Quadratures for oscillatory and singular integrals

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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, as well as Gaussian quadratures with respect to the oscillatory weight $w(x) = xe^{im\pi x}$, $x \in [-1, 1]$. Numerical examples are included.*

Keywords: Numerical integration, Orthogonal polynomials, Product rules, Gaussian quadratures, Oscillatory kernel, Singular kernel.

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, some new approaches, as well as a few applications of quadrature formulas. 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

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

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

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

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.

There is a MATHEMATICA package for numerical and symbolic construction of orthogonal polynomials and quadrature formulas under title "OrthogonalPolynomials" (see [3], [4]). The package has implemented almost all the classes of orthogonal polynomials studied up to date.

This paper is organized as follows. In Section 2 we introduce a class of orthogonality with respect to an oscillatory weight. Section 3 discusses the methods for oscillatory functions, including the standard methods, the product rules, as well as some complex integration methods. Section 4 is dedicated to constructions and applications of some efficient quadratures, including Gaussian quadratures with respect to the oscillatory weight $w(x) = xe^{im\pi x}$, $x \in [-1, 1]$.

2. ORTHOGONALITY WITH RESPECT TO AN OSCILLATORY WEIGHT

Let a complex valued linear functional $\mathcal{L}$ be given on the linear space of all algebraic polynomials $\mathcal{P}$. The values of the linear functional $\mathcal{L}$ at the set of monomials are called moments and they are denoted by μ_k. Thus, $\mathcal{L}[x^k] = \mu_k$, $k \in \mathbb{N}_0$. A sequence of polynomials $\{P_n(x)\}_{n=0}^{\infty}$ is called a *formal orthogonal polynomial sequence* with respect to a *moment functional* $\mathcal{L}$ provided for all nonnegative integers k and n,

 $1°$ $P_n(x)$ is a polynomial of degree n,
 $2°$ $\mathcal{L}[P_n(x)P_k(x)] = 0$ for $k \neq n$,
 $3°$ $\mathcal{L}[P_n(x)^2] \neq 0$.

If a sequence of orthogonal polynomial exists for a given linear functional $\mathcal{L}$, then $\mathcal{L}$ is called *quasi-definite linear functional*. Under condition $\mathcal{L}[P_n^2(x)] > 0$, the functional $\mathcal{L}$ is called positive definite. For details see Chihara [5, pp. 6–17].

The necessary and sufficient conditions for the existence of a sequence of orthogonal polynomials with respect to the linear functional $\mathcal{L}$ are that for each $n \in \mathbb{N}$ the Hankel determinants

$$\Delta_n = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} \\ \mu_1 & \mu_2 & & \mu_n \\ \vdots & & & \\ \mu_{n-1} & \mu_n & & \mu_{2n-2} \end{vmatrix} \neq 0. \tag{2.1}$$

In the case of positive definiteness of $\mathcal{L}$, we can define $(p, q) := \mathcal{L}[p(x)\overline{q(x)}]$ for all algebraic polynomials $p(x)$ and $q(x)$, so that the orthogonality with respect to the moment functional $\mathcal{L}$ is consistent with the standard definition of orthogonality with respect to an inner product. On the other side, there are several interesting quasi-definite cases when the moments are non-real. We mention here only *orthogonality with respect to an oscillatory weight* [6].

Let $w(x) = xe^{im\pi x}$, where $x \in [-1, 1]$ and $m \in \mathbb{Z}$. Putting

$$\mathcal{L}[p] := \int_{-1}^{1} p(x)w(x)\, dx \quad (p \in \mathcal{P}), \tag{2.2}$$

i.e.,

$$\mu_k = \frac{(-1)^{m+k}(k+1)!}{(im\pi)^{k+1}} \sum_{\nu=0}^{k} \frac{(1 + (-1)^\nu)(-im\pi)^\nu}{(\nu+1)!},$$

in [6] it was proved that for every integer $m\ (\neq 0)$, the sequence of formal orthogonal polynomials with respect to the functional $\mathcal{L}$ exists uniquely. Such orthogonal polynomials have several interesting properties and they can be applied in numerical integration of highly oscillatory functions (see [6]). The corresponding case with Chebyshev weight, i.e., when $w(x) = x(1 - x^2)^{-1/2}e^{i\zeta x}$, $\zeta \in \mathbb{R}$, was recently investigated in [7].

