} \int_0^{\infty} t^{2k} e^{-x\cosh t} \cosh \frac{t}{2} dt =$$
$$= K_{\frac{1}{2}}(x) - \frac{\beta^2}{2!} \int_0^{\infty} t^2 e^{-x\cosh t} \cosh \frac{t}{2} dt$$
$$+ \frac{\beta^4}{4!} \int_0^{\infty} t^4 e^{-x\cosh t} \cosh \frac{t}{2} dt + \cdots , \tag{1.17}$$
$$ImK_{\frac{1}{2}+i\beta}(x) = \sum_{k=0}^{\infty} \frac{\beta^{2k+1}}{(2k+1)!} \int_0^{\infty} t^{2k+1} e^{-x\cosh t} \sinh \frac{t}{2} dt =$$
$$= \beta \int_0^{\infty} t e^{-x\cosh t} \sinh \frac{t}{2} dt - \frac{\beta^3}{3!} \int_0^{\infty} t^3 e^{-x\cosh t} \sinh \frac{t}{2} dt + \cdots . \tag{1.18}$$

These functions are entire functions in the variable β, and therefore the series converge for all real values of β. From these expansions it is possible to obtain the series for the derivatives and for the integrals of these functions with respect to the variable β, which will converge for all real β also. Similar integrals for the spherical functions are stated in [23].

It's possible to rewrite the expansions (1.16)–(1.18) in terms of Laplace transforms as follows,

$$K_{i\beta}(x) = e^{-x} \sum_{k=0}^{\infty} (-1)^k L\left[\frac{\operatorname{arccosh}^{2k}(y+1)}{\sqrt{(y+1)^2-1}}; y \to x\right] \frac{\beta^{2k}}{(2k)!}, \tag{1.19}$$

$$ReK_{\frac{1}{2}+i\beta}(x) = e^{-x} \sum_{k=0}^{\infty} (-1)^k L\left[\frac{\operatorname{arccosh}^{2k}(y+1)}{\sqrt{2y}}; y \to x\right] \frac{\beta^{2k}}{(2k)!}, \tag{1.20}$$

$$ImK_{\frac{1}{2}+i\beta}(x) = e^{-x} \sum_{k=0}^{\infty} (-1)^k L\left[\frac{\operatorname{arccosh}^{2k+1}(y+1)}{\sqrt{2(y+2)}}; y \to x\right] \frac{\beta^{2k+1}}{(2k+1)!}, \tag{1.21}$$

This form of writing may be more convenient since it is possible to use numerical methods for evaluating Laplace transforms.

The expansions (1.19)–(1.21) are convenient for the calculation of the kernels of Kontorovitch-Lebedev integral transforms for small values β.

2. Inequalities for the MacDonald functions $K_{i\beta}(x)$, $ReK_{\frac{1}{2}+i\beta}(x)$ and $ImK_{\frac{1}{2}+i\beta}(x)$. It follows from (1.1) that for all $\beta \in [0, \infty)$

$$|ReK_{\frac{1}{2}+i\beta}(x)| \le K_{\frac{1}{2}}(x) = \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} e^{-x},$$

and it follows from (1.2) that for all $\beta \in [0, \infty)$

$$|ImK_{\frac{1}{2}+i\beta}(x)| \le \int_0^{\infty} e^{-x\cosh t} \sinh \frac{t}{2} dt = \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} e^{x} \left[1 - \phi((2x)^{\frac{1}{2}})\right] \le B\frac{e^{-x}}{x},$$

where B is some positive constant [10],[11].

In [4], for arbitrary $\nu = \sigma + i\beta$, $\sigma \ge 0$, the following inequality is derived

$$|I_\nu(x)| \le e^{\frac{\pi|\beta|}{2}} I_\sigma(x).$$

Taking advantage of the formula [4]

$$|K_\nu(x)| \le \left(C_1(x,\sigma) + C_2(x,\sigma)|\beta|^{\sigma-\frac{1}{2}}\right) e^{-\frac{\pi|\beta|}{2}},$$

we obtain that beginning with some $T, |\beta| > T$,

$$|K_{\frac{1}{2}+i\beta}(x)| \le C(x)e^{-\frac{\pi|\beta|}{2}}.$$

But this inequality is too rough and may be insufficient for conducting various proofs. To obtain more refined inequalities, we use [5]

$$|K_{i\beta}(x)| \le Ax^{-\frac{1}{4}}e^{-\frac{\pi|\beta|}{2}}, \tag{2.1}$$

where A is some positive constant, and the representations [8]

