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THE NUMERICAL COMPUTATION OF SPECIAL FUNCTIONS BY USE OF QUADRATURE RULES FOR SADDLE POINT INTEGRALS

II. GAMMA FUNCTIONS, MODIFIED BESSEL FUNCTIONS AND PARABOLIC CYLINDER FUNCTIONS

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Errata for the ALGOL 60 procedures

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N.M. Temme

In transferring the programs from the test version to the printing version some errors were made.

p. 38, line 20, read: eps := 10↑(-.6 × d);

line 21, delete: m := 0; tt := 0; include: g := .5;

line 31, read: knux (instead of inux)

p. 49, line 9, delete: tt := tt + 1;

Furthermore, on page 14, line 2, read: doubled (instead of doubted).

AMS(MOS) subject classification scheme (1970): 33-04, 33A15, 33A40, 33A70, 41A60, 65D20, 65D30

The numerical computation of special functions by use of quadrature rules
for saddle point integrals

II. Gamma functions, modified Bessel functions and parabolic cylinder fun

by

N.M. Temme

ABSTRACT

This is a second paper in a series in which quadrature rules are use
for the computation of special functions. The functions considered here a
the Euler gamma function, modified Bessel functions and parabolic cylinde
functions.

KEY WORDS & PHRASES: *mechanical quadrature, trapezoidal integration rules*
saddle point methods, computation of special functio
gamma function, modified Bessel function, parabolic
cylinder function

5D20, 65D30

CONTENTS

2.0. INTRODUCTION

This is a second report in a series on the computation of special functions. It contains applications of the methods of part I. The functions considered here are the gamma function $\Gamma(x)$ with $x > 0$, the modified Bessel functions $K_\nu(x)$ and $I_\nu(x)$ (with $\nu \geq 0$, $x > 0$) and a parabolic cylinder function $D_\nu(x)$ (with $\nu \leq 0$, $x \in \mathbb{R}$). The starting point is an integral, the quadrature method for evaluating the integral is the trapezoidal rule. In the fourth report the Bessel functions and the parabolic cylinder functions will be treated for other ranges of the parameters. In the third report incomplete gamma functions (among others) will be considered.

In the present paper the range of the parameters is chosen such that in the saddle point integrals to be used the procedure is not disturbed for some combinations of the variables of the functions. To be more specific, in the saddle point analysis of the Bessel functions and the parabolic cylinder functions more than one saddle point of the integrand may be considered. For certain combinations of the parameters ν and x these saddle points will coincide. This gives rise to non-uniform behaviour of these functions (especially if the parameters are large). These situations will be excluded in this paper. They will be considered in the fourth one.

In the third paper we will give examples in which a saddle point may coincide with a pole of the integrand. A major example for that case is the incomplete gamma function.

In the underlying paper we start with the Euler gamma function. It is a simple example (a function of one variable, considered real here), but it will explain our methods to be used in the subsequent examples. Moreover, the results are to be used in our third report on the incomplete gamma functions.

Sometimes the results of the first report TEMME (1977[a]) are used. We refer to formulae, theorems, remarks and sections of that paper by using simply the numbers of the first report, i.e., with the first digit 1. The formulae, etc. in the present report have numbers with first digit 2.

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2.1. THE GAMMA FUNCTION

For Re $z > 0$ the gamma function is defined by

$$(2.1.1) \qquad \Gamma(z) = \int_0^\infty e^{-t} t^{z-1} dt$$

As is well known, excellent numerical approximations may be obtained from the asymptotic series for $\Gamma(z)$ or from Stirling's series for $\ln \Gamma(z)$. For Stirling's series sharp error bounds for the remainder are known, even for complex values of z. By recursion the gamma function can be computed for small or intermediate values of z. The reflexion formula

$$\Gamma(1+z)\Gamma(1-z) = \pi z/\sin(\pi z)$$

can be used when Re z is negative. Apart from results based on asymptotic methods, expansions are available based on other principles. For instance, LUKE (1969) discusses in detail an expansion given by LANCZOS (1964) for complex argument. Consequently, from a computational point of view there is no problem. However, we consider the gamma function since it is a nice example for explaining our methods. Moreover the results of this section can be used for other special functions in subsequent papers, especially for the incomplete gamma functions.