According to (2.2) we can define

$$(p, q) := \int_{-1}^{1} p(x)q(x)w(x)\,dx \quad (p, q \in \mathcal{P}),$$

but, as we can see, (p, q) is not Hermitian and not positive definite.

3. INTEGRATION OF OSCILLATING FUNCTIONS

In this section we consider integrals of the form

$$I(f, K) = I(f(\cdot), K(\cdot; x)) = \int_{a}^{b} w(t)f(t)K(t; x)\,dt, \tag{3.1}$$

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

$$c_k(f) = a_k(f) + ib_k(f) = \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) e^{ikt}\,dt, \tag{3.2}$$

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

$$H_m(x) = \int_{0}^{+\infty} t^{\mu} f(t) H_{\nu}^{(m)}(\omega t)\,dt \qquad (m = 1, 2), \tag{3.3}$$

where ω is a real parameter and $H_{\nu}^{(m)}(t)$, $m = 1, 2$, are the Hankel functions (see Wong [8]). Also, we mention here a type of integrals involving Bessel functions

$$I_{\nu}(f; \omega) = \int_{0}^{+\infty} e^{-t^2} J_{\nu}(\omega t) f(t^2) t^{\nu+1}\,dt, \quad \nu > -1, \tag{3.4}$$

where ω is a large positive parameter. Such integrals appear in some problems of high energy nuclear physics (cf. [9]).

$2°$ 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 (3.1) is taken to be a Cauchy principal value integral.

In this section we consider only integration of oscillatory functions.

3.1. 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 [10].

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,

$$f(x) \approx P_k(x) = P_k(x_{2k-1} + ht) = \phi_k(t), \tag{3.5}$$

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 (3.5) 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.,

$$A = \frac{(\theta^2 - 2)\sin\theta + 2\theta\cos\theta}{\theta^3} + i\frac{\theta\cos\theta - \sin\theta}{\theta^2},$$

$$B = \frac{4}{\theta^3}(\sin\theta - \theta\cos\theta),$$

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 [11] and Ehrenmark [12].

Improvements of the previous technique have been done by Flinn [13], Luke [14], Buyst and Schotsmans [15], Tuck [16], Einarsson [17], Van de Vooren and Van Linde [18], etc. For example, Flinn [13] 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 [19] used the idea of approximating the transformed function by polynomials in $1/t$. Miklosko [20] 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 [21], Piessens [22], [23], [24]). 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 (3.2) 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 [21] 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 [25].

Quadrature formulas for the Fourier and the Bessel transforms (3.3) were derived by Wong [8].

Other formulas are based on the integration between the zeros of $\cos mx$ or $\sin mx$ (cf. [26], [27], [28], [29], and [30]). 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 $a \leq x_1 < x_2 < \cdots < x_m \leq b$, 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 [26, 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 [31], Hurwitz and Zweifel [32]).

3.2. Product Integration Rules

Consider the integral (3.1) with a "well-behaved" function f on (a, b). The main idea in the method of product integration is to determine the adverse behavior 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 $L_n(f; \cdot)\pi_\nu(\cdot) \leq 2n - 2$, we can apply Gaussian formula (1.2), and then

$$a_\nu = \frac{1}{\|\pi_\nu\|^2} \sum_{k=1}^{n} \lambda_k f(\tau_k) \pi_\nu(\tau_k), \tag{3.6}$$

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

Putting $L_n(f; t)$ in (3.1) 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.,

$$Q_n(f; x) = \sum_{\nu=0}^{n-1} a_\nu \int_a^b w(t) \pi_\nu(t) K(t; x) \, dt \tag{3.7}$$

and $R_n^{PR}(f; x)$ is the corresponding remainder. By $b_\nu(x)$ we denote the integrals in (3.7),

$$b_\nu(x) = \int_a^b w(t) \pi_\nu(t) K(t; x) \, dt, \quad \nu = 0, 1, \ldots, n - 1. \tag{3.8}$$

