Numerical Calculation of Integrals Involving Oscillatory and Singular Kernels and Some Applications of Quadratures

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Dedicated to Professor Mario Rosario Occorsio on the occasion of his 65th birthday

Abstract—Numerical methods for strongly oscillatory and singular functions are given in this paper. Beside a summary of standard methods and product integration rules, we consider a class of complex integration methods. Several applications of quadrature processes in problems in telecommunications and physics are also presented. Numerical examples are included.

Keywords—Numerical integration, Oscillatory kernel, Singular kernel, Orthogonal polynomials, Product rules, Gaussian quadratures, Error function, Bessel functions, Legendre functions.

1. INTRODUCTION

Integrals of strongly oscillatory or singular functions appear in many branches of mathematics, physics and other applied and computational sciences. The standard methods of numerical integration often require too much computation work and cannot be successfully applied. Therefore, for problems with singularities, for integrals of strongly oscillatory functions and others, there are a large number of special approaches. In this paper we give an account on some special – fast and efficient – quadrature methods, as well as some new approaches. Also, we give a few applications of quadrature formulas in telecommunications and physics. Such methods require a knowledge of orthogonal polynomials (cf. [1]).

Let $\mathcal{P}_n$ be the set of all algebraic polynomials P $(\not\equiv 0)$ of degree at most n and let $d\lambda(t)$ be a nonnegative measure on $\mathbb{R}$ with finite support or otherwise, for which the all moments $\mu_\nu = \int_{\mathbb{R}} t^\nu \, d\lambda(t)$ exist for every ν and $\mu_0 > 0$. Then there exists a unique system of orthogonal (monic) polynomials $\pi_k(\cdot) = \pi_k(\,\cdot\,; d\lambda)$, $k = 0, 1, \ldots$, defined by

$$\pi_k(t) = t^k + \text{lower degree terms}, \qquad (\pi_k, \pi_m) = \|\pi_k\|^2 \delta_{km},$$

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where the inner product is given by

$$(f,g) = \int_{\mathbb{R}} f(t)g(t)\,d\lambda(t) \qquad (f,g \in L^2(\mathbb{R}) = L^2(\mathbb{R};d\lambda))$$

and the norm by $\|f\| = \sqrt{(f,f)}$.

Such orthogonal polynomials $\{\pi_k\}$ satisfy a three-term recurrence relation

$$\pi_{k+1}(t) = (t-\alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), \quad k \geq 0, \tag{1.1}$$

$$\pi_0(t) = 1, \quad \pi_{-1}(t) = 0,$$

with the real coefficients α_k and $\beta_k > 0$. Because of orthogonality, we have that

$$\alpha_k = \frac{(t\pi_k,\pi_k)}{(\pi_k,\pi_k)}, \quad \beta_k = \frac{(\pi_k,\pi_k)}{(\pi_{k-1},\pi_{k-1})}.$$

The coefficient β_0, which multiplies $\pi_{-1}(t) = 0$ in three-term recurrence relation may be arbitrary. Sometimes, it is convenient to define it by $\beta_0 = \int_{\mathbb{R}} d\lambda(t)$.

The n-point Gaussian quadrature formula

$$\int_{\mathbb{R}} f(t)\,d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) + R_n(f), \tag{1.2}$$

has maximum algebraic degree of exactness $2n-1$, in the sense that $R_n(f) = 0$ for all $f \in \mathcal{P}_{2n-1}$. The nodes $\tau_\nu = \tau_\nu^{(n)}$ are the eigenvalues of the symmetric tridiagonal Jacobi matrix $J_n(w)$, given by

$$J_n(w) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \mathbf{0} \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{n-1}} \\ \mathbf{0} & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix},$$

while the weights $\lambda_\nu = \lambda_\nu^{(n)}$ are given in terms of the first components $v_{\nu,1}$ of the corresponding normalized eigenvectors by $\lambda_\nu = \beta_0 v_{\nu,1}^2$, $\nu = 1,\ldots,n$, where $\beta_0 = \int_{\mathbb{R}} d\lambda(t)$. There are well-known and efficient algorithms, such as the QR algorithm with shifts, to compute eigenvalues and eigenvectors of symmetric tridiagonal matrices (cf. [2]). A simple modification of the previous method can be applied to the construction of Gauss-Radau and Gauss-Lobatto quadrature formulas.

The paper is organized as follows. Section 2 discusses the methods for oscillatory functions, including the standard methods, the product rules, as well as some complex integration methods. Section 3 is dedicated to applications of quadratures in some problems in telecommunications and physics.

2. INTEGRATION OF OSCILLATING FUNCTIONS

In this section we consider integrals of the form

$$I(f,K) = I(f(\cdot),K(\cdot;x)) = \int_a^b w(t)f(t)K(t;x)\,dt, \tag{2.1}$$

where (a, b) is an interval on the real line, which may be finite or infinite, $w(t)$ is a given weight function as before, and the kernel $K(t; x)$ is a function depending on a parameter x and such that it is highly oscillatory or has singularities on the interval (a, b) or in its nearness. Usually, an application of standard quadrature formulas to $I(f; K)$ requires a large number of nodes and too much computation work in order to achieve a modest degree of accuracy. A few typical examples of such kernels are:

1° Oscillatory kernel $K(t; x) = e^{ixt}$, where $x = \omega$ is a large positive parameter. In this class we have Fourier integrals over $(0, +\infty)$ (Fourier transforms)

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

or Fourier coefficients

$$c_k(f) = a_k(f) + ib_k(f) = \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) e^{ikt}\, dt, \tag{2.2}$$

where $\omega = k \in \mathbb{N}$. There are also some other oscillatory integral transforms like the Bessel transforms

$$H_m(x) = \int_0^{+\infty} t^\mu f(t) H_\nu^{(m)}(\omega t)\, dt \qquad (m = 1, 2), \tag{2.3}$$

where ω is a real parameter and $H_\nu^{(m)}(t)$, $m = 1, 2$, are the Hankel functions (see Wong [3]). Also, we mention here a type of integrals involving Bessel functions

$$I_\nu(f; \omega) = \int_0^{+\infty} e^{-t^2} J_\nu(\omega t) f(t^2) t^{\nu+1}\, dt, \quad \nu > -1, \tag{2.4}$$

where ω is a large positive parameter. Such integrals appear in some problems of high energy nuclear physics (cf. [4]).

2° Logarithmic singular kernel $K(t; x) = \log |t - x|$, where $a \le x \le b$.

3° 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 (2.1) is taken to be a Cauchy principal value integral.

In this section we consider only integration of oscillatory functions.

2.1. A Summary of Standard Methods

The earliest formulas for numerical integration of rapidly oscillatory function are based on the piecewise approximation by the low degree polynomials of $f(x)$ on the integration interval. The resulting integrals over subintervals are then integrated exactly. A such method was obtained by Filon [5].

