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Numerical Computation of an Integral Appearing in the Fröman–Fröman Phase-Integral Formula for Calculation of Quantal Matrix Elements without the Use of Wave Functions

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In this paper we present an efficient method for the numerical treatment of an integral appearing in the Fröman–Fröman phase-integral formula. Realistic error bounds are developed. The stability and convergence of the method are verified for a large class of integrands.

1. INTRODUCTION

On the basis of certain phase-integral approximations of arbitrary order introduced by Fröman [1, 2] and generalized by Fröman and Fröman [3] (cf. also pp. 126–131 in [4]) the same authors have been able to derive a simple and accurate formula for the calculation of quantal matrix elements without the use of wave functions [5]. The purpose of the present paper is to devise a method for the numerical computation of the kind of integral which appears in the Fröman–Fröman formula for matrix elements.

2. COMPUTATIONAL SCHEME

We want to evaluate numerically integrals of the general form

$$I_0(f_0, g_0) = \int_a^b f_0(x') \exp\left\{\int_a^{x'} g_0(t')\,dt'\right\} dx' \tag{1}$$

where a, b are real numbers and f_0, g_0 are given complex-valued functions defined on the real interval $[a, b]$. Making the substitutions

$$x' = a + \frac{b-a}{2}(x+1) \qquad t' = a + \frac{b-a}{2}(t+1)$$

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and defining

$$f(x) = \frac{b-a}{2} f_0(x') \qquad g(t) = \frac{b-a}{2} g_0(t')$$

we transform (1) to the standard form

$$I(f, g) = \int_{-1}^{1} f(x) \exp\left\{\int_{-1}^{x} g(t)\, dt\right\} dx. \tag{2}$$

We often need to treat the special case $g = 0$. Then we are faced with the simpler task to evaluate

$$\int_{-1}^{1} f(x)\, dx. \tag{3}$$

In order to facilitate the computer work we use real arithmetic. Writing

$$f = f_1 + if_2, \qquad g = g_1 + ig_2 \tag{4}$$

and putting

$$G_i(x) = \int_{-1}^{x} g_i(t)\, dt, \qquad i = 1, 2,$$

we get

$$I(f, g) = \int_{-1}^{1} \{f_1(x) \cos G_2(x) - f_2(x) \sin G_2(x)\} \exp\{G_1(x)\}\, dx$$
$$+ i \int_{-1}^{1} \{f_1(x) \sin G_2(x) + f_2(x) \cos G_2(x)\} \exp\{G_1(x)\}\, dx.$$

Hence our result is obtained by evaluating two real integrals. Many different quadrature schemes are conceivable. We want to use methods which are efficient in a situation characterized as follows:

(1) The functions f_i and g_i may be evaluated at any point.

(2) The labor to determine these functional values is great in comparison to the effort to perform an arithmetic operation.

(3) The work to evaluate $f_i(u)$ and $g_i(u)$ for some u is appreciably less than the combined effort to determine $f_i(u)$ and $g_i(v)$ for $u \neq v$.

We are given an error tolerance and the problem is to determine integral (1) with an error which does not exceed the tolerance. Thus we generate a sequence of approximations whose accuracy generally increases with the labor spent. We consider a general class of quadrature schemes where the calculations are performed by carrying out Steps (a) through (e) below:

(a) Select an integer n and a corresponding set of abscissas x_{nk}, $k = 1, 2,..., n$.

(b) The functions g_1 and g_2 are approximated by the polynomials p_1 and p_2 of degree less than n which interpolate g_1 and g_2 in the abscissas x_{nk} defined in the previous step.

(c) Put

$$P_i(x) = \int_{-1}^{x} p_i(t)\,dt, \qquad i = 1, 2. \tag{5}$$

This integration is done analytically.

(d) Approximate G_i with P_i, $i = 1, 2$.

(e) The integral

$$\hat{I}(f, g) = \int_{-1}^{1} \{f_1(x) \cos P_2(x) - f_2(x) \sin P_2(x)\} \exp\{P_1(x)\}\,dx$$
$$+ i \int_{-1}^{1} \{f_1(x) \sin P_2(x) + f_2(x) \cos P_2(x)\} \exp\{P_1(x)\}\,dx$$

is computed numerically using the same abscissas x_{nk} introduced in Step (a).

If the estimated error in the computed integral exceeds a preselected tolerance, n is increased. The new n-value and the corresponding abscissas are selected in such a way that all old points are retained.

In the method implemented in the computer program [6]

$$x_{nk} = \cos(k\pi/(n + 1)), \qquad k = 1, 2,..., n \tag{6}$$

and n is advanced according to the rule

$$n_{\text{new}} = 2n_{\text{old}} + 1 \tag{7}$$

and the first n-value is always taken to be odd. Thus if we start with $n = 11$, the sequence 11, 23, 47,... is generated.