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

$$Q_n(f; x) = \sum_{\nu=0}^{n-1} a_\nu b_\nu(x), \tag{3.9}$$

where the coefficients a_ν and $b_\nu(x)$ are given by (3.6) and (3.8), respectively. Another form of (3.9) is

$$Q_n(f; x) = \sum_{k=1}^{n} \Lambda_k(x) f(\tau_k), \tag{3.10}$$

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 (3.8), 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.,

$$K_n(t; x) = \sum_{\nu=0}^{n-1} \frac{b_\nu(x)}{\|\pi_\nu\|^2} \pi_\nu(t). \tag{3.11}$$

We can see that the product integration rule (3.9), i.e., (3.10), 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 (3.11). Now, we give some of such examples.

In [33, 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,

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

where $x \in [-1,1]$. In this case, (3.10) 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 [34]; (2) For $\lambda = 0$ and $\lambda = 1$ – the method of Patterson [35]. An approximation by Chebyshev polynomials was considered by Piessens and Poleunis [36].

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 (3.4), 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

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

Thus, in this case the the coefficients (3.8) become

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

In 1979 Gabutti [9] 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,

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

The imaginary part of this gives the previous example. An asymptotic behaviour of this integral was investigated by Frenzen and Wong [37]. 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 [38] and Gabutti and Lepora [39].

A significant progress in product quadrature rules (and interpolation processes) was made in the last twenty years (see Elliott and Paget [40]–[41], Sloan and Smith [42]–[44], Smith and Sloan [45], Nevai [46]–[48], Mastroianni and Vértesi [49]–[50], Mastroianni and Monegato [51], Mastroianni [52], and others).

3.3. 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. 3.1). Following [53] we consider the Fourier integral on the finite interval

$$I(f;\omega) = \int_{-1}^{1} f(x)e^{i\omega x}\,dx, \qquad (3.12)$$
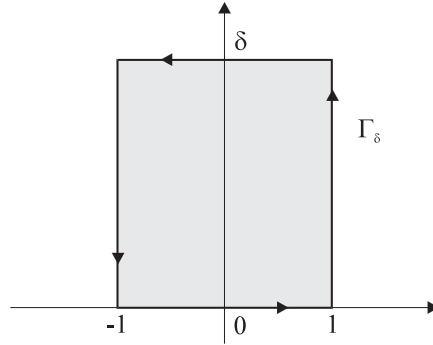
with an analytic real-valued function f.

Figure 3.1: The contour of integration

THEOREM 3.1. *Let f be an analytic real-valued function in the half-strip of the complex plane, $-1 \le \mathrm{Re}\,z \le 1$, $\mathrm{Im}\,z \ge 0$, with singularities z_ν ($\nu = 1,\ldots,m$) in the region $G = \mathrm{int}\,\Gamma$, and let*

$$2\pi i \sum_{\nu=1}^{m} \mathop{\mathrm{Res}}_{z=z_\nu}\left\{f(z)e^{i\omega z}\right\} = P + iQ.$$

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

$$\int_{-1}^{1} |f(x+i\delta)|\,dx \le Me^{\xi\delta}. \qquad (3.13)$$

Then

$$\int_{-1}^{1} f(x)\cos\omega x\,dx = P + \frac{2}{\omega}\int_{0}^{+\infty} \mathrm{Im}\left[e^{i\omega}f_e\left(1+i\frac{t}{\omega}\right)\right]e^{-t}\,dt,$$

$$\int_{-1}^{1} f(x)\sin\omega x\,dx = Q - \frac{2}{\omega}\int_{0}^{+\infty} \mathrm{Re}\left[e^{i\omega}f_o\left(1+i\frac{t}{\omega}\right)\right]e^{-t}\,dt,$$

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

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

Since

$$
\begin{aligned}
|I_\delta| &= \Big|\int_{-1}^1 f(x+i\delta)e^{i\omega(x+i\delta)}\,dx\Big| = e^{-\omega\delta}\Big|\int_{-1}^1 f(x+i\delta)e^{i\omega x}\,dx\Big| \\
&\le e^{-\omega\delta}\int_{-1}^1 |f(x+i\delta)|\,dx \le M e^{(\xi-\omega)\delta} \to 0 \quad \text{(because of (3.13))},
\end{aligned}
$$

