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Computing Integrals of Highly Oscillatory Special Functions Using Complex Integration Methods and Gaussian Quadratures

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Abstract

An account on computation of integrals of highly oscillatory functions based on the so-called *complex integration methods* is presented. Beside the basic idea of this approach some applications in computation of Fourier and Bessel transformations are given. Also, Gaussian quadrature formulas with a modified Hermite weight are considered, including some numerical examples.

1 Introduction and Preliminaries

In this paper we give an account on computing integrals of highly oscillatory functions based on the so-called *complex integration methods* and using quadrature processes in general, as well as some new results and numerical examples. Some of these results have been recently presented during author's lecture at the *4th Dolomites Workshop on Constructive Approximation and Applications*, Session: *Numerical integration, integral equations and transforms* (September 8–13, 2016, Alba di Canazei, Italy).

We deal here with integration of functions of the form

$$I(f,K)=I(f(\cdot),K(\cdot;x))=\int_a^b w(t)f(t)K(t;x)\,\mathrm{d}t, \tag{1}$$

where (a,b) is an interval on the real line, which may be finite or infinite, $w(t)$ is a given weight function, and the kernel $K(t;x)$ is a function depending on a parameter x and such that it is highly oscillatory or/and has singularities on the interval (a,b) or in its nearness. Typical examples of such kernels are:

(a) Oscillatory kernel $K(t;x)=\mathrm{e}^{\mathrm{i}xt}$, where $x=\omega$ is a large positive parameter. Then we have Fourier integrals over $(0,+\infty)$ (*Fourier transforms*)

$$\mathcal{F}(f;\omega)=\int_0^{+\infty} t^{\mu}f(t)\mathrm{e}^{\mathrm{i}\omega t}\,\mathrm{d}t \qquad (\mu>-1)$$

or *Fourier coefficients* (on a finite interval)

$$c_k(f)=a_k(f)+\mathrm{i}b_k(f)=\frac{1}{\pi}\int_{-\pi}^{\pi} f(t)\mathrm{e}^{\mathrm{i}kt}\,\mathrm{d}t, \tag{2}$$

where $\omega=k\in\mathbb{N}$.

(b) Oscillatory kernels $K(t;x)=H_\nu^{(m)}(xt)$, where $x=\omega$ is also a large positive parameter. These integral transforms are known as *Hankel* (or *Bessel*) *transforms* (see Wong [51]),

$$\mathcal{H}_m(x)=\int_0^{+\infty} t^{\mu}f(t)H_\nu^{(m)}(\omega t)\,\mathrm{d}t \qquad (m=1,2), \tag{3}$$

where $H_\nu^{(m)}(t)$, $m=1,2$, are the Hankel functions of first and second type and order ν,

$$H_\nu^{(1)}(z)=J_\nu(z)+\mathrm{i}Y_\nu(z) \quad \text{and} \quad H_\nu^{(2)}(z)=J_\nu(z)-\mathrm{i}Y_\nu(z),$$

where J_ν is the *Bessel* function of the first kind and order (index) ν, defined by

$$J_\nu(z)=\sum_{k=0}^{+\infty}\frac{(-1)^k}{k!\Gamma(k+\nu+1)}\Big(\frac{z}{2}\Big)^{2k+\nu}, \qquad J_{-n}(z)=(-1)^nJ_n(z).$$

Otherwise, J_ν is a particular solution of the so-called *Bessel* differential equation

$$z^2y''+zy'+(z^2-\nu^2)y=0.$$

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The second linearly independent solution of this equation is the *Bessel* function of the second kind Y_ν (sometimes known as *Weber* or *Neumann* function),

$$Y_\nu(z) = \frac{J_\nu(z)\cos(\nu\pi) - J_{-\nu}(z)}{\sin(\nu\pi)}.$$

(c) Logarithmic singular kernel $K(t;x) = \log|t-x|$, where $a \le x \le b$.

(d) Algebraic singular kernel $K(t;x) = |t-x|^\alpha$, where $\alpha > -1$ and $a < x < b$.

Also, we mention here an important case when $K(t;x) = 1/(t-x)$, where $a < x < b$ and the integral (1) is taken to be a Cauchy principal value integral.

Integrals of rapidly oscillating functions appear mainly in the theory of special functions and Fourier analysis, but also in other applied and computational sciences and engineering, e.g., in theoretical physics (in particular, theory of scattering), acoustic scattering, quantum chemistry, theory of transport processes, electromagnetics, telecommunication, fluid mechanics, etc. For example, in the last time, a very attractive problem is the numerical solution of *Volterra* integral equation of the second (or first) kind with highly oscillatory kernel

$$y(x) + \int_0^x \frac{J_\nu(\omega(x-t))}{(x-t)^\alpha}\, y(t)\,\mathrm{d}t = \varphi(x),$$

or

$$\lambda y(x) + \int_0^x \frac{\mathrm{e}^{\mathrm{i}\omega g(x-t)}}{(x-t)^\alpha}\, y(t)\,\mathrm{d}t = \varphi(x),$$

where $x \in [0,1]$, $0 \le \alpha < 1$, $\omega \gg 1$, $\varphi(x)$ and $g(x)$ are given functions, and $y(x)$ is unknown function.

We mention also a type of integrals involving Bessel functions

$$I_\nu(f;\omega) = \int_0^{+\infty} \mathrm{e}^{-t^2} J_\nu(\omega t) f(t^2) t^{\nu+1}\,\mathrm{d}t, \quad \nu > -1,$$

with a large positive parameter ω. Such integrals appear in some problems of high energy nuclear physics (cf. [14]).

In Fig. 1 we present the graphics of $J_3(\omega x)$ and $Y_3(\omega x)$ on $[1,10]$ for some values of the parameter ω

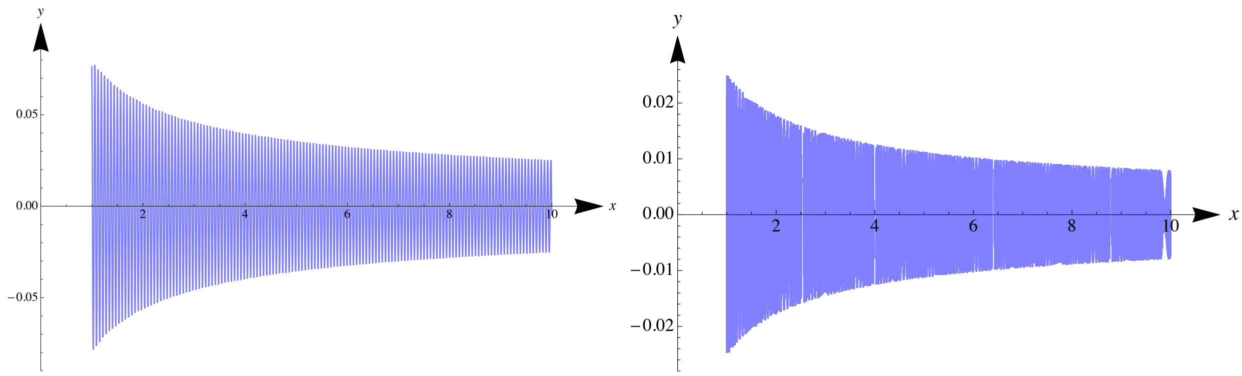


Figure 1: The graphics of $J_3(100x)$ *(left)* and $Y_3(1000x)$ *(right)* on $[1,10]$

Conventional techniques for computing values of special functions are power series, Chebyshev expansions, asymptotic expansions, recurrence relations, sequence transformations, continued fractions and best rational approximations, differential and difference equations, quadrature methods, etc. A nice survey on these methods, including a list of recent software for special functions as well as a list of new publications on computational aspects of special functions is given recently by Gil, Segura and Temme [18]. An application of standard quadrature formulas to $I(f;K)$ usually requires a large number of nodes and too much computation work in order to achieve a modest degree of accuracy. In a recent joint survey paper with M. Stanić [40] we discussed some specific nonstandard methods for numerical integration of highly oscillating functions, mainly based on some contour integration methods and applications of some kinds of Gaussian quadratures, including complex oscillatory weights. In particular, Filon-type quadratures for weighted Fourier integrals, exponential-fitting quadrature rules, Gaussian-type quadratures with respect to some complex oscillatory weights, methods for irregular oscillators, as well as two methods for integrals involving highly oscillating Bessel functions have been considered, including some numerical examples. In addition, we mention also the so-called integrals with *irregular oscillators*

$$I[f;g] = \int_a^b f(x)\mathrm{e}^{\mathrm{i}\omega g(x)}\,\mathrm{d}x, \tag{4}$$

where $-\infty < a < b < +\infty$, $|\omega|$ is large, and both f and g are sufficiently smooth functions. In a special case when $g(x) = x$, we have the so-called regular oscillators. Numerical calculation of the integrals 4 has been treated in a large number of papers (cf. [10, 11, 12], [22], [24], [26, 27, 28, 29], [31], [43, 44, 45, 46], etc.). The most important are asymptotic methods, Filon–type methods, and Levin–type methods. Asymptotic method was presented by Iserles and Nørsett [29].

Using suitable *integral representations of special functions*, in this paper, we show how existing or specially developed quadrature rules can be successfully applied to effectively calculation of highly oscillatory integrals (Fourier type integrals, oscillatory Bessel transformation, Bessel-Hilbert transformation, etc.). The procedure is based on an idea from our paper [35] from 1998, where, beside an account on some special – fast and efficient – quadrature methods for weighted integrals of strongly oscillatory functions, we introduced the so-called *Complex Integration Methods* for some classes of oscillatory integrals (1).

This paper is organized as follows. In Section 2 we give some basic facts on the *Complex Integration Methods*. Applications of these methods to integrals of highly oscillatory special functions are treated in Section 3. Finally, in Section 4 we consider Gaussian quadrature formuals with respect to a modified Hermite weight on $\mathbb{R}$.

2 Complex Integration Methods – Basic Idea

The basic idea of the *Complex Integration Methods* is to transform the integral of an oscillatory function to a weighed integral with respect to the exponentially decreasing weight function on $(0,+\infty)$.

First we illustrate this idea to calculation of the Fourier integrals on the finite interval $[-1,1]$,

$$I(f;\omega)=\int_{-1}^{1} f(x)\mathrm{e}^{\mathrm{i}\omega x}\,\mathrm{d}x, \tag{5}$$

assuming that f is an analytic real-valued function in the half-strip of the complex plane, $-1\le \operatorname{Re} z\le 1$, $\operatorname{Im} z\ge 0$, with possible singularities at the points z_ν $(\nu=1,\ldots,m)$ inside the region

$$G_\delta=\Big\{z\in\mathbb{C}\ \Big|\ -1\le \operatorname{Re} z\le 1,\ 0\le \operatorname{Im} z\le\delta\Big\},$$

where δ is sufficiently large.

Now we suppose that the corresponding residues of these singularities give

$$2\pi\mathrm{i}\sum_{\nu=1}^{m}\operatorname*{Res}_{z=z_\nu}\Big\{f(z)\mathrm{e}^{\mathrm{i}\omega z}\Big\}=P+iQ, \tag{6}$$

as well as that there exist the constants $M>0$, $\delta_0>0$ and $\xi<\omega$ such that

$$\int_{-1}^{1}|f(x+\mathrm{i}\delta)|\,\mathrm{d}x\le M\mathrm{e}^{\xi\delta}\quad(\delta>\delta_0>0). \tag{7}$$