DEFINITION. 1. $a \ll b$ means that a is much less than b, i.e., a/b is negligible in comparison with 1. ||

DEFINITION. 2. Assume that $x < b$ and $a \approx b$. Then we write $x \lesssim a$ ("x is approximately less than a"). ||

Thus if $x < 2^{1/2}$, we could write $x \lesssim 1.4$ and $x \ll 10^6$.

We next explain how the error in the computed value of (2) is estimated. Let n_0 be a given number and generate by (7) the sequence $\{n_l\}_0^\infty$, i.e., $n_l = 2n_{l-1} + 1$, $l = 1, 2,...$. Denote by $I_l(f, g)$ the estimate of (2) corresponding to n_l. Hence the absolute value of the error is

$$| I_l(f, g) - I(f, g)|. \tag{8}$$

We use the approximation

$$| I_l(f, g) - I(f, g)| \lesssim | I_l(f, g) - I_{l-1}(f, g)|. \tag{9}$$

This is a pessimistic assessment, if the sequence $\{I_l(f, g)\}_0^\infty$ is "rapidly converging."

By this concept we mean that

$$| I_l(f, g) - I(f, g)| \ll | I_{l-1}(f, g) - I(f, g)| \tag{10}$$

when l is larger than some number l_0. For then we have

$$\begin{aligned} | I_{l-1}(f, g) - I(f, g)| &\leqslant | I_{l-1}(f, g) - I_l(f, g)| + | I_l(f, g) - I(f, g)| \\ &\approx | I_{l-1}(f, g) - I_l(f, g)| \end{aligned}$$

giving instead of (9)

$$| I_{l-1}(f, g) - I(f, g)| \approx | I_l(f, g) - I_{l-1}(f, g)|.$$

We illustrate the effectiveness of our method on the numerical examples accounted for in the Appendix. Since the exact values of these integrals are known we can determine the actual errors and compare with the error bounds (9). We make the following observations.

(i) The error decreases exponentially in n, i.e., there are positive constants A and B, with $B < 1$, such that

$$| I_l(f, g) - I(f, g)| < A \cdot B^{n_l} \tag{11}$$

where A and B depend on the integrands.

(ii) If we increase n according to (7), condition (10) is met, i.e., our error bound is, as a rule, too conservative.

(iii) The presence of round-offs limits the obtainable accuracy of the computed value. As illustrated by the examples in the Appendix this ultimate accuracy is different for different integrands.

Thus it is of no use to select n_l too large. As described in [6] the calculations are stopped when for the first time condition (12a) is met while (12b) is violated

$$| I_l(f, g) - I_{l-1}(f, g)| \leqslant 10^{-3} | I_l(f, g)|, \tag{12a}$$

$$| I_l(f, g) - I_{l-1}(f, g)| \leqslant | I_{l-1}(f, g) - I_{l-2}(f, g)|. \tag{12b}$$

It could be that the estimates for very low values of n behave irregularly and do not obey (11). Therefore condition (12a) is imposed in order to prevent a premature stop for this reason. However, as long as (11) prevails then (12b) is met. Therefore if (12b) is violated while (12a) holds we must have reached the noise level where round-offs prevent further improvement in the accuracy of the computed value. In the following sections we shall show that the computational methods implemented in [6] work for a general class of functions.

3. Convergence Properties

In this section we show that the error bound (11) is valid for a wide class of functions, if x_{nk} are chosen according to (6).

DEFINITION 3. Let $\rho \geqslant 1$ be a given number. We define E_ρ as the ellipse in the complex plane given by

$$E_\rho = \{z = \tfrac{1}{2}(\xi + \xi^{-1}),\ \xi = \rho e^{i\theta},\ 0 \leqslant \theta < 2\pi\}. \quad \| \tag{13}$$

Thus E_ρ is an ellipse with foci at $+1$ and -1. Its half-axes have the lengthe $\frac{1}{2}(\rho + \rho^{-1})$ and $\frac{1}{2}(\rho - \rho^{-1})$, respectively.