Consider the Fourier integral on the finite interval

$$I(f; \omega) = \int_a^b f(x) e^{i\omega x}\, dx$$

and divide that interval $[a, b]$ into $2N$ subintervals of equal length $h = (b - a)/(2N)$, so that $x_k = a + kh$, $k = 0, 1, \ldots, 2N$. The Filon's construction of the formula is based upon a quadratic fit for $f(x)$ on every subinterval $[x_{2k-2}, x_{2k}]$, $k = 1, \ldots, N$ (by interpolation at the mesh points). Thus,

$$f(x) \approx P_k(x) = P_k(x_{2k-1} + ht) = \phi_k(t), \tag{2.5}$$

where $t \in [-1,1]$ and $P_k \in \mathcal{P}_2$, $k = 1,\ldots,N$. It is easy to get

$$\phi_k(t) = f_{2k-1} + \frac{1}{2}(f_{2k} - f_{2k-2})t + \frac{1}{2}(f_{2k} - 2f_{2k-1} + f_{2k-2})t^2,$$

where $f_r \equiv f(x_r)$, $r = 0,1,\ldots,2N$. Using (2.5) we have

$$I(f;\omega) \approx \sum_{k=1}^{N} \int_{x_{2k-2}}^{x_{2k}} f(x)e^{i\omega x}\,dx = h\sum_{k=1}^{N} e^{i\omega x_{2k-1}} \int_{-1}^{1} \phi_k(t)e^{i\theta t}\,dt,$$

where $\theta = \omega h$. Since

$$\int_{-1}^{1} \phi_k(t)e^{i\theta t}\,dt = Af_{2k-2} + Bf_{2k-1} + Cf_{2k},$$

where

$$A = \overline{C} = \frac{1}{2}\int_{-1}^{1}(t^2 - t)e^{i\theta t}\,dt, \quad B = \int_{-1}^{1}(1 - t^2)e^{i\theta t}\,dt,$$

i.e.,

$$\begin{aligned} A &= \frac{(\theta^2 - 2)\sin\theta + 2\theta\cos\theta}{\theta^3} + i\frac{\theta\cos\theta - \sin\theta}{\theta^2}, \\ B &= \frac{4}{\theta^3}(\sin\theta - \theta\cos\theta), \end{aligned}$$

we obtain

$$I(f;\omega) \approx h\Big\{i\alpha(e^{i\omega a}f(a) - e^{i\omega b}f(b)) + \beta E_{2N} + \gamma E_{2N-1}\Big\},$$

with $\alpha = (\theta^2 + \theta\sin\theta\cos\theta - 2\sin^2\theta)/\theta^3$, $\beta = 2(\theta(1+\cos^2\theta) - \sin^2\theta)/\theta^3$, $\gamma = 4(\sin\theta - \theta\cos\theta)/\theta^3$, and

$$E_{2N} = \sum_{k=0}^{N}{}'' f(x_{2k})e^{i\omega x_{2k}}, \quad E_{2N-1} = \sum_{k=1}^{N} f(x_{2k-1})e^{i\omega x_{2k-1}},$$

where the double prime indicates that both the first and last terms of the sum are taken with factor $1/2$. The limit $\theta \to 0$ leads to the Simpson's rule. The error estimate was given by Håvie [6] and Ehrenmark [7].

Improvements of the previous technique have been done by Flinn [8], Luke [9], Buyst and Schotsmans [10], Tuck [11], Einarsson [12], Van de Vooren and Van Linde [13], etc. For example, Flinn [8] used fifth-degree polynomials in order to approximate $f(x)$ taking values of function and values of its derivative at the points x_{2k-2}, x_{2k-1}, and x_{2k}, and Stetter [14] used the idea of approximating the transformed function by polynomials in $1/t$. Miklosko [15] proposed to use an interpolatory quadrature formula with the Chebyshev nodes.

The construction of Gaussian formulae for oscillatory weights has also been considered (cf. Gautschi [16], Piessens [17], [18], [19]). Defining nonnegative functions on $[-1,1]$,

$$u_k(t) = \frac{1}{2}(1 + \cos k\pi t), \quad v_k(t) = \frac{1}{2}(1 + \sin k\pi t),$$

the Fourier coefficients (2.2) can be expressed in the form

$$a_k(f) = 2\int_{-1}^{1} f(\pi t)u_k(t)\,dt - \int_{-1}^{1} f(\pi t)\,dt$$

and

$$b_k(f) = 2\int_{-1}^{1} f(\pi t)v_k(t)\,dt - \int_{-1}^{1} f(\pi t)\,dt.$$

Now, the Gaussian formulae can be obtained for the first integrals on the right-hand side in these equalities. For $k = 1(1)12$ Gautschi [16] obtained n-point Gaussian formulas with 12 decimal digits when $n = 1(1)8$, $n = 16$, and $n = 32$. We mention, also, that for the interval $[0, +\infty)$ and the weight functions $w_1(t) = (1+\cos t)(1+t)^{-(2n-1+s)}$ and $w_2(t) = (1 + \sin t)(1 + t)^{-(2n-1+s)}$, $n = 1(1)10$, $s = 1.05(0.05)4$, the n-point formulas were constructed by Krilov and Kruglikova [20].

Quadrature formulas for the Fourier and the Bessel transforms (2.3) were derived by Wong [3].

Other formulas are based on the integration between the zeros of $\cos mx$ or $\sin mx$ (cf. [21], [22], [23], [24], and [25]). In general, if the zeros of the oscillatory part of the integrand are located in the points x_k, $k = 1, 2, \ldots, m$, on the integration interval $[a, b]$, where $a \le x_1 < x_2 < \cdots < x_m \le b$, then we can calculate the integral on each subinterval $[x_k, x_{k+1}]$ by an appropriate rule. A Lobatto rule is good for this purpose (see Davis and Rabinowitz [21, p. 121]) because of use the end points of the integration subintervals, where the integrand is zero, so that more accuracy can be obtained without additional computation.

There are also methods based on the Euler and other transformations to sum the integrals over the trigonometric period (cf. Longman [26], Hurwitz and Zweifel [27]).

2.2. Product Integration Rules

Consider the integral (2.1) with a "well-behaved" function f on (a, b). The main idea in the method of product integration is to determine the adverse behaviour of the kernel K in an analytic form.

Let $\pi_k(\,\cdot\,)$, $k = 0, 1, \ldots$, be orthogonal polynomials with respect to the weight $w(t)$ on (a, b), and let λ_ν and τ_ν ($\nu = 1, \ldots, n$) be Christoffel numbers and nodes, respectively, of the n-point Gaussian quadrature formula (1.2). Further, let $L_n(f; \cdot)$ be the Lagrange interpolation polynomial for the function f, based on the zeros of $\pi_n(t)$, i.e.,

$$L_n(f; t) = \sum_{\nu=1}^{n} f(\tau_\nu)\ell_\nu(t),$$

where $\ell_\nu(t) = \pi_n(t)/((t - \tau_\nu)\pi_n'(\tau_\nu))$, $\nu = 1, \ldots, n$. Expanding it in terms of orthogonal polynomials $\{\pi_\nu\}$, we have

$$L_n(f; t) = \sum_{\nu=0}^{n-1} a_\nu \pi_\nu(t),$$

where the coefficients a_ν, $\nu = 0, 1, \ldots, n-1$, are given by

$$a_\nu = \frac{1}{\|\pi_\nu\|^2}(L_n(f; \cdot), \pi_\nu) = \frac{1}{\|\pi_\nu\|^2}\int_a^b w(t)L_n(f; t)\pi_\nu(t)\,dt.$$

Since the degree of $L_n(f; \cdot)\pi_\nu(\cdot) \le 2n - 2$, we can apply Gaussian formula (1.2), and then

$$a_\nu = \frac{1}{\|\pi_\nu\|^2}\sum_{k=1}^{n} \lambda_k f(\tau_k)\pi_\nu(\tau_k), \tag{2.6}$$

because of $L_n(f;\tau_k)=f(\tau_k)$ for each $k=1,\ldots,n$.

Putting $L_n(f;t)$ in (2.1) instead of $f(t)$ we obtain

$$I(f,K)=Q_n(f;x)+R_n^{PR}(f;x),$$

where

$$Q_n(f;x)=\int_a^b w(t)L_n(f;t)K(t;x)\,dt,$$

i.e.,

$$Q_n(f;x)=\sum_{\nu=0}^{n-1} a_\nu \int_a^b w(t)\pi_\nu(t)K(t;x)\,dt \tag{2.7}$$

and $R_n^{PR}(f;x)$ is the corresponding remainder. By $b_\nu(x)$ we denote the integrals in (2.7),

$$b_\nu(x)=\int_a^b w(t)\pi_\nu(t)K(t;x)\,dt, \quad \nu=0,1,\ldots,n-1. \tag{2.8}$$

Finally, we obtain so-called the *product integration rule*

$$Q_n(f;x)=\sum_{\nu=0}^{n-1} a_\nu b_\nu(x), \tag{2.9}$$

where the coefficients a_ν and $b_\nu(x)$ are given by (2.6) and (2.8), respectively. Another form of (2.9) is

$$Q_n(f;x)=\sum_{k=1}^{n} \Lambda_k(x)f(\tau_k), \tag{2.10}$$

where

$$\Lambda_k(x)=\lambda_k\sum_{\nu=0}^{n-1}\frac{1}{\|\pi_\nu\|^2}\pi_\nu(\tau_k)b_\nu(x), \quad k=1,\ldots,n.$$

As we mentioned on the beginning of this subsection, it is very important in this method to have $b_\nu(x)$ in an analytic form. It is very convenient if we have a Fourier expansion of the kernel $K(\cdot;x)$ in terms of orthogonal polynomials π_ν,

$$K(t;x)=\sum_{\nu=0}^{+\infty} B_\nu(x)\pi_\nu(t).$$

Because of (2.8), we see that $B_\nu(x)=b_\nu(x)/\|\pi_\nu\|^2$.