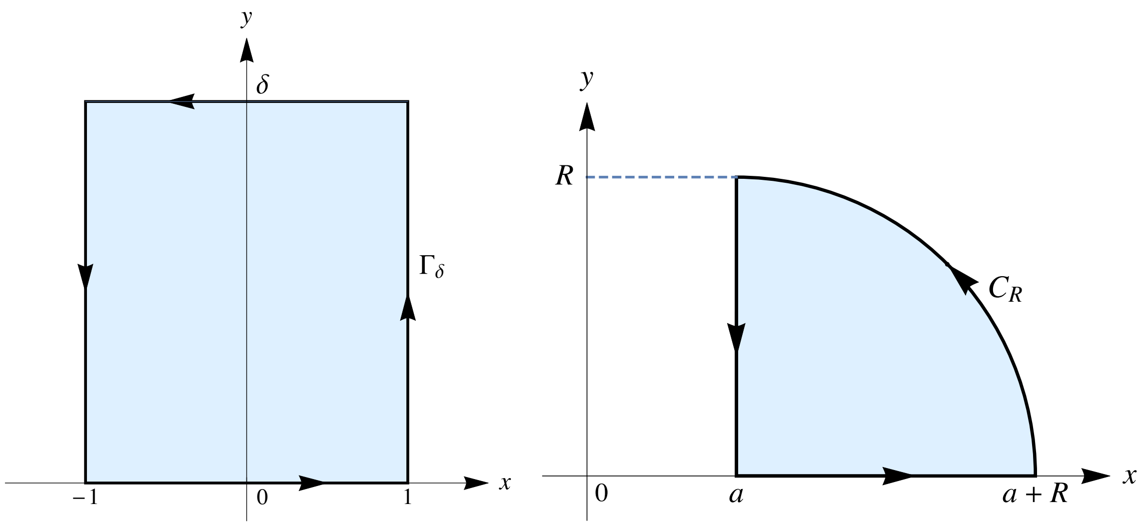


Figure 2: The contours of integration Γ_δ *(left)* and C_R *(right)*

By integrating the function $z\mapsto f(z)\mathrm{e}^{\mathrm{i}\omega z}$ over the contour $\Gamma_\delta=\partial G_\delta$ (see Fig. 2 (left)), we have

$$\begin{aligned}\oint_{\Gamma_\delta} f(z)\mathrm{e}^{\mathrm{i}\omega z}\,\mathrm{d}z &= \int_0^\delta f(1+\mathrm{i}y)\mathrm{e}^{\mathrm{i}\omega(1+\mathrm{i}y)}\mathrm{i}\,\mathrm{d}y+\int_1^{-1} f(x+\mathrm{i}\delta)\mathrm{e}^{\mathrm{i}\omega(x+\mathrm{i}\delta)}\,\mathrm{d}x+\int_\delta^0 f(-1+\mathrm{i}y)\mathrm{e}^{\mathrm{i}\omega(-1+\mathrm{i}y)}\mathrm{i}\,\mathrm{d}y+I(f;\omega)\\ &= 2\pi\mathrm{i}\sum_{\nu=1}^{m}\operatorname*{Res}_{z=z_\nu}\Big\{f(z)\mathrm{e}^{\mathrm{i}\omega z}\Big\}=P+\mathrm{i}Q,\end{aligned}$$

i.e.,

$$I(f;\omega)=P+\mathrm{i}Q+\mathrm{i}\int_0^\delta\Big[\mathrm{e}^{-\mathrm{i}\omega}f(-1+\mathrm{i}y)-\mathrm{e}^{\mathrm{i}\omega}f(1+\mathrm{i}y)\Big]\mathrm{e}^{-\omega y}\,\mathrm{d}y+\int_{-1}^{1}(x+\mathrm{i}\delta)\mathrm{e}^{\mathrm{i}\omega}f(x+\mathrm{i}\delta)\,\mathrm{d}x.$$

Because of (7) we conclude that

$$\begin{aligned} |I_\delta| &= \left|\int_{-1}^{1} f(x+\mathrm{i}\delta)\mathrm{e}^{\mathrm{i}\omega(x+\mathrm{i}\delta)}\,\mathrm{d}x\right| = \mathrm{e}^{-\omega\delta}\left|\int_{-1}^{1} f(x+\mathrm{i}\delta)\mathrm{e}^{\mathrm{i}\omega x}\,\mathrm{d}x\right| \\ &\leq \mathrm{e}^{-\omega\delta}\int_{-1}^{1} |f(x+\mathrm{i}\delta)|\,\mathrm{d}x \leq M\mathrm{e}^{(\xi-\omega)\delta}. \end{aligned}$$

Thus, $I_\delta \to 0$ when $\delta \to +\infty$, and

$$I(f;\omega) = P + \mathrm{i}Q + \frac{1}{\mathrm{i}\omega}\int_0^{+\infty}\left[\mathrm{e}^{\mathrm{i}\omega} f\left(1+\mathrm{i}\frac{t}{\omega}\right) - \mathrm{e}^{-\mathrm{i}\omega} f\left(-1+\mathrm{i}\frac{t}{\omega}\right)\right]\mathrm{e}^{-t}\,\mathrm{d}t. \tag{8}$$

In this way we proved the following result:

Theorem 2.1 ([35]). *Let f be an analytic real-valued function in the half-strip of the complex plane, $-1 \leq \operatorname{Re} z \leq 1$, $\operatorname{Im} z \geq 0$, with possible singularities z_ν ($\nu = 1,\ldots,m$) in the region $G_\delta = \operatorname{int}\Gamma_\delta$, such that (6) holds. Supposing that there exist the constants $M > 0$ and $\xi < \omega$ such that the condition (7) holds for sufficiently large δ, we have (8).*

The obtained integral (8) in Theorem 2.1 can be solved by using the Gauss-Laguerre rule.

In order to illustrate the efficiency of this method we consider a simple example – Fourier coefficients (2), with $f(t) = 1/(t^2+\varepsilon^2)^m$ ($m \in \mathbb{N}$, $\varepsilon > 0$). Thus, we are interested in the integrals

$$c_k(f) = \int_{-1}^{1} f(x)\mathrm{e}^{\mathrm{i}k\pi x}\,\mathrm{d}x, \qquad \omega = k\pi.$$

According to (8), for $1 \leq m \leq 3$, we have

$$c_k(f) = P + \mathrm{i}Q + \frac{(-1)^k}{\mathrm{i}k\pi}\int_0^{+\infty}\left[f\left(1+\mathrm{i}\frac{t}{k\pi}\right) - f\left(-1+\mathrm{i}\frac{t}{k\pi}\right)\right]\mathrm{e}^{-t}\,\mathrm{d}t,$$

where, in our case, we have

$$f(z) = \frac{1}{(z^2+\varepsilon^2)^m}, \quad P + \mathrm{i}Q = 2\pi\mathrm{i}\operatorname*{Res}_{z=\mathrm{i}\varepsilon}\left\{f(z)\mathrm{e}^{\mathrm{i}k\pi z}\right\} = \begin{cases} \dfrac{\pi}{\varepsilon}\mathrm{e}^{-k\pi\varepsilon}, & m = 1, \\ \dfrac{\pi(1+k\pi\varepsilon)}{2\varepsilon^3}\mathrm{e}^{-k\pi\varepsilon}, & m = 2, \\ \dfrac{\pi(3+3k\pi\varepsilon+k^2\pi^2\varepsilon^2)}{8\varepsilon^5}\mathrm{e}^{-k\pi\varepsilon}, & m = 3. \end{cases}$$

For calculating $c_5(f)$, $c_{10}(f)$ and $c_{40}(f)$, when $\varepsilon = 1$ and $\varepsilon = 10^{-2}$, we apply the n-point Gauss-Laguerre rule for $n = 1,\ldots,7$ nodes. The corresponding relative errors in quadrature approximations are given in Table 1. Numbers in parentheses indicate decimal exponents. As we can see the convergence is faster for larger k (and smaler ε).

Table 1: Relative errors in n-point Gauss-Laguerre approximations of $c_k(f)$ for $k = 5, 10, 40$ and $\varepsilon = 1$ and 10^{-2}

	$k=5$		$k=10$		$k=40$	
n	$\varepsilon=1$	$\varepsilon=10^{-2}$	$\varepsilon=1$	$\varepsilon=10^{-2}$	$\varepsilon=1$	$\varepsilon=10^{-2}$
1	1.11(−2)	1.69(−9)	2.60(−3)	1.28(−10)	1.59(−4)	7.91(−13)
2	3.48(−4)	1.38(−10)	2.56(−5)	3.40(−12)	1.04(−7)	1.45(−15)
3	2.12(−5)	8.83(−12)	2.71(−7)	1.02(−13)	5.78(−11)	3.35(−18)
4	3.84(−7)	1.03(−13)	3.25(−9)	3.21(−15)	5.45(−14)	9.92(−21)
5	3.49(−8)	7.80(−14)	1.29(−10)	8.69(−17)	8.20(−13)	4.48(−22)
6	8.46(−9)	9.35(−15)	4.06(−12)	2.94(−19)	4.77(−12)	2.39(−21)
7	1.61(−9)	6.62(−16)	1.65(−13)	2.21(−19)	5.40(−14)	2.75(−23)

Table 2: Gaussian approximation of the integral $c_k(f)$

k	$\varepsilon=1$	$\varepsilon=10^{-2}$
5	$4.0039258\underline{346130827412}(-3)$	$1.55333209782728\underline{2899812027}(+6)$
10	$-1.010071027052\underline{0897087}(-3)$	$1.507753137017524820\underline{873537}(+6)$
40	$-6.331369411209\underline{4129150}(-5)$	$1.0088603450377737040756\underline{38}(+6)$

Approximative values obtained by 7-point Gauss-Laguerre rule are presented in Table 2. Digits in error are underlined.

Now we consider the Fourier integral on $(0,+\infty)$,

$$F(f;\omega)=\int_0^{+\infty} f(x)\mathrm{e}^{\mathrm{i}\omega x}\,\mathrm{d}x,$$

which can be transformed to

$$F(f;\omega)=\frac{1}{\omega}\int_0^{+\infty} f\left(\frac{x}{\omega}\right)\mathrm{e}^{\mathrm{i}x}\,\mathrm{d}x=\frac{1}{\omega}F\left(f\left(\frac{\cdot}{\omega}\right);1\right),$$

which means that is enough to consider only the case $\omega=1$.

In order to calculate $F(f;1)$ we select a positive number a and divide the integral over $(0,+\infty)$ into two integrals,

$$F(f;1)=\int_0^{a} f(x)\mathrm{e}^{\mathrm{i}x}\,\mathrm{d}x+\int_a^{+\infty} f(x)\mathrm{e}^{\mathrm{i}x}\,\mathrm{d}x=L_1(f)+L_2(f),$$

where

$$L_1(f)=a\int_0^{1} f(at)\mathrm{e}^{\mathrm{i}at}\,\mathrm{d}t \quad\text{and}\quad L_2(f)=\int_a^{+\infty} f(x)\mathrm{e}^{\mathrm{i}x}\,\mathrm{d}x.$$

For calculating the second integral $L_2(f)$ we use the complex integration method over the closed circular contour C_R presented in Fig. 2 (right).

Theorem 2.2 ([35]). *Suppose that the function $z\mapsto f(z)$ is defined and holomorphic in the region $D=\{z\in\mathbb{C}\,|\,\mathrm{Re}\,z\geq a>0,\ \mathrm{Im}\,z\geq 0\}$, and such that*

$$|f(z)|\leq\frac{A}{|z|},\quad \textit{when } |z|\to+\infty, \tag{9}$$

for some positive constant A. Then

$$L_2(f)=\mathrm{i}\mathrm{e}^{\mathrm{i}a}\int_0^{+\infty} f(a+\mathrm{i}y)\mathrm{e}^{-y}\,\mathrm{d}y \qquad (a>0). \tag{10}$$

In this case, by Cauchy's residue theorem, we have

$$\int_a^{a+R} f(x)\mathrm{e}^{\mathrm{i}x}\,\mathrm{d}x+\int_0^{\pi/2}\left[f(z)\mathrm{e}^{\mathrm{i}z}\right]_{z=a+R\mathrm{e}^{\mathrm{i}\theta}}R\mathrm{i}\mathrm{e}^{\mathrm{i}\theta}\,\mathrm{d}\theta+\int_R^{0} f(a+\mathrm{i}y)\mathrm{e}^{\mathrm{i}(a+\mathrm{i}y)}\mathrm{i}\,\mathrm{d}y=0. \tag{11}$$

Let $z=a+R\mathrm{e}^{\mathrm{i}\theta}$, $0\leq\theta\leq\pi/2$. Because of (9), we have that

$$|f(z)|\leq\frac{A}{|a+R\cos\theta+\mathrm{i}\sin\theta|}=\frac{A}{\sqrt{a^2+2aR\cos\theta+R^2}}\leq\frac{A}{\sqrt{a^2+R^2}} \quad (0\leq\theta\leq\pi/2).$$

Using Jordan's inequality $\sin\theta\geq 2\theta/\pi$, when $0\leq\theta\leq\pi/2$, we obtain the following estimate for the integral over the arc

$$\left|\int_0^{\pi/2}\left[f(z)\mathrm{e}^{\mathrm{i}z}\right]_{z=a+R\mathrm{e}^{\mathrm{i}\theta}}R\mathrm{i}\mathrm{e}^{\mathrm{i}\theta}\,\mathrm{d}\theta\right|\leq\int_0^{\pi/2}\left|f(a+R\mathrm{e}^{\mathrm{i}\theta})\right|\mathrm{e}^{-R\sin\theta}R\,\mathrm{d}\theta\leq\frac{\pi}{2}\cdot\frac{A}{\sqrt{a^2+R^2}}\cdot\frac{\pi}{2}\left(1-\mathrm{e}^{-R}\right)\to 0,$$

when $R\to+\infty$, and then (10) follows directly from (11).

In the numerical implementation we use the Gauss-Legendre rule on $(0,1)$ and Gauss-Laguerre rule for calculating $L_1(f)$ and $L_2(f)$, respectively.

3 Computing Integrals of Highly Oscillatory Special Functions

The idea on complex integration methods has been exploited in many papers, which are dealing with integrals of special functions, in particular with a highly oscillatory Bessel kernels (cf. Chen [4, 5, 6, 7, 8], Kang and Xiang [30], Xu, Milovanović and Xiang [53], Xu and Milovanović [52], Xu and Xiang [54], etc.). For example, Chen [4] considered the numerical evaluation of the integrals on (a,b), $0<a<b$, involving highly oscillatory Bessel kernel $J_\nu(\omega x)$, where $J_\nu(\omega x)$ is the Bessel function of the first kind and of order $\nu(>0)$ and ω is a large positive parameter. Using the integral form of Bessel function and its analytic continuation, he applied the complex integration methods to transform these integrals into the forms on $[0,+\infty)$ that the integrand does not oscillate and decays exponentially fast, and which can be efficiently computed by using Gauss-Laguerre quadrature rule.