$$\begin{aligned} ReK_{\frac{1}{2}+i\beta}(x) &= \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} \frac{e^{-x}}{\cosh(\pi\beta)} \\ &+\frac{\beta\tanh(\pi\beta)}{(2\pi)^{\frac{1}{2}}}\int_0^x \left[\frac{e^{-(x-y)}}{\sqrt{x-y}} - \frac{e^{-(x+y)}}{x^{\frac{1}{2}}}\right] K_{i\beta}(y)dy \\ &-\frac{\beta\tanh(\pi\beta)}{(2\pi)^{\frac{1}{2}}}\int_x^\infty \frac{e^{-(x+y)}}{x^{\frac{1}{2}}}\frac{K_{i\beta}(y)}{y}\,dy, \\ ImK_{\frac{1}{2}+i\beta}(x) &= \frac{\beta e^x}{(2\pi)^{\frac{1}{2}}}\int_x^\infty \frac{e^{-y}K_{i\beta}(y)}{y(y-x)^{\frac{1}{2}}}\,dy. \end{aligned} \tag{2.2}$$

LEMMA 2.1. *The following inequalities hold for $x > 0$*

$$|ReK_{\frac{1}{2}+i\beta}(x)| \le c|\beta|e^{-\frac{\pi|\beta|}{2}}x^{-\frac{3}{4}} + \left(\frac{2\pi}{x}\right)^{\frac{1}{2}} e^{-x}e^{-\pi|\beta|},$$
$$|ImK_{\frac{1}{2}+i\beta}(x)| \le c_0|\beta|e^{-\frac{\pi|\beta|}{2}}x^{-\frac{3}{4}},$$

where c_0 and c are some positive constants.

Proof. We estimate the second additive term in (2.2), using the inequality (2.1),

$$\begin{aligned} &|\frac{\beta\tanh(\pi\beta)}{(2\pi)^{\frac{1}{2}}}\int_0^x \left[\frac{e^{-(x-y)}}{(x-y)^{\frac{1}{2}}} - \frac{e^{-(x+y)}}{x^{\frac{1}{2}}}\right]\frac{K_{i\beta}(y)}{y}dy| \\ &\le A|\beta|e^{-\frac{\pi|\beta|}{2}}\frac{e^{-x}}{\sqrt{x}}\int_0^x \frac{\frac{e^y}{\sqrt{1-\frac{y}{x}}} - e^y}{y}y^{-\frac{1}{4}}dy \le A|\beta|e^{-\frac{\pi|\beta|}{2}}x^{-\frac{3}{4}}. \end{aligned} \tag{2.3}$$

We next estimate the third additive term,

$$\begin{aligned} |\frac{\beta\tanh(\pi\beta)}{\sqrt{2\pi}}\int_x^\infty \frac{e^{-(x+y)}}{\sqrt{x}}\frac{K_{i\beta}(y)}{y}dy| &\le B|\beta|e^{-\frac{\pi|\beta|}{2}}\frac{e^{-x}}{\sqrt{x}}\int_x^\infty e^{-y}y^{-\frac{5}{4}}dy \\ &\le B|\beta|e^{-\frac{\pi|\beta|}{2}}e^{-2x}x^{-\frac{3}{4}}. \end{aligned} \tag{2.4}$$

Combining the first term and estimates (2.3) and (2.4), we obtain the required inequality.

Furthermore, we obtain

$$\begin{aligned} |ImK_{\frac{1}{2}+i\beta}(x)| &\le |\frac{\beta e^x}{\sqrt{2\pi}}\int_0^\infty \frac{e^{-y}K_{i\beta}(y)}{y\sqrt{y-x}}dy| \\ &\le c_0|\beta|e^{-\frac{\pi|\beta|}{2}}e^x\int_x^{infty}\frac{e^{-y}y^{-\frac{5}{4}}}{\sqrt{y-x}}dy \le c_0|\beta|e^{-\frac{\pi|\beta|}{2}}x^{-\frac{3}{4}}. \end{aligned}$$

For future use, an analysis of the behavior of the modified Bessel function $K_{\sigma+i\beta}(x)$ for large values of β is necessary. □

LEMMA 2.2. *For* $0 \le \sigma \le \frac{1}{2}$, $|\beta| \ge \beta_0 \ge 1$, $x \ge x_0 \ge 1$, *the following inequality holds,*

$$|K_{\sigma+i\beta}(x)| \le \left(c_1 x^{\sigma-\frac{1}{2}} + c_2 x^{\frac{1}{2}-\sigma}|\beta|^{\sigma-\frac{1}{2}}\right) e^{x-\frac{\pi|\beta|}{2}},$$

where $c_1 > 0$, $c_2 > 0$, c_1, c_2, β_0, x_0 *are some constants.*

Proof. We use the formula [6]

$$K_\mu(x) = \frac{\pi}{2\sin(\pi\mu)}(I_{-\mu}(x) - I_\mu(x)), \qquad \mu = \sigma + i\beta.$$