LEMMA 1. *Let φ be analytic in the interior and continuous at the boundary of the ellipse E_ρ defined by* (13) *and let Q_n be the polynomial of degree less than n which interpolates φ at the points x_{nk} given by* (6). *Then there is a constant A_0 independent of n such that*

$$\max_{-1\leqslant x\leqslant 1} | \varphi(x) - Q_n(x)| \leqslant A_0 n\rho^{-n}. \tag{14}$$

Proof. Clearly $\prod_{k=1}^{n} (x - x_{nk}) = 2^{-n}U_n(x)$, where $U_n(x)$ is the Čebyšev polynomial of the second kind of degree n (see e.g. [8, p. 49]). Using this result, it follows from Theorem 3.6.1, page 68 of [7] that

$$\phi(x) - Q_n(x) = \frac{1}{2\pi i}\int_{E_\rho} \frac{\phi(\xi)\, U_n(x)}{[\xi - x][U_n(\xi)]}\, d\xi. \tag{15}$$

Since $| U_n(x)| \leqslant n + 1$ on $[-1, 1]$, we get the bound

$$| \phi(x) - Q_n(x)| \leqslant \frac{n+1}{2\pi}\int_{E_\rho} \frac{| \phi(\xi)|}{| \xi - x |\, | U_n(\xi)|}\, | d\xi |. \tag{16}$$

Using the result $U_n(x) = T'_{n+1}(x)/(n + 1)$ and expression (4.4.2), page 83 of [7], we see that

$$U_n(\zeta) = \frac{\xi^{n+1} - \xi^{-n-1}}{\xi - \xi^{-1}} \qquad \text{with} \quad \zeta = \tfrac{1}{2}(\xi + \xi^{-1}).$$

Hence, putting $\xi = \rho e^{i\theta}$

$$U_n(\zeta) = \frac{(\rho^{n+1} - \rho^{-n-1})\cos(n + 1)\,\theta + i(\rho^{n+1} + \rho^{-n-1})\sin(n + 1)\,\theta}{(\rho - \rho^{-1})\cos\theta + i(\rho + \rho^{-1})\sin\theta}$$

and

$$| U_n(\zeta)|^2 = (\rho^{2n+2} + \rho^{-2n-2} - 2\cos(2n + 2)\,\theta)/(\rho^2 + \rho^{-2} - 2\cos 2\theta).$$

Therefore

$$| U_n(\zeta)| \geqslant (\rho^{n+1} - \rho^{-n-1})/(\rho + \rho^{-1}).$$

Entering this result into (16) we easily reach the desired conclusion. $\|$

Put

$$\varphi(x) = f(x)\exp\left\{\int_{-1}^{x} g(t)\, dt\right\},$$

Then (2) takes the form

$$\int_{-1}^{+1} \varphi(x)\, dx. \tag{17}$$

By Lemma 1 Steps (b), (c), and (d) entail that φ in (17) is replaced by $\varphi + \Delta_n$ where

$$|\Delta_n(x)| \leqslant C \cdot D^n \tag{18}$$

where C and D are constants and $0 \leqslant D < 1$.

Interpolating in the abscissas x_{nk} given by (6) and integrating the resulting polynomial is equivalent to using Filippi's rule [9],

$$\int_{-1}^{+1} \varphi(x)\, dx = \sum_{k=1}^{n} A_{nk}\varphi(x_{nk}), \tag{19}$$

which has nonnegative weights A_{nk}. It is also known that provided φ meets the same conditions as in Lemma 1, then there are constants C_0 and D_0 with $0 \leqslant D_0 < 1$ such that

$$\left| \int_{-1}^{+1} \varphi(x)\, dx - \sum_{k=1}^{n} A_{nk}\varphi(x_{nk}) \right| \leqslant C_0 D_0^{\,n}. \tag{20}$$

See [10, 11].

We now prove

LEMMA 2. *Let E_ρ and φ be as in Lemma* 1 *and let Δ_n meet* (18). *Then there are constants K and L, $0 \leqslant L < 1$, such that*

$$R = \left| \int_{-1}^{+1} \varphi(x)\, dx - \sum_{k=1}^{n} A_{nk}[\varphi(x_{nk}) + \Delta_n(x_{nk})] \right| \leqslant KL^n$$

where x_{nk} is given by (6) *and A_{nk} is the corresponding weight in Filippi's rule.*

Proof. Due to (20) we have

$$\left| \int_{-1}^{+1} \varphi(x)\, dx - \sum_{k=1}^{n} A_{nk}\varphi(x_{nk}) \right| \leqslant C_0 D_0^{\,n}.$$

Since $A_{nk} \geqslant 0$ and Filippi's rule gives exact results for $\varphi(x) = 1$ we get

$$\sum_{k=1}^{n} A_{nk} = \sum_{k=1}^{n} |A_{nk}| = 2.$$

Therefore

$$\begin{aligned} R &\leqslant \left| \int_{-1}^{+1} \varphi(x)\, dx - \sum_{k=1}^{n} A_{nk}\varphi(x_{nk}) \right| + \sum_{k=1}^{n} |A_{nk}|\, |\Delta_n(x_{nk})| \\ &\leqslant C_0 D_0^{\,n} + 2CD^n \end{aligned}$$

and hence the assertion follows. ||

Thus by combining Lemmas 1 and 2 we obtain

THEOREM 1. *Let f_i and g_i, $i=1,2$ meet the assumptions of Lemma* 1 *and let x_{nk} be given by* (6). *Then the truncation error* $| I_n(f, g) - I(f, g)|$ *after performing Steps* (a) *through* (e) *of the computational scheme satisfies* (11). ||

This result is also confirmed by the numerical examples in the Appendix.