Since our results obtained by trapezoidal quadrature rules are connected with asymptotic expansions we give the following well-known results

$$(2.1.2) \qquad \begin{aligned} \Gamma(z) &\sim e^{-z} z^{z-\frac{1}{2}} (2\pi)^{\frac{1}{2}} \sum_{k=0}^{\infty} c_k z^{-k}, \\ 1/\Gamma(z) &\sim e^{z} z^{-z+\frac{1}{2}} (2\pi)^{-\frac{1}{2}} \sum_{k=0}^{\infty} (-1)^k c_k z^{-k}, \end{aligned}$$

with $c_0 = 1$, $c_1 = 1/12$, $c_2 = 1/288, \ldots$. These are asymptotic expansions for $z \to \infty$, as $|\arg z| \le \pi - \varepsilon < \pi$. The connection between the coefficients in both series becomes clear in later subsections by considering appropriate integral representations of $\Gamma(z)$ and $1/\Gamma(z)$. Exact rational values for c_k, $k = 1,\ldots,20$, have been given by WRENCH (1968). He also gives these coefficients to 50 D. For k = 21,...,30, SPIRA (1971) gives exact rational values for c_k and also their 45 D equivalent.

2.1.1. THE RECIPROCAL GAMMA FUNCTION

In the first place we confine our attention to the reciprocal gamma function defined for all complex z by Hankel's integral

$$(2.1.3)\qquad 1/\Gamma(z) = \frac{1}{2\pi i}\int_{-\infty}^{(0^+)} e^t t^{-z}\,dt,$$

where the branch-cut of the many-valued function t^{-z} runs from 0 to $-\infty$; t^{-z} takes for $|\arg z| < \pi$ its principal value. The symbol $\int_{-\infty}^{(0^+)}$ denotes an integral taken over a loop coming from the point $-\infty$, encircling the origin counter-clockwise and returning to its starting point. Other versions of (2.3) are obtained by turning around the branch-cut and by introducing additional parameters. Then we have

$$(2.1.4)\qquad 1/\Gamma(z) = \frac{(\sigma e^{-i\pi})^{1-z}}{2\pi i}\int_{\infty e^{i\delta}}^{(0^+)} e^{-\sigma t} t^{-z}\,dt,$$

where

$$-\tfrac{1}{2}\pi - \delta < \arg \sigma < \tfrac{1}{2}\pi - \delta, \qquad \delta \le \arg t \le 2\pi + \delta,$$

and, again, z is an arbitrarily complex number.

Let temporarily z be positive. Then the integral in (2.3) can be written as

$$(2.1.5)\qquad 1/\Gamma(z) = \frac{e^z z^{1-z}}{2\pi i}\int_{-\infty}^{(0^+)} e^{z\phi(t)}\,dt,$$

where

$$(2.1.6)\qquad \phi(t) = t - 1 - \ln t.$$

We look for a suitable contour of integration for (2.1.5). Guided by the saddle point method we select a contour L such that

(2.1.7) $\quad \mathrm{Im}[z\phi(t)] = \text{constant} \quad \text{for} \quad t \in L.$

(Detailed information on this method can be obtained from the literature, see for instance DE BRUIJN (1968) or LAUWERIER (1974).) If L is chosen such that (2.1.7) is satisfied, we can take $\exp\{i\ \mathrm{Im}[z\phi(t)]\}$ before the integral and as a consequence the remaining part of the integrand has a constant sign. Hence, the integral is well suited for numerical quadrature. Generally, there is some freedom in choosing the constant in (2.1.7), but it is convenient to take the path through the saddle point t_0 of $\phi(t)$, given by the solution of $\phi'(t) = 0$. Hence, $t_0 = 1$. The contour is then called a saddle point contour and for large values of z a small neighbourhood of t_0 contributes significantly to the integral.