Evaluation of Cauchy principal value integrals of oscillatory functions was also considered in such a way by Wang and Xiang [50], as well as applications to the computation of highly oscillatory Bessel Hilbert transforms [52]. We mention also the corresponding applications in solving Volterra and Fredholm integral equations with highly oscillatory kernels (cf. [13], [23], [32]).

Recently, Xu, Milovanović and Xiang [53] developed a method for efficient computation of highly oscillatory integrals with Hankel kernel,

$$I_1[f]=\int_a^{b} f(x)H_\nu^{(1)}(\omega x)\,\mathrm{d}x \quad\text{and}\quad I_2[f]=\int_a^{+\infty} f(x)H_\nu^{(1)}(\omega x)\,\mathrm{d}x, \tag{12}$$

for $\omega \gg 1$ and $b > a > 0$. Using the integral form of the Hankel function for $x > 0$ (see [20, p. 915])

$$H_\nu^{(1)}(\omega x) = \sqrt{\frac{2}{\pi\omega x}} \frac{e^{i(\omega x - \frac{\pi}{2}\nu - \frac{\pi}{4})}}{\Gamma(\nu+\frac{1}{2})} \int_0^{+\infty} \left(1 + \frac{it}{2\omega x}\right)^{\nu-\frac{1}{2}} t^{\nu-\frac{1}{2}} e^{-t}\, dt,$$

they obtained the following integral representations for the previous integrals:

$$I_1[f] = \sqrt{\frac{2}{\pi\omega}} \frac{e^{-i\pi(2\nu+1)/4}}{\Gamma(\nu+\frac{1}{2})} \int_a^b f(x) x^{-1/2} g(x) e^{i\omega x}\, dx \quad \text{and} \quad I_2[f] = \sqrt{\frac{2}{\pi\omega}} \frac{e^{-i\pi(2\nu+1)/4}}{\Gamma(\nu+\frac{1}{2})} \int_a^{+\infty} f(x) x^{-1/2} g(x) e^{i\omega x}\, dx,$$

where

$$g(x) = \int_0^{+\infty} \left(1 + \frac{it}{2\omega x}\right)^{\nu-\frac{1}{2}} t^{\nu-\frac{1}{2}} e^{-t}\, dt. \tag{13}$$

Supposing that f be a holomorphic function in the half-strip of the complex plane, $a \le \mathrm{Re}(z) \le b$, $\mathrm{Im}(z) \ge 0$, as well as that there exist two constants C and ω_0, such that $|f(x+iR)| \le Ce^{\omega_0 R}$, $a \le x \le b$, with $0 < \omega_0 < \omega$, the integral $I_1[f]$ can be reduced to (see [53])

$$I_1[f] = \frac{i}{\omega} \sqrt{\frac{2}{\pi\omega}} \frac{e^{-i\pi(2\nu+1)/4}}{\Gamma\left(\nu+\frac{1}{2}\right)} (G(a) - G(b)), \tag{14}$$

where

$$G(c) = e^{i\omega c} \int_0^{+\infty} F\left(c + \frac{i}{\omega} t\right) e^{-t}\, dt. \tag{15}$$

Really, (14) follows after an application of the complex integration method over the contour $\Gamma = \partial D = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_4$ (see Fig. 3 (left)), where D is the region

$$D = \left\{ z \in \mathbb{C} \;\middle|\; a \le \mathrm{Re}(z) \le b,\ 0 \le \mathrm{Im}(z) \le R \right\}.$$

In this case, the integrand $F(z) = f(z) z^{-1/2} g(z)$ is a holomorphic function in D, such that $\int_{\Gamma_1\cup\Gamma_2\cup\Gamma_3\cup\Gamma_4} F(z) e^{i\omega z}\, dz = 0$.

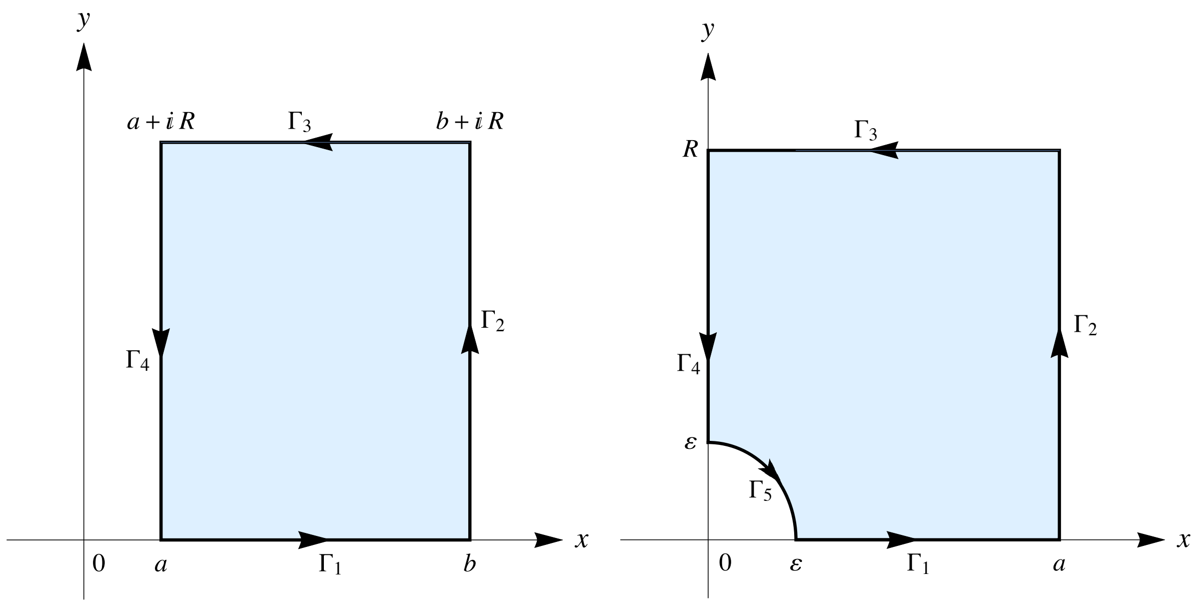


Figure 3: The contours of integration $\Gamma = \partial D$ (*left*) and $\Gamma = \partial(G \setminus G')$ (*right*)

Regarding the assumptions we can see that

$$\left| \int_{\Gamma_3} F(z) e^{i\omega z}\, dz \right| \le \int_{\Gamma_3} |F(z) e^{i\omega z}| |dz| \le CM e^{-(\omega-\omega_0)R} (b-a) \to 0 \quad \text{as} \quad R \to +\infty,$$

i.e., $\int_{\Gamma_3} F(z)\mathrm{e}^{\mathrm{i}\omega z}\,\mathrm{d}z \to 0$ as $R \to +\infty$, so that

$$\begin{aligned}
\int_{\Gamma_1} F(z)\mathrm{e}^{\mathrm{i}\omega z}\,\mathrm{d}z &= -\lim_{R\to+\infty}\int_{\Gamma_2\cup\Gamma_3\cup\Gamma_4} F(z)\mathrm{e}^{\mathrm{i}\omega z}\,\mathrm{d}z \\
&= \lim_{R\to+\infty}\left\{\mathrm{i}\int_0^R F(a+\mathrm{i}y)\mathrm{e}^{\mathrm{i}\omega(a+\mathrm{i}y)}\,\mathrm{d}y - \mathrm{i}\int_0^R F(b+\mathrm{i}y)\mathrm{e}^{\mathrm{i}\omega(b+\mathrm{i}y)}\,\mathrm{d}y\right\} \\
&= \frac{\mathrm{i}}{\omega}\int_0^{+\infty} \mathrm{e}^{\mathrm{i}\omega a}F\Big(a+\mathrm{i}\frac{t}{\omega}\Big)\mathrm{e}^{-t}\,\mathrm{d}t - \frac{\mathrm{i}}{\omega}\int_0^{+\infty} \mathrm{e}^{\mathrm{i}\omega b}F\Big(b+\mathrm{i}\frac{t}{\omega}\Big)\mathrm{e}^{-t}\,\mathrm{d}t \\
&= \frac{\mathrm{i}}{\omega}(G(a)-G(b)),
\end{aligned}$$

where

$$G(c) = \mathrm{e}^{\mathrm{i}\omega c}\int_0^{+\infty} F\Big(c+\frac{\mathrm{i}}{\omega}t\Big)\mathrm{e}^{-t}\,\mathrm{d}t.$$

Thus, we have

$$I_1[f] = \int_a^b f(x)H_\nu^{(1)}(\omega x)\,\mathrm{d}x = \sqrt{\frac{2}{\pi\omega}}\frac{\mathrm{e}^{-\mathrm{i}\pi(2\nu+1)/4}}{\Gamma\big(\nu+\frac{1}{2}\big)}\int_{\Gamma_1} F(z)\mathrm{e}^{\mathrm{i}\omega z}\,\mathrm{d}z,$$

i.e., (14).

Similarly, using a circular contour like one in Fig. 2 (right), the second integral in (12) can be reduced to

$$I_2[f] = \int_a^{+\infty} f(x)H_\nu^{(1)}(\omega x)\,\mathrm{d}x = \frac{\mathrm{i}}{\omega}\sqrt{\frac{2}{\pi\omega}}\frac{\mathrm{e}^{-\mathrm{i}\pi(2\nu+1)/4}}{\Gamma\big(\nu+\frac{1}{2}\big)}G(a).$$

Since $F(z) = f(z)z^{-1/2}g(z)$ and $g(x)$ defined in (13), after certain transformations, $G(c)$ can be transformed to (see [53])

$$G(c) = \mathrm{e}^{\mathrm{i}\omega c}\int_0^{+\infty}\int_0^{+\infty} \frac{f\big(c+\frac{\mathrm{i}}{\omega}t\big)}{\big(c+\frac{\mathrm{i}}{\omega}t\big)^\nu}\Big(c+\frac{\mathrm{i}}{\omega}t+\frac{\mathrm{i}}{2\omega}s\Big)^{\nu-1/2}\mathrm{e}^{-t}s^{\nu-1/2}\mathrm{e}^{-s}\,\mathrm{d}t\,\mathrm{d}s.$$

For computing this double integral, in [53] we used two classical Gaussian quadrature rules

$$\int_0^{+\infty} h(x)w_\ell(x)\,\mathrm{d}x = \sum_{k=1}^n A_{n,k}^{(\ell)}h(x_{n,k}^{(\ell)}) + R_n^{(\ell)}[h], \quad \ell = 1,2; \tag{16}$$

one with respect to the Laguerre weight $w_1(t) = \mathrm{e}^{-t}$ and the second one to the generalized Laguerre weight $w_2(s) = s^{\nu-1/2}\mathrm{e}^{-s}$. The coefficients in the three-term recurrence relations for the corresponding orthogonal polynomials,

$$\pi_{k+1}^{(\ell)}(x) = (x-\alpha_k^{(\ell)})\pi_k^{(\ell)}(x) - \beta_k^{(\ell)}\pi_{k-1}^{(\ell)}(x), \quad k = 0,1,\ldots,$$

with $\pi_0^{(\ell)}(x) = 1$, $\pi_{-1}^{(\ell)}(x) = 0$, are given by

$$\begin{aligned}
&\alpha_k^{(1)} = 2k+1, && \beta_0^{(1)} = 1,\ \ \beta_k^{(1)} = k^2; \\
&\alpha_k^{(2)} = 2k+\nu+\frac{1}{2}, && \beta_0^{(2)} = \Gamma\Big(\nu+\frac{1}{2}\Big),\ \ \beta_k^{(2)} = k\Big(k+\nu-\frac{1}{2}\Big),
\end{aligned}$$

respectively. With these recursive coefficients, it is easy to compute quadrature parameters in (16), the nodes $x_{n,k}^{(\ell)}$ and the weights (Christoffel numbers) $A_{n,k}^{(\ell)}$, using the well-known Golub-Welsch algorithm [19] (see also [33, p. 100]), with the Jacobi matrices

$$J_n(w_\ell) = \begin{bmatrix}
\alpha_0^{(\ell)} & \sqrt{\beta_1^{(\ell)}} & & & \mathbf{O} \\
\sqrt{\beta_1^{(\ell)}} & \alpha_1^{(\ell)} & \sqrt{\beta_2^{(\ell)}} & & \\
& \sqrt{\beta_2^{(\ell)}} & \alpha_2^{(\ell)} & \ddots & \\
& & \ddots & \ddots & \sqrt{\beta_{n-1}^{(\ell)}} \\
\mathbf{O} & & & \sqrt{\beta_{n-1}^{(\ell)}} & \alpha_{n-1}^{(\ell)}
\end{bmatrix} \quad (\ell = 1,2).$$

This algorithm is implemented in our MATHEMATICA package `OrthogonalPolynomials` (see [9], [38]), which is freely downloadable from the web site: `http://www.mi.sanu.ac.rs/~gvm/`.