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. $\blacksquare$

The obtained integrals in Theorem 3.1 can be solved by using Gauss-Laguerre rule. In order to illustrate the efficiency of this method we consider a simple example – Fourier coefficients (3.2), 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

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

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

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

and

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

we get

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

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

In Table 3.1 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 3.1: 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 3.2 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

Table 3.2: Relative errors in N-point GLa-approximations of $a_k(f)$

N	$\varepsilon = 1$			$\varepsilon = 0.01$
	$k = 5$	$k = 10$	$k = 40$	$k = 20$
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)			

column of Table 3.2 we give the corresponding relative errors in the case when $\varepsilon = 0.01$ and $k = 20$, where $a_{20}(f) = -1.023459866383(-4)$.

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

$$a_k(f) = \frac{1}{\pi} \int_{-\pi}^{\pi} \frac{\cos kt}{t^2 + \varepsilon^2} \, dt, \tag{3.14}$$

gives bed results with a slow convergence (see Table 3.3).

The rapidly oscillatory integrand in (3.14) is displayed in Figure 3.2 for $\varepsilon = 1$ and $k = 40$.

Table 3.3: Relative errors in N-point GLe-approximations of $a_k(f)$

N	$\varepsilon = 1$			$\varepsilon = 0.01$
	$k = 5$	$k = 10$	$k = 40$	$k = 20$
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)

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

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

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

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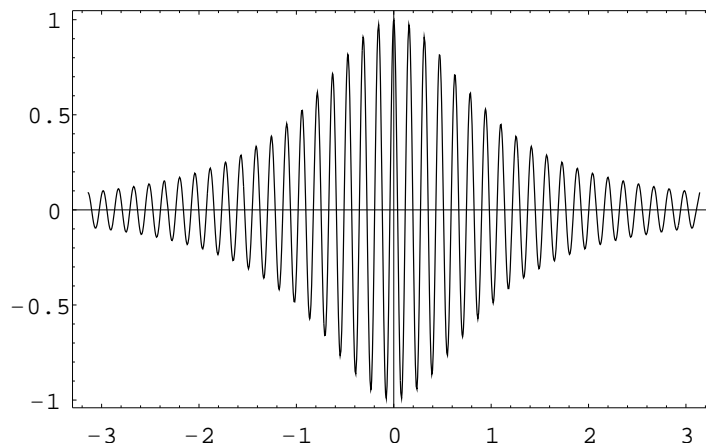
where

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

THEOREM 3.2. *Suppose that the function $f(z)$ is defined and holomorphic in the region $D = \{z \in \mathbb{C} \,|\, \operatorname{Re} z \geq a > 0, \operatorname{Im} z \geq 0\}$, and such that*

$$|f(z)| \leq \frac{A}{|z|}, \quad \text{when } |z| \to +\infty, \tag{3.15}$$

for some positive constant A. Then

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

Figure 3.2: The case $\varepsilon = 1$ and $k = 40$

PROOF. Taking $a > 0$ and the closed contour C_R in D (see Fig. 3.3) we get, by Cauchy's residue theorem,

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

Because of (3.15), 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

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

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 3.4.
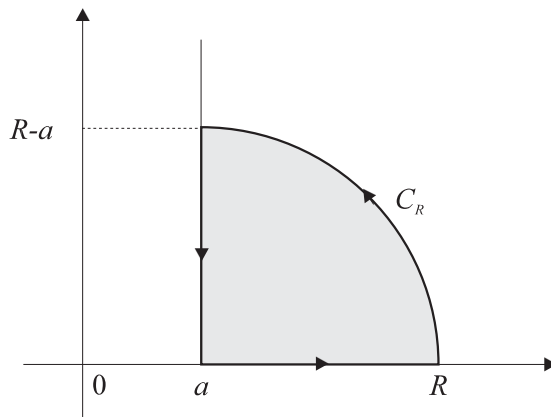
Figure 3.3: The contour of integration

Table 3.4: 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)

4. CONSTRUCTIONS AND APPLICATIONS OF SOME QUADRATURES

In this section we give constructions and applications of some Gaussian quadrature rules for calculating integrals with 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.

