# Computing the Macdonald function for complex orders

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# Integral representation

$$K_\nu(x) = \int_0^\infty e^{-x\cosh t} \cosh \nu t \, \mathrm{d}t, \;\; x > 0$$

complex order $\nu = \alpha + \mathrm{i}\beta$

$$\mathrm{Re}\, K_{\alpha+\mathrm{i}\beta}(x) = \int_0^\infty e^{-x\cosh t} \cosh \alpha t \cos \beta t \, \mathrm{d}t,$$

$$\mathrm{Im}\, K_{\alpha+\mathrm{i}\beta}(x) = \int_0^\infty e^{-x\cosh t} \sinh \alpha t \sin \beta t \, \mathrm{d}t.$$

it suffices to consider $0 \le \alpha \le 1$; assume $|\beta| \le 10$

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$K_{\mathrm{i}\beta}$ and $K_{1/2+\mathrm{i}\beta}$ are the kernels in the ordinary and modified Kontorovich–Lebedev integral transform

# Gauss quadrature

weight function

$$w(u) = \exp(-e^u), \quad 0 \le u < \infty$$

recurrence coefficients for orthogonal polynomials

computed by a multiple-component discretization method based on $[0, \infty] = [0, .75] \cup [.75, 1.5] \cup [1.5, 3] \cup [3, \infty]$

```
global mc mp iq idelta irout DM uv AB
N=100; eps0=.5e-12;
mc=4; mp=0; iq=0; idelta=2; Mmax=900;
AB=[[0 .75];[.75 1.5];[1.5 3];[3 Inf]];
[ab,Mcap,kount]=mcdis(N,eps0,@quadgp,Mmax);
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```

n-point Gauss formula for $\mathtt{n} \le \mathrm{N}$