Now, an application of quadrature formulas (16) to (14) gives

$$I_1[f] = Q_{n_1,n_2}[f] + R_{n_1,n_2}[f],$$

where the cubature sum $Q_{n_1,n_2}[f]$ (with n_1 nodes in the first quadrature and n_2 nodes in the second one) is given by

$$Q_{n_1,n_2}[f] = \frac{\mathrm{i}}{\omega}\sqrt{\frac{2}{\pi\omega}}\,\frac{\mathrm{e}^{-\mathrm{i}\pi(2\nu+1)/4}}{\Gamma\left(\nu+\frac{1}{2}\right)}\sum_{k=1}^{n_1}\sum_{j=1}^{n_2} A_{n_1,k}^{(1)} A_{n_2,j}^{(2)}\left[\varphi(x_{n_1,k}^{(1)}, x_{n_2,j}^{(2)}; a) - \varphi(x_{n_1,k}^{(1)}, x_{n_2,j}^{(2)}; b)\right],$$

where

$$\varphi(t,s;c) = \mathrm{e}^{\mathrm{i}\omega c}\frac{f\left(c+\frac{\mathrm{i}}{\omega}t\right)}{\left(c+\frac{\mathrm{i}}{\omega}t\right)^{\nu}}\left(c+\frac{\mathrm{i}}{\omega}t+\frac{\mathrm{i}}{2\omega}s\right)^{\nu-1/2}.$$

Theorem 3.1 ([53]). *Suppose that f is a holomorphic function in the half-strip of the complex plane, $a \le \mathrm{Re}(z) \le b$, $\mathrm{Im}(z) \ge 0$, and there exist two constants C and ω_0, such that $|f(x+\mathrm{i}R)| \le Ce^{\omega_0 R}$, $a \le x \le b$, with $0 < \omega_0 < \omega$. Then the error bound of the method for the integral $I_1[f]$ is given by*

$$I_1[f] - Q_{n_1,n_2}[f] = O\left(\omega^{-\frac{3}{2}-2\tau}\right), \quad \omega \gg 1,$$

where $\tau = \min\{n_1, n_2\}$.

A similar result has been proved for the quadrature method

$$\overline{Q}_{n_1,n_2}[f] = \frac{\mathrm{i}}{\omega}\sqrt{\frac{2}{\pi\omega}}\,\frac{\mathrm{e}^{-\mathrm{i}\pi(2\nu+1)/4}}{\Gamma\left(\nu+\frac{1}{2}\right)}\sum_{k=1}^{n_1}\sum_{j=1}^{n_2} A_{n_1,k}^{(1)} A_{n_2,j}^{(2)}\varphi\left(x_{n_1,k}^{(1)}, x_{n_2,j}^{(2)}; a\right)$$

for calculating $I_2[f]$.

Theorem 3.2 ([53]). *Suppose that f is a holomorphic function in the complex plane $\left\{0 \le \arg(z) \le \pi/2\right\}$, and there exists some constant C_1, such that $|f(z)| \le C_1$ as $|z| \to +\infty$. Then the error bound of the method for the integral $I_2[f]$ is given by*

$$I_2[f] - \overline{Q}_{n_1,n_2}[f] = O\left(\omega^{-\frac{3}{2}-2\tau}\right), \quad \omega \gg 1,$$

where $\tau = \min\{n_1, n_2\}$.

As we can see the convergence of quadrature sums $Q_{n_1,n_2}[f]$ and $\overline{Q}_{n_1,n_2}[f]$ to $I_1[f]$ and $I_2[f]$, respectively, is very fast, especially for larger ω.

In the sequel we mention another approach for computing the Bessel transformations

$$I_1[f] = \int_0^a f(x)J_\nu(\omega x)\,\mathrm{d}x \quad \text{and} \quad I_2[f] = \int_0^{+\infty} f(x)J_\nu(\omega x)\,\mathrm{d}x,$$

where $a > 0$ and ν is an arbitrary nonnegative number. The method has been recently developed in a joint paper by Xu [52] and it is based on the use of the following important identity

$$J_\nu(z) = \frac{1}{(2\pi z)^{1/2}}\left\{\mathrm{e}^{\frac{1}{2}(\nu+\frac{1}{2})\pi\mathrm{i}}W_{0,\nu}(2\mathrm{i}z) + \mathrm{e}^{-\frac{1}{2}(\nu+\frac{1}{2})\pi\mathrm{i}}W_{0,\nu}(-2\mathrm{i}z)\right\}, \tag{17}$$

where $W_{\kappa,\mu}(z)$ is the *Whittaker W* function, as well as its asymptotic property as $z \to 0$,

$$W_{0,\nu}(z) \sim \begin{cases} z^{1/2}\log z, & \nu = 0, \\ z^{1/2-\nu}, & \nu > 0. \end{cases} \tag{18}$$

Based on an idea of Chen [8], we rewrite the integral $I_1[f]$ as a sum $I_1[f] = I_1'[f] + I_1''[f]$, where

$$I_1'[f] = \int_0^a F(x)J_\nu(\omega x)\,\mathrm{d}x \quad \text{and} \quad I_1''[f] = \sum_{k=0}^{2n-1+n_1}\frac{f^{(k)}(0)}{k!}\int_0^a x^k J_\nu(\omega x)\,\mathrm{d}x, \tag{19}$$

where $n_1 = \lceil \nu \rceil$ is the smallest integer not less than ν, and

$$F(x) = f(x) - \sum_{k=0}^{2n-1+n_1}\frac{f^{(k)}(0)}{k!}x^k. \tag{20}$$

The integral in $I_1''[f]$ can be expressed in the explicit form [20, p. 676]

$$\int_0^a x^k J_\nu(\omega x)\,\mathrm{d}x = \frac{2^k\Gamma(\frac{k+\nu+1}{2})}{\omega^{k+1}\Gamma(\frac{\nu-k+1}{2})} + \frac{a}{\omega^k}\left\{(k+\nu-1)J_\nu(\omega a)s_{k-1,\nu-1}^{(2)}(\omega a) - J_{\nu-1}(\omega a)s_{k,\nu}^{(2)}(\omega a)\right\},$$

where $s_{k,\nu}^{(2)}(z)$ denotes the second kind of Lommel function.

For the integral $I_1'[f]$ we put

$$F_1(x) = F(x)x^{-1/2}\mathrm{e}^{-\mathrm{i}\omega x}W_{0,\nu}(-2\mathrm{i}\omega x) \quad \text{and} \quad F_2(x) = F(x)x^{-1/2}\mathrm{e}^{\mathrm{i}\omega x}W_{0,\nu}(2\mathrm{i}\omega x), \tag{21}$$

where F is defined in (20). Now, according to the identity (17), we can see that

$$\begin{aligned} F(z)J_\nu(\omega z) &= \frac{1}{\sqrt{2\pi\omega}}\Big\{\mathrm{e}^{\frac{1}{2}(\nu+\frac{1}{2})\pi\mathrm{i}}F(z)z^{-1/2}W_{0,\nu}(2\mathrm{i}\omega z) + \mathrm{e}^{-\frac{1}{2}(\nu+\frac{1}{2})\pi\mathrm{i}}F(z)z^{-1/2}W_{0,\nu}(-2\mathrm{i}\omega z)\Big\} \\ &= \frac{1}{\sqrt{2\pi\omega}}\Big\{\mathrm{e}^{-\frac{1}{2}(\nu+\frac{1}{2})\pi\mathrm{i}}F_1(z)\mathrm{e}^{\mathrm{i}\omega z} + \mathrm{e}^{\frac{1}{2}(\nu+\frac{1}{2})\pi\mathrm{i}}F_2(z)\mathrm{e}^{-\mathrm{i}\omega z}\Big\}. \end{aligned}$$

In order to calculate the integral $I_1'[f]$ defined in (19) we suppose that f is a holomorphic function in the half-strip of the complex plane $0 \le \mathrm{Re}(z) \le a$ and define we define the regions $G = \Big\{z \in \mathbb{C} \;\Big|\; 0 \le \mathrm{Re}(z) \le a,\ 0 \le \mathrm{Im}(z) \le R\Big\}$ and $G' = \Big\{z \in \mathbb{C} \;\Big|\; |z| \le \varepsilon,\ 0 \le \arg(z) \le \pi/2\Big\}$, such that G contains G', i.e., $0 < \varepsilon < \min\{a, R\}$ (see Fig. 3 (right)). Then, we note that $z \mapsto F_1(z)\mathrm{e}^{\mathrm{i}\omega z}$ is holomorphic in $G \setminus G'$ (see (18) for behaviour at $z = 0$), as well as the function $z \mapsto F_2(z)\mathrm{e}^{-\mathrm{i}\omega z}$ in a symmetric region with respect to the real axis. Therefore, by the Cauchy Residue Theorem, $\int_\Gamma F_1(z)\mathrm{e}^{\mathrm{i}\omega z}\,\mathrm{d}z = 0$, where $\Gamma = \partial(G \setminus G') = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_4 \cup \Gamma_5$ (displayed in Fig. 3 (right)), as well as $\int_{\Gamma^*} F_2(z)\mathrm{e}^{-\mathrm{i}\omega z}\,\mathrm{d}z = 0$ over the symmetric contour Γ^* (w.r.t. the real axis).

Applying the complex integration method Xu and Milovanović proved the following result:

Theorem 3.3 ([53]). *Assume that f is a holomorphic function in the half-strip of the complex plane, $0 \le \mathrm{Re}(z) \le a$, and there exist two constants C and ω_0, such that for $0 < \omega_0 < \omega$, the inequalities*

$$\int_0^a |F_1(x+\mathrm{i}R)|\,\mathrm{d}x \le C\mathrm{e}^{\omega_0 R} \quad \textit{and} \quad \int_0^a |F_2(x+\mathrm{i}R)|\,\mathrm{d}x \le C\mathrm{e}^{\omega_0 R}$$

hold, where F_1 and F_2 are defined in (21). Then the integral $I_1'[f]$ can be rewritten in the following form

$$\int_0^a F(x)J_\nu(\omega x)\,\mathrm{d}x = \frac{1}{\sqrt{2\pi\omega}}\Big\{\mathrm{e}^{\frac{1}{2}(\nu+\frac{1}{2})\pi\mathrm{i}}\Big[I[F_2,a] - I[F_2,0]\Big] + \mathrm{e}^{-\frac{1}{2}(\nu+\frac{1}{2})\pi\mathrm{i}}\Big[I[F_1,0] - I[F_1,a]\Big]\Big\},$$

where

$$I[F_1,y] = \frac{\mathrm{i}\mathrm{e}^{\mathrm{i}\omega y}}{\omega}\int_0^{+\infty} F_1\Big(y + \frac{\mathrm{i}p}{\omega}\Big)\mathrm{e}^{-p}\,\mathrm{d}p \quad \textit{and} \quad I[F_2,y] = \frac{\mathrm{i}\mathrm{e}^{-\mathrm{i}\omega y}}{\omega}\int_0^{+\infty} F_2\Big(y - \frac{\mathrm{i}p}{\omega}\Big)\mathrm{e}^{-p}\,\mathrm{d}p, \tag{22}$$

and F_1 and F_2 are defined in (21).

A similar result has been obtained for the integral $I_2[f]$ over $(0, +\infty)$ [53]. Also, numerical quadrature rules of Gaussian type for computing the line integrals $I[F_j, a]$ and $I[F_j, 0]$ $(j = 1, 2)$ have been analyzed in detail in [53].

In the case $a > 0$ these integrals can be evaluated by the n-point Gauss-Laguerre quadrature rule as

$$I[F_1,a] \approx Q^n_{I[F_1,a]} = \frac{\mathrm{i}\mathrm{e}^{\mathrm{i}\omega a}}{\omega}\sum_{k=1}^n w_k F_1\Big(a + \frac{\mathrm{i}x_k}{\omega}\Big) \quad \text{and} \quad I[F_2,a] \approx Q^n_{I[F_2,a]} = \frac{\mathrm{i}\mathrm{e}^{-\mathrm{i}\omega a}}{\omega}\sum_{k=1}^n w_k F_2\Big(a - \frac{\mathrm{i}x_k}{\omega}\Big).$$

However, when $a = 0$ the behavior of the functions F_1 and F_2 at $z = 0$ should be taken into account. According to (18) we have introduced the functions

$$L_j(x) = \begin{cases} \dfrac{F_j(x)}{\log x}, & \nu = 0, \\[2mm] \dfrac{F_j(x)}{x^\alpha}, & \nu > 0, \end{cases}$$

for $j = 1, 2$, where $\alpha = \lceil \nu \rceil - \nu$, and then we concluded that for $\nu > 0$ the previous integrals can be evaluated by the generalized Gauss-Laguerre quadrature rule (with the parameter α), e.g.,

$$I[F_1,0] = \frac{\mathrm{i}}{\omega}\int_0^{+\infty} F_1\Big(\frac{\mathrm{i}p}{\omega}\Big)\mathrm{e}^{-p}\,\mathrm{d}p = \Big(\frac{\mathrm{i}}{\omega}\Big)^{1+\alpha}\int_0^{+\infty} L_1\Big(\frac{\mathrm{i}p}{\omega}\Big)p^\alpha\mathrm{e}^{-p}\,\mathrm{d}p \approx Q^n_{I[F_1,0]} = \Big(\frac{\mathrm{i}}{\omega}\Big)^{1+\alpha}\sum_{k=1}^n w_k^\alpha L_1\Big(\frac{\mathrm{i}x_k^\alpha}{\omega}\Big).$$

Finally, the most complicated case is when $a = 0$ and $\nu = 0$. Then for the integral $I[F_1, 0]$ we have

$$I[F_1,0] = \frac{\mathrm{i}}{\omega}\int_0^{+\infty} F_1\Big(\frac{\mathrm{i}p}{\omega}\Big)\mathrm{e}^{-p}\,\mathrm{d}p = \frac{\mathrm{i}}{\omega}\int_0^{+\infty} L_1\Big(\frac{\mathrm{i}p}{\omega}\Big)\log\Big(\frac{\mathrm{i}p}{\omega}\Big)\mathrm{e}^{-p}\,\mathrm{d}p. \tag{23}$$

Evidently, the Gauss-Laguerre (GL) quadrature rule is not feasible, because of logarithmic singularity. However, if we rewrite the integral $I[F_1, 0]$ as a linear combination of two integrals,

$$I[F_1,0] = \frac{\mathrm{i}}{\omega}\Big\{\int_0^{+\infty} L_1\Big(\frac{\mathrm{i}p}{\omega}\Big)\Big[\log\Big(\frac{\mathrm{i}}{\omega}\Big) - 1 + p\Big]\mathrm{e}^{-p}\,\mathrm{d}p - \int_0^{+\infty} L_1\Big(\frac{\mathrm{i}p}{\omega}\Big)(p - 1 - \log p)\mathrm{e}^{-p}\,\mathrm{d}p\Big\},$$

then, we can apply the ordinary Gauss-Laguerre rule to the first integral and the so-called *logarithmic Gauss-Laguerre* (logGL) rule to the second one. Thus, the application of such two n-point rules leads to the following approximate formula

$$I[F_1,0] \approx Q^n_{I[F_1,0]} = \frac{\mathrm{i}}{\omega}\Big\{\sum_{k=1}^{n} w_k L_1\Big(\frac{\mathrm{i}x_k}{\omega}\Big)\Big[\log\Big(\frac{\mathrm{i}}{\omega}\Big)-1+x_k\Big]-\sum_{k=1}^{n} w_k^G\Big(\frac{\mathrm{i}x_k^G}{\omega}\Big)\Big\},$$

where x_k^G and w_k^G, $k=1,\ldots,n$, are the nodes and weights of the n-point logGL-rule. A similar formula can be done for $I[F_2,0]$ (see [53]).