4. NUMERICAL STABILITY

We next discuss the problem of estimating how sensitive the computed results are to round-off errors in given functional values and committed during the course of the computations.

Influence of the Round-Offs in the Given Functional Values

In Steps (a) and (b) we interpolate the integrand g_i at x_{nk} which gives the polynomial p_i of degree less than n. We can write

$$p_i(t) = \sum_{k=1}^{n} l_k(t)\, g_i(x_{nk}), \tag{21}$$

where by Lagrange's interpolation formula l_k is the polynomial of degree less than n satisfying

$$l_k(x_{nj}) = \delta_{kj}\,.$$

Integrating (21) we get

$$P_i(x) = \sum_{k=1}^{n} L_k(x)\, g_i(x_{nk}),$$

where

$$L_k(x) = \int_{-1}^{x} l_k(t)\, dt, \tag{22}$$

and P_i is defined by (5).

Assume now that the values $g_i(x_{nk})$ are perturbed by an amount not exceeding ϵ in absolute value. Denote by $\Delta P_i(x)$ the resulting error in $P_i(x)$. We find immediately

$$| \Delta P_i(x)| \leqslant \epsilon \Lambda(x)$$

where

$$\Lambda(x) = \sum_{r=1}^{n} | L_r(x)|. \tag{23}$$

For the special choice of x_{nk} defined by (6) we get $L_r(1) = A_{rk}$ in (19), the weights in Filippi's rule. Hence we conclude $\Lambda(1) = 2$. We show the more general result

LEMMA 3. *Define* Λ *by* (23), L_k *by* (22), *and* x_{nk} *by* (6). *Then there is a constant* C *such that*

$$\Lambda(x_{nk}) = \sum_{r=1}^{n} | L_r(x_{nk})| \leqslant C \tag{24}$$

for all k *and odd* n.

Remark. The meaning of this result is that errors in the input data $g_i(x_{nk})$ are at most magnified by a factor C in the process of computing $P_i(x_{nk})$. We note that the more general result

$$\Lambda(x) \leqslant C, \qquad x \in [-1, 1]$$

may be established using the same argument as in the proof of this lemma.

Proof of Lemma 3. Instead of x_{nk} we simply write t_k. l_k of (21) may be written

$$l_k(t) = \frac{U_n(t)}{(t - t_k)\, U_n{}'(t_k)}$$

where as before U_n is the Čebyšev polynomial of the second kind. Thus

$$L_k(t_j) = \frac{1}{U_n{}'(t_k)} \int_0^{t_j} \frac{U_n(t)}{t - t_k}\, dt. \tag{25}$$

We now put $t = \cos\theta$, $\theta_j = j\pi/(n+1)$, and $\theta_k = k\pi/(n+1)$. Using the fact that

$$U_n(\cos\theta) = \frac{\sin(n+1)\,\theta}{\sin\theta}$$

we find after straightforward calculations

$$| L_k(t_j)| = \frac{\sin^2\theta_k}{n+1} \left| \int_0^{\theta_j} z_k(\theta) \sin(n+1)\,\theta\, d\theta \right| \tag{26}$$

where

$$z_k(\theta) = \frac{1}{\cos\theta - \cos\theta_k}.$$

We seek an upper bound for the integral in (26). We write

$$\int_0^{\theta_j} z_k(\theta) \sin(n+1)\,\theta\, d\theta = \sum_{l=1}^{j} a_l \tag{27}$$

where

$$a_l = \int_{\theta_{l-1}}^{\theta_l} z_k(\theta) \sin(n+1)\,\theta\, d\theta.$$

We note that z_k is increasing in the interval $[0, \pi]$ and has a simple pole at θ_k. Thus $a_{l-1} \cdot a_l < 0$ for $l = 2, 3,..., k$ and $a_{l-1} \cdot a_l < 0$ for $l = k + 2, k + 3,..., n$. Further $| a_l | > | a_{l-1} |$, $l = 2, 3,..., k$ and $| a_l | < | a_{l-1} |$, $l = k + 2, k + 3,..., n$. Thus

$$\left| \sum_{l=1}^{j} a_l \right| \leqslant | a_k | \qquad \text{if } j \leqslant k$$

and

$$\left| \sum_{l=1}^{j} a_l \right| \leqslant | a_k | + | a_{k+1} | \qquad \text{if } j > k.$$