```
load -ascii ab;
xw=gauss(n,ab);
```

# The function $K_\nu(x)$ for $x \geq 1$

change of variables

$$e^{-x\cosh t} = e^{-\frac{1}{2}xe^{t}} \cdot e^{-\frac{1}{2}xe^{-t}} = e^{-\frac{1}{2}x} \cdot e^{-\frac{1}{2}x(e^{t}-1)} \cdot e^{-\frac{1}{2}xe^{-t}}$$

new variable

$$\tfrac{1}{2}x(e^{t}-1) = e^{u}-1, \quad 0 \leq u < \infty$$

transformed formulae

$$\operatorname{Re} K_{\alpha+\mathrm{i}\beta}(x) = \tfrac{1}{2}(2/x)^{\alpha} e^{1-\frac{1}{2}x} \int_0^\infty e^{-e^{u}} f(u;\alpha,\beta,x)\,\mathrm{d}u,$$

$$\operatorname{Im} K_{\alpha+\mathrm{i}\beta}(x) = \tfrac{1}{2}(2/x)^{\alpha} e^{1-\frac{1}{2}x} \int_0^\infty e^{-e^{u}} g(u;\alpha,\beta,x)\,\mathrm{d}u,$$

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for 9-digit accuracy, Gauss quadrature with $n = 30$ suffi ces

diffi culty: for much smaller $x$, steep boundary layer phenomena develop in $f(u;\alpha,\beta,x)$, $g(u;\alpha,\beta,x)$

# The function $K_\nu(x)$ for $x < 1$

$$K_\nu(x) = \left( \int_0^c + \int_c^\infty \right) e^{-x\cosh t} \cosh \nu t \, \mathrm{d}t \qquad c > 0$$

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second integral

$$\int_c^\infty e^{-x\cosh t}\cosh \nu t = \int_0^\infty e^{-x\cosh(\tau+c)}\cosh \nu(\tau + c)\mathrm{d}\tau$$

change of variables with $\xi := xe^c$

$$e^{-x\cosh(\tau+c)} = e^{-\frac{1}{2}\xi} \cdot e^{-\frac{1}{2}\xi(e^\tau - 1)} \cdot e^{-\frac{1}{2}\xi e^{-2c} e^{-\tau}}$$

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looks very much like before with $\xi$ replacing $x$. Since $x = 1$ was OK before, $\xi = 1$ should be OK now. This determines $c = \ln(1/x)$.

