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CALCULATING A CLASS OF INTEGRALS ENCOUNTERED IN THEORETICAL CHEMISTRY

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A b s t r a c t. *The methods for numerical calculating the Cauchy principal value integrals of the form* v.p. $\int_{-\infty}^{+\infty} \log |P(ix)/Q(ix)|\, dx$ *are developed, where* $P(x)$ *and* $Q(x)$ *are monic polynomials of equal degrees with integer coefficients, and* $i = \sqrt{-1}$ *. These integrals play a distinguished role in theoretical chemistry.*

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1. *Introduction*

In this paper we are concerned with the Cauchy principal value integrals of the form

$$\text{v.p.} \int_{-\infty}^{+\infty} \log \left| \frac{P(ix)}{Q(ix)} \right| dx, \tag{1}$$

where

$$P(x) = \sum_{k=0}^{n} a_k\, x^k \qquad \text{and} \qquad Q(x) = \sum_{k=0}^{n} b_k\, x^k \tag{2}$$

are polynomials of equal degree whose coefficients are integers, $a_n = b_n = 1$, and $i = \sqrt{-1}$.

Integrals of this kind play a significant role in theoretical (quantum) chemistry. It seems that such integrals were first considered by Coulson and Jacobs [10], who showed that the difference between the total π-electron energy of two conjugated hydrocarbons with equal number of carbon atoms is given by

$$E(G_2) - E(G_1) = \frac{1}{\pi}\,\text{v.p.}\int_{-\infty}^{+\infty} \log\left|\frac{\phi(G_1, ix)}{\phi(G_2, ix)}\right| dx \tag{3}$$

where G_1 and G_2 are the corresponding molecular graphs [67], and ϕ stands for their characteristic polynomial. This formula is an immediate consequence of Coulson's classic integral expression for the total π-electron energy [9, 67]:

$$E(G) = \frac{1}{\pi}\,\text{v.p.}\int_{-\infty}^{+\infty} \left[n - \frac{ix\,\phi'(G, ix)}{\phi(G, ix)}\right] dx \tag{4}$$

where ϕ' denotes the first derivative of ϕ.

Several variants of Eq. (3), pertaining to energy differences, were considered in the chemical literature [18, 19, 28, 42]. Of these, the so-called "topological resonance energy" should especially be mentioned [60, 60]:

$$TRE(G) = \frac{1}{\pi}\,\text{v.p.}\int_{-\infty}^{+\infty} \log\left|\frac{\phi(G, ix)}{\alpha(G, ix)}\right| dx \tag{5}$$

where α is the matching polynomial.

It should be noted that in actual chemical applications (which are very numerous) both the total π-electron energy and the topological resonance energy are not computed by means of the formulas (3)–(5), but by using other computational techniques. However, there is another chemical theory in which calculation of numerical values of integrals of the type (1) cannot be avoided.

In 1977 one of the present authors [7, 17, 43] developed a novel theory of cyclic conjugation which made it possible to assess the effect of an individual cycle on the thermodynamic stability of a polycyclic conjugated molecule. Details of this theory can be found in several expository articles [27, 36, 37, 38], whereas its mathematical formalism is outlined in [66, 67]. Almost in the same time Aihara [1] proposed a similar, yet not equivalent, theory, in which no integrals of the type (1) were used. The advantage of our approach over Aihara's was recognized only many years later [2]

Within our theory of cyclic conjugation, the energy-effect of a cycle Z of a polycyclic conjugated molecule whose molecular graph is G is computed as:

$$ef(G,Z) = \frac{1}{\pi}\,\text{v.p.}\int\limits_{-\infty}^{+\infty} \log\left|\frac{\phi(G,ix)}{\phi(G,ix)+2\,\phi(G-Z,ix)}\right| dx. \qquad (6)$$

Recently, analogous expressions for the effects of pairs, triplets, quartets, etc. of cycles were deduced [74], as well as for the effect of conjugation in one cycle on conjugation in another cycle [91, 68, 16, 92, 39].