In order to bound the integral (26) we must estimate a_k and a_{k+1}. We find

$$\begin{aligned} | a_k | &= \left| \int_{\theta_{k-1}}^{\theta_k} z_k(\theta) \sin(n+1)\,\theta \, d\theta \right| \\ &= \frac{1}{n+1} \int_{-\pi}^{0} | \sin \lambda | \frac{d\lambda}{\cos\left(\theta_k + \dfrac{\lambda}{n+1}\right) - \cos \theta_k}. \end{aligned}$$

Now put

$$D_{nk} = \sin \theta_k \, | a_k |.$$

Next we apply the simple results

$$2x/\pi \leqslant \sin x < x, \qquad x \in [0, \pi/2],$$
$$| \cos(x + h) - \cos x | \geqslant h \min_{x \leqslant \lambda \leqslant x+h} | \sin \lambda |.$$

Then

$$D_{n1} \leqslant (\pi^2/2) \int_{-\pi}^{0} \lambda^{-1} \sin \lambda/(\pi + \lambda)\, d\lambda, \tag{28}$$

$$D_{nk} \leqslant \pi \int_{-\pi}^{0} \lambda^{-1} \sin \lambda \, d\lambda, \qquad 1 < k \leqslant (n+1)/2, \tag{29}$$

$$D_{nk} \leqslant \int_{-\pi}^{0} \lambda^{-1} \sin \lambda \, d\lambda, \qquad (n+1)/2 < k \leqslant n.$$

Thus $D_{nk} \leqslant D$ where D is the larger of the two integrals (28), (29). Returning to (26) we arrive at

$$| L_k(\theta_j)| \begin{array}{ll} \leqslant \dfrac{\sin \theta_k}{n+1} D, & j \leqslant k \\ \leqslant \dfrac{2 \sin \theta_k}{n+1} D, & j > k. \end{array}$$

Thus

$$\Lambda(x_j) = \sum_{k=1}^{n} | L_k(x_j)| \leqslant \frac{D}{n+1} \left\{ 2 \sum_{k=1}^{j-1} \sin \theta_k + \sum_{k=j}^{n} \sin \theta_k \right\} < 2D.$$

Hence the lemma is proved, if we take $C = 2D$. ||

Influence of Round-Offs Committed During the Computations

In the computer program p_i is represented as an expansion in Čebyšev polynomials of the second kind

$$p = \sum_{r=1}^{n} c_r{}^n U_{r-1}$$

(p stands for p_1 or p_2). We observe that $c_r{}^n$ depends both on r and n. Thus

$$P(x) = \sum_{r=1}^{n} c_r{}^n v_r(x), \qquad v_r(x) = \int_{-1}^{x} U_{r-1}(t)\,dt.$$

Both $c_r{}^n$ and $v_r(x)$ are computed and stored with a relative accuracy which we denote by η. We find immediately that the relative error $\delta P(x)$ caused by a relative error η in $c_r{}^n$ and $v_r(x)$ satisfies the relation

$$|\,\delta P(x)| \leqslant 2\eta \sum_{r=1}^{n} |\,c_r{}^n v_r(x)| \Big/ \Big| \sum_{r=1}^{n} c_r{}^n v_r(x) \Big|. \tag{30}$$

The right-hand side of (30) is easily evaluated during the calculations, and high values indicate loss in precision in the calculated values.

We observe that of the entities in (30) $v_r(x)$ is the same for all integrands while c_r reflects the properties of the function to be integrated.

We prove

LEMMA 4. *Let φ and Q_n be as in Lemma* 1 *and put*

$$Q_n = \sum_{r=1}^{n} c_r{}^n U_{r-1}(x). \tag{31}$$

Then

$$\lim_{n\to\infty} \sum_{r=1}^{n} (c_r{}^n)^2 = \frac{2}{\pi} \int_{-1}^{+1} (1 - t^2)^{1/2}\,\varphi^2(t)\,dt.$$

Proof. Q_n interpolates φ at $x_{1n}, x_{2n}, \ldots, x_{nn}$ and has the expansion (31). Since

$$\int_{-1}^{+1} (1 - t^2)^{1/2}\,U_r{}^2(t)\,dt = \pi/2, \qquad r = 0, 1, 2, \ldots,$$

$$\sum_{r=1}^{n} (c_r{}^n)^2 = \frac{2}{\pi} \int_{-1}^{+1} (1 - t^2)^{1/2}\,Q_n{}^2(t)\,dt.$$