Since $\mathrm{Im}[z\phi(t_0)] = 0$ we solve (2.1.7) with constant = 0. By writing

$$t = \rho\, e^{i\theta}, \quad \rho > 0, \quad -\pi < \theta < \pi,$$

the solution is given by

$$\rho = \theta/\sin\theta, \qquad -\pi < \theta < \pi.$$

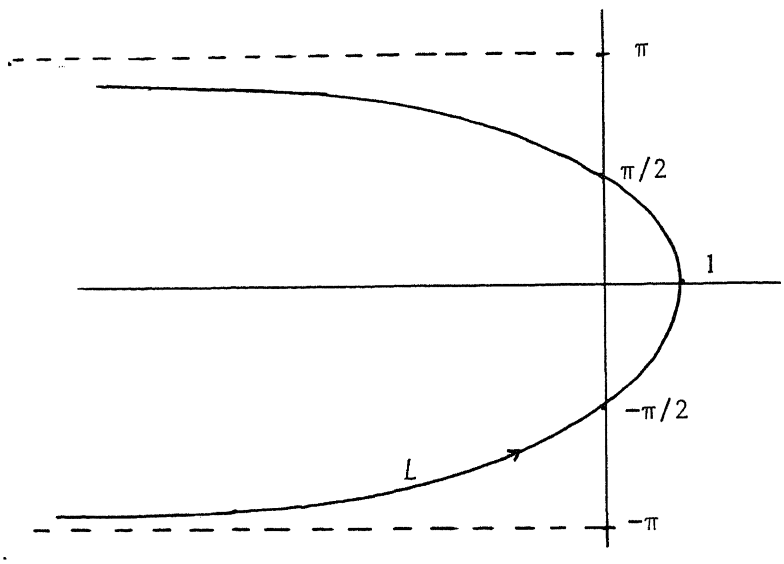

Fig. 2.1.1. Contour for (2.1.5)

By choosing θ as a variable of integration we obtain (since $dt/d\theta = d[e^{i\theta}\theta/\sin\theta]/d\theta = i$ + a real odd function of θ)

$$(2.1.8) \qquad 1/\Gamma(z) = \frac{z^{1-z}e^{z}}{2\pi}\int_{-\pi}^{\pi} e^{z\phi_1(\theta)}\,d\theta, \qquad z > 0.$$

where

$$(2.1.9) \qquad \phi_1(\theta) = \theta \operatorname{cotg}\theta - \ln(\theta/\sin\theta) - 1.$$

The function $\Phi\colon \mathbb{R} \to \mathbb{R}$ defined by

$$(2.1.10) \qquad \Phi(\theta) = \begin{cases} \exp[z\phi_1(\theta)], & |\theta| \le \pi \\ 0 & |\theta| \ge \pi \end{cases}$$

is a C^{∞}-function with compact support. In the notation of Definition 1.2 we can write $\Phi \in C_c^{\infty}([-\pi,\pi])$. The integral

$$(2.1.11) \qquad \int_{-\pi}^{\pi} \Phi(\theta)\,d\theta$$

corresponding to the integral in (2.1.8) can be computed with algorithms based on the trapezoidal rule described in Section 1.2 for the finite intervals. By interpreting $z^{1-z} = ze^{-z\ln z}$ as 0 at $z = 0$, (2.1.8) can be defined for $z \ge 0$. The integral in (2.1.8) is slowly varying for $z \to \infty$. In fact, the factor before the integral is almost equal to the dominant factor of the asymptotic expansion (see 2.1.2)).

In the following tables we give the results of numerical experiments. In order to show the rate of convergence of the iterative algorithm described in Subsection 1.3.3, we computed the integral for several positive z-values using the trapezoidal rule. The value of ε in the iterative algorithm is taken as 0.05. Function values of the integrand smaller than 0.0005 are neglected. Table I shows the computed values of $\Gamma(z)$ and the number of function values $\Phi(\theta)$ of (2.1.11) greater than 0.0005. The initial value of the discretization parameter h is $\pi/4$.