4.1. 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 [54] stated a problem[1] of finding a computationally effective approximations for the integral

$$I_{m,n}^{\alpha,\beta} = \int_{-\infty}^{+\infty} \hat{H}_m(t)\hat{H}_n(t)w^{(\alpha,\beta)}(t)\,dt, \tag{4.1}$$

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 $m \neq n$.
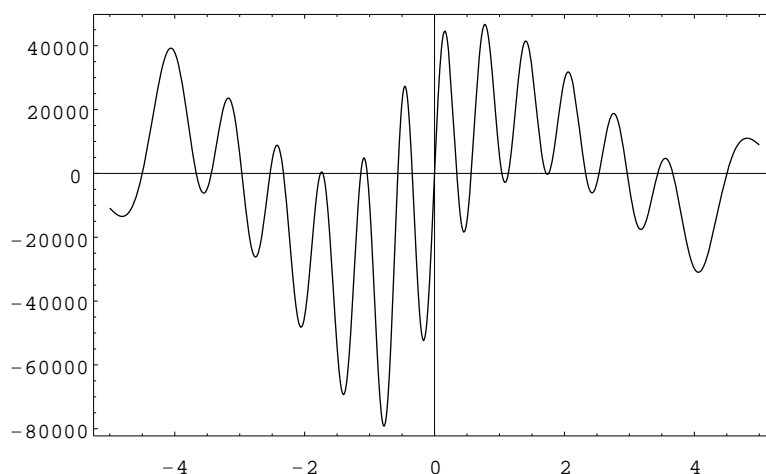

Figure 4.1: The case $\alpha = \beta = 1$ and $m = 10$, $n = 15$

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,

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

$$\cong \sum_{k=1}^{N} \frac{\lambda_k^H P(\tau_k^H)}{\sqrt{1+\alpha\tau_k^H + \beta(\tau_k^H)^2}},$$

---

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

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 4.1: 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 (4.1) 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 4.1.

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

$$I_{m,n}^{\alpha,\beta} \approx Q_{m,n}^{\alpha,\beta} = \sum_{\nu=1}^{N} \lambda_\nu^{(\alpha,\beta)} \hat{H}_m(\tau_\nu^{(\alpha,\beta)}) \hat{H}_n(\tau_\nu^{(\alpha,\beta)}). \tag{4.2}$$

In Table 4.2 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 quadrature formula

Table 4.2: 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)

(4.2) was $N = 5, 10, 15, 20$. Since the N-point Gaussian quadrature formula (4.2) has maximum algebraic degree of exactness $2N - 1$, we see that obtained results are exact for every N such that $2N - 1 \geq m + n$.

4.2. Gaussian Quadrature Rules With Oscillatory Weight

We return to orthogonal polynomials with respect to the oscillatory weight $w(x) = xe^{im\pi x}$ on $[-1, 1]$ (see Section 2) and we want to construct the corresponding quadrature of Gaussian type. Since we cannot claim that the zeros of orthogonal polynomials are simple, in applications we should be ready to apply Gaussian quadrature rules which deal with multiplicities. In the case of multiple zeros of orthogonal polynomials, the Gaussian quadrature rule has the following form (see [55], [56])

$$G_n(f) = \sum_{\nu=1}^{n} \sum_{k=0}^{m_\nu - 1} w_{\nu,k}^n f^{(k)}(x_\nu^n). \tag{4.3}$$

According to considerations in [6], at most two nodes in (4.3) may have multiplicities. However, in all our examples we have encountered simple nodes and we have used the standard Gaussian quadrature rule

$$G_n(f) = \sum_{\nu=1}^{n} w_\nu^n f(x_\nu^n). \tag{4.4}$$

Distributions of the zeros of the orthogonal polynomials for $m = 2$ and $m = 22$ are presented in Figure 4.2. Only the zeros of polynomials with degrees $n = 5(5)35$ are displayed. The corresponding distribution of the zeros for $m = 1000$ is given in Figure 4.3 (left). For better visibility in the same figure (right) only the main group of zeros is presented.