The last quadrature rule on $(0,+\infty)$ with respect to the weight function

$$w_\alpha^G(x) = x^\alpha(x-1-\log x)\mathrm{e}^{-x} \quad \text{on} \quad (0,+\infty),$$

has been constructed recently by Gautschi [16], using his MATLAB package `SOPQ` for symbolic/variable-precision calculations (see Appendix B in [17]). Graphics of this weight for $\alpha=-1/2,0,1/2$ are presented in Fig. 4. Following Gautschi [16], the

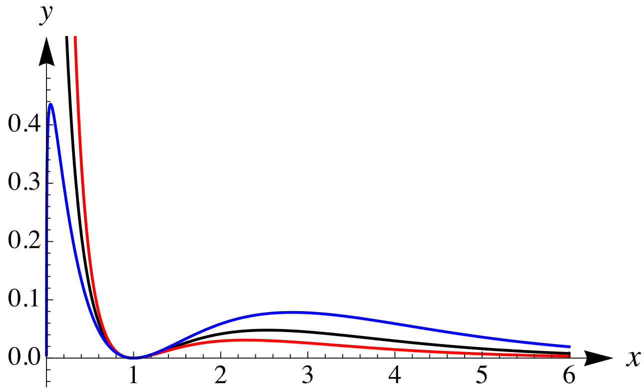


Figure 4: Gautschi's logGL weight function for $\alpha=-1/2$ (*red line*), $\alpha=0$ (*black line*), and $\alpha=1/2$ (*blue line*)

moments with of the weight function $x \mapsto w_\alpha^G(x)$ on $\mathbb{R}^+$ are

$$\mu_k = \int_0^{+\infty} x^{k+\alpha}(x-1-\log x)\mathrm{e}^{-x}\,\mathrm{d}x = \Gamma(\alpha+k+1)[\alpha+k-\psi(\alpha+k+1)], \quad k\ge 0,$$

where $\psi(x)=\Gamma'(x)/\Gamma(x)$ is the logarithmic derivative of the gamma function, as well as the modified moments relative to the system of monic generalized monic Laguerre polynomials $\widehat{L}_k^{(\alpha)}(x)$,

$$m_k = \int_0^{+\infty} x^\alpha(x-1-\log x)\widehat{L}_k^{(\alpha)}(x)\mathrm{e}^{-x}\,\mathrm{d}x \begin{cases} [\alpha-\psi(\alpha+1)]\Gamma(\alpha+1), & k=0,\\ \alpha\,\Gamma(\alpha+1), & k=1,\\ (-1)^k(k-1)!\Gamma(\alpha+1), & k\ge 2. \end{cases}$$

Using these moments and the previous mentioned MATHEMATICA package `OrthogonalPolynomials` we can obtain the recursive coefficients α_k^G and β_k^G. For example for $\alpha=0$, we have

$$\alpha_0^G=1,\quad \alpha_1^G=\frac{3\gamma+5}{\gamma+1},\quad \alpha_2^G=\frac{20\gamma^4+106\gamma^3+111\gamma^2+32\gamma-1}{(\gamma+1)(4\gamma^3+14\gamma^2+5\gamma-1)},$$

$$\alpha_3^G=\frac{4032\gamma^7+48480\gamma^6+176768\gamma^5+237320\gamma^4+72624\gamma^3-31006\gamma^2-8839\gamma+2489}{(4\gamma^3+14\gamma^2+5\gamma-1)(144\gamma^4+1104\gamma^3+1652\gamma^2+184\gamma-237)};$$

$$\beta_0^G=\gamma,\quad \beta_1=\frac{\gamma+1}{\gamma},\quad \beta_2^G=\frac{4\gamma^3+14\gamma^2+5\gamma-1}{\gamma(\gamma+1)^2},\quad \beta_3^G=\frac{\gamma(\gamma+1)\big(144\gamma^4+1104\gamma^3+1652\gamma^2+184\gamma-237\big)}{(4\gamma^3+14\gamma^2+5\gamma-1)^2},\quad \text{etc.},$$

where γ is the well-known Euler's constant (see [53]).

Theorem 3.4 ([53]). *If the functions $F_1(x)$ and $F_2(x)$ defined by (21) satisfy the condition of Theorem 3.3, the error bound of the method for the integral $I_1[f]$ can be estimated as*

$$\left|Q^n_{I_1[f]}-I_1[f]\right| = \begin{cases} O\big(\omega^{-2n-3/2}(1+\log\omega)\big), & \nu=0,\\ O\big(\omega^{-2n-3/2}\big), & \nu>0. \end{cases}$$

An alternative approach for computing the integral (23) has been also developed in [53]. Namely, we constructed the so-called *universal* (*direct*) quadrature formulas of Gaussian type

$$\int_0^{+\infty} g(t)\mathrm{e}^{-t}\,\mathrm{d}t = \sum_{k=1}^{n} A_k g(\tau_k) + R_n(g), \tag{24}$$

which are exact for each $g(t) = p(t) + q(t)\log t$, where $p(t)$ and $q(t)$ are algebraic polynomials of degree at most $n-1$. These quadrature rules can calculate integrals with a sufficient accuracy, regardless of whether their integrands contain a logarithmic singularity, or they do not. Thus, an application of such rules avoids the separation into singular and non-singular parts in integrands, as well as an additional integration of such a singular part using some special logarithmically weighted quadrature formula like one w.r.t. the weight function $w_\alpha^G(t)$. Thus, with the universal quadrature formula (24) we can directly calculate the integrals $I[F_1, y]$ and $I[F_2, y]$ given by (22) in Theorem 3.3; for example,

$$I[F_1, y] \approx \frac{\mathrm{i}\mathrm{e}^{\mathrm{i}\omega y}}{\omega} \sum_{k=1}^{n} A_k F_1\Big(y + \frac{\mathrm{i}\tau_k}{\omega}\Big).$$

Unfortunately, the construction of such universal quadrature formulas is not simple. Namely, there are not elegant tools for their construction like Golub-Welsch procedure in the case of construction quadrature rules with a polynomial degree of precision. In this non-polynomial case, in order to construct the quadrature formula (24), we must solve the following system of $2n$ nonlinear equations

$$\sum_{k=1}^{n} A_k \varphi_j(\tau_k) = \int_0^{+\infty} \varphi_j(t)\mathrm{e}^{-t}\,\mathrm{d}t, \quad j = 1, 2, \ldots, 2n, \tag{25}$$

in τ_k and A_k, $k = 1, \ldots, n$, taking an orthonormal system $\{\varphi_1, \varphi_2, \ldots, \varphi_{2n}\}$ obtained from the system of $2n$ linearly independent functions $U = \{1, t, \ldots, t^{n-1}, \log t, t\log t, \ldots, t^{n-1}\log t\}$ by an orthogonalization process (cf. [33, pp. 75–77]). Since $\varphi_1(t) = 1$, the right-hand side in the previous system of Eqs. becomes

$$\int_0^{+\infty} \varphi_j(t)\varphi_1(t)\mathrm{e}^{-t}\,\mathrm{d}t = \begin{cases} 1, & j = 0, \\ 0, & j \neq 0. \end{cases}$$

Otherwise, a direct use of the non-orthogonal system of the basis functions U leads to a very ill-conditioned iterative process.

The orthonormal system of functions $\{\varphi_1, \varphi_2, \ldots, \varphi_{2n}\}$ can be considered as a Müntz system $\{t^{\lambda_0}, t^{\lambda_1}, \ldots, t^{\lambda_{2n-1}}\}$ on $(0, +\infty)$, with $\lambda_j = \lambda_{n+j} = j$, $j = 0, 1, \ldots, n-1$. Then, we can see that $\varphi_j(t) = \overline{L}_{j-1}(t)$, $j = 1, \ldots, n$, are normalized classical Laguerre polynomials. So, for different $n \in \mathbb{N}$, we obtain the following orthogonal functions:

1° $n = 1$:

$$\varphi_1(t) = 1, \quad \varphi_2(t) = \frac{\sqrt{6}}{\pi}(\gamma + \log t);$$

2° $n = 2$:

$$\varphi_1(t) = 1, \quad \varphi_2(t) = t - 1, \quad \varphi_3(t) = \sqrt{\frac{6}{\pi^2 - 6}}\big(\gamma + 1 - t + \log t\big),$$

$$\varphi_4(t) = \sqrt{\frac{6}{216 - 12\pi^4 + \pi^6}}\Big\{6 - \gamma(\pi^2 - 12) - \big[\pi^2 + \gamma(6 - \pi^2)\big]t + \big[12 - \pi^2 + (\pi^2 - 6)t\big]\log t\Big\};$$

3° $n = 3$:

$$\varphi_1(t) = 1, \quad \varphi_2(t) = t - 1, \quad \varphi_3(t) = \frac{1}{2}\big(t^2 - 4t + 2\big), \quad \varphi_4(t) = \frac{1}{2}\sqrt{\frac{3}{2\pi^2 - 15}}\big(6 + 4\gamma - 8t + t^2 + 4\log t\big),$$

$$\varphi_5(t) = C_5\Big\{24 - 2\pi^2 + \gamma(21 - 2\pi^2) + \big[2\pi^2 - 27 + \gamma(2\pi^2 - 15)\big]t + (9 - \pi^2)t^2 + \big[(2\pi^2 - 15)t - 2\pi^2 + 21\big]\log t\Big\},$$

$$\begin{aligned}\varphi_6(t) = C_6\Big\{&504 - 51\pi^2 + 2\gamma\big(279 - 48\pi^2 + 2\pi^4\big) + 2\big[4\pi^4 - 24\pi^2 - 153 - \gamma(4\pi^4 - 66\pi^2 + 261)\big]t \\ &+ \big[54 + 24\pi^2 - 3\pi^4 + \gamma(72 - 27\pi^2 + 2\pi^4)\big]t^2 \\ &+ \big[\big(72 - 27\pi^2 + 2\pi^4\big)t^2 - 2\big(261 - 66\pi^2 + 4\pi^4\big)t + 2(2\pi^4 - 48\pi^2 + 279)\big]\log t\Big\},\end{aligned}$$

where

$$C_5 = \sqrt{\frac{6}{-1080 + 549\pi^2 - 84\pi^4 + 4\pi^6}} \quad \text{and} \quad C_6 = \sqrt{\frac{3}{159408 - 65610\pi^2 + 2727\pi^4 + 1584\pi^6 - 216\pi^8 + 8\pi^{10}}},$$

etc.

For solving the system of equations (25) we use the well-known Newton-Kantorovich method, with quadratic convergence, but the main problem which then arises is how to provide sufficiently good starting values. Our strategy in the construction is based on the method of continuation, starting from the corresponding standard Gauss-Laguerre formula (with a polynomial degree of exactness). Numerical values of parameters τ_k and A_k, $k = 1, \ldots, n$, for $1 \le n \le 6$ was presented in [53]. For some additional details on the generalized Gaussian quadratures on a finite interval and for Müntz systems of functions see [36], [39] and [37].

4 Gaussian Quadrature Formulas with a Modified Hermite Weight

I this section we consider the Gaussian quadrature formula on $\mathbb{R}$ with respect to a modified Hermite weight $x \mapsto e^{-x^2}$ by the square root term $x \mapsto \sqrt{1+\alpha x+\beta x^2}$, i.e.,

$$w^{(\alpha,\beta)}(x) = \frac{e^{-x^2}}{\sqrt{1+\alpha x+\beta x^2}}, \tag{26}$$

with the real parameters α and β such that $\alpha^2 < 4\beta$.