The quantity *ef* was extensively studied and applied to a variety of chemical problems. These researches were done either by finding some generally valid mathematical properties of *ef* [20, 21, 22, 24, 30, 65] or by performing numerical calculations [12, 25, 26, 29, 31, 32, 33, 34, 35, 41, 44, 45, 50, 51, 52, 53, 54, 56, 57, 61, 62, 63, 64, 69, 70, 71, 75, 72, 74, 76, 77, 78, 79, 5, 73, 81, 90, 4, 49, 48, 47, 3, 15, 55, 82, 46, 13, 14].

In the general case, the polynomials $P(x) \equiv \phi(G,x)$ and $Q(x) \equiv \phi(G,x) + 2\,\phi(G-Z,x)$, occurring in the expression on the right–hand side of Eq. (6) are monic, of equal degree, and have integer coefficients. The zeros of $Q(x)$ may be complex-valued and in practical applications are not known.

For $x \to \pm\infty$ the integrand in (6) tends to zero as $x^{-|Z|}$, where $|Z| \geq 3$ is the size of the cycle Z. At $x = 0$ the integrand may possess a singularity.

In standard chemical applications of the integrals of the form (1) it is assumed that the coefficients a_1 and b_1 in the polynomials $P(x)$ and $Q(x)$ are equal to zero. If this is not the case, then pertinent corrections need to be made [58, 85].

The hitherto reported *ef*-values were computed by means of a Simpson–type integration [40], in which the integrand is computed for $x = \frac{1}{2}\,h + kh$ for $k = 0, 1, 2, \ldots$, up to the point at which the integrand is smaller than a critical value C. By empirical testing it was found that $h = 0.004$ and $C = 0.00001$ yield *ef*-values accurate to 3 or 4 decimal places. However, this latter accuracy could be tested only for the few (simple) examples for which the right–hand side of (6) can be solved analytically.

In the subsequent sections we show how integrals of the type (1) can be calculated in a much more efficient and much more accurate manner. Two methods are presented. In both cases a previous reduction to an integral with a rational function is provided (Section 2). In Section 3 we apply the trapezoidal rule after the so-called double exponential ransformation of the integrand. Such ideas have been appeared in papers of Japanese mathematicians (cf. Takahasi and Mori [93, 94], Iri, Moriguti, and Takasawa [80], Mori [89]). The second method, presented in Section 4, is based on a transformation of the integral over the real line to an integral over the finite interval $(-1,1)$, with respect to the Chebyshev weights. An application of the corresponding quadratures of Gaussian type is also presented.

2. *Reduction to integrals of rational functions*

In this section we reduce the Cauchy principal value integral (1) to an improper integral of a rational function over $\mathbb{R}$.

Let $\mathcal{P}_n$ be a set of all real algebraic polynomials of degree at most n and $\hat{\mathcal{P}}_n$ be its subset of monic polynomials of degree n. With $\mathcal{R}[m,n]$ we denote the set of all rational functions of the form $u(t)/v(t)$ such that $u \in \mathcal{P}_m$, $v \in \hat{\mathcal{P}}_n$, and $\gcd(u(t),v(t)) = 1$ (i.e., the polynomials $u(t)$ and $v(t)$ are relatively prime).

According to (2) we have

$$P(ix)P(-ix) = (a_0 - a_2x^2 + a_4x^4 - \cdots)^2 + x^2(a_1 - a_3x^2 + a_5x^4 - \cdots)^2,$$

i.e., $|P(ix)|^2 = P(ix)P(-ix) = p(x^2)$ and similarly $|Q(ix)|^2 = Q(ix)Q(-ix) = q(x^2)$. Such polynomials

$$p(t) = t^n + \alpha t^{n-1} + \cdots \qquad \text{and} \qquad q(t) = t^n + \beta t^{n-1} + \cdots$$

are real monic polynomials of degree n and nonnegative for $t \geq 0$. Without loss of generality, we can suppose that they are relatively prime. In addition, we suppose that they have not positive zeros, i.e., $p(t), q(t) > 0$ for $t > 0$.