TABLE I

Trapezoidal rule for (2.1.8)

z	computed value of $\Gamma(z)$	n
1	1.00029	5
2	0.999999923	9
3	2.0000000047	8
4	6.0000000048	8
5	24.999999995	8
6	120.00000006	13
7	720.00039	10
8	5040.00041	10
9	40320.00050	10
10	362880.00068	10

In Table II we give the results in the successive steps of the iterative algorithm for the computation of $\Gamma(z)$. For $z = 1,5,10$ we give the values of $T_0(h)$, $T_{\frac{1}{2}h}(h)$ and $T_0^{(2)}(h)$, where $T_d(h)$ is introduced in Subsection 1.3.1 and $T_0^{(2)}(h)$ is the trapezoidal rule including the second derivative (i.e., $I_{2,n}(f)$ of (1.44)). The initial value of h is $\pi/4$ and h is halved in each following step. The process is finished when h is so small that

$$|T_0(h) - T_{\frac{1}{2}h}(h)| < 10^{-12}.$$

Also the number of function values larger than 10^{-16} is shown: n for $T_0(h)$, m for $T_0^{(2)}(h)$. We used a CDC-computer with machine accuracy 2^{-47}.

TABLE II

Trapezoidal rule for (2.1.8) (with second derivative)

	h/π	$T_0(h)$	$T_{\frac{1}{2}h}(h)$	$T_0^{(2)}(h)$	n	m
	1/4	1.00028744418149	0.99970189815628	1.0000148181276	7	7
	1/8	0.99999458426980	1.0000054580636	0.99999994027512	15	15
z=1	1/16	1.0000000211371	0.99999997892468	0.99999999990698	31	31
	1/32	1.0000000000310	0.99999999996900	1.0000000000000	62	62
	1/64	1.0000000000000	0.99999999999998	1.0000000000000	124	125
	1/4	23.961601888067	24.038521364259	24.000000014976	6	6
z=5	1/8	23.999999995010	24.000000004990	24.000000000000	13	13
	1/16	24.000000000000	24.000000000000	24.000000000000	26	27
	1/4	335722.81282098	394816.94265830	362880.64633633	5	5
z=10	1/8	362879.78455509	362880.21544520	362880.00000001	11	11
	1/16	362880.00000001	362880.00000001	362880.00000001	22	23

REMARK 2.1. From Table I it follows that the computed result is much more accurate than the prescribed value of ε (= 0.05). Also, the effect of neglecting the function values smaller than 0.0005 does not result in relative errors of the same size. From Table II we see the role of $T_0(h)$ and $T_{\frac{1}{2}h}(h)$: the exact value lies always between these two quantities. Furthermore it follows that $T_0^{(2)}(2h)$ roughly gives the same error as $T_0(h)$ or $T_{\frac{1}{2}h}(h)$.

REMARK 2.2. Representation (2.1.8) is also valid for complex values of z with Re $z > 0$, but in that case oscillations in the integrand will occur. By considering θ as a complex variable as well, the optimal path of integration in the θ-plane is given by

$$\mathrm{Im}[z\phi_1(\theta)] = 0.$$

This path is sketched in Figure 2.1.2. Since this equation cannot be solved explicitly with respect to θ it is rather difficult to make use of it.