We can see that the distribution of the zeros is such that all zeros are with positive imaginary part, except for one zero of polynomials of odd degree for which its real part is zero. From the figures we can also conclude that all zeros are in the half-strip $\{z \in \mathbb{C} : |\operatorname{Re} z| < 1 \wedge \operatorname{Im}(z) > 0\}$, except maybe one zero for polynomials of odd degree with real part equal to zero. Also, it is obvious that if m is increasing, then the zeros of the polynomials are grouped around the
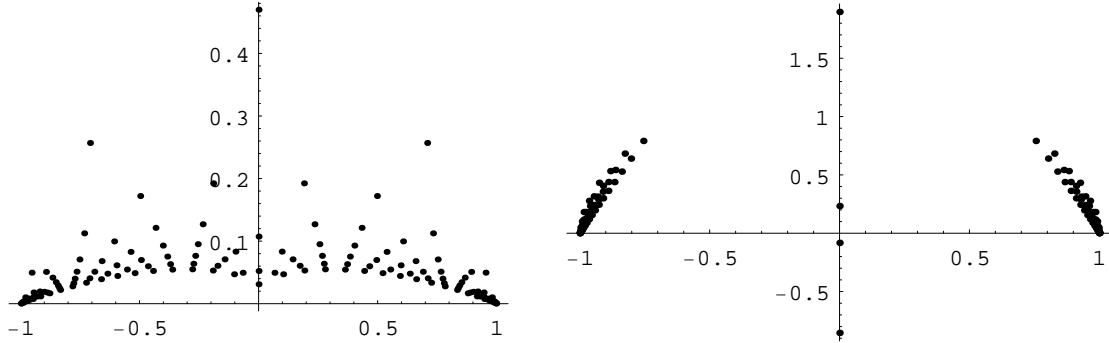
Figure 4.2: Distribution of zeros for $m = 2$ (left) and $m = 22$ (right)
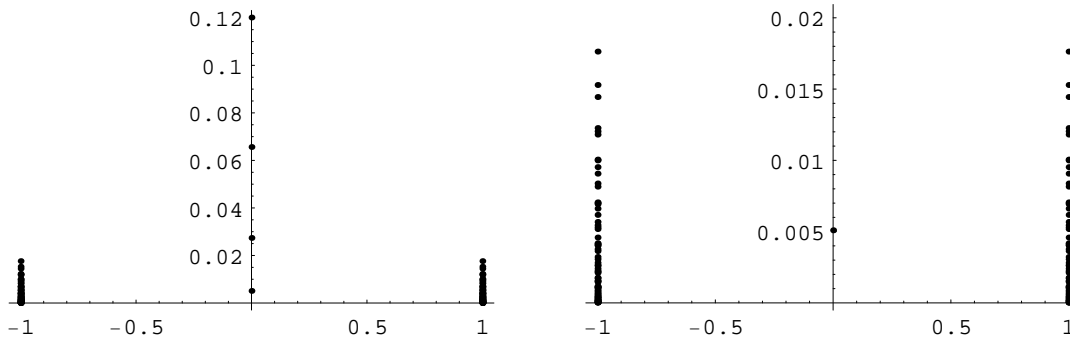
Figure 4.3: Distribution of zeros for $m = 1000$: all zeros (left) and selected zeros (right)

points ± 1. This is the reason why the QR-algorithm in D-arithmetic cannot be used for a construction of zeros with a large m (for example, $m = 10^9$). Zeros of polynomials for very large m are very close to each other, so that they cannot be distinguished in D-arithmetic.

Also, it can be seen that for a fixed m, if we increase degree of a polynomial, then the zeros tend to cover the interval $(-1, 1)$. This is, however, less obvious for larger m, because of the mentioned behavior of their grouping near the points ± 1.

Since the zeros of the orthogonal polynomials are not contained in the supporting set of the measure μ, we cannot expect the quadrature rule (4.3) to converge, except for functions which are analytic in a certain complex domain $\mathcal{D} \supset [-1, 1]$. Spurious zeros (see [57]) for our sequence of orthogonal polynomials were not detected.