Then

$$\text{v.p.} \int_{-\infty}^{+\infty} \log\left|\frac{P(ix)}{Q(ix)}\right| dx = \frac{1}{2}\ \text{v.p.} \int_{-\infty}^{+\infty} \log\left|\frac{P(ix)}{Q(ix)}\right|^2 dx = \frac{1}{2}\ \text{v.p.} \int_{-\infty}^{+\infty} \log\frac{p(x^2)}{q(x^2)}\, dx.$$

An integration by parts gives

$$\frac{1}{2}\int \log\frac{p(x^2)}{q(x^2)} dx = \frac{x}{2}\log\frac{p(x^2)}{q(x^2)} - \int x^2\left(\frac{p'(x^2)}{p(x^2)} - \frac{q'(x^2)}{q(x^2)}\right) dx. \tag{7}$$

Defining a rational function $R(t)$ by

$$R(t) = t\left(\frac{q'(t)}{q(t)} - \frac{p'(t)}{p(t)}\right) = \frac{h(t)}{p(t)q(t)}, \tag{8}$$

where $h(t) = t(p(t)q'(t) - q(t)p'(t))$, we get

$$\begin{aligned} R(t) &= t\left\{\frac{nt^{n-1} + (n-1)\beta t^{n-2} + \cdots}{t^n + \beta t^{n-1} + \cdots} - \frac{nt^{n-1} + (n-1)\alpha t^{n-2} + \cdots}{t^n + \alpha t^{n-1} + \cdots}\right\} \\ &= t\,\frac{(\alpha-\beta)t^{2n-2} + \cdots}{p(t)q(t)} \quad \in \mathcal{R}[2n-1, 2n]. \end{aligned}$$

Precisely, $R(t) \in \mathcal{R}[m, 2n]$ for some m between 0 and $2n-1$.

Thus, $R(x^2) = o(x^{-2r})$ as $x \to +\infty$, where $r \geq 1$. For $t > 0$ the denominator of the rational function $R(t)$ is strictly positive, except $t = 0$, but this function $R(t)$ cannot have a pole at the origin. Namely, if $p(t)$ or $q(t)$ (not both) has a zero at the origin, then such a pole is eliminated by the factor t in $h(t)$. Regarding these facts, we have the existence of the improper integral

$$\int_{-\infty}^{+\infty} R(x^2)\,dx.$$

Also, by definition of the Cauchy principal value integral, it is easy to conclude that the first term on the right hand side in (7) has no contribution in the integral (1), so that the following result holds:

Lemma 1 *For the integral* (1) *we have*

$$\text{v.p.}\int_{-\infty}^{+\infty} \log\left|\frac{P(ix)}{Q(ix)}\right| dx = \int_{-\infty}^{+\infty} R(x^2)\,dx, \tag{9}$$

where the function $R(t) \in \mathcal{R}[m, 2n]$ $(0 \leq m \leq 2n-1)$ *has the form* (8), *where* $h \in \mathcal{P}_m$ *and* $p, q \in \hat{\mathcal{P}}_n$.

For example, for $p(t) = t^2 + 4t$ and $q(t) = t^2 + 4t + 2$, according to (8) and (9), we get

$$\text{v.p.}\int_{-\infty}^{+\infty} \log\frac{x^4 + 4\,x^2}{x^4 + 4\,x^2 + 2}\,dx = \int_{-\infty}^{+\infty} \frac{-8(x^2+2)}{(x^2+4)(x^4+4x^2+2)}\,dx.$$

Thus, it is reduced to an improper integral, which value is

$$-2\pi\Big(\sqrt{4+2\sqrt{2}}-2\Big) = -3.852383833273321\dots\ .$$

Thus, our starting problem (1) is reduced to an integration of rational functions over $\mathbb{R}$. It is well known that in the eighteenth century Johan Bernoulli solved the problem of indefinite integration of rational functions by their partial decomposition. The main computational problem with this method is computing the factorization of a polynomial. However, in the middle of the nineteenth century the Russian mathematician Mikhail Vasilyevich Ostrogradsky presented an algorithm for finding the rational part of the integral without factoring. Some similar approaches were latter discovered. The problem of computing the transcendental part of the primitive was recently solved. The recent development of symbolic computations made also a progress in this area (for details see a book of Bronstein [8], as well as some papers dealing with Landen transformation for rational functions [6] and [83]).