Thus

$$\sum_{r=1}^{n} (c_r{}^n)^2 - \frac{2}{\pi} \int_{-1}^{1} (1 - t^2)^{1/2}\,\varphi^2(t)\,dt = \frac{2}{\pi} \int_{-1}^{1} (1 - t^2)^{1/2}\,(Q_n{}^2(t) - \varphi^2(t))\,dt.$$

By Lemma 1 we find, using the maximum norm $\| \|_\infty$.

$$| Q_n^2(t) - \varphi^2(t)| = |(Q_n(t) + \varphi(t))(Q_n(t) - \varphi(t))| \leqslant (\| Q_n \|_\infty + \| \varphi \|_\infty) A_0\rho^{-n}$$

and hence the assertion follows. $\|$

Returning now to (30) we use Schwarz' inequality and get

$$\left(\sum_{r=1}^{n} | c_r^n v_r(x)|\right)^2 \leqslant \left(\sum_{r=1}^{n} v_r^2(x)\right)\left(\sum_{r=1}^{n} (c_r^n)^2\right)$$

$$\approx \left(\sum_{r=1}^{n} v_r^2(x)\right)^2 \frac{2}{\pi} \int_{-1}^{+1} (1 - t^2)^{1/2} \varphi^2(t)\, dt.$$

Hence Lemma 4 can be used to assess the loss in accuracy caused by the fact that intermediate results are stored with a finite precision.

5. Conclusions

We have presented a method to calculate the integral (1) in an efficient manner under the conditions specified in (1), (2), and (3) in Section 2. We have shown convergence of the method and investigated its sensitivity for errors in input data and in intermediate results. Our theoretical conclusions are supported by many numerical experiments some of which are reported in the appendix.

APPENDIX: Numerical Examples

Below we present four different examples of functions f_0 and g_0, for which the analytical solution of (1) in Section 2 is known.

Example 1.

$$f_0(x) = \frac{1}{2 + x}; \qquad g_0(t) = \frac{1}{2 + t}; \qquad [a, b] = [-1, 1]; \qquad I_0(f_0, g_0) = 2.$$

Example 2.

$$f_0(x) = \frac{1}{(1.1 + x)^5}; \qquad g_0(t) = \frac{1}{1.1 + t}; \qquad [a, b] = [-1, 1];$$

$$I_0(f_0, g_0) = 3332.97340063749.$$

Example 3.

$$f_0(x) = 1 + \tan^2 x - 2 \sin x \cos x - 5 \cos x \sin^4 x,$$

$$g_0(t) = f_0(t); \qquad [a, b] = [-1, 1],$$

$$I_0(f_0, g_0) = \exp\{2 \tan 1 - 2 \sin^5 1\} - 1 = 8.689494503013295.$$

EXAMPLE 4. In connection with tests of the formula for calculating matrix elements [5] an application to the linear harmonic oscillator was studied in [12]. Here one certainly knows the exact matrix elements, but as a measure of the accuracy of the formula this and corresponding applications have been of great help. The formula can in this case, except for a constant factor, be written as

$$I_1 = \int_\Gamma \frac{z^{1/2(\lambda-\mu)+2p}}{(Q_\lambda(z))^{1/2}\,(Q_\mu(z))^{1/2}} \exp\{i\omega_\lambda(z) - i\omega_\mu(z)\}\, dz$$

where $p = 0, 1, 2$, $\lambda = 2n + 1$, $\mu = 2m + 1$, and n, m are the principal quantum numbers under consideration and where

$$\begin{aligned} Q_\lambda(z) &= -i(z^2 - \lambda)^{1/2}, \qquad \lambda > 0, \quad \lambda \text{ real}, \\ (Q_\lambda(z))^{1/2} &= e^{-i\pi/4}(z^2 - \lambda)^{1/4}, \\ i\omega_\lambda(z) &= \int_{\lambda^{1/2}}^{z} (z^2 - \lambda)^{1/2}\, dz, \end{aligned}$$

and Γ is a circle with radius $A > \max(\lambda^{1/2}, \mu^{1/2})$ and with its center at the origin. The analytical solution of I_1 is

$$\begin{aligned} I_1 &= -\,2\pi \exp\left\{\frac{\lambda}{4}\ln\frac{\lambda}{4} - \frac{\mu}{4}\ln\frac{\mu}{4} - \frac{\lambda-\mu}{4}\right\} A_{2p}, \\ A_0 &= 1, \\ A_2 &= \frac{\lambda+\mu}{4}\left(1 + \frac{\lambda-\mu}{4}\right), \\ A_4 &= \frac{3(\lambda+\mu)^2 + 2(\lambda-\mu)^2}{32} + \frac{(\lambda-\mu)[7(\lambda+\mu)^2 + (\lambda-\mu)^2]}{256} \\ &\quad + \frac{(\lambda-\mu)^2(\lambda+\mu)^2}{512}. \end{aligned}$$