For a construction of the Gaussian quadrature rule the QR-algorithm is used, but in a modified form [58] (for details see [6]). In Table 4.3 we give the nodes and the weights of the

x_ν^n	w_ν^n
$\pm 0.99833323072985 + i8.0272939519631(-3)$	$\pm 2.6219203933839(-3)\ -i1.6185441353473(-2)$
$\pm 0.99100855292260 + i4.3127353860182(-2)$	$\mp 4.2536667302542(-4)\ -i1.3094541072322(-2)$
$\pm 0.97687553159991 + i1.1013718224261(-1)$	$\mp 1.0621304335557(-3)\ -i2.4769593783534(-3)$
$\pm 0.95373342919595 + i2.1833923751031(-1)$	$\mp 1.2031273072243(-4)\ -i7.4485602824591(-5)$
$\pm 0.91584375790176 + i3.9367290146258(-1)$	$\mp 8.9861059280033(-7)\ +i4.3878859382919(-7)$
$\pm 0.99846411789590 + i3.8408078263538(-3)$	$\pm 3.1046382565034(-3)\ -i8.8805764375599(-3)$
$\pm 0.99183153354877 + i2.0347206579223(-2)$	$\pm 1.9244416480364(-3)\ -i1.2968640292577(-2)$
$\pm 0.97957734645900 + i5.0510187350466(-2)$	$\mp 1.6177820964010(-3)\ -i7.9111318842472(-3)$
$\pm 0.96109698530124 + i9.5210986930994(-2)$	$\mp 1.8324015346507(-3)\ -i2.0568347704191(-3)$
$\pm 0.93538991039429 + i1.5590937196538(-1)$	$\mp 5.3091855800340(-4)\ -i5.9554706994496(-5)$
$\pm 0.90085641267460 + i2.3495811423141(-1)$	$\mp 3.6520885773394(-5)\ +i4.3342540474941(-5)$
$\pm 0.85489295111768 + i3.3624578190485(-1)$	$\pm 1.7102442502967(-6)\ +i2.4540197057364(-6)$
$\pm 0.79298840127057 + i4.6668799320411(-1)$	$\pm 4.5156899615527(-8)\ -i4.7151995083521(-8)$
$\pm 0.70627510516459 + i6.4046420228669(-1)$	$\mp 3.9409685347890(-10)+i6.5422096655704(-11)$
$\pm 0.57200700024404 + i8.9689758832390(-1)$	$\pm 1.3302611178019(-13)-i1.8953246644963(-13)$

Table 4.3: Nodes x_ν^n and weights w_ν^n for $n = 10$ and $n = 20$, when $m = 10$

Gaussian formulas (4.4) (to 14 decimals only, to save space) for $n = 10$ and $n = 20$ points, when the weight function is $w(x) = x \exp(i10\pi x)$ ($m = 10$).

A possible application of these quadratures is in numerical calculation of integrals involving highly oscillatory integrands. We consider here the calculation of Fourier coefficients:

$$F_m(f) = C_m(f) + iS_m(f) = \int_{-1}^{1} f(x)e^{im\pi x}dx.$$

Since $\int_{-1}^{1} \exp(im\pi x)dx = 0$, we have

$$F_m(f) = \int_{-1}^{1} \frac{f(x) - f(0)}{x} x e^{im\pi x}dx = \int g(x)d\mu(x),$$

so that we can compute it using the Gaussian quadrature rules (4.4) of the function g defined by

$$g(x) = \frac{f(x) - f(0)}{x}, \quad g(0) = f'(0).$$

Under the assumption that f is analytic in some domain $\mathcal{D} \supset [-1, 1]$, the numerical integration can be safely applied, since g is also analytic in $\mathcal{D}$.

n	$G_n(f)$	$\widetilde{G}_n(f)$
10	-0.0509124802888631	-0.0509120068454231
20	-0.0509124798498521	-0.0509120064064121
30	-0.0509124699339274	-0.0509119964904873
40	-0.0509120078597894	
50	-0.0509120064014030	
60	-0.0509120064013063	
70	-0.0509120064013063	