For our specific kind of integrals in the subsequent sections we give two efficient methods for their numerical calculating.

3. *Double exponential transformation and trapezoidal rule*

We start this section with some classical rules for calculating the integral $I(f) := \int_a^b f(x)\,dx$.

Taking $h := (b-a)/n$ and equally spaced points $x_k := a + kh$, $k = 0, 1, \dots, n$, we have the well-known composite trapezoidal rule

$$I(f) \approx T_n(f;h) := h\left(\frac{1}{2}f_0 + f_1 + \cdots + f_{n-1} + \frac{1}{2}f_n\right), \tag{10}$$

where $f_k := f(x_k)$, $k = 0, 1, \dots, n$. If $f \in C^2[a,b]$ it is easy to prove that

$$I(f) - T_n(f;h) = -\frac{(b-a)h^2}{12}f''(\xi), \qquad a < \xi < b. \tag{11}$$

As we can see this rule converges very slowly with respect to step refinement as $O(h^2)$.

Another simple rule is the classical composite Simpson rule

$$I(f) \approx S_n(f;h) := \frac{h}{3}\Big[f_0 + 4(f_1 + \cdots + f_{2n-1}) + 2(f_2 + \cdots + f_{2n-2}) + f_{2n}\Big],$$

where $h := (b-a)/2n$, $x_k := a + kh$, $f_k := f(x_k)$, $k = 0, 1, \dots, 2n$, which is slightly faster, but complicated than the previous one. Namely, if $f \in C^4[a, b]$,

$$I(f) - S_n(f; h) = -\frac{(b-a)h^4}{180} f^{(4)}(\xi), \qquad a < \xi < b.$$

For functions with continuous derivatives of order at least $2m-1$, a generalization of (11) is the well-known Euler-Maclaurin summation formula

$$\begin{aligned} I(f) - T_n(f; h) &= -\frac{h^2}{12}(f'(b) - f'(a)) + \frac{h^4}{720}(f'''(b) - f'''(a)) \\ &- \cdots - \frac{h^{2m} B_{2m}}{(2m)!}\Big(f^{(2m-1)}(b) - f^{(2m-1)}(a)\Big) - E_m(f), \end{aligned}$$

where B_{2m} is the Bernoulli number of order $2m$ and

$$E_m(f) = (b-a)\frac{B_{2m+2} h^{2m+2}}{(2m+2)!} f^{(2m+2)}(\xi), \quad a < \xi < b.$$

If we restrict our analysis to analytic functions with all derivatives of f which vanish at $x = a$ and $x = b$, then the discretization error is given only by remainder $E_m(f)$ as $m \to +\infty$. Then the convergence with respect to step refinement is faster than any finite order and the trapezoidal rule becomes a method of choice. Such a convergence is known as *exponential convergence*.

In order to calculate the integral (9) with the trapezoidal rule with the previous property we first apply the so-called double-exponential transformation $x = u(t) = \sinh((\pi/2)\sinh t)$, reducing it to

$$I = \int_{-\infty}^{+\infty} R(x^2)\, dx = \int_{-\infty}^{+\infty} R(u(t)^2) u'(t)\, dt,$$

i.e.,

$$I = \frac{\pi}{2} \int_{-\infty}^{+\infty} R\left(\sinh^2\left(\frac{\pi}{2}\sinh t\right)\right) \cosh\left(\frac{\pi}{2}\sinh t\right) \cosh t\, dt. \tag{12}$$

The crucial point in this transformation is the decay of the integrand be double exponential, i.e.,

$$|R(u(t)^2) u'(t)| \approx \exp(-C \exp|t|) \quad \text{as } |t| \to +\infty,$$

where C is some positive constant. For an integral of such form of an analytic function on $(-\infty, +\infty)$, it is known that the trapezoidal formula with an equal mesh size gives an optimal formula (cf. [80, 87, 88, 89, 93, 94, 95]).