In order to compute I_1 numerically we must rewrite it into the required form (1). Put $I_1 = I_{10}I_{20}$ where

$$\begin{aligned} I_{10} &= \exp\left\{\int_{\lambda^{1/2}}^{a} (z^2 - \lambda)^{1/2}\, dz - \int_{\mu^{1/2}}^{a} (z^2 - \mu)^{1/2}\, dz\right\}, \\ I_{20} &= \int_\Gamma \frac{z^{1/2(\lambda-\mu)+2p}}{(Q_\lambda(z))^{1/2}\,(Q_\mu(z))^{1/2}} \exp\left\{\int_a^z ((z'^2 - \lambda)^{1/2} - (z'^2 - \mu)^{1/2})\, dz'\right\} dz. \end{aligned}$$

I_{10} can be evaluated analytically, because

$$\int_{\lambda^{1/2}}^{z} (z^2 - \lambda)^{1/2}\, dz = \frac{z}{2}(z^2 - \lambda)^{1/2} - \frac{\lambda}{2}\ln\left\{\frac{z + (z^2 - \lambda)^{1/2}}{\lambda^{1/2}}\right\}.$$

I_{20} can be written in the required form (1) by integrating around the circle Γ, $z = A(\cos x + i \sin x)$, $0 \leqslant x < 2\pi$. This is not complicated but the exact formulas for $f_0(x)$ and $g_0(x)$ are omitted here. Six different subcases are reported (4a–f).

	λ	μ	p	A
4a, d	23	21	0	20,8
4b, e	21	23	1	20,8
4c, f	21	25	2	20,8

These four examples illustrate the following theoretical results.

(a) The error decreases exponentially in n_l. If ϵ_l is the relative error in $I_l(f, g)$, formula (11) tells us to expect

$$\ln \epsilon_l = C + Dn_l$$

C, D are constants, for sufficiently large n_l and until other kinds of errors will dominate. This is illustrated in Fig. 1.

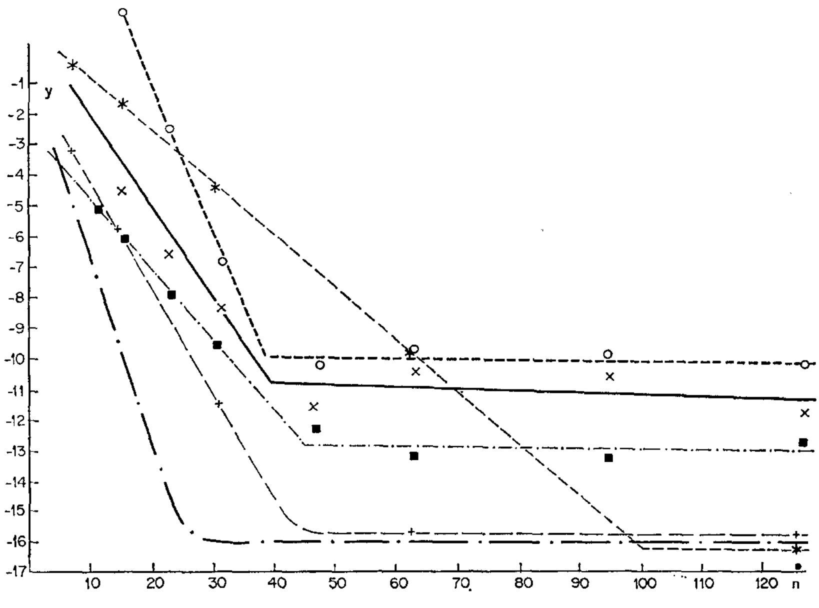

FIG. 1. y = logarithm of relative error.

Example	C_n^2	
1	≈ 1	•, —— · ——
2		+, — —
3	≈ 5	*, - - -
4a	≈ 2	■, — · — ·
4b	≈ 120	×, ———
4c	≈ 19000	○, - - -

(b) The speed with which the error decreases is dependent on the functions.

(c) The accuracy of the best estimate, depends on the functions f_0 and g_0 since intermediate results are stored with finite precision. Compare the discussion at the end of Section 4. The loss of accuracy depends on the size of C_n

$$C_n^2 = \sum_{r=1}^{n} (c_r{}^n)^2.$$

See Lemma 4. We have computed C_n^2 for examples 1, 3, 4a–c. As can be seen from Table I, high values of C_n^2 (example 4b and 4c) are followed by worse accuracy of the best approximation.