## transformed formulae

$$\mathrm{Re}\, K_{\alpha+\mathrm{i}\beta}(x) = c \int_0^1 e^{-x\cosh(\tau c)} \cosh(\alpha c\tau)\cos(\beta c\tau)\mathrm{d}\tau + \tfrac{1}{2}(2/x)^{\alpha} e^{\frac{1}{2}} \int_0^{\infty} e^{-e^u} \varphi(u;\alpha,\beta,x)\mathrm{d}u,$$

$$\mathrm{Im}\, K_{\alpha+\mathrm{i}\beta}(x) = c \int_0^1 e^{-x\cosh(\tau c)} \sinh(\alpha c\tau)\sin(\beta c\tau)\mathrm{d}\tau + \tfrac{1}{2}(2/x)^{\alpha} e^{\frac{1}{2}} \int_0^{\infty} e^{-e^u} \psi(u;\alpha,\beta,x)\mathrm{d}u,$$

$n_1$-point Gauss-Legendre resp. $n_2$-point Gauss

for $.01 \le x \le 1$ and 9-digit accuracy, $n_1 = 30$ and $n_2 = 30$ suffice

# The function $K_\nu(x)$ for $x \le .01$

$$K_\nu(x) = \frac{\pi/2}{\sin \nu\pi} \left(I_{-\nu}(x) - I_\nu(x)\right), \quad \nu \notin \mathbb{N}$$

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combine power series expansions for $I_{\pm\nu}$ with reflection formula for the gamma function

$$\Gamma(\nu)\Gamma(1-\nu) = \frac{\pi}{\sin \nu\pi}$$

three-term approximation

$$K_\nu(x) \approx \tfrac{1}{2}\left(\tfrac{x}{2}\right)^{-\nu}\Gamma(\nu)\left[1 + \tfrac{x^2}{4(1-\nu)} + \tfrac{x^4}{32(1-\nu)(2-\nu)}\right] + \tfrac{1}{2}\left(\tfrac{x}{2}\right)^{\nu}\Gamma(-\nu)\left[1 + \tfrac{x^2}{4(1+\nu)} + \tfrac{x^4}{32(1+\nu)(2+\nu)}\right]$$

# The function $K_{\alpha+\mathrm{i}\beta}$ for $|\beta| > 10$

computationally difficult and complex

alternative   symbolic computation

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Matlab

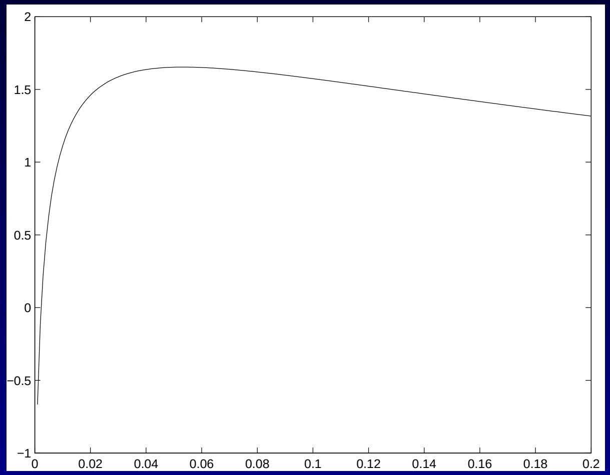
```
K=mfun('BesselK',a+b*i,x)