In our case we apply the trapezoidal formula with an equal mesh size h, so that we obtain

$$I_h = \frac{\pi h}{2} \sum_{k=-\infty}^{+\infty} R\left(\sinh^2\left(\frac{\pi}{2}\sinh kh\right)\right)\cosh\left(\frac{\pi}{2}\sinh kh\right)\cosh kh.$$

Since the integrand decays double exponentially, in actual computation of the previous sum we truncate the infinite summation at $k = -M$ and $k = M$, so that we obtain the double-exponential (DE) formula for our integral

$$I \approx I_h^{(N)} = \frac{\pi h}{2} \sum_{k=-M}^{M} R\left(\sinh^2\left(\frac{\pi}{2}\sinh kh\right)\right)\cosh\left(\frac{\pi}{2}\sinh kh\right)\cosh kh,$$

where $N = 2M + 1$.

Example 1 Let $\phi(G, x) = x^{10} - 11x^8 + 41x^6 - 65x^4 + 43x^2 - 9$ and $\phi(G - Z, x) = x^4 - 3x^2 + 1$. Then we have $P(x) = \phi(G, x)$ and $Q(x) = \phi(G, x) + 2\phi(G - Z, x)$, so that

$$\begin{aligned} |P(ix)|^2 &= P(ix)P(-ix) = (9 + 43x^2 + 65x^4 + 41x^6 + 11x^8 + x^{10})^2, \\ |Q(ix)|^2 &= Q(ix)Q(-ix) = (7 + 37x^2 + 63x^4 + 41x^6 + 11x^8 + x^{10})^2, \end{aligned}$$

i.e.,

$$\left|\frac{P(ix)}{Q(ix)}\right|^2 = \left(\frac{9 + 16x^2 + 8x^4 + x^6}{7 + 16x^2 + 8x^4 + x^6}\right)^2,$$

because of $\gcd(|P(ix)|^2, |Q(ix)|^2) = (1 + 3x^2 + x^4)^2$. The problem can be additionally simplified by taking (see Lemma 1): $p(t) = 9 + 16t + 8t^2 + t^3$, $q(t) = 7 + 16t + 8t^2 + t^3$, $h(t) = 2t(p(t)q'(t) - q(t)p'(t)) = 2t(16 + 16t + 3t^2)$, and

$$R(t) = 2\frac{h(t)}{p(t)q(t)} = \frac{4t(16 + 16t + 3t^2)}{(7 + 16t + 8t^2 + t^3)(9 + 16t + 8t^2 + t^3)}.$$

Thus, $R(t) \in \mathcal{R}[3, 6]$. The behavior of the function $R(x^2)$ is presented in Fig. 1. Its values for $x = \pm 5, \pm 10, \pm 15, \pm 20$ are 0.000518, 0.0000108, 1.005×10^{-6}, 1.826×10^{-7}, respectively.

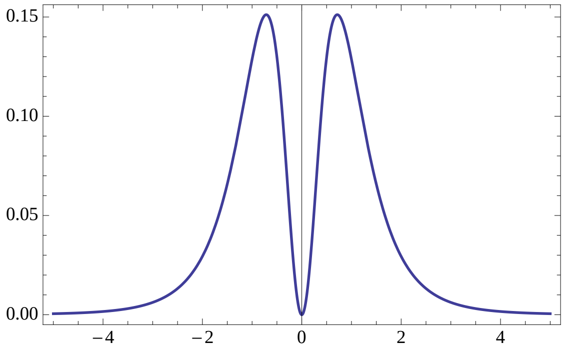

Fig. 1. The function $R(x^2)$

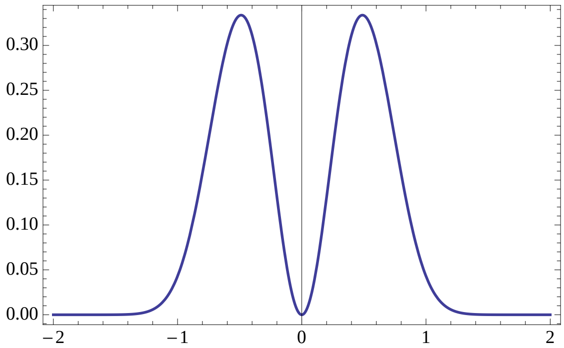

Fig. 2. The function $R(u(t)^2)u'(t)$

However, after DE transformation $x = u(t) = \sinh((\pi/2)\sinh t)$, the integrand $R(u(t)^2)u'(t)$ decays double exponentially (see Fig. 2). For example, its values for $t = \pm 1, \pm 2, \pm 3 \pm 4$ are 0.04298, 9.654×10^{-10}, 4.102×10^{-31}, 1.357×10^{-89}, respectively.