Let $K_n(\cdot;x)$ be the best L^2-approximation of $K(\cdot;x)$ in $\mathcal{P}_{n-1}$, i.e.,

$$K_n(t;x)=\sum_{\nu=0}^{n-1}\frac{b_\nu(x)}{\|\pi_\nu\|^2}\pi_\nu(t). \tag{2.11}$$

We can see that the product integration rule (2.9), i.e., (2.10), is equivalent to the Gaussian rule applied to the function $f(\cdot)K_n(\cdot;x)$. Indeed, since $\Lambda_k(x)=\lambda_k K_n(\tau_k;x)$, we have

$$Q_n^G(f(\cdot)K_n(\cdot;x))=\sum_{k=1}^{n}\lambda_k f(\tau_k)K_n(\tau_k;x)=Q_n(f;x).$$

In some applications $K_n(\tau_k;x)$ can be computed conveniently by Clenshaw's algorithm based on the recurrence relation (1.1) for the orthogonal polynomials π_ν.

In some cases we know analytically the coefficients in an expansion of (2.11). Now, we give some of such examples.

In [28, p. 560] we used

$$\int_{-1}^{1} C_k^\lambda(t)e^{i\omega t}(1-t^2)^{\lambda-1/2}\,dt = i^k \frac{2\pi\Gamma(2\lambda+k)}{k!\Gamma(\lambda)(2\omega)^\lambda}\,J_{k+\lambda}(\omega),$$

where $C_k^\lambda(t)$ ($\lambda > -1/2$) is the Gegenbauer polynomial of degree k. Taking this exact value of the integral we find the following expansion of $e^{i\omega t}$ in terms of Gegenbauer polynomials,

$$K(t;\omega) = e^{i\omega t} \sim \Big(\frac{2}{\omega}\Big)^\lambda \Gamma(\lambda) \sum_{k=0}^{+\infty} i^k(k+\lambda)J_{k+\lambda}(\omega)C_k^\lambda(t),$$

where $x \in [-1,1]$. In this case, (2.10) reduces to the product rule with respect to the Gegenbauer weight.

In some special cases we get: (1) For $\lambda = 1/2$ – the method of Bakhvalov-Vasil'eva [29]; (2) For $\lambda = 0$ and $\lambda = 1$ – the method of Patterson [30]. An approximation by Chebyshev polynomials was considered by Piessens and Poleunis [31].

Taking the expansion

$$e^{i\omega t} \sim e^{-(\omega/2)^2} \sum_{k=0}^{+\infty} i^k \frac{(\omega/2)^k}{k!}\,H_k(t), \quad |t| < +\infty,$$

where H_k is the Hermite polynomial of degree n, we can calculate integrals of the form

$$\int_{-\infty}^{+\infty} e^{-t^2}e^{i\omega t}f(t)\,dt.$$

In a similar way we can use the expansion

$$e^{i\omega t^2} \sim \sum_{k=0}^{+\infty} \frac{(i\omega)^k}{k!2^{2k}(1-i\omega)^{k+1/2}}\,H_{2k}(x), \quad |t| < +\infty.$$

Consider now the integral $I_\nu(f;\omega)$ given by (2.4), which can be reduced to the following form

$$\begin{aligned} I_\nu(f;\omega) &= \frac{1}{2}\int_0^{+\infty} e^{-t}J_\nu(\omega\sqrt{t})f(t)t^{\nu/2}\,dt \\ &= \frac{1}{2}\int_0^{+\infty} t^\nu e^{-t}[t^{-\nu/2}J_\nu(\omega\sqrt{t})]f(t)t^{\nu/2}\,dt, \end{aligned}$$

where we put the oscillatory kernel in the brackets. Using the monic generalized Laguerre polynomials $\hat{L}_n^\nu(t)$, which are orthogonal on $(0,+\infty)$ with respect to the weight $t^\nu e^{-t}$, we get the expansion

$$t^{-\nu/2}J_\nu(\omega\sqrt{t}) \sim \Big(\frac{\omega}{2}\Big)^\nu e^{-(\omega/2)^2} \sum_{k=0}^{+\infty} \frac{(-1)^k(\omega/2)^{2k}}{k!\Gamma(k+\nu+1)}\,\hat{L}_n^\nu(t).$$

Thus, in this case the the coefficients (2.8) become

$$b_k(\omega) = (-1)^k\Big(\frac{\omega}{2}\Big)^{\nu+2k} e^{-(\omega/2)^2}.$$

In 1979 Gabutti [4] investigated in details the case $\nu = 0$. Using a special procedure in D-arithmetic on an IBM 360/75 computer he illustrated the method taking an example with $f(t) = \sin t$ and $\omega = 20$.

At the end we mention that it is possible to find exactly $I_\nu(f;\omega)$ when $f(t) = e^{i\alpha t}$. Namely,

$$I_\nu(e^{i\alpha t};\omega) = \frac{1}{2}\Big(\frac{\omega}{2}\Big)^\nu \frac{1}{(1-i\alpha)^{\nu+1}} \exp\Big[-\frac{(\omega/2)^2}{1-i\alpha}\Big].$$

The imaginary part of this gives the previous example. An asymptotic behaviour of this integral was investigated by Frenzen and Wong [32]. They showed that $I_0(f;\omega)$ decays exponentially like $e^{-\gamma\omega^2}$, $\gamma > 0$, when $f(z)$ is an entire function subject to a suitable growth condition. Further considerations were given by Gabutti [33] and Gabutti and Lepora [34].

A significant progress in product quadrature rules (and interpolation processes) was made in the last twenty years (see Elliott and Paget [35]–[36], Sloan and Smith [37]–[39], Smith and Sloan [40], Nevai [41]–[43], Mastroianni and Vértesi [44]–[45], Mastroianni and Monegato [46], Mastroianni [47], and others).

2.3. Complex Integration Methods

Let

$$G = \{z \in \mathbb{C} \mid -1 \le \operatorname{Re} z \le 1,\ 0 \le \operatorname{Im} z \le \delta\}$$

where $\Gamma_\delta = \partial G$ (see Fig. 2.1). Consider the Fourier integral on the finite interval

$$I(f;\omega) = \int_{-1}^{1} f(x)e^{i\omega x}\,dx, \tag{2.12}$$

with an analytic real-valued function f.

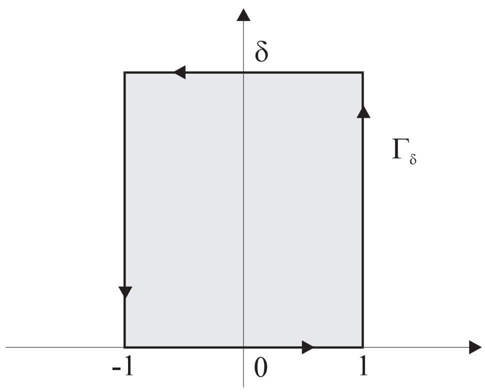

Figure 2.1: The contour of integration

Theorem 2.1. *Let f be 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 singularities z_ν $(\nu = 1,\dots,m)$ in the region $G = \operatorname{int}\Gamma$, and let*

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

Suppose that there exist the constants $M > 0$ and $\xi < \omega$ such that

$$\int_{-1}^{1} |f(x+i\delta)|\, dx \le M e^{\xi\delta}. \tag{2.13}$$

Then

$$\begin{aligned}\int_{-1}^{1} f(x)\cos\omega x\, dx &= P + \frac{2}{\omega}\int_0^{+\infty} \mathrm{Im}\Big[e^{i\omega} f_e\Big(1+i\frac{t}{\omega}\Big)\Big] e^{-t}\, dt,\\ \int_{-1}^{1} f(x)\sin\omega x\, dx &= Q - \frac{2}{\omega}\int_0^{+\infty} \mathrm{Re}\Big[e^{i\omega} f_o\Big(1+i\frac{t}{\omega}\Big)\Big] e^{-t}\, dt,\end{aligned}$$

where $f_o(z)$ and $f_e(z)$ are the odd and even part in $f(z)$, respectively.