1. We first estimate $\sin(\pi\mu)$. It is possible to show that for $|\beta| \ge \beta_0^{(1)} > 0$, $\beta_0^{(1)}$ some constant, the following inequality is valid

$$a_1 e^{\pi|\beta|} \le |\sin(\pi\mu)| \le a_2 e^{\pi|\beta|}, \tag{2.5}$$

where $a_1 > 0$, $a_2 > 0$, a_1, a_2 are some constants.

2. We next estimate $I_\mu(x)$, $\mu = \sigma + i\beta$, $\sigma \ge 0$. The following inequality is derived for $\sigma \ge 0$ in [4]

$$|I_\mu(x)| \le I_0(x)\frac{(\frac{x}{2})^\sigma e^{\frac{\pi|\beta|}{2}}}{\Gamma(\sigma+1)}.$$

It follows from the asymptotics of $I_0(x)$ [10] for large x that for $x \ge x_0^{(1)} > 0$, $x_0^{(1)}$ some constant,

$$|I_\mu(x)| \le a_3 x^{\sigma-\frac{1}{2}} e^{x+\frac{\pi\ |\beta|}{2}}, \tag{2.6}$$

where $a_3 > 0,\ a_3$ some constant.

3. We finally estimate $I_{-\mu}(x)$, $\mu = \sigma + i\beta$, $\sigma \ge 0$. Proceeding analogously [4], we can rewrite $I_{-\mu}(x)$ in the form

$$I_{-\mu}(x) = \frac{(\frac{x}{2})^{-\mu}}{\Gamma(1-\mu)}\psi(x,\mu),$$

where

$$\psi(x,\mu) = 1 + \sum_{s=1}^{\infty}\frac{(\frac{x}{2})^{2s}}{s!\prod_{k=1}^{k=s}(-\mu+k)}.$$

Then $|k-\mu| = \sqrt{(k-\sigma)^2+\beta^2} \ge k-1$ for $0 \le \sigma \le \frac{1}{2}$, $k = 2, 3, \ldots$, and $\sqrt{(1-\sigma)^2+\beta^2} \ge \frac{1}{2}$, β arbitrary. Therefore, $\prod_{k=1}^{k=s}\sqrt{(k-\sigma)^2+\beta^2} \ge \frac{(s-1)!}{2}$. We obtain, after some calculations, that

$$\psi(x,\mu) \le 1 + 2\sum_{s=1}^{\infty}\frac{(\frac{x}{2})^{2s}}{s!(s-1)!} \le 2\left(1 + \frac{x}{2}I_1(x)\right).$$

Using for $|\beta| \ge \beta_0^{(2)} \ge 1$, $0 \le \sigma \le \frac{1}{2}$, the expansion of the gamma-function from [5] and the asymptotics [6] for $I_1(x)$ we obtain that beginning with some $x_0^{(2)}$, $x \ge x_0^{(2)} \ge 1$, the following estimation holds,

$$|I_{-\mu}(x)| \le a_4 x^{\frac{1}{2}-\sigma}|\beta|^{\sigma-\frac{1}{2}} e^{x+\frac{\pi|\beta|}{2}}, \tag{2.7}$$

$a_4 > 0$, a_4 some constant.

Combining the estimations (2.5)–(2.7), we obtain that for $0 \le \sigma \le \frac{1}{2}$, $|\beta| \ge \beta_0 \ge 1$, $x \ge x_0 \ge 1$, $\beta_0 = \max(\beta_0^{(1)}, \beta_0^{(2)})$, $x_0 = \max(x_0^{(1)}, x_0^{(2)})$ the following inequality is valid,

$$|K_\mu(x) \le \frac{\pi}{2a_1} e^{-\pi|\beta|} |I_{-\mu}(x) - I_\mu(x)| \le \frac{\pi}{2a_1}\left(a_3 x^{\sigma-\frac{1}{2}} + a_4 x^{\frac{1}{2}-\sigma}|\beta|^{\sigma-\frac{1}{2}}\right) e^{x-\frac{\pi|\beta|}{2}}.$$

Denoting $c_1 = \frac{\pi}{2a_1}a_3$, $c_2 = \frac{\pi}{2a_1}a_4$, we obtain the statement of the lemma. □

The properties of the modified Kontorovitch–Lebedev integral transforms are considered in [7]–[15].