Taking the bounds in the integral as $a = -3$ and $b = 3$ (corresp. value of integrand 4.102×10^{-31}), for $N = 10(10)100$ we get the trapezoidal approximations $I_h^{(N+1)}$. Table 1 shows these approximations, together with the relative errors. In each entry of the second column the first digit in error is underlined. In the third column numbers in parentheses indicate decimal exponents, for example $1.40(-2) = 1.40 \times 10^{-2}$.

The exact value (to 33 significant digits), as determined by the method in the next section, is 0.380477864729266685437345222424304. The corresponding exact value of (6) is $ef(G, Z) = 0.12110986581742458176900 7\ldots$.

Table 1. Numerical approximations $I_h^{(N+1)}$ and the corresponding relative errors for $N = 10(10)100$

N	$I_h^{(N+1)}$	e_{rel}
10	0.385796	1.40(−2)
20	0.38049435	4.33(−5)
30	0.38047789486	7.92(−8)
40	0.38047786477677	1.25(−10)
50	0.3804778647293509	2.21(−13)
60	0.3804778647292668368	3.98(−16)
70	0.3804778647292666856998	6.90(−19)
80	0.3804778647292666854378032	1.20(−21)
90	0.3804778647292666854373346027	2.11(−24)
100	0.3804778647292666854373452238	3.70(−27)

4. *Transformation to the finite interval and Gaussian formulae*

In this section we propose another transformation $x = -t/\sqrt{1-t^2}$ (cf. [88]) in order to reduce (9) to the following integral over the finite interval $(-1, 1)$,

$$\int_{-\infty}^{+\infty} R(x^2)\, dx = \int_{-1}^{1} R\left(\frac{t^2}{1-t^2}\right) \frac{dt}{(1-t^2)^{3/2}}, \tag{13}$$

where $R(t)$ is defined in (8). This suggests us to apply some of Gaussian formulas for numerical calculation of (13). Namely, the Gaussian quadrature rule with respect to the Gegenbauer weight $w^\lambda(t) = (1-t^2)^{\lambda-1/2}$, $\lambda > -1/2$,

$$\int_{-1}^{1} \varphi(t)\, w^\lambda(t)\, dt = \sum_{k=1}^{N} A_k^\lambda \varphi(\tau_k^\lambda) + R_N(\varphi), \tag{14}$$

could be appropriate for this purpose. The nodes τ_k^λ, $k = 1, \ldots, N$, are zeros of the Gegenbauer polynomial $C_N^\lambda(t)$ of degree N, and the weights A_k^λ, $k = 1, \ldots, N$, are the corresponding Christoffel numbers (cf. [84, Chap. 5]). They can be calculated in an efficient way by using the Mathematica Package "`OrthogonalPolynomials`" [11].

Example 2 Consider again the integral from Example 1. In this case, the integral (13), written as a weighted integral with respect to the Gegenbauer weight $w^\lambda(t)$, becomes

$$\int_{-1}^{1} \frac{4t^2\left(3t^4-16t^2+16\right)\left(1-t^2\right)^{2-\lambda}}{\left(3t^4-11t^2+9\right)\left(2t^6-3t^4-5t^2+7\right)}\, w^\lambda(t)\, dt.$$

The complete integrand $R(t^2/(1-t^2))(1-t^2)^{-3/2}$ is presented in Fig. **??**. Applying the corresponding Gaussian formula (14) for $\lambda = 0, 1/2, 1, 3/2, 2$ to the previous integral we obtain results with the relative errors presented in Table 2. Note that this parameter λ must be such that $-1/2 < \lambda \le 2$.