Proof. By Cauchy's residue theorem, we have

$$\begin{aligned}\oint_{\Gamma_\delta} f(z)e^{i\omega z}\, dz &= \int_0^{\delta} f(1+iy)e^{i\omega(1+iy)} i\, dy + \int_1^{-1} f(x+i\delta)e^{i\omega(x+i\delta)}\, dx\\ &\quad + \int_\delta^0 f(-1+iy)e^{i\omega(-1+iy)} i\, dy + I(f;\omega)\\ &= 2\pi i \sum_{\nu=1}^{m} \operatorname*{Res}_{z=z_\nu}\Big\{f(z)e^{i\omega z}\Big\} = P + iQ.\end{aligned}$$

Since

$$\begin{aligned}|I_\delta| &= \Big|\int_{-1}^{1} f(x+i\delta)e^{i\omega(x+i\delta)}\, dx\Big| = e^{-\omega\delta}\,\Big|\int_{-1}^{1} f(x+i\delta)e^{i\omega x}\, dx\Big|\\ &\le e^{-\omega\delta}\int_{-1}^{1} |f(x+i\delta)|\, dx \le M e^{(\xi-\omega)\delta} \to 0 \ \ \text{(because of (2.13))},\end{aligned}$$

when $\delta \to +\infty$, we obtain

$$I(f;\omega) = P + iQ + \frac{1}{i\omega}\int_0^{+\infty} \Big[e^{i\omega} f\Big(1+i\frac{t}{\omega}\Big) - e^{-i\omega} f\Big(-1+i\frac{t}{\omega}\Big)\Big] e^{-t}\, dt.$$

Taking $f(z) = f_o(z) + f_e(z)$ and separating the real and imaginary part in the previous formula, we get the statement of theorem. ■

The obtained integrals in Theorem 2.1 can be solved by using Gauss-Laguerre rule. In order to illustrate the efficiency of this method we consider a simple example – Fourier coefficients (2.2), with $f(t) = 1/(t^2+\varepsilon^2)$, $\varepsilon > 0$.

Since

$$c_k(f) = \int_{-1}^{1} f(\pi x)e^{ik\pi x}\, dx, \qquad \omega = k\pi,$$

and

$$e^{i\omega} f\Big(1+i\frac{t}{\omega}\Big) - e^{-i\omega} f\Big(-1+i\frac{t}{\omega}\Big) = (-1)^k\Big[f\Big(\pi+i\frac{t}{k}\Big) - f\Big(-\pi+i\frac{t}{k}\Big)\Big],$$

we get

$$c_k(f) = P + iQ - i\frac{(-1)^k}{\pi k}\int_0^{+\infty} \Big[f\Big(\pi+i\frac{t}{k}\Big) - f\Big(-\pi+i\frac{t}{k}\Big)\Big] e^{-t}\, dt.$$

In our case, we have

$$f(\pi z) = \frac{1}{\pi^2 z^2+\varepsilon^2}, \quad P + iQ = 2\pi i \operatorname*{Res}_{z=i\varepsilon/\pi}\Big\{f(\pi z)e^{ik\pi z}\Big\} = \frac{1}{\varepsilon}\, e^{-k\varepsilon},$$

and

$$f\Big(\pi + i\frac{t}{k}\Big) - f\Big(-\pi + i\frac{t}{k}\Big) = -\frac{4\pi i\,(t/k)}{\left(\varepsilon^2 + \pi^2 - (t/k)^2\right)^2 + 4\pi^2(t/k)^2},$$

we get

$$a_k(f) = e^{-k} - 4\frac{(-1)^k}{k}\int_0^{+\infty} \frac{t/k}{\left(\varepsilon^2 + \pi^2 - (t/k)^2\right)^2 + 4\pi^2(t/k)^2}\, e^{-t}\, dt.$$

Of course, $b_k(f) = 0$.

In Table 2.1 we give coefficients for $k = 5, 10, 40$ obtained for $\varepsilon = 1$ in D-arithmetic (with machine precision 2.22×10^{-16}). Numbers in parentheses indicate decimal exponents.

Table 2.1: Fourier coefficients $a_k(f)$ for $f(t) = 1/(t^2 + \varepsilon^2)$, $\varepsilon = 1$

k	$a_k(f)$
5	8.0466954304415(-3)
10	-2.9016347088212(-4)
40	-2.1147947576924(-5)

Table 2.2 shows relative errors in Gaussian approximation of Fourier coefficients $a_k(f)$ for $\varepsilon = 1$ and $k = 5, 10, 40$, when we apply the N-point Gauss-Laguerre rule (GLa). In the last column of Table 2.2 we give the correponding relative errors in the case when $\varepsilon = 0.01$ and $k = 20$, where $a_{20}(f) = -1.023459866383(-4)$.

Table 2.2: Relative errors in N-point GLa-approximations of $a_k(f)$

	$\varepsilon = 1$			$\varepsilon = 0.01$
N	$k = 5$	$k = 10$	$k = 40$	$k = 20$
1	4.7(−3)	8.6(−3)	4.7(−4)	3.2(−9)
2	1.6(−4)	8.1(−5)	2.9(−7)	1.2(−11)
3	6.0(−6)	8.5(−7)	1.6(−10)	6.8(−14)
4	2.6(−7)	7.3(−9)	3.4(−14)	
5	1.7(−8)	1.6(−11)		
10	2.8(−13)			

On the other side, a direct application of N-point Gauss-Legendre rule (GLe) ($N = 5(5)40$) to the integral

$$a_k(f) = \frac{1}{\pi}\int_{-\pi}^{\pi} \frac{\cos kt}{t^2 + \varepsilon^2}\, dt, \tag{2.14}$$

gives bed results with a slow convergence (see Table 2.3).

The rapidly oscillatory integrand in (2.14) is displyed in Figure 2.2 for $\varepsilon = 1$ and $k = 40$.

Consider now the Fourier integral on $(0, +\infty)$,

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

Table 2.3: Relative errors in N-point GLe-approximations of $a_k(f)$

	$\varepsilon = 1$			$\varepsilon = 0.01$
N	$k = 5$	$k = 10$	$k = 40$	$k = 20$
5	5.2(1)	1.5(3)	3.0(4)	5.6(7)
10	2.5(1)	2.3(1)	1.4(4)	2.8(4)
15	1.1(0)	2.2(3)	2.4(4)	2.0(7)
20	4.9(−2)	2.0(2)	2.6(4)	3.7(3)
25	2.1(−3)	8.8(0)	4.1(3)	1.2(7)
30	9.3(−5)	3.8(−1)	2.5(4)	9.0(4)
35	4.6(−6)	1.7(−2)	8.9(2)	8.7(6)
40	1.8(−7)	7.3(−4)	2.1(3)	6.9(4)