```

Example

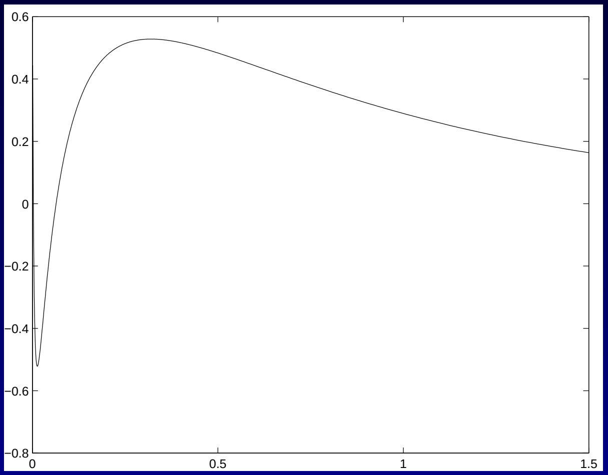
```
>> K=mfun('BesselK',15*i,2)
K =
     3.697490757619081e-11
```

# Plots of $K_{\mathrm{i}\beta}$

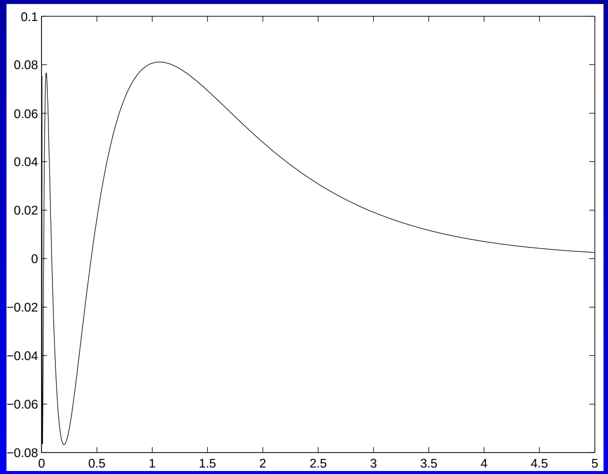
$\beta = 1/2$



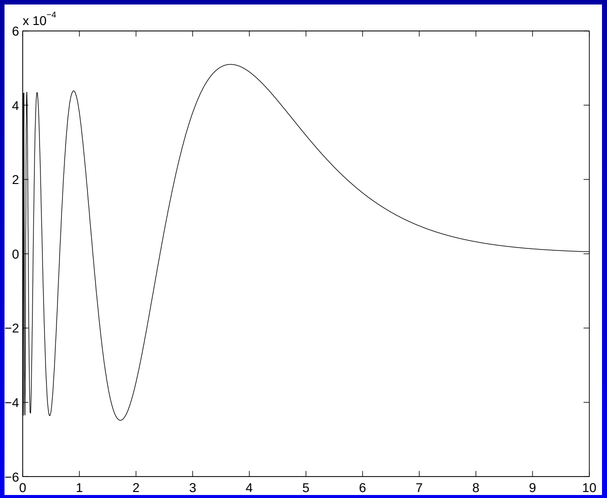

$\beta = 1$




$\beta = 2$

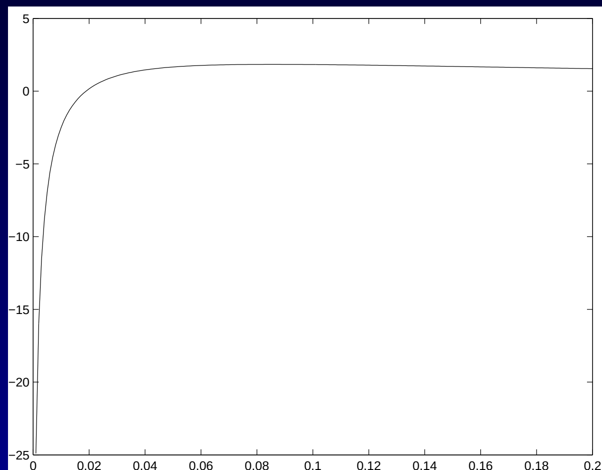


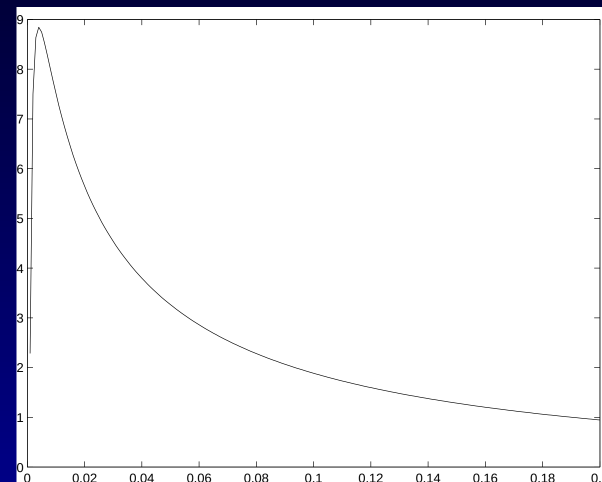

$\beta = 5$



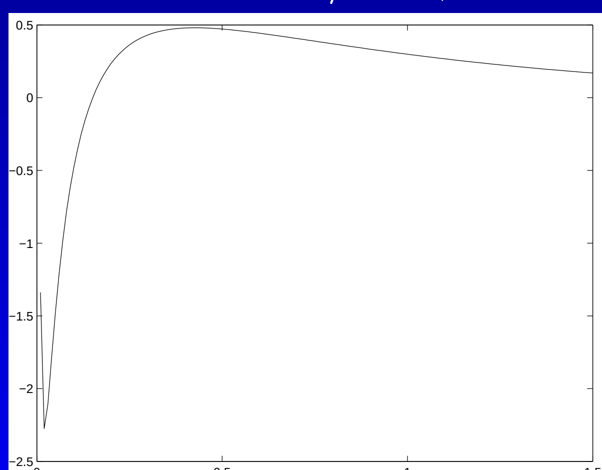
# Plots of $K_{1/2+\mathrm{i}\beta}$

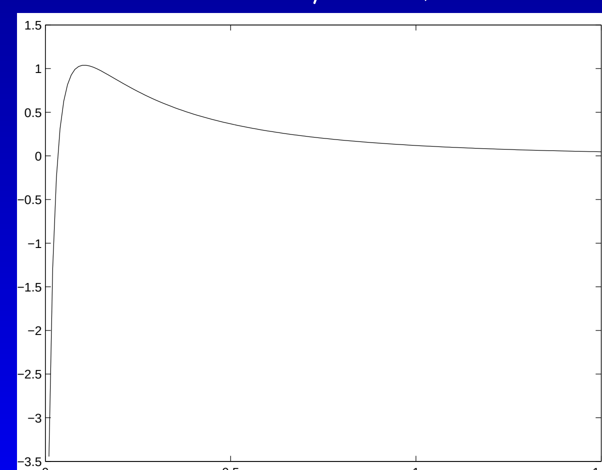
$\mathrm{Re}\, K_{1/2+\mathrm{i}\beta}$ $\beta = 1/2$ $\mathrm{Im}\, K_{1/2+\mathrm{i}\beta}$



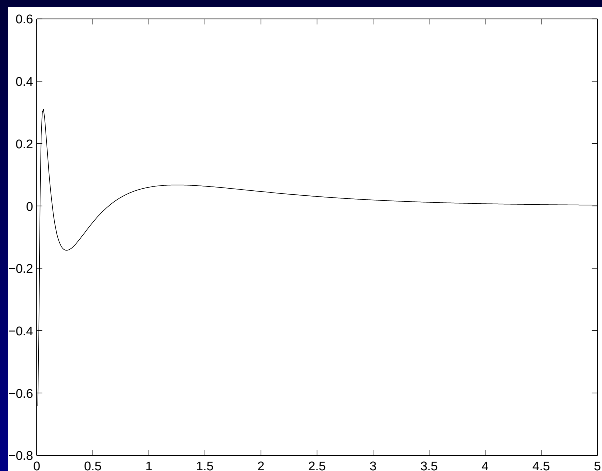

$\mathrm{Re}\, K_{1/2+\mathrm{i}\beta}$ $\beta = 1$ $\mathrm{Im}\, K_{1/2+\mathrm{i}\beta}$

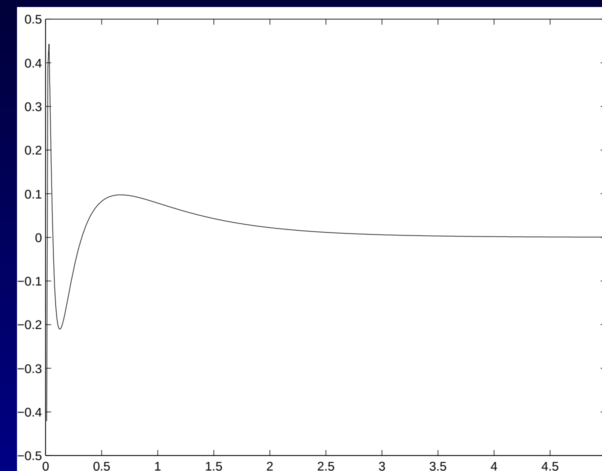


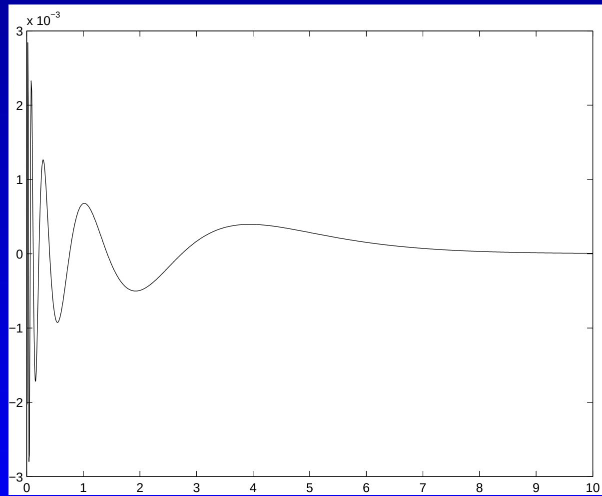
# Plots of $K_{1/2+\mathrm{i}\beta}$ (cont')

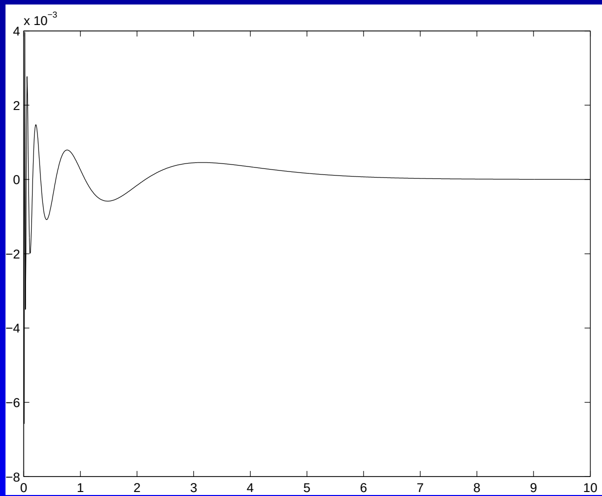
$\mathrm{Re}\, K_{1/2+\mathrm{i}\beta}$ $\beta = 2$ $\mathrm{Im}\, K_{1/2+\mathrm{i}\beta}$




$\mathrm{Re}\, K_{1/2+\mathrm{i}\beta}$ $\beta = 5$ $\mathrm{Im}\, K_{1/2+\mathrm{i}\beta}$



# Behavior at infinity and zero of $K_{\mathrm{i}\beta}$

$$K_{\mathrm{i}\beta}(x) \sim \sqrt{\frac{\pi}{2x}}\, e^{-x}, \quad x \to \infty$$

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$$K_{\mathrm{i}\beta}(x) \sim \sqrt{\frac{\pi}{\beta \sinh \beta\pi}}\, k(x,\beta), \quad x \downarrow 0$$

where

$$k(x,\beta) = \sin(\beta \ln(2/x) + \arg\Gamma(1+\mathrm{i}\beta))$$

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note