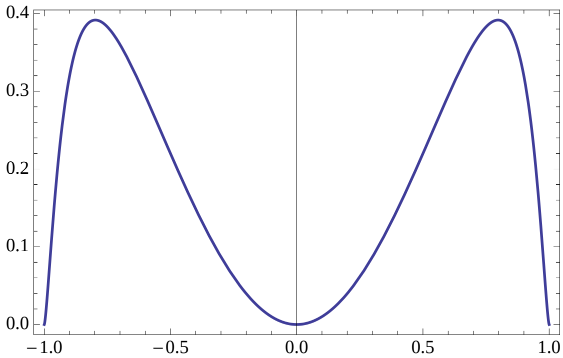

Fig. 3. The function $R(t^2/(1-t^2))(1-t^2)^{-3/2}$ in Example 2

Table 2. Relative errors in Gauss-Gegenbauer quadrature sums for some selected values of λ

N	$\lambda = 0$	$\lambda = 1/2$	$\lambda = 1$	$\lambda = 3/2$	$\lambda = 2$
10	9.99(−4)	1.18(−3)	4.28(−4)	1.24(−3)	2.75(−4)
20	1.64(−7)	2.77(−5)	6.72(−8)	3.75(−5)	3.42(−8)
30	2.06(−11)	3.39(−6)	8.34(−12)	5.16(−6)	3.90(−12)
40	2.33(−15)	7.95(−7)	9.35(−16)	1.27(−6)	4.20(−16)
50	2.48(−19)	2.60(−7)	9.91(−20)	4.27(−7)	4.33(−20)
60	2.54(−23)	1.04(−7)	1.01(−23)	1.75(−7)	4.35(−24)
70	2.54(−27)	4.84(−8)	1.01(−27)	8.19(−8)	4.28(−28)
80	2.49(−31)	2.48(−8)	9.89(−32)	4.25(−8)	4.16(−32)
90	2.41(−35)	1.38(−8)	9.56(−36)	2.38(−8)	3.99(−36)
100	2.31(−39)	8.16(−9)	9.14(−40)	1.41(−8)	3.79(−40)

As we can see, the convergence is slow only if the integrand has an irrational factor. In these cases it is the factor "$\sqrt{1-t^2}$" which appears for $\lambda = 1/2$ (Gauss-Legendre quadrature) and $\lambda = 3/2$. In other cases this factor is included in the weight function and the corresponding function $\varphi(t)$ is a pure rational function. Regarding this fact we prefer to use Gauss-Chebyshev quadrature formulas (for $\lambda = 0$ and $\lambda = 1$), because of their simplicity.

In a general case, the rational function $R(t)$ belongs to $\mathcal{R}[m, 2n]$, where $0 \le m \le 2n - 1$ (see Lemma 1), and therefore it has the following form

$$R(t) = \frac{\sum\limits_{k=0}^{m} r_k t^k}{\sum\limits_{k=0}^{2n} s_k t^k}.$$

Regarding (13), we have

$$\int_{-\infty}^{+\infty} R(x^2)\, dx = \int_{-1}^{1} \frac{\sum\limits_{k=0}^{m} r_k t^{2k}(1-t^2)^{m-k}}{\sum\limits_{k=0}^{2n} s_k t^{2k}(1-t^2)^{2n-k}} (1-t^2)^{\ell} \cdot \frac{dt}{\sqrt{1-t^2}},$$

where $\ell = 2n - m - 1 \ge 0$. Thus, the Gauss-Chebyshev quadrature of the first kind ($\lambda = 0$) can be always applied to the integral (13). However, the corresponding Gauss-Chebyshev quadrature of the second kind ($\lambda = 1$) can be applied if $m \le 2n - 2$.

Now, we derive explicit expressions for these Gaussian quadrature sums

$$\int_{-\infty}^{+\infty} R(x^2)\, dx \approx S_N^{\lambda}(R) \qquad (\lambda = 0, 1). \tag{15}$$

Number of functional evaluations in these sums is reduced to $N/2$.

Theorem 1 *Let $N \in \mathbb{N}$, $R(t) \in \mathcal{R}[m, 2n]$, $0 \le m \le 2n - 1$, and $\xi_k = \cot^2 \dfrac{(2k-1)\pi}{2N}$, $k = 1, \ldots, [N/2]$. Then*

$$S_N^0(R) = \frac{2\pi}{N} \sum_{k=1}^{[N/2]} (1 + \xi_k) R(\xi_k) + \varepsilon_N \frac{\pi}{N} R(0), \tag{16}$$

where $\varepsilon_N = 0$ if N is even, and $\varepsilon_N = 1$ if N is odd.