Remark 1. The weight function $w^{(\alpha,\beta)}(x)$ has the quasi-singularities near to the real axis if $\alpha^2 \to 4\beta$. In the limit case, $w^{(\alpha,\alpha^2/4)}(x)$ has a singularity, i.e., a pole of the first order at the point $-\alpha/(2\beta)$ on the real line.

Several methods for modified weights (measures) by the rational terms (linear and quadratic factors and divisors) can be found in [15, Subsection 2.4], as well as the corresponding MATLAB software in [17, pp. 19–27].

Thus, we are interested here in constructing Gaussian quadrature rules of the form

$$\int_{-\infty}^{+\infty} \frac{f(x)}{\sqrt{1+\alpha x+\beta x^2}} e^{-x^2}\,dx = \sum_{\nu=1}^{N} A_\nu f(x_\nu) + R_N(f), \tag{27}$$

where $A_\nu = A_\nu^{(\alpha,\beta)}$ are weight coefficients (Christoffel numbers), and $R_n(f)$ is the corresponding remainder term, such that $R_N(f) = 0$ for each $f \in \mathcal{P}_{2N-1}$.

Remark 2. In 1997 Bandrauk [3] stated a problem how to evaluate the integral

$$I_{m,n}^{\alpha,\beta} = \int_{-\infty}^{+\infty} \frac{H_m(x)H_n(x)}{\sqrt{1+\alpha x+\beta x^2}} e^{-x^2}\,dx, \tag{28}$$

where $H_m(x)$ is the Hermite polynomial of degree m, defined by

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}\left(e^{-x^2}\right), \quad n \ge 0.$$

Alternatively, the question was how to find computationally effective approximations for the integral (28). The function $x \mapsto H_m(x)e^{-x^2/2}$ is the quantum-mechanical wave function of m photons, the quanta of the electromagnetic field. The integral (28) expresses the modification of atomic Coulomb potentials by electromagnetic fields. In the case $m = n = 0$, the integral $I_{0,0}^{\alpha,\beta}$ represents the vacuum or zero-field correction (for details see [2, Chaps. 1 and 3]).

Evidently, for $\alpha = \beta = 0$, the integral $I_{m,n}^{0,0}$ expresses the orthogonality of the Hermite polynomials, i.e, $I_{m,n}^{0,0} = 2^m m!\sqrt{\pi}\delta_{m,n}$, where $\delta_{m,n}$ is the Kronecker delta.

A solution for $I_{0,0}^{\alpha,\beta}$ was derived by Grosjean [21] in the following form

$$I_{0,0}^{\alpha,\beta} = \frac{1}{\beta}\sum_{j=0}^{+\infty} \frac{\left[(4\beta-\alpha^2)/4\beta^2\right]^j}{2^{2j}(j!)^2} \sum_{r=0}^{+\infty} (-1)^r \frac{(2r+2j)!}{(2r)!(r+j)!}\left(\frac{\alpha}{2\beta}\right)^{2r} c_{r,j},$$

where

$$c_{r,j} = -\gamma + \log 4 - \log\left(\frac{4\beta-\alpha^2}{4\beta^2}\right) + 2H_j + H_{r+j} - 2H_{2r+2j},$$

γ $(= 0.57721566490\ldots)$ is Euler's constant, and H_j is the j-th harmonic number,

$$H_j = 1 + \frac{1}{2} + \cdots + \frac{1}{j}.$$

Also, he gave a study of $I_{m,0}^{\alpha,\beta}$, $m = 1, 2, \ldots$, as well as a five-term recurrence relation for these integrals.

The problem from Remark 2 was also considered in [35], with the monic Hermite polynomials $\widehat{H}_k(x) = 2^{-k}H_k(x)$ in (28). For constructing the coefficients α_k and β_k, $k = 0, 1, \ldots$, in the three-term recurrence relation

$$\pi_{k+1}(x) = (x-\alpha_k)\pi_k(x) - \beta_k\pi_{k-1}(x), \quad k \ge 0 \quad (\pi_0(x) = 1,\ p_{-1}(x) = 0) \tag{29}$$

for polynomials $\pi_k(x)$ orthogonal on $(-\infty, \infty)$ with respect to the modified Hermite weight function (26), it was used the *discretized Stieltjes-Gautschi procedure* with the discretization based on the standard Gauss-Hermite quadratures,

$$\begin{aligned} \int_{-\infty}^{+\infty} P(t)w^{(\alpha,\beta)}(x)\,dx &= \int_{-\infty}^{+\infty} \frac{P(x)}{\sqrt{1+\alpha x+\beta x^2}} e^{-x^2}\,dx \\ &\cong \sum_{k=1}^{N} \frac{\lambda_k^H P(\tau_k^H)}{\sqrt{1+\alpha\tau_k^H + \beta(\tau_k^H)^2}}, \end{aligned}$$

where P is an arbitrary algebraic polynomial, and $\tau_k^H = \tau_k$ are nodes (zeros of $H_N(x)$) and

$$\lambda_k^H = \frac{2^{N-1}(N-1)!\sqrt{\pi}}{NH_{N-1}(\tau_k)^2}$$

are the weights (Christoffel numbers) of the N-point Gauss-Hermite quadrature formula (cf. [33, p. 325]). Such a procedure is needed for each of selected pairs (α,β). The recurrence coefficients for $k<20$ and $\alpha=\beta=1$ were presented in [35]. The corresponding Gaussian approximations were tested in double precision arithmetic in two cases: $m=3$, $n=6$, and $m=10$, $n=15$.

In this section we give a simple way for constructing the coefficients in the three-term recurrence relation (29), using the modified method of moments, realized in the MATHEMATICA package `OrthogonalPolynomials` ([9], [38]) in variable-precision arithmetic in order to overcome the numerical instability. All that is required is a procedure for numerical calculation of the modified moments in variable-precision arithmetic. In the same time, we give answer to the problem stated in Remark 2.

In our case we use the first $2N$ modified moments with respect to the sequence of the monic Hermite polynomials, i.e.,

$$m_k = m_k^{(\alpha,\beta)} = \int_{-\infty}^{+\infty} \frac{\widehat{H}_k(x)}{\sqrt{1+\alpha x+\beta x^2}} \mathrm{e}^{-x^2}\,\mathrm{d}x, \quad k=0,1,\ldots,2N-1, \tag{30}$$

in order to get quadrature rules of Gaussian type (27) for each $n \le N$, using the Golub-Welsch algorithm [19]. For the sequence $\{\widehat{H}_k(x)\}_{k\in\mathbb{N}_0}$ the following recurrence relation $\widehat{H}_{k+1}(x) = x\widehat{H}_k(x) - (k/2)\widehat{H}_{k-1}(x)$ holds, with $\widehat{H}_0(x)=1$ and $\widehat{H}_1(x)=x$.

First we transform the trinomial in the integral (30) to a canonical form

$$1+\alpha x+\beta x^2 = \beta\left[(x-p)^2+q^2\right], \quad p=-\frac{\alpha}{2\beta}, \quad q=\frac{4\beta-\alpha^2}{2\beta} \quad (p^2+q^2=\beta),$$

and then we apply the so-called *double-exponential* (*DE*) *transformation*

$$x = u(t) = p + q\sinh\left(\frac{\pi}{2}\sinh t\right),$$

in order to reduce the modified moments (30) to

$$m_k = m_k^{(\alpha,\beta)} = \frac{\pi}{2}\sqrt{p^2+q^2}\int_{-\infty}^{+\infty} \widehat{H}_k(u(t))\mathrm{e}^{-u(t)^2}\cosh t\,\mathrm{d}t, \quad k=0,1,\ldots,2N-1. \tag{31}$$

The crucial point in this DE transformation is the decay of the integrand be at least double exponential ($\approx \exp(-C\exp|t|)$ as $|t|\to+\infty$, where C is some positive constant. For integrals of such form of an analytic function on $\mathbb{R}$, it is known that the trapezoidal formula with an equal mesh size gives an optimal formula (cf. [25, 34, 41, 42, 47, 48, 49]).

For calculating the modified moments (31) we apply the trapezoidal formula with an equal mesh size h, i.e.,

$$m_k[h] = \frac{\pi h}{2}\sqrt{p^2+q^2}\sum_{j=-\infty}^{+\infty} \widehat{H}_k(u(jh))\mathrm{e}^{-u(jh)^2}\cosh jh, \quad k=0,1,\ldots,2N-1.$$

Since the integrand decays double exponentially, in actual computation of these sums we can truncate the infinite summation at $k=-M$ and $k=M$, so that

$$m_k \approx m_k[h;M] = \frac{\pi h}{2}\sqrt{p^2+q^2}\sum_{j=-M}^{M} \widehat{H}_k(u(jh))\mathrm{e}^{-u(jh)^2}\cosh jh, \quad k=0,1,\ldots,2N-1. \tag{32}$$

Because of some symmetry in the expression for $m_k[h;M]$, (32) can be implemented in the following way. Namely, if we put

$$t_j = jh, \quad \xi_j = q\sinh\left(\frac{\pi}{2}\sinh t_j\right), \quad c_j = 2\cosh(2p\xi_j), \quad s_j = 2\sinh(2p\xi_j),$$

we have $u(t_j)=p+\xi$, $u(-t_j)=p-\xi$, $u(0)=p$, and therefore

$$m_k[h;M] = \frac{\pi h}{2}\sqrt{p^2+q^2}\,\mathrm{e}^{-p^2}\left\{\widehat{H}_k(p) + \sum_{j=1}^{M}\mathrm{e}^{-\xi_j^2}\cosh(t_j)\left[\widehat{H}_k(p+\xi_j)\mathrm{e}^{-2p\xi_j} + \widehat{H}_k(p-\xi_j)\mathrm{e}^{2p\xi_j}\right]\right\}, \quad k=0,1,\ldots,2N-1.$$

Lemma 4.1. *Let*

$$\varphi_k(p,\xi) = \widehat{H}_k(p+\xi)\mathrm{e}^{-2p\xi} + \widehat{H}_k(p-\xi)\mathrm{e}^{2p\xi}, \quad \psi_k(p,\xi) = \widehat{H}_k(p+\xi)\mathrm{e}^{-2p\xi} - \widehat{H}_k(p-\xi)\mathrm{e}^{2p\xi}, \quad k=0,1,\ldots.$$

Then, the following recurrence relations

$$\varphi_{k+1}(p,\xi) = p\varphi_k(p,\xi) - \frac{k}{2}\varphi_{k-1}(p,\xi) - \xi\psi_k(p,\xi), \quad k=0,1,\ldots, \tag{33}$$

$$\psi_{k+1}(p,\xi) = p\psi_k(p,\xi) - \frac{k}{2}\psi_{k-1}(p,\xi) - \xi\varphi_k(p,\xi), \quad k=0,1,\ldots, \tag{34}$$

hold, where $\varphi_0(p,\xi) = 2\cosh(2p\xi)$, $\psi_0((p,\xi) = 2\sinh(2p\xi)$, *and* $\varphi_{-1}(p,\xi) = \psi_{-1}(p,\xi) = 0$.

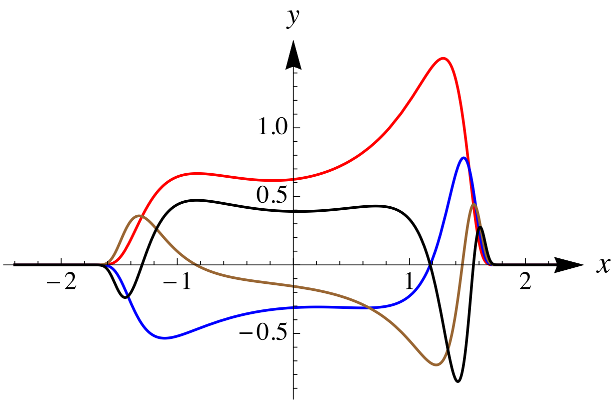
A proof of this lemma can be done using the three-term recurrence relation of the monic Hermite polynomials.
According to Lemma 4.1 we see that

$$m_k[h;M] = \frac{\pi h}{2}\sqrt{p^2+q^2}\,\mathrm{e}^{-p^2}\left\{\widehat{H}_k(p) + \sum_{j=1}^{M}\mathrm{e}^{-\xi_j^2}\cosh(t_j)\varphi_k(p,\xi)\right\}, \quad k=0,1,\ldots,2N-1. \tag{35}$$