$$\gamma := \arg\Gamma(1+\mathrm{i}\beta) = \operatorname{Im}\left[\ln\Gamma(1+\mathrm{i}\beta)\right]$$

# Computing the Kontorovich-Lebedev transform

$$F(\beta) = \int_0^\infty K_{\mathrm{i}\beta}(x) f(x) \mathrm{d}x, \quad \beta > 0$$

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Gauss–Laguerre on

$$\int_2^\infty K_{\mathrm{i}\beta}(x) f(x) \mathrm{d}x = \int_0^\infty [e^t K_{\mathrm{i}\beta}(2+t) f(2+t)] e^{-t} \mathrm{d}t$$

## computing the KL transform (cont')

special treatment of

$$\int_0^2 K_{\mathrm{i}\beta}(x) f(x) \mathrm{d}x = \int_0^2 [K_{\mathrm{i}\beta}(x) - \sqrt{\frac{\pi}{\beta \sinh \beta\pi}}\, k(x,\beta)]$$

$$f(x)\mathrm{d}x + \sqrt{\frac{\pi}{\beta \sinh \beta\pi}} \int_0^2 f(x) \sin(\beta \ln(2/x) + \gamma) \mathrm{d}x$$

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Gauss–Legendre on first, and Gauss–Laguerre on second integral,

$$\int_0^2 f(x) \sin(\beta \ln(2/x) + \gamma)\mathrm{d}x = 2\int_0^\infty f(2e^{-t}) \sin(\beta t + \gamma) e^{-t}\mathrm{d}t$$

## Special Gaussian quadrature

$$\int_0^1 f(2t)\sin(\beta\ln(1/t)+\gamma)\mathrm{d}t$$
$$= \int_0^1 f(2t)w_\beta(t)\mathrm{d}t - \int_0^1 f(2t)\mathrm{d}t$$

where

$$w_\beta(t) = 1+\sin(\beta\ln(1/t)+\gamma) \ \text{ on } [0,1]$$

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moments of $w_\beta$

$$m_k = \int_0^1 t^k w_\beta(t)\mathrm{d}t = \frac{1}{k+1} + \frac{1}{(k+1)^2+\beta^2}\left((k+1)\sin\gamma + \beta\cos\gamma\right), \quad k = 0, 1, 2, \ldots$$

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symb/vpa-Chebyshev algorithm

$\Longrightarrow$ orthogonal polynomials $\Longrightarrow$ Gauss formula