Table 4.4: Gaussian approximations $G_n(f)$ and $\widetilde{G}_n(f)$ for $S_{10}(f)$ and $f(x) = x/(x^2 + 1/4)$

In general, for some analytic function f, the approximation of the integral with respect to the measure $\exp(im\pi x)dx$, can be given as

$$F_m(f) = \int_{-1}^{1} f(x)e^{im\pi x}dx \approx \sum_{\nu=1}^{n} \frac{w_\nu^n}{x_\nu^n}(f(x_\nu^n) - f(0)). \qquad (4.5)$$

We can get an interesting result if we apply our quadrature rule for $m = 10$ to the function $f(x) = \dfrac{x}{x^2 + 1/4}$. According to (4.5), we consider

$$S_{10}(f) = \int_{-1}^{1} \frac{x}{x^2 + 1/4} \sin(10\pi x)dx \approx G_n(f) = \mathrm{Im}\left\{\sum_{\nu=1}^{n} \frac{w_\nu^n}{(x_\nu^n)^2 + 1/4}\right\}.$$

The Gaussian approximations for $n = 10(10)70$ are given in Table 4.4. The function f has simple poles at $z = \pm i/2$. Finding the residuum at the point $\lambda = i/2$, we obtain $R = \mathrm{Im}\left\{2\pi i \, \mathrm{Res}_{z=i/2}[f(z)e^{i10\pi z}]\right\} = 4.734434401198 \times 10^{-7}$.

If we simply add this value to $G_n(f)$, we can significantly improve the results for $n < 40$, as can be checked in Table 4.4 (the column $\widetilde{G}_n(f) = G_n(f) + R$). The reason for such behavior of the quadrature rules we can find in the zero distribution for polynomials orthogonal with respect to the weight $w(x) = x \exp(i10\pi x)$ on $[-1, 1]$ (see Figure 4.4). As we can see, while the convex hull of the zeros includes the point $\lambda = i/2$ (cases for $n \leq 30$), this singularity has an influence on the Gaussian approximations $G_n(f)$. But, when zeros drop below λ (for $n \geq 40$), this influence ceases.

If we increase m, for example taking $m = 30, 100, 10^6$, the convergence is rather faster. Table 4.5 shows $G_n(f)$ for $m = 30$ and $m = 100$. For $m = 10^6$, the relative error in $G_{10}(f)$ is smaller than 10^{-60}.
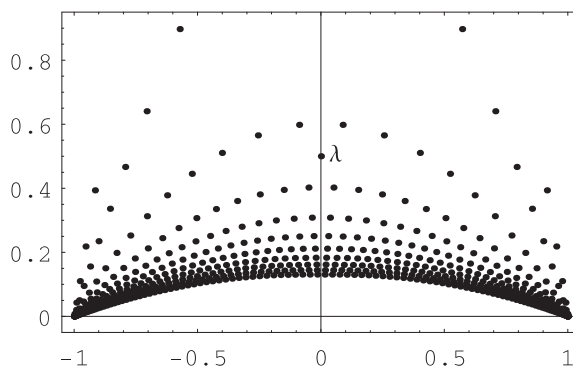
Figure 4.4: Distribution of zeros for polynomials orthogonal with respect to the weight function $w(x) = x \exp(i10\pi x)$ on $[-1, 1]$

m	n	$G_n(f)$
30	10	$-0.016975913176678720 7976$
	20	$-0.016975913176678046 0809$
	30	$-0.016975913176678046 0809$
100	10	$-0.00050929580138121841037438653708$
	20	$-0.00050929580138121841037438653707$

Table 4.5: Gaussian approximations $G_n(f)$ for $S_{30}(f)$ and $S_{100}(f)$

This faster convergence can be understood easily, since values of the residuum at $z = i/2$ are decreasing exponentially with m, so it cannot harm the convergence.

5. CONCLUSION

In this paper we presented some numerical methods which can be used to calculate integrals with oscillatory and singular weight functions. Section 3 presents classical methods used so far for the integration of the mentioned integrals. Section 4 describes the method based on the orthogonal polynomials. This method, used for the integration of such integrals, is rather new and its investigation is not completed yet.

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