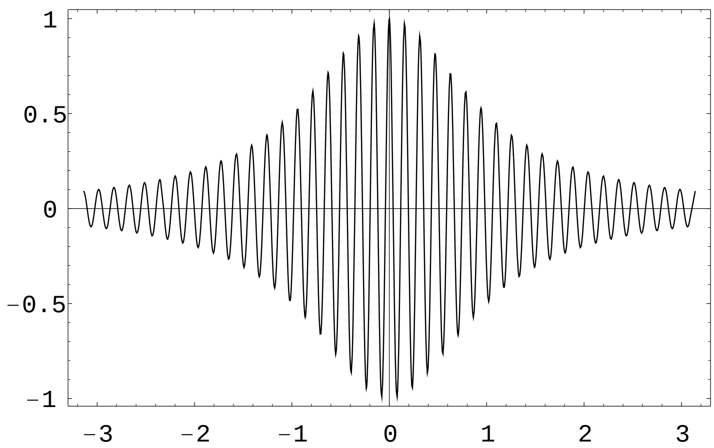

Figure 2.2: The case $\varepsilon = 1$ and $k = 40$

which can be transformed to

$$F(f;\omega) = \frac{1}{\omega}\int_0^{+\infty} f(x/\omega)e^{ix}\,dx = F(f(\cdot/\omega);1),$$

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 put

$$K(f;1) = \int_0^a f(x)e^{ix}\,dx + \int_a^{+\infty} f(x)e^{ix}\,dx = L_1(f) + L_2(f),$$

where

$$L_1(f) = a\int_0^1 f(at)e^{iat}\,dt \quad \text{and} \quad L_2(f) = \int_a^{+\infty} f(x)e^{ix}\,dx.$$

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

$$|f(z)| \leq \frac{A}{|z|}, \quad \text{when } |z| \to +\infty, \tag{2.15}$$

for some positive constant A. Then

$$L_2(f) = ie^{ia} \int_0^{+\infty} f(a+iy)e^{-y}\, dy \qquad (a > 0).$$

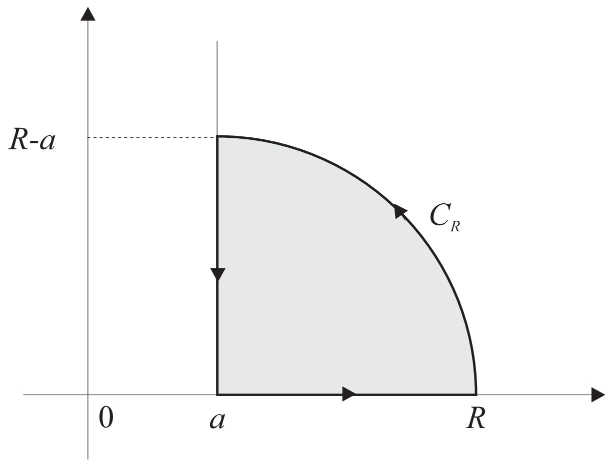

Figure 2.3: The contour of integration

Proof. Taking $a > 0$ and the closed contour C_R in D (see Fig. 2.3) we get, by Cauchy's residue theorem,

$$\int_a^R f(x)e^{ix}\, dx \; + \; \int_0^{\pi/2} [f(z)e^{iz}]_{z=a+(R-a)e^{i\theta}} (R-a)ie^{i\theta}\, d\theta \\ + \; i\int_{R-a}^0 f(a+iy)e^{i(a+iy)}\, dy = 0.$$

Because of (2.15), we have that $|f(z)| \le a/(R-2a)$, when $R \to +\infty$. Using the Jordan's lemma we obtain the following estimate for the integral over the arc

$$\Big| \int_0^{\pi/2} [f(z)e^{iz}]_{z=a+(R-a)e^{i\theta}} (R-a)ie^{i\theta}\, d\theta \Big| \le \frac{\pi}{2} \cdot \frac{A}{R-2a} (1 - e^{-(R-a)}) \to 0,$$

when $R \to +\infty$, and then desired result follows. ∎

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. In order to illustrate the numerical results, we consider the integral

$$F(\cos(\cdot); 1) = \int_0^{+\infty} \frac{\cos x}{1+x^3}\, dx = 0.70888800613933\ldots$$

The relative errors in approximations using N-point quadrature rules, with different values of a, are shown in Table 2.4.

3. SOME APPLICATIONS OF QUADRATURES

In this section we give a few applications of Gaussain quadrature rules in some problems in physics and telecommunications, where is very important to calculate integrals with

Table 2.4: Relative errors in N-point Gaussian approximations of $F(\cos(\cdot);1)$

N	$a=1$	$a=2$	$a=3$	$a=4$	$a=5$
10	4.7(−3)	2.3(−4)	1.1(−6)	8.4(−5)	1.3(−4)
20	1.2(−2)	8.8(−6)	4.9(−8)	1.1(−9)	1.5(−8)
30	2.7(−3)	4.8(−9)	1.1(−9)	8.8(−12)	1.2(−12)
40	9.9(−4)	4.5(−8)	3.8(−11)	6.3(−14)	4.1(−15)

a high precision. If we want to have a good quadrature process with a reasonable convergence, then the integrand should be sufficiently regular. Furthermore, singularities in its first or second derivative can be disturbing. Also, the quasi singularities, i.e., singularities near to the integration interval, cause remarkable decelerate of the convergence.

3.1. Integration of the Error Function

We consider now an integral which appears in telecommunications (see [48]),

$$P_e = \frac{1}{\pi^m}\int_0^{\pi}\cdots\int_0^{\pi} \operatorname{erfc}\Big[c\Big(1+\sum_{k=1}^{m} c_k\cos\theta_k\Big)\Big]\,d\theta_1\ldots d\theta_m,$$

where c and c_k are positive constants, and the error function $\operatorname{erfc}(t)$ is defined by

$$w(t) = \operatorname{erfc}(t) = \frac{1}{\sqrt{2\pi}}\int_t^{+\infty} e^{-x^2/2}\,dx. \tag{3.1}$$

In our calculation, we used the following approximation $(0 \le t < +\infty)$

$$\operatorname{erfc}(t) = (a_1x + a_2x^2 + a_3x^3 + a_4x^4 + a_5x^5)e^{-t^2/2} + \varepsilon, \tag{3.2}$$

where $x = 1/(1+pt)$, $p = 0.23164189$, and $|\varepsilon| \le 0.75\times 10^{-7}$. The coefficients a_k are given by:

$$\begin{aligned} a_1 &= 0.127414796, & a_2 &= -0.142248368,\\ a_3 &= 0.7107068705, & a_4 &= -0.7265760135,\\ a_5 &= 0.5307027145. \end{aligned}$$

In order to calculate P_e (the error probability in telecommunications), we put $x_k = \cos\theta_k$ $(k=1,\ldots,m)$. Then, we get

$$P_e = \frac{1}{\pi^m}\int_{-1}^{1}\frac{dx_1}{\sqrt{1-x_1^2}}\cdots\int_{-1}^{1}\frac{1}{\sqrt{1-x_1^m}}\operatorname{erfc}\Big[c\Big(1+\sum_{k=1}^{m}c_kx_k\Big)\Big]\,dx_m.$$

Applying the Gauss-Chebyshev quadrature formula

$$\int_{-1}^{1}\frac{f(t)}{\sqrt{1-t^2}}\,dt = \frac{\pi}{n}\sum_{\nu=1}^{n} f(\tau_\nu) + R_n(f), \tag{3.3}$$

where τ_ν $(\nu = 1,\ldots,n)$ are zeros of the Chebyshev polynomial $T_n(t)$, i.e.,

$$\tau_\nu = \cos\frac{(2\nu-1)\pi}{2n}, \qquad \nu = 1,\ldots,n,$$

successively m times, we obtain

$$P_e = \frac{1}{n^m} \sum_{\nu_1=1}^{n} \cdots \sum_{\nu_m=1}^{n} \operatorname{erfc}\Big[c\Big(1 + \sum_{k=1}^{m} c_k \tau_{\nu_k}\Big)\Big] + E_n^{(m)}, \tag{3.4}$$

where $E_n^{(m)}$ is the corresponding error. Notice that for $f \in C^{2n}[-1,1]$ the remainder $R_n(f)$ in (3.3) can be represented in the form