In the sequel, as an example, we take $\alpha=\beta=50/13$ in the weight function (26) and $N=40$. Then we have $p=-1/2$ and $q=1/10$, which means that the integrands in (30) have quasi-singularites at $p\pm iq$ in the complex plane.
In order to illustrate the effect of the before mentioned double-exponential decay of integrands, we present the graphics of integrands for $k=0,1,2,3$ (left) and $k=65$ (right) in Figure 5. The values of all integrands in (31), $k=0,1,\ldots,79$, at $t=2.1$, are:

$$\{1.\times10^{-321},\ 3.\times10^{-320},\ 7.\times10^{-319},\ 2.\times10^{-317},\ 5.\times10^{-316},\ 1.\times10^{-314},\ 4.\times10^{-313},\ 1.\times10^{-311},\ 3.\times10^{-310},\ 8.\times10^{-309},$$
$$2.\times10^{-307},\ 6.\times10^{-306},\ 2.\times10^{-304},\ 4.\times10^{-303},\ 1.\times10^{-301},\ 3.\times10^{-300},\ 8.\times10^{-299},\ 2.\times10^{-297},\ 6.\times10^{-296},\ 2.\times10^{-294},$$
$$4.\times10^{-293},\ 1.\times10^{-291},\ 3.\times10^{-290},\ 8.\times10^{-289},\ 2.\times10^{-287},\ 6.\times10^{-286},\ 2.\times10^{-284},\ 4.\times10^{-283},\ 1.\times10^{-281},\ 3.\times10^{-280},$$
$$8.\times10^{-279},\ 2.\times10^{-277},\ 6.\times10^{-276},\ 1.\times10^{-274},\ 4.\times10^{-273},\ 1.\times10^{-271},\ 3.\times10^{-270},\ 7.\times10^{-269},\ 2.\times10^{-267},\ 5.\times10^{-266},$$
$$1.\times10^{-264},\ 4.\times10^{-263},\ 1.\times10^{-261},\ 3.\times10^{-260},\ 7.\times10^{-259},\ 2.\times10^{-257},\ 5.\times10^{-256},\ 1.\times10^{-254},\ 3.\times10^{-253},\ 8.\times10^{-252},$$
$$2.\times10^{-250},\ 6.\times10^{-249},\ 2.\times10^{-247},\ 4.\times10^{-246},\ 1.\times10^{-244},\ 3.\times10^{-243},\ 7.\times10^{-242},\ 2.\times10^{-240},\ 5.\times10^{-239},\ 1.\times10^{-237},$$
$$3.\times10^{-236},\ 9.\times10^{-235},\ 2.\times10^{-233},\ 6.\times10^{-232},\ 2.\times10^{-230},\ 4.\times10^{-229},\ 1.\times10^{-227},\ 3.\times10^{-226},\ 7.\times10^{-225},\ 2.\times10^{-223},$$
$$5.\times10^{-222},\ 1.\times10^{-220},\ 3.\times10^{-219},\ 8.\times10^{-218},\ 2.\times10^{-216},\ 5.\times10^{-215},\ 1.\times10^{-213},\ 4.\times10^{-212},\ 9.\times10^{-211},\ 2.\times10^{-209}\},$$

and their maximal value is $2.\times10^{-209}$. Similarly, the maximal absolute value of all values at $t=-2.1$ is $4.\times10^{-232}$.



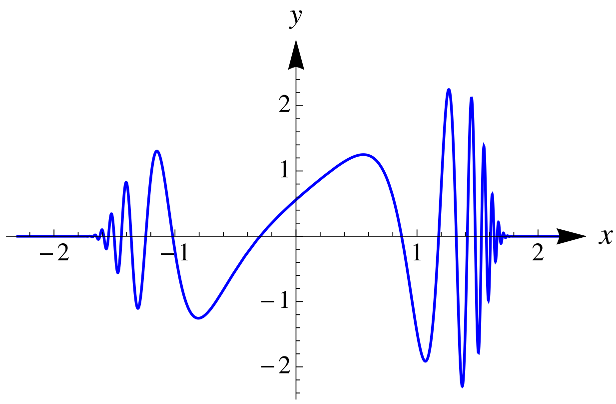


Figure 5: (*Left*) The integrands in $m_k^{(\alpha,\beta)}$ for $k=0$ (*red line*), $k=1$ (*blue line*), $k=2$ (*brown line*), and $k=3$ (*black line*) for $\alpha=\beta=50/13$; (*Right*) The integrand in $m_{65}^{(\alpha,\beta)}\times10^{-35}$ for $\alpha=\beta=50/13$

The corresponding MATHEMATICA code, which includes our package `OrthogonalPolynomials`, can be done in the following form:

```
<< orthogonalPolynomials`
(* Input of parameters alpha, beta, and Nmax *)
alpha = 50/13; beta = 50/13; Nmax = 40;
alphaH = Table[0,{k,0,2 Nmax}]; betaH = Prepend[Table[k/2,{k,1,2 Nmax}],Sqrt[Pi]];
HerM[x_] := aMakePolynomial[2 Nmax,alphaH,betaH,x,ReturnList -> True];
p=-alpha/(2 beta); q= Sqrt[4 beta-alpha^2]/(2 beta);
u[t_] := p + q Sinh[Pi/2 Sinh[t]];
fMH[t_,k_] := Pi/2 Sqrt[p^2+q^2] HerM[u[t]][[k+1]]Exp[-u[t]^2]Cosh[t];
(* Print values of integrands of all moments at t=2.1 *)
Tp = Table[N[fMH[21/10, k], 1], {k, 0, 2 Nmax-1}]; Print[Tp]; Max[Abs[Tp]]
```

The following code represents a procedure (DExpT) for calculating all moments (35), using the recurrence relations (33) and (34), as well as a command for calculating the recursive coefficients in (29), α_k and β_k, $k=0,1,\ldots,N-1$ (lists `alphaM` and `betaM`), by the Chebyshev methods of modified moments (`aChebyshevAlgorithmModified`):

```
Options[DExpT] = {WorkingPrecision -> $MachinePrecision};
DExpT[Pol_,b_,M_,p_,q_,Nmax_,Ops___] :=
Module[{wp,h,fac,momM,vt,j,xi,cvt,ec,c,s,phi0,phi1,phi2,psi0,psi1,psi2,k},
 {wp} = {WorkingPrecision} /. {Ops} /. Options[DExpT];
 Block[{$MinPrecision = wp}, h = b/M; fac = N[Pi/2 Sqrt[p^2+q^2]Exp[-p^2],wp];
 momM = N[Pol[p], wp]; vt = N[Table[j h, {j,1,M}], wp];
```

```
  xi = q Sinh[Pi/2 Sinh[vt]]; cvt = Cosh[vt]; ec = Exp[-xi^2] cvt;
  c = 2 Cosh[2 p xi]; s = 2 Sinh[2 p xi]; phi0 = c;
  phi1 = p c - xi s; psi0 = s; psi1 = p s - xi c;
  momM[[1]] = momM[[1]] + Total[ec  phi0];
  momM[[2]] = momM[[2]] + Total[ec  phi1];
  For[k = 1, k <= 2 Nmax - 2, k++,
   phi2 = p phi1 - k/2 phi0 - xi psi1;
   psi2 = p psi1 - k/2 psi0 - xi phi1;
   momM[[k + 2]] = momM[[k + 2]] + Total[ec phi2];
   phi0 = phi1; psi0 = psi1; phi1 = phi2; psi1 = psi2;]; momM = h fac  momM;
  Return[momM];];];

momM = DExpT[Function[x,HerM[x]], 21/10, 800, p, q, Nmax, WorkingPrecision -> 52];
{alphaM, betaM} = aChebyshevAlgorithmModified[momM, alphaH, betaH, WorkingPrecision -> 52];
```

As we can see, in this case, the moment integrals are calculated by the trapezoidal rule, taking $M = 800$ (positive) equidistant nodes on the finite interval $[0, b] = [0, 21/10]$. In in order to overcome the numerical instability and obtain the first $N = 40$ recursion coefficients α_k and β_k with 40 exact decimal digits, we had used the working precision of 52 decimal digits (`WorkingPrecision -> 52`). These recursion coefficients for $\alpha = \beta = 50/13$ are shown in Table 3.

Table 3: Recursion coefficients for the polynomials $\{\pi_k(\,\cdot\,; w^{(\alpha,\beta)})\}$, $\alpha = \beta = 50/13$

k	alpha(k)	beta(k)
0	-3.0560076509895536100068588364455558057864E-01	2.3726193810771496093571467350452699993374E+00
1	1.0911359011720707250487957309040316368823E-01	2.2454688633719411071620026054065378981 64E-01
2	-6.3936507510446131845102135415317140049 55E-02	7.4640454924927157560618068755593701523 32E-01
3	2.8960936229143833904624964510226566409 30E-02	1.3029428971216445235528772314081925071 39E+00
4	-1.2093084233603055348402594151655921375 50E-02	1.7091139329036035875556545168901035909 42E+00
5	-1.7188377540003917226509457353321000580 77E-03	2.3096757110778460316376173557080759845 24E+00
6	7.7507204891690992338119496420627733374 94E-03	2.7119331282511538010718506106202112559 24E+00
7	-1.2984389683308394867611148815032725291 07E-02	3.2954239107684012557598526844155868819 92E+00
8	1.4122418311016240896164840089746665219 98E-02	3.7270671650305351907509681231281186349 84E+00
9	-1.5369296343256451777227013179320914575 88E-02	4.2766500740989692456287760265786747613 72E+00
10	1.4293721164007635808630480107580039951 97E-02	4.7437917326958795700818331901004032041 12E+00
11	-1.3716547022765080690748128254731191641 51E-02	5.2596930494054701721042031735358113361 96E+00
12	1.1767982227705046550682459197984680671 42E-02	5.7577914193917633795867733160348970764 18E+00
13	-1.0473359108090817800000345742952550031 76E-02	6.2467929778469215650574990441078583144 70E+00
14	8.3409819540661877392483076122823413199 47E-03	6.7676702761673761927290008348867259613 25E+00
15	-6.9021530582831119211503389867836308106 28E-03	7.2383443080036916585602331948613946060 57E+00
16	4.9299454378191965322854800211733267895 08E-03	7.7734065671596672998860987939240018085 22E+00
17	-3.6313756265433288270994463102298420100 77E-03	8.2339100006766672226539081484291531901 99E+00
18	1.9728478730882523085624759960479915535 34E-03	8.7755874233409274450767266630372417313 81E+00
19	-9.3823159783545611452695525907379976469 37E-04	9.2327219785170299152308291463655602984 91E+00
20	-3.5906811236743286694555714043242000785 43E-04	9.7750148532633871067153085332412784385 28E+00
21	1.0953586785984604767185025770773857308 42E-03	1.0233936625406388452468600306356025083 13E+01
22	-2.0414616792837724926617951519910131748 94E-03	1.0772504280735150756509219731823159993 94E+01
23	2.4930380182530235273131311998759570199 16E-03	1.1236763057954451682159460771801084621 15E+01
24	-3.1271577618503186377845581264789899243 99E-03	1.1768787193096505407802472785279804286 97E+01
25	3.3313076973733716674600056538520874909 94E-03	1.2240522034132642998113448670716557632 80E+01
26	-3.7050664017550122307034767824496379341 30E-03	1.2764470948222814689108823027711736825 94E+01
27	3.7084726133556384640863028892083442662 82E-03	1.3244666345057854257652857430055229029 19E+01
28	-3.8761182828115932329789391673142944892 51E-03	1.3760029711861713684118097343263719162 64E+01
29	3.7266295219703985388460326690917817971 21E-03	1.4248780063109610354891935360706860571 43E+01
30	-3.7395412812046427609702914327570187220 20E-03	1.4755811734025935487486100736082301630 91E+01
31	3.4816479573684036226878054282369690379 66E-03	1.5252566765623526654825010573456430554 99E+01
32	-3.3854932406565042541448460892097094182 70E-03	1.5752054466886660486047698662018073230 07E+01
33	3.0580773603279798783873103509530181149 09E-03	1.6255832715153425841969839990750920160 28E+01
34	-2.8916025838249893037500006609635060686 01E-03	1.6748902654297145826008607559683409103 84E+01
35	2.5270727732482490370286481702391243879 33E-03	1.7258468516678656959150380358779200628 09E+01
36	-2.3218822187049788243484092145974302034 17E-03	1.7746426654500641421844095940608043193 41E+01
37	1.9461332674600153835169914755296932815 66E-03	1.8260431269253820434882000280532237821 16E+01
38	-1.7270432612575685395480733213795047405 00E-03	1.8744639524018636905241767814754233843 54E+01
39	1.3598844333452107406243923066605778540 45E-03	1.9261728299065298204470764273123969408 27E+01

These recursive coefficients enable us to construct the Gaussian formulas (27) for each $N \le 40$.

We return now to the problem (28) given in Remark 2. Note that the integrand $x \mapsto H_m(x)H_n(x)w^{(\alpha,\beta)}(x)$ in (28) has $m+n$ zeros on $\mathbb{R}$ and very large oscillations (see graphics in Fig. 6).