Proof: Let $\lambda = 0$ and $\varphi(t)$ be defined as

$$\varphi(t) = \frac{1}{1-t^2}\; R\left(\frac{t^2}{1-t^2}\right).$$

Then for the N-point Gauss-Chebyshev quadrature sum of the first kind in (14), with the nodes $\tau_k = \tau_k^0 = \cos\theta_k$, where $\theta_k = \dfrac{(2k-1)\pi}{2N}$, $k = 1, \ldots, N$, all weight coefficients are equal, i.e., $A_k = A_k^0 = \pi/N$ (cf. [86, p. 174]). Therefore,

$$S_N^0(R) = \frac{\pi}{N}\sum_{k=1}^{N} \frac{1}{1-\cos^2\theta_k}\; R\left(\frac{\cos^2\theta_k}{1-\cos^2\theta_k}\right) = \frac{\pi}{N}\sum_{k=1}^{N}\frac{1}{\sin^2\theta_k}\, R(\cot^2\theta_k),$$

i.e.,

$$S_N^0(R) = \frac{\pi}{N}\sum_{k=1}^{N}(1+\cot^2\theta_k)\, R(\cot^2\theta_k),$$

which reduces to (16). □

Theorem 2 *Let $N \in \mathbb{N}$, $R(t) \in \mathcal{R}[m, 2n]$, $0 \le m \le 2n-2$, and $\eta_k = \cot^2 \dfrac{k\pi}{N+1}$, $k = 1, \ldots, [N/2]$. Then*

$$S_N^1(R) = \frac{2\pi}{N+1}\sum_{k=1}^{[N/2]}(1+\eta_k)R(\eta_k) + \varepsilon_N \frac{\pi}{N+1} R(0), \tag{17}$$

where $\varepsilon_N = 0$ if N is even, and $\varepsilon_N = 1$ if N is odd.

Proof: In this case $\lambda = 1$ and

$$\varphi(t) = \frac{1}{(1-t^2)^2}\; R\left(\frac{t^2}{1-t^2}\right).$$

Nodes of the corresponding N-point quadrature are zeros of the Chebyshev polynomial of the second kind $U_N(t) = \sin[(N+1)\arccos t]/\sqrt{1-t^2}$, i.e., $\tau_k = \tau_k^1 = \cos\theta_k$, where $\theta_k = \dfrac{k\pi}{N+1}$, $k = 1, \ldots, N$, and the weight coefficients are $A_k = A_k^1 = \dfrac{\pi}{N+1}\sin^2\theta_k$, $k = 1, \ldots, N$ (cf. [86, p. 174]). Therefore,

$$S_N^1(R) = \frac{\pi}{N+1}\sum_{k=1}^{N}\frac{\sin^2\theta_k}{(1-\cos^2\theta_k)^2}\; R\left(\frac{\cos^2\theta_k}{1-\cos^2\theta_k}\right)$$

reduces to (17). □

The obtained formulas (16) and (17) are very simple for implementing and using in integration. For example, the function $R(t)$ from Examples 1 and 2 belongs to $\mathcal{R}[3,6]$ and Theorem 2 can be applied. The quadrature sums $S_N^1(R)$ for $N = 10(10)100$ are presented in Table **??**.

Table 3. Quadrature sums $S_N^1(R)$ for $N = 10(10)100$

N	Quadrature sum $S_N^1(R)$
10	$0.380\underline{6}407$
20	$0.3804778\underline{9}027$
30	$0.38047786447\underline{3}243$
40	$0.38047786472926\underline{7}041$
50	$0.3804778647292666854\underline{7}505$
60	$0.3804778647292666854373\underline{4}9077$
70	$0.3804778647292666854373452228\underline{8}086$
80	$0.38047786472926668543734522242\underline{4}3\underline{4}194$
90	$0.3804778647292666854373452224243043\underline{0}6513$
100	$0.380477864729266685437345222424304302875\underline{6}715$

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