$$R_n(f) = \frac{\pi}{2^{2n-1}(2n)!}\, f^{(2n)}(\xi) \qquad (-1 < \xi < 1).$$

In order to estimate $E_n^{(m)}$ we take $f(t) = \operatorname{erfc}(a+bt)$ $(z = a+bt,\ a, b > 0)$. Then we can find

$$f^{(2n)}(t) = -\frac{b^{2n}}{\sqrt{2\pi}} \cdot \frac{d^{2n-1}}{dz^{2n-1}}(e^{-z^2/2}) = \frac{b^{2n}}{2^n\sqrt{\pi}} e^{-s^2} H_{2n-1}(s),$$

where $s = z/\sqrt{2}$ and $H_{2n-1}(s)$ is the Hermite polynomial of degree $2n-1$. Then, for the remainder term in the Gauss-Chebyshev formula (3.3) we get

$$r_n = R_n(f) = \frac{\sqrt{\pi}\, b^{2n}}{2^{3n-1}(2n)!}\, e^{-v^2} H_{2n-1}(v),$$

where $v = (a+b\xi)/\sqrt{2}$ $(-1 < \xi < 1)$. Since (see [49])

$$|H_{2n-1}(v)| \le |v| e^{v^2/2} \frac{(2n)!}{n!}\,,$$

we conclude that

$$|r_n| \le \frac{\sqrt{\pi} b^{2n}}{2^{3n-1} n!}\, |v| e^{-v^2} \le \pi K_n b^{2n},$$

not depending on a. By induction, we can prove:

THEOREM 3.1. *For the remainder $E_n^{(m)}$ in (3.4) the following estimate*

$$|E_n^{(m)}| \le \frac{c^{2n}}{2^{3n-1} n! \sqrt{\pi e}} \sum_{k=1}^{m} c_k^{2n} \tag{3.5}$$

holds.

Thus, basing on (3.4) we have a formula for numerical calculation of the integral P_e in the form

$$P_e \approx P_e^{(n)} = \frac{1}{n^m} \sum_{\nu_1=1}^{n} \cdots \sum_{\nu_m=1}^{n} \operatorname{erfc}\Big[c\Big(1 + \sum_{k=1}^{m} c_k \tau_{\nu_k}\Big)\Big]. \tag{3.6}$$

If the error in (3.2) is such that $|\varepsilon| \le E$, then for the total error in the approximation (3.6) we have

$$|\varepsilon_T| \le E + |E_n^{(m)}|.$$

The number of nodes in the Gauss-Chebyshev formula (3.3) should be taken so that the upper bound of the error $E_n^{(m)}$, given in (3.5), be the same order as E.

3.2. Singular Integrals in Analysis of Antennas

A numerical procedure for a class of singular integrals which appear in the analysis of a monopole antenna, coaxially located along the axis of a infinite conical reflector was given in [50]. Namely, the authors considered the integral

$$I(a,\nu)=\int_0^a \frac{j_\nu(x)}{x}\sin(a-x)\,dx, \tag{3.7}$$

where $j_\nu(x)$ is the spherical Bessel function of the index ν, defined by

$$j_\nu(x)=\frac{\sqrt{\pi}}{2}\Big(\frac{x}{2}\Big)^\nu\sum_{k=0}^{+\infty}\frac{(-1)^k(x/2)^{2k}}{k!\Gamma(\nu+k+3/2)},$$

and the index ν is a solution of the equation

$$P_\nu(\cos\theta_1)=0, \tag{3.8}$$

where $P_\nu(\cos\theta)$ is the Legendre function of the the first kind defined by

$$P_\nu(\cos\theta)=\frac{\sqrt{2}}{\pi}\int_0^\theta\frac{\cos(\nu+1/2)\varphi}{\sqrt{\cos\varphi-\cos\theta}}\,d\vartheta, \tag{3.9}$$

and θ_1 is the flare angle of the cone. Equation (3.8) has an infinite number of solutions ν_k $(k\in\mathbb{N})$.

Since

$$\lim_{x\to 0+}\frac{j_\nu(x)}{x}=\begin{cases}0, & \nu>1,\\ 1/3, & \nu=1,\\ +\infty, & \nu<1,\end{cases}$$

we see that the integrand in (3.7) is singular when $\nu<1$. This case occurs when $\theta_1>\pi/2$. Namely, then the first solution of (3.8) is less than 1 ($\nu_1<1$). An analysis of this equation was done in [51] (see also [52]).

The integration problem (3.7) was solved in [50] by extraction of singularity in the form

$$I(a,\nu)=C_\nu(a)\frac{a^\nu}{\nu}+\int_0^a\frac{j_\nu(x)\sin(a-x)-C_\nu(a)x^\nu}{x}\,dx,$$

where $C_\nu(a)=2^{-\nu-1}\sqrt{\pi}\sin a/\Gamma(\nu+3/2)$. For calculation of the spherical Bessel function the authors used a procedure given in [52].

We give here an alternative procedure for (3.7) using only Gaussian quadratures. In our approach we take an integral representation of the Bessel functions.

Since

$$j_\nu(z)=\sqrt{\frac{\pi}{2z}}\,J_{\nu+1/2}(z),$$

using the following representation for the cylindric Bessel functions (see [53, p. 360, Eq. 9.1.20])

$$J_\nu(z)=\frac{2(z/2)^\nu}{\sqrt{\pi}\Gamma(\nu+1/2)}\int_0^1(1-t^2)^{\nu-1/2}\cos(zt)\,dt\quad(\operatorname{Re}\nu>-1/2),$$

we find

$$j_\nu(x)=\frac{(x/2)^\nu}{2\Gamma(\nu+1)}\int_{-1}^1(1-t^2)^\nu\cos(xt)\,dt$$

and then

$$I(a,\nu) = \frac{1}{4\Gamma(\nu+1)} \int_0^a \Big(\frac{x}{2}\Big)^{\nu-1} \sin(a-x)dx \int_{-1}^1 (1-t^2)^\nu \cos(xt)\,dt,$$

i.e.,

$$I(a,\nu) = \frac{1}{4\Gamma(\nu+1)} \int_{-1}^1 (1-t^2)^\nu G_\nu(t)\,dt,$$

where

$$G_\nu(t) = \int_0^a \Big(\frac{x}{2}\Big)^{\nu-1} \sin(a-x)\cos(xt)\,dx \quad (\nu>0).$$

After integration by parts, this formula reduces to

$$G_\nu(t) = \frac{2}{\nu}\int_0^a \Big(\frac{x}{2}\Big)^{\nu} [\cos(a-x)\cos xt + t\sin(a-x)\cos xt]dx.$$

Changing variables $x = a(1-\xi^2)$ $(\xi \ge 0)$, we get

$$G_\nu(t) = \frac{8}{\nu}\Big(\frac{a}{2}\Big)^{\nu+1} \int_0^1 \xi(1-\xi^2)^\nu g(\xi,t)\,d\xi,$$

where

$$g(\xi,t) = \cos[a\xi^2]\cos[at(1-\xi^2)] + t\sin[a\xi^2]\sin[at(1-\xi^2)].$$

Notice that $g(\pm\xi,\pm t) = g(\xi,t)$. Because of that, we have

$$I(a,\nu) = \frac{(a/2)^{\nu+1}}{\nu\Gamma(\nu+1)} \int_{-1}^1\int_{-1}^1 w^{(\nu,1)}(\xi) w^{(\nu,0)}(t) g(\xi,t)\,d\xi dt,$$

where $w^{(\nu,\mu)}(t) = |t|^\mu (1-t^2)^\nu$ is the *generalized Gegenbauer weight.*

The (monic) generalized Gegenbauer polynomials $W_k^{(\alpha,\beta)}(t)$, orthogonal on $(-1,1)$ with respect to the weight $w^{(\alpha,\mu)}(t) = |t|^\mu(1-t^2)^\alpha$, $\beta = (\mu-1)/2$, $(\alpha,\mu > -1)$, were introduced by Lascenov [54] (see, also, Chihara [55, pp. 155–156]). These polynomials can be expressed in terms of the Jacobi polynomials,

$$\begin{aligned} W_{2k}^{(\alpha,\beta)}(t) &= \frac{k!}{(k+\alpha+\beta+1)_k} P_k^{\alpha,\beta)}(2t^2-1), \\ W_{2k+1}^{(\alpha,\beta)}(t) &= \frac{k!}{(k+\alpha+\beta+2)_k} xP_k^{\alpha,\beta+1)}(2t^2-1). \end{aligned}$$