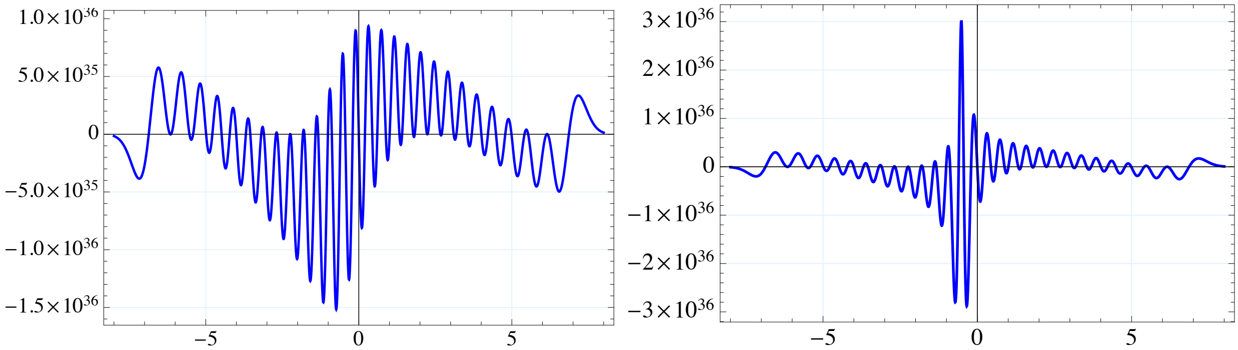


Figure 6: The integrand $x \mapsto H_{30}(x)H_{25}(x)w^{(\alpha,\beta)}(x)$ for $\alpha=\beta=1$ (*left*) and $\alpha=\beta=50/13$ (*right*)

Using the well-known Feldheim's linearization formula for Hermite polynomials (cf. Askey [1, p. 42])

$$H_m(x)H_n(x) = \sum_{\nu=0}^{\min(m,n)} \binom{m}{\nu}\binom{n}{\nu} 2^\nu \nu! H_{m+n-2\nu}(x),$$

we can transform (28) to

$$I_{m,n}^{\alpha,\beta} = 2^{m+n} \sum_{\nu=0}^{\min(m,n)} \binom{m}{\nu}\binom{n}{\nu} \frac{\nu!}{2^\nu} \int_{-\infty}^{+\infty} \frac{\widehat{H}_{m+n-2\nu}(x)}{\sqrt{1+\alpha x+\beta x^2}} \mathrm{e}^{-x^2}\,\mathrm{d}x = 2^{m+n} \sum_{\nu=0}^{\min(m,n)} \binom{m}{\nu}\binom{n}{\nu} \frac{\nu!}{2^\nu} m_{m+n-2\nu}^{(\alpha,\beta)},$$

i.e., $I_{m,n}^{\alpha,\beta}$ can be expressed in terms of the modified moments (30) or approximately by $m_k[h;M]$, i.e.,

$$I_{m,n}^{\alpha,\beta} \approx 2^{m+n} \sum_{\nu=0}^{\min(m,n)} \binom{m}{\nu}\binom{n}{\nu} \frac{\nu!}{2^\nu} m_{m+n-2\nu}[h;M],$$

with some appropriate h and M.

Table 4: Gaussian approximations $Q_{30,25}^{(N)}$ of the integral $I_{30,25}^{\alpha,\beta}$ for $\alpha=\beta=50/13$ and $N=25(1)30$

N	$Q_{30,25}^{(N)}$
25	3.898244052558028200823864546757694876758 (+35)
26	−1.427237521561725565254536466961946087101 (+36)
27	−3.385708554339398400919137631484156473271 (+35)
28	−6.866138084691156226517445794601480146019 (+35)
29	−6.866138084691156226517445794601480146019 (+35)
30	−6.866138084691156226517445794601480146019 (+35)

Alternatively, $I_{m,n}^{\alpha,\beta}$ can be exactly calculated (up to rounding errors) by applying the N-point Gaussian formula (27), for a given parameters α and β, taking the number of nodes N to be such that $m+n \le 2N-1$. Thus,

$$I_{m,n}^{\alpha,\beta} \approx Q_{m,n}^{(N)} = \sum_{\nu=1}^{N} A_\nu H_m(x_\nu)H_n(x_\nu). \tag{36}$$

For example, to calculate $I_{30,25}^{\alpha,\beta}$ we need $N \ge 28$.

Taking recursion coefficients from Table 3 we can evaluate nodes and weights (x_ν and A_ν) in the quadrature formula (27) by the function `aGaussianNodesWeights` from our MATHEMATICA package `OrthogonalPolynomials`, in this case, up to $N \le 40$. The corresponding Gaussian approximations of the integral $I_{30,25}^{50/13,50/13}$ are presented in Table 4 for $N=25(1)30$. As we can see, the obtained results for $N \ge 28$ are exact (up to rounding errors). Results in error are displayed in red.

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References

[1] R. Askey. *Orthogonal Polynomials and Special Functions*. Regional Conference Series in Applied Mathematics, Vol. 21. SIAM, Philadelphia, PA, 1975.

[2] A. D. Bandrauk. *Molecules in Laser Fields*. Marcel Dekker, New York, 1994.

[3] A. D. Bandrauk. Problem 97-7: A family of integrals occurring in quantum mechanics. *SIAM Rev.* 39:317–318, 1997.

[4] R. Chen. Numerical approximations to integrals with a highly oscillatory Bessel kernel. *Appl. Numer. Math.*, 62:636–648, 2012.

[5] R. Chen. On the evaluation of Bessel transformations with the oscillators via asymptotic series of Whittaker functions. *J. Comput. Appl. Math.*, 250:107–121, 2013.

[6] R. Chen. On the implementation of the asymptotic Filon-type method for infinite integrals with oscillatory Bessel kernels. *Appl. Math. Comput.*, 228:477–488, 2014.

[7] R. Chen. On the evaluation of infinite integrals involving Bessel functions. *Appl. Math. Comput.*, 235:212–220, 2014.

[8] R. Chen. Numerical approximations for highly oscillatory Bessel transforms and applications. *J. Math. Anal. Appl.*, 421:1635–1650, 2015.

[9] A. S. Cvetković, G. V. Milovanović. The Mathematica Package "OrthogonalPolynomials". *Facta Univ. Ser. Math. Inform.*, 19:17–36, 2004.

[10] G. A. Evans. Two robust methods for irregular oscillatory integrals over a finite range. *Appl. Numer. Math.*, 14:383–395, 1994.

[11] G. A. Evans. An expansion method for irregular oscillatory integrals. *Internat. J. Comput. Math.*, 63:137–148, 1997.

[12] G. A. Evans, J. R. Webster. A high order, progressive method for the evaluation of irregular oscillatory integrals. *Appl. Numer. Math.*, 23:205–218, 1997.

[13] C. Fang, J. Ma, M. Xiang. On Filon methods for a class of Volterra integral equations with highly oscillatory Bessel kernels. *Appl. Math. Comput.*, 268:783–792, 2015.

[14] B. Gabutti. On high precision methods for computing integrals involving Bessel functions. *Math. Comp.*, 147:1049–1057, 1979.

[15] W. Gautschi. *Orthogonal Polynomials: Computation and Approximation*. Numerical Mathematics and Scientific Computation. Oxford Science Publications. Oxford University Press, New York, 2004.

[16] W. Gautschi. Gauss quadrature routines for two classes of logarithmic weight functions. *Numer. Algorithms*, 55:265–277, 2010.

[17] W. Gautschi. *Orthogonal Polynomials in MATLAB: Exercises and Solution*. Software – Environments – Tools. SIAM, Philadelphia, PA, 2016.

[18] A. Gil, J. Segura, N. M. Temme. Basic methods for computing special functions. In: *Recent Advances in Computational and Applied Mathematics* (T.E. Simos, ed.), 67–121, Springer, 2011.

[19] G. Golub, J. H. Welsch. Calculation of Gauss quadrature rules. *Math. Comp.*, 23: 221–230, 1969.

[20] I. S. Gradshteyn, I. M. Ryzhik. *Integrals, Series, and Products*. 7th ed. Academic Press, New York, 2007.

[21] C. C. Grosjean. Solution of Problem 97-7: A family of integrals occurring in quantum mechanics. *SIAM Rev.* 40:374–381, 1998.

[22] A. I. Hascelik. Suitable Gauss and Filon–type methods for oscillatory integrals with an algebraic singularity. *Appl. Numer. Math.*, 59:101–118, 2009.

[23] G. He, S. Xiang, Z. Xu. A Chebyshev collocation method for a class of Fredholm integral equations with highly oscillatory kernels. *J. Comput. Appl.Math.*, 300:354–368, 2016.

[24] D. Huybrechs, S. Vandewalle. On the evaluation of highly oscillatory integrals by analytic continuation. *SIAM J. Numer. Anal.*, 44:1026–1048, 2006.

[25] M. Iri, S. Moriguti, Y. Takasawa. On certain quadrature formula. *J. Comput. Appl. Math.*, 17:3–20, 1987.

[26] A. Iserles. On the numerical quadrature of highly–oscillating integrals I: Fourier transforms. *IMA J. Numer. Anal.*, 24:365–391, 2004.

[27] A. Iserles. On the numerical quadrature of highly–oscillating integrals II: Irregular oscillators. *IMA J. Numer. Anal.*, 25:25–44, 2005.

[28] Iserles, A., Nørsett, S.P.: On quadrature methods for highly oscillatory integrals and their implementation. BIT **44**, 755–772 (2004)

[29] A. Iserles, S. P. Nørsett. Efficient quadrature of highly–oscillatory integrals using derivatives. *Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci.*, 461:1383–1399, 2005.

[30] H. Kang, S. Xiang. On the calculation of highly oscillatory integrals with an algebraic singularity. *Appl. Math. Comput.*, 217:3890–3897, 2010.

[31] J. Li, X. Wang, T. Wang, S. Xiao. An improved Levin quadrature method for highly oscillatory integrals. *Appl. Numer. Math.*, 60:833–842, 2010.

[32] J. Ma. Oscillation-free solutions to Volterra integral and integro-differential equations with periodic force terms. *Appl. Math. Comput.*, 294:294–298, 2017.

[33] G. Mastroianni, G. V. Milovanović. *Interpolation Processes – Basic Theory and Applications*. Springer Monographs in Mathematics, Springer Verlag, Berlin – Heidelberg – New York, 2008.

[34] G. V. Milovanović. Expansions of the Kurepa function. *Publ. Inst. Math. (Beograd) (N.S.)*, 57(71):81–90, 1995.

[35] G. V. Milovanović. Numerical calculation of integrals involving oscillatory and singular kernels and some applications of quadratures. *Comput. Math. Appl.*, 36:19–39, 1998.

[36] G. V. Milovanović. Generalized Gaussian quadratures for integrals with logarithmic singularity. FILOMAT, 30:1111–1126, 2016.

[37] G. V. Milovanović, A. S. Cvetković. Gaussian type quadrature rules for Müntz systems. *SIAM J. Sci. Comput.*, 27:893–913, 2005.

[38] G. V. Milovanović, A. S. Cvetković. Special classes of orthogonal polynomials and corresponding quadratures of Gaussian type. *Math. Balkanica*, 26:169–184, 2012.

[39] G. V. Milovanović, T. S. Igić, D. Turnić. Generalized quadrature rules of Gaussian type for numerical evaluation of singular integrals. *J. Comput. Appl. Math.*, 278:306–325, 2015.

[40] G. V. Milovanović, M. Stanić. Numerical integration of highly-oscillating functions. In: *Analytic Number Theory, Approximation Theory, and Special Functions – In Honor of Hari M. Srivastava* (G.V. Milovanović, M.Th. Rassias, eds.), 613–649, Springer, New York, 2014.

[41] G. Monegato, L. Scuderi. Quadrature rules for unbounded intervals and their application to integral equations. In: *Approximation and Computation: In Honor of Gradimir V. Milovanović* (W. Gautschi, G. Mastroianni, Th. M. Rassias, eds.), 185–208, Springer Optimization and its Applications, Vol. 42, Springer, New York, 2011.

[42] M. Mori. Quadrature formulas obtained by variable transformation and DE-rule. *J. Comput. Appl. Math.*, 12&13:119–130, 1985.

[43] S. Olver. Moment-free numerical integration of highly oscillatory functions. *IMA J. Numer. Anal.*, 26:213–227, 2006.

[44] T. Sauter. Computation of irregularly oscillating integrals. *Appl. Numer. Math.*, 35:245–264, 2000.

[45] L. F. Shampine. Integrating oscillatory functions in Matlab. *Int. J. Comput. Math.*, 88(11):2348–2358, 2011.

[46] L. F. Shampine. Integrating oscillatory functions in Matlab, II. *Electron. Trans. Numer. Anal.*, 39:403–413, 2012.

[47] H. Takahasi, M. Mori. Error estimation in the numerical integration of analytic functions. *Report Computer Centre University of Tokyo*, 3:41–108, 1970.

[48] H. Takahasi, M. Mori. Quadrature formulas obtained by variable transformation. *Numer. Math.*, 21:206–219, 1973.

[49] J. Waldvogel. Towards a general error theory of the trapezoidal rule. In: *Approximation and Computation: In Honor of Gradimir V. Milovanović* (W. Gautschi, G. Mastroianni, Th. M. Rassias, eds.), 267–282, Springer Optimization and its Applications, Vol. 42, Springer, New York, 2011.

[50] H. Wang, S. Xiang. On the evaluation of Cauchy principal value integrals of oscillatory functions. *J. Comput. Appl. Math.*, 234:95–100, 2010.

[51] R. Wong. Quadrature formulas for oscillatory integral transforms. *Numer. Math.*, 39:351–360, 1982.

[52] Z. Xu, G. V. Milovanović. Efficient method for the computation of oscillatory Bessel transform and Bessel Hilbert transform. *J. Comput. Appl. Math.*, 308:117–137, 2016.

[53] Z. Xu, G. V. Milovanović, S. Xiang. Efficient computation of highly oscillatory integrals with Hankel kernel. *Appl. Math. Comput.*, 261:312–322, 2015.

[54] Z. Xu, S. Xiang. On the evaluation of highly oscillatory finite Hankel transform using special functions. *Numer. Algorithms*, 72:37–56, 2016.