TABLE I

		Relative error				Relative error	
Example	n	Estimate	Actual	Example	n	Estimate	Actual
1	7	$0.57 \cdot 10^{-2}$	$0.13 \cdot 10^{-4}$	4c	7	$0.32 \cdot 10$	$-0.53 \cdot 10^{3}$
	15	$0.13 \cdot 10^{-4}$	$0.16 \cdot 10^{-9}$		15	$0.43 \cdot 10^{2}$	$0.14 \cdot 10^{2}$
	31	$0.16 \cdot 10^{-9}$	$-0.11 \cdot 10^{-15}$		31	$0.14 \cdot 10^{2}$	$-0.88 \cdot 10^{-7}$
	63	$0.12 \cdot 10^{-16}$	$-0.12 \cdot 10^{-15}$		63	$-0.88 \cdot 10^{-7}$	$0.11 \cdot 10^{-9}$
					127	$0.54 \cdot 10^{-10}$	$0.53 \cdot 10^{-10}$
2	7	0.90	0.44	4d	7	$0.86 \cdot 10^{-1}$	$-0.29 \cdot 10^{-2}$
	15	0.42	$0.25 \cdot 10^{-1}$		15	$-0.30 \cdot 10^{-2}$	$0.15 \cdot 10^{-3}$
	31	$0.25 \cdot 10^{-1}$	$0.50 \cdot 10^{-4}$		31	$0.14 \cdot 10^{-3}$	$0.12 \cdot 10^{-4}$
	63	$0.50 \cdot 10^{-4}$	$0.11 \cdot 10^{-9}$		63	$0.12 \cdot 10^{-4}$	$0.24 \cdot 10^{-7}$
	127	$0.11 \cdot 10^{-9}$	$-0.51 \cdot 10^{-16}$		127	$0.24 \cdot 10^{-7}$	$0.52 \cdot 10^{-12}$
3	7	0.22	$0.53 \cdot 10^{-3}$	4e	7	$-0.69 \cdot 10^{1}$	$0.97 \cdot 10^{-1}$
	15	$0.53 \cdot 10^{-3}$	$0.12 \cdot 10^{-5}$		15	$0.99 \cdot 10^{-1}$	$-0.25 \cdot 10^{-2}$
	31	$0.12 \cdot 10^{-5}$	$0.32 \cdot 10^{-11}$		31	$-0.25 \cdot 10^{-2}$	$0.20 \cdot 10^{-4}$
	63	$0.32 \cdot 10^{-11}$	$-0.18 \cdot 10^{-15}$		63	$0.20 \cdot 10^{-4}$	$0.51 \cdot 10^{-7}$
	127	$0.10 \cdot 10^{-16}$	$-0.19 \cdot 10^{-15}$		127	$0.51 \cdot 10^{-7}$	$-0.70 \cdot 10^{-12}$
4a	7	$0.21 \cdot 10^{-1}$	$-0.63 \cdot 10^{-3}$	4f	7	$0.12 \cdot 10^{1}$	$-0.25 \cdot 10^{2}$
	15	$-0.63 \cdot 10^{-3}$	$-0.68 \cdot 10^{-6}$		15	$-0.34 \cdot 10^{2}$	0.28
	31	$-0.68 \cdot 10^{-6}$	$0.31 \cdot 10^{-9}$		31	0.28	$-0.79 \cdot 10^{-4}$
	63	$0.31 \cdot 10^{-9}$	$-0.72 \cdot 10^{-13}$		63	$-0.79 \cdot 10^{-4}$	$0.22 \cdot 10^{-6}$
	127	$-0.29 \cdot 10^{-12}$	$0.22 \cdot 10^{-12}$		127	$0.22 \cdot 10^{-6}$	$0.37 \cdot 10^{-11}$
4b	7	$0.55 \cdot 10^{2}$	$0.13 \cdot 10$				
	15	$0.13 \cdot 10$	$0.39 \cdot 10^{-4}$				
	31	$0.39 \cdot 10^{-4}$	$0.48 \cdot 10^{-8}$				
	63	$0.48 \cdot 10^{-8}$	$0.39 \cdot 10^{-10}$				
	127	$0.37 \cdot 10^{-10}$	$0.16 \cdot 10^{-11}$				

(d) Finally, Table I shows that our error estimate is in general pessimistic, as expected. For large n though, when the roundoff errors are larger than the truncation errors, formula (9) does not give a strict error estimate. Compare examples 1 and 3 where we even get an error estimate below the computer accuracy, $\approx 10^{-16}$ which of course is absurd. For all other results the error estimate is either pessimistic or approximately, as shown in Table I.

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