Notice that $W_{2k+1}^{(\alpha,\beta)}(t) = tW_{2k}^{(\alpha,\beta+1)}(t)$. The coefficients in their three-term recurrence relation

$$\begin{aligned} W_{k+1}^{(\alpha,\beta)}(t) &= tW_k^{(\alpha,\beta)}(t) - \beta_k W_{k-1}^{(\alpha,\beta)}(t), \quad k=0,1,\ldots, \\ W_{-1}^{(\alpha,\beta)}(t) &= 0, \;\; W_0^{(\alpha,\beta)}(t) = 1, \end{aligned}$$

are known in the explicit form. Namely,

$$\begin{aligned} \beta_{2k} &= \frac{k(k+\alpha)}{(2k+\alpha+\beta)(2k+\alpha+\beta+1)}, \\ \beta_{2k-1} &= \frac{(k+\beta)(k+\alpha+\beta)}{(2k+\alpha+\beta-1)(2k+\alpha+\beta)}, \end{aligned}$$

for $k = 1, 2, \ldots$, except when $\alpha+\beta = -1$; then $\beta_1 = (\beta+1)/(\alpha+\beta+2)$. Some applications of these polynomials in numerical quadratures and least square approximation with constraint were given in [56] and [57], respectively.

The construction of the corresponding Gaussian quadratures is very simple in this case with regard to the knowledge of recursion coefficients. Here also, there is a convenience in a number of the integrand evaluations. Since the integrand is even, we can get the Gaussian quadrature of degree of exactness $4N-1$, taking only N (positive) points $\tau_1^{(\mu,\nu)}, \ldots, \tau_N^{(\mu,\nu)}$, as zeros of the polynomial $W_{2N}^{(\alpha,\beta)}(t)$, where $\alpha = \nu$, $\beta = (\mu-1)/2$. Thus,

$$\int_1^1 w^{(\mu,\nu)}(t)\phi(t)\,dt \approx Q_N^{(\mu,\nu)}(\phi) = 2\sum_{i=1}^{N} A_k^{(\mu,\nu)}\phi(\tau_k^{(\mu,\nu)}),$$

and we finally get

$$I(a,\nu) \approx I_N(a,\nu) = \frac{4(a/2)^{\nu+1}}{\nu\Gamma(\nu+1)}\sum_{i=1}^{N}\sum_{j=1}^{N} A_i B_j g(x_i, y_j),$$

where, because of simplicity, we put

$$A_k = A_k^{(1,\nu)}, \quad x_k = \tau_k^{(1,\nu)}, \quad B_k = A_k^{(0,\nu)}, \quad y_k = \tau_k^{(0,\nu)},$$

for $k = 1, \ldots, n$. This quadrature formula is based on N^2 nodes and gives good approximation of the integral $I(\pi/2,\nu)$. The obtained results rounded to 12 decimal places, for $a = \pi/2$ and $\nu = 0.1(0.1)1.0$, are displayed in Table 3.1. We used our quadrature formula for $N = 7$. All digits in approximation $I_7(\pi/2,\nu)$ are correct.

Table 3.1: Approximation of $I(\pi/2,\nu)$ for $\nu = 0.1(0.1)1.0$

ν	Approximation $I_7(\pi/2,\nu)$
0.1	9.092660539259
0.2	4.113983342491
0.3	2.470467111313
0.4	1.661658513482
0.5	1.187153595723
0.6	0.879930124888
0.7	0.668250458550
0.8	0.516135176348
0.9	0.403518784385
1.0	0.318309886184

Table 3.2 shows the relative errors in approximations $I_N(\pi/2,\nu)$ for $N = 2(1)6$ and again $\nu = 0.1(0.1)1.0$. As we can see, the convergence of approximations is fast and we can take relatively small N in order to get a satisfactory result.

3.3. Calculation of Legendre Functions

Numerical calculation of the Legendre function of the first order is also possible using Gaussian quadratures. We start with Dirichlet-Mehler integral representation (3.9). The functions $P_\nu(x)$ satisfy the three-term recurrence relation

$$(\nu+2)P_{\nu+2}(t) = (2\nu+3)tP_{\nu+1}(t) - (\nu+1)P_\nu(t). \tag{3.10}$$

Table 3.2: Relative errors in approximations $I_N(\pi/2,\nu)$ for $\nu = 0.1(0.1)1.0$ and $N = 2(1)6$

ν	$N=2$	$N=3$	$N=4$	$N=5$	$N=6$
0.1	9.2(−3)	1.5(−4)	1.3(−6)	7.6(−9)	3.0(−11)
0.2	8.2(−3)	1.3(−4)	1.1(−6)	6.3(−9)	2.5(−11)
0.3	7.2(−3)	1.1(−4)	9.4(−7)	5.3(−9)	2.1(−11)
0.4	6.5(−3)	9.5(−5)	8.0(−7)	4.4(−9)	1.7(−11)
0.5	5.8(−3)	8.3(−5)	6.9(−7)	3.7(−9)	1.4(−11)
0.6	5.2(−3)	7.3(−5)	5.9(−7)	3.1(−9)	1.2(−11)
0.7	4.6(−3)	6.4(−5)	5.1(−7)	2.6(−9)	9.8(−12)
0.8	4.2(−3)	5.6(−5)	4.4(−7)	2.2(−9)	8.2(−12)
0.9	3.8(−3)	4.9(−5)	3.8(−7)	1.9(−9)	6.9(−12)
1.0	3.4(−3)	4.4(−5)	3.3(−7)	1.6(−9)	5.8(−12)

When ν is an nonnegative integer, the functions $P_\nu(t)$ reduce to the Legendre polynomials orthogonal on $(-1,1)$.

The integrand in (3.9) is quasi-singular at $\theta = 0$, i.e., when $t = 1$. Therefore, we use an extraction in the form

$$\begin{aligned} P_\nu(\cos\theta) &= \cos[(\nu+1/2)\theta]P_{-1/2}(\cos\theta) \\ &\quad +\frac{\sqrt{2}}{\pi}\int_0^\theta \frac{\cos(\nu+1/2)\varphi-\cos(\nu+1/2)\theta}{\sqrt{\cos\varphi-\cos\theta}}\,d\theta, \end{aligned}$$

and then we change variables $\varphi = \theta(1-x^2)$ in order to get an integral on $(0,1)$. Thus, we find

$$P_\nu(\cos\theta) = \frac{2}{\pi}\cos[(\nu+1/2)\theta]K\Big(\sin\frac{\theta}{2}\Big) + \frac{4}{\pi}\int_0^1 S(\theta,x)\,dx,$$

where

$$S(\theta,x) = \frac{(\theta x)\sin[(\nu+1/2)(\theta-\xi)]\sin\xi}{\sin^{1/2}(\theta-\xi)\sin^{1/2}\xi}\,, \quad \xi = \frac{\theta x^2}{2}\,,$$

and K is the complete elliptic integral of the first kind.