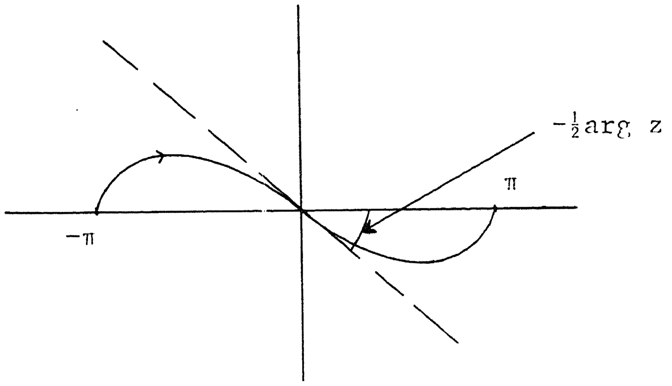

Fig. 2.1.2. Contour for (2.1.8) if z is complex

REMARK 2.3. (Confer Remark 1.12.) Asymptotic estimations based on representations of the remainder given in (1.40), as was done in Subsection 1.2.5, cannot explicitly be given for all possible values of z and h. For limiting values of $\mu = zh$ the same phenomena occur as in 1.2.5. For large μ there is a saddle point near $\theta = 0$, for small μ there are saddle points near $\theta = \pm\pi$.

Another integral representation based on the method of saddle points is obtained by introducing a new variable of integration, say u, in (2.1.5) (with contour of integration L) by way of the following definition

(2.1.12) $\quad -\frac{1}{2}u^2 = \phi(t).$

(It is possible to use (2.1.8) with $-\frac{1}{2}u^2 = \phi_1(\theta)$ but the transformation via (2.1.5) gives more information on the singularities of the mapping in (2.1.2)). The condition in (2.1.12) is that $t \in L$ corresponds with $u \in \mathbb{R}$, such that $\mathrm{sign}(u) = \mathrm{sign}[\mathrm{Im}(t)]$. From this condition imposed on the relation between u and t defined in (2.1.12) it follows that

(2.1.13) $\quad u = i(1-t)[2(t-1-\ln t)/(1-t)^2]^{\frac{1}{2}},$

where the square root is positive for positive values of its argument.

Substitution of (2.1.12) in (2.1.5) gives

(2.1.14) $$1/\Gamma(z) = \frac{z^{1-z}e^z}{2\pi i}\int_{-\infty}^{\infty} e^{-\frac{1}{2}zu^2}\, g(u)du,$$

with

(2.1.15) $$g(u) = \frac{dt}{du}\ .$$

Singularities of the integrand are due to the function g, which by using (2.1.12) and (2.1.6) can be written as

(2.1.16) $$g(u) = \frac{dt}{du} = \frac{ut}{1-t}\ .$$

It follows (for more details on this point see TEMME (1977^b)) that singular points occur in the u-plane at $2\sqrt{\pi}\, e^{\pm i\pi/4}$.

The asymptotic expansion of $1/\Gamma(z)$ given in (2.1.2) can be obtained by substituting the Taylor series for g(u) in (2.1.14) and termwise integration. The Taylor series can easily be obtained by using (2.1.16).

From the position of the singularities of g(u) in the u-plane, it follows that the integrand of (2.1.14) belongs to H_a (see Definition 1.1) with $a = \sqrt{2\pi}$. Hence, the integral can be computed by using the trapezoidal rule for the infinite interval. The integrand is as in (1.13) with $0 < \omega < \frac{1}{2}z$.

From (1.14) it follows that the rate of convergence is given by

$$e^{-2\pi a/h + \omega a^2}, \qquad a = \sqrt{2\pi}$$

and ω any positive number smaller than $\frac{1}{2}z$. It follows that for all $z > 0$ the trapezoidal rule effectively can be applied on (2.1.14).

The efficiency of the use of (2.1.14) is somewhat disturbed by the lack of an explicit expression of t as a function of u. Since the same function is also encountered in a following paper, where the incomplete gamma functions are discussed, we give some details for the computation.

The inversion problem can be solved by using the relation between t and θ given by

$$t = \frac{\theta}{\sin\theta} e^{i\theta}, \qquad t \in L, \quad -\pi < \theta < \pi,$$

from which follows that in fact the equation

$$\text{(2.1.17)} \qquad \tfrac{1}{2}u^2 = -\phi_1(\theta)$$

must be solved, with ϕ_1 given in (2.1.9), for real u and θ, sign(u) = sign(θ). (From this remark it is also obvious that (2.1.14) can be obtained by using