3. Tau method approximation for modified Bessel function of imaginary order. Several approaches for the evaluation of the modified Bessel functions are elaborated in [1]–[2]. The Tau method [3] realization, with minimal residue choice for the determination of the polynomial approximations of the solutions of the second order differential equations with polynomial coefficients [16] of the following form

$$(a_0y^2 + a_5y)v''(y) + (a_1y + a_2)v'(y) + a_3v(y) = 0,\ v(0) = a_4, \quad y \in [0, 1],$$

is supposed. An n-th approximation of the solution is sought in the form of the n-th degree polynomial $v_n(y)$, which is the solution of the equation

$$(b_0y^2 + b_5y)v(y) = \int_0^y (b_1x + b_2y + b_3)v(x)dx + b_4y + \tau_{n+2}T^*_{n+2}[(1 - \alpha_{n+2})y + \alpha_{n+2}],$$

where the coefficients a_i, $i = 0, \ldots, 5$, may be expressed by coefficients b_i, $i = 0, \ldots, 5$, $\alpha_{n+2} = \sin^2 \frac{\pi}{4(n+2)}$ — the leftmost root of the shifted Chebyshev polynomial of the $n+2$-th degree $T^*_{n+2}(y)$ in the interval $[0, 1]$, τ_{n+2} — undefined coefficient.

The problem about determination of the polynomial $P_n(y) = \sum_{k=0}^{n} p_k y^k$, which is the least deviated from zero on the interval $[0, 1]$ among all n-th degree polynomials, satisfying the pair of linear correlations on the coefficients $p_0 = 0$, $\sum_{i=1}^{n} c_i^{(n)} p_i = 1$ was considered. The following theorem is proved [16]:

THEOREM 3.1. *If the sequence of numbers $c_i^{(n)}$, $i = 1, \ldots, n$, is alternating, then the polynomial $\tau_n T^*_n[(1 - \alpha_n)y + \alpha_n]$ is the polynomial least deviating from zero in the uniform metric on $[0, 1]$ among all polynomials of degree n, satisfying the indicated pair of linear relations.*

On the basis of this theorem it's shown (as suggested by us) in the Tau method residue, in a number of significant cases, is a minimal in the uniform metric on $[0, 1]$, among all possible polynomial residues permitting the Volterra integral equations solution.

We have the following differential equation with polynomial coefficients for the approximation and computing of the second kind modified Bessel function $K_{i\beta}(x)$:

$$y^2v''(y) + 2(y + 1)v'(y) + (1/4 + \beta^2)v(y) = 0,$$

$$v(0) = 1,$$

and the Volterra integral equation

$$y^2v(y) = \int_0^y \left[\left(\frac{9}{4} + \beta^2\right)x - \left(\frac{1}{4} + \beta^2\right)y - 2\right] v(x)dx + 2y.$$

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We obtain the following recurrence formulas for the coefficients of canonical polynomials $Q_m(y) = \sum_{k=0}^{m} q_{km} y^k$ in this case:

$$q_{00} = \frac{2}{\frac{1}{4} + \beta^2}, \quad q_{0k} = -\frac{2(k+2)}{k^2 + k + \frac{1}{4} + \beta^2} q_{0k-1}, \quad k = 1, \ldots$$

The minimality of the residue suggested by us follows from the Theorem 3.1 as $\frac{q_{0m}}{|q_{0m}|} = (-1)^m, m = 0, 1, \ldots$

The advantages of this modification, as compared with usual and other tau-methods, is shown.

4. Tau method approximation for modified Bessel function of complex order. A new numerical scheme of the Tau method application is proposed for the solution of the second order linear differential equations systems, with the second order polynomial coefficients of the following kind:

$$(a_0^{(j)} y^2 + a_1^{(j)} y) v_j''(y) + \sum_{i=1}^{k} [(a_{3i-1}^{(j)} y - a_{3i}^{(j)}) v_i'(y) + a_{3i+1}^{(j)} v_i(y)] = 0,$$
$$v_j(0) = a_{3k+2}^{(j)}, \quad j = 1, \ldots, k, \quad y \in [0, 1],$$

in the unknown vector-function $v(y) = (v_1(y), \ldots, v_k(y))$. It is assumed to have only one solution. Integrating twice and carrying an addition in the right part in the kind of the vector-polynomial $P_n(y)$, we derive for the determination of the n-th approximation of the solution $v(y) = (v_1(y), \ldots, v_k(y))$ the system of Volterra integral equations with polynomial kernels