Table 3.3: Maximal absolute errors in calculation of $P_\nu(\cos\theta)$, $0 \le \theta \le \vartheta$, $0 \le \nu < 2$

N	$\vartheta=\pi/3$	$\vartheta=\pi/2$	$\vartheta=2\pi/3$	$\vartheta=5\pi/6$
5	8.9(−7)	3.1(−6)	1.7(−4)	1.5(−3)
10	4.7(−13)	5.9(−13)	7.1(−11)	1.5(−9)

For numerical calculation of the integral $\int_0^1 S(\theta,x)\,dx$ we use the standard N-point Gauss-Legendre quadrature formula transformed before to $(0,1)$, while for the complete elliptic integral

$$K(\sin\alpha) = \int_0^{\pi/2}(1-\sin^2\alpha\sin^2\theta)^{-1/2}\,d\theta$$

we use the well-known process of the arithmetic-geometric mean (cf. [53, pp. 598–599]). An analysis of this quadrature process shows that we must take $N = 20$ in the Gauss-Legendre rule in order to get the values of $P_\nu(\cos\theta)$ for $0 \le \nu < 2$ and $0 \le \theta < \pi$

with an absolute error less than 10^{-10}. Some computational problems can occur when $\theta \to \pi$. By certain restrictions on θ, for example $0 \le \theta \le \vartheta < \pi$, our approximation for $P_\nu(\cos\theta)$ gives better results. The corresponding maximal absolute errors in calculation of $P_\nu(\cos\theta)$ are given in Table 3.3.

When the index $\nu \ge 2$ it is convenient to use three-term recurrence relation (3.10), starting by two values $P_\mu(\cos\theta)$ and $P_{\mu+1}(\cos\theta)$, where $0 \le \mu < 1$. One similar procedure was given in [51].

3.4. Integrals Occurring in Quantum Mechanics

Let α and β be real parameters such that $\alpha^2 < 4\beta$, and let $w^{(\alpha,\beta)}(t)$ be a modified exponential weight on $(-\infty, +\infty)$, given by

$$w^{(\alpha,\beta)}(t) = \frac{e^{-t^2}}{\sqrt{1+\alpha t+\beta t^2}}\,.$$

Recently Bandrauk [58] stated a problem[1] of finding a computationally effective approximations for the integral

$$I_{m,n}^{\alpha,\beta} = \int_{-\infty}^{+\infty} \hat{H}_m(t)\hat{H}_n(t)w^{(\alpha,\beta)}(t)\,dt, \tag{3.11}$$

where $\hat{H}_n(t)$ is the monic Hermite polynomial of degree n. The function $t \mapsto H_m(t)e^{-t^2/2}$ is the quantum-mechanical wave function of m photons, the quanta of the electromagnetic field. The integral express the modification of atomic Coulomb potentials by electromagnetic fields. The integral $I_{0,0}^{\alpha,\beta}$ is of interest in its own right. It represents the vacuum or zero-field correction.

Evidently, for $\alpha = \beta = 0$, the integral $I_{m,n}^{\alpha,\beta}$ expresses the orthogonality of the Hermite polynomials, and $I_{m,n}^{0,0} = 0$ for $m \ne n$.

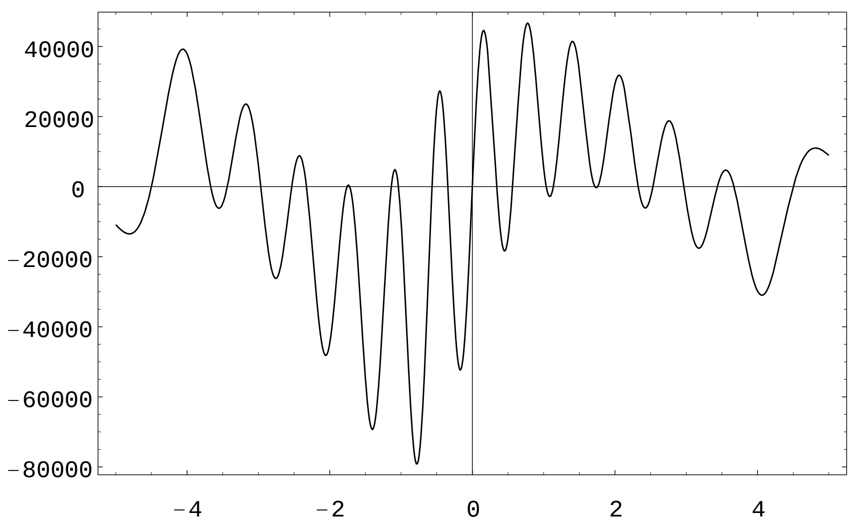

Figure 3.1: The case $\alpha = \beta = 1$ and $m = 10$, $n = 15$

[1] The original problem was stated with the Hermite polynomials $H_k(t) = 2^k\hat{H}_k(t)$ $(k \ge 0)$.

In order to compute the recursion coefficients in three-term recurrence relation (1.1) for the weight $w^{(\alpha,\beta)}(t)$ on $\mathbb{R}$, we use the discretized Stieltjes procedure, with the discretization based on the Gauss-Hermite quadratures,

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

where P is an arbitrary algebraic polynomial, and τ_k^H and λ_k^H are the parameters of the N-point Gauss-Hermite quadrature formula. We need such a procedure for each of selected pairs (α,β). The recursion coefficients for $\alpha=\beta=1$ are shown in Table 3.4.

Table 3.4: Recursion coefficients for the polynomials $\{\pi_k(\,\cdot\,;w^{(1,1)})\}$

k	alpha(k)	beta(k)
0	-1.13718980227451884899E-01	1.60766630028944893121E+00
1	-2.98816813129032592761E-02	3.97745941390277354575E-01
2	-1.85679035713552418458E-02	8.59017858999744830059E-01
3	-1.11233908951155754459E-02	1.34150020202713424624E+00
4	-7.92784095565612963769E-03	1.82832224474490311965E+00
5	-5.94481593708158274332E-03	2.32049028595201023201E+00
6	-4.61320306236083269485E-03	2.81392714298467724481E+00
7	-3.77400607804653998726E-03	3.30922646548235467381E+00
8	-3.10374039370687352784E-03	3.80522704177833428173E+00
9	-2.65108641700060815508E-03	4.30202508196469245713E+00
10	-2.26842278846161700443E-03	4.79927392312629547184E+00
11	-1.98912530996355941798E-03	5.29692873475598728737E+00
12	-1.74932773647048079346E-03	5.79488527243872611520E+00
13	-1.56237000002809778848E-03	6.29308070865561292494E+00
14	-1.40104941875887432738E-03	6.79148342996299101450E+00
15	-1.26885269546785898765E-03	7.29004317825168070747E+00
16	-1.15424028426112948617E-03	7.78874923730844163954E+00
17	-1.05691742533931946106E-03	8.28756682324525295902E+00
18	-9.71970640332240357136E-04	8.78649067850541708346E+00
19	-8.98019722632390496377E-04	9.28549797716577173470E+00

The integrand $t\mapsto \hat{H}_m(t)\hat{H}_n(t)w^{(\alpha,\beta)}(t)$ in (3.11) has $m+n$ zeros in the integration interval and very big oscillations. The case $\alpha=\beta=1$ and $m=10$, $n=15$ is displayed in Figure 3.1.

Applying the corresponding Gaussian formulas, with respect to the weight $w^{(\alpha,\beta)}(t)$, to $I_{m,n}^{\alpha,\beta}$ we get approximative formulas

$$I_{m,n}^{\alpha,\beta} \approx Q_{m,n}^{\alpha,\beta} = \sum_{\nu=1}^{N} \lambda_\nu^{(\alpha,\beta)} \hat{H}_m(\tau_\nu^{(\alpha,\beta)})\hat{H}_n(\tau_\nu^{(\alpha,\beta)}). \tag{3.12}$$

In Table 3.5 we present the obtained results for $\alpha=\beta=1$ in double precision arithmetic in two cases: $m=3$, $n=6$, and $m=10$, $n=15$. The number of nodes in

Table 3.5: Gaussian approximation of the integral $I_{m,n}^{\alpha,\beta}$

N	$Q_{3,6}^{1,1}$	$Q_{10,15}^{1,1}$
5	2.63168167926273(-1)	-4.01134148759825(4)
10	2.63168167926273(-1)	3.20721013272847(4)
15	2.63168167926273(-1)	-2.06784419769247(4)
20	2.63168167926273(-1)	-2.06784419769247(4)

quadrature formula (3.12) was $N = 5, 10, 15, 20$. Since the N-point Gaussian quadrature formula (3.12) has maximum algebraic degree of exactness $2N - 1$, we see that obtained results are exact for every N such that $2N - 1 \geq m + n$.

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