$$(b_0^{(j)} y^2 + b_1^{(j)} y) v_j(y) = \int_0^y [\sum_{i=1}^{k} (b_{3i-1}^{(j)} x + b_{3i}^{(j)} y + b_{3i+1}^{(j)}) v_i(x)] dx + P_{jn+2}(y),$$
$$j = 1, \ldots, k,$$

where the coefficients $b_i^{(j)}$ and $a_i^{(j)}, i = 0, \ldots, 3k+2$ and $j = 1, \ldots, k$, are connected in a definite way and $P_{jn+2}(y)$, $j = 1, \ldots, k$, are $n+2$-th degree polynomials. The different variables of the vector residue choice and its minimization are analyzed. The recurrence formulas for the canonical vector-polynomials coefficients convenient for the calculations are given.

Consider the system of two second order differential equations ($k = 2$) in more detail. This case is of particular interest for differential equations with complex coefficients.

The scheme of the integral form of the Tau Method described in this paper can be used for deriving polynomial approximations of hypergeometric and confluent hypergeometric functions of the first kind with complex parameters.

The modified Kontorovich–Lebedev integral transforms [7] with kernels $ReK_{\frac{1}{2}+i\beta}(x) = \frac{K_{\frac{1}{2}+i\beta}(x) + K_{\frac{1}{2}-i\beta}(x)}{2}$ and $ImK_{\frac{1}{2}+i\beta}(x) = \frac{K_{\frac{1}{2}+i\beta}(x) - K_{\frac{1}{2}-i\beta}(x)}{2i}$, where $K_s(x)$ is MacDonald's function, is of great importance in solving some problems of mathematical physics, in particular mixed boundary value problems for the HELMHOLTZ equation in wedge and cone domains. We find it necessary to compute $ReK_{\frac{1}{2}+i\beta}(x)$ and $ImK_{\frac{1}{2}+i\beta}(x)$ to use this transform in practice [13]. These functions also occur in solving some classes of dual integral equations with kernels which contain MacDonald's function of imaginary index $K_{i\beta}(x)$ [7]. Therefore, now we consider the second kind modified Bessel function $K_{\frac{1}{2}+i\beta}(x)$ in more detail.

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We have a system of two second order differential equations

$$y^2v_1'' + 2(y+1)v_1' + \beta^2 v_1 + \beta v_2 = 0,$$

$$y^2v_2'' + 2(y+1)v_2' - \beta v_1 + \beta^2 v_2 = 0,$$

$$v_1(0) = 1, v_2(0) = 0,$$

or the system of Volterra integral equations

$$y^2v_1(y) = \int_0^y ((2+\beta^2)x - (2+\beta^2 y))v_1(x)dx + \beta\int_0^y (x-y)v_2(x)dx + 2y,$$

$$y^2v_2(y) = \beta\int_0^y (y-x)v_1(x)dx + \int_0^y ((2+\beta^2)x - (2+\beta^2 y))v_2(x)dx,$$

$$K_{\frac{1}{2}+i\beta}(x) = (\frac{\pi}{2x})^{\frac{1}{2}} e^{-x}(v_1(\frac{1}{x}) + iv_2(\frac{1}{x}),\ x \geq 1.$$

The following formulas for the coefficients of canonical vector-polynomials are derived [16]

$$q_{1m}^{(1)} = \frac{(\beta^2 + m(m+1))(m+1)(m+2)}{(\beta^2 + m(m+1))^2 + \beta^2}, \qquad q_{2m}^{(1)} = \frac{\beta(m+2)(m+1)}{(\beta^2 + m(m+1))^2 + \beta^2},$$

$$q_{1m}^{(2)} = -q_{2m}^{(1)}, \qquad q_{2m}^{(2)} = q_{1m}^{(1)},$$

$$q_{1i}^{(j)} = -\frac{2(i+1)((\beta^2 + i(i+1))q_{1i+1}^{(j)} - \beta q_{2i+1}^{(j)})}{(\beta^2 + i(i+1))^2 + \beta^2},$$

$$q_{2i}^{(j)} = -\frac{2(i+1)(\beta q_{1i+1}^{(j)} + (\beta^2 + i(i+1))q_{2i+1}^{(j)})}{(\beta^2 + i(i+1))^2 + \beta^2},$$

$$i = m-1, \ldots, 0, \quad j = 1, 2.$$

By means of computations is shown that the choice of the residue in the form $P_{jn+2}(y) = \tau_{jn+2}T_{n+2}[(1-\alpha_{n+2})y + \alpha_{n+2}]$, $j = 1, 2$, is optimal as compared with other known variants in this case too.

The applications for the numerical solution of boundary value problems in wedge domains are given in [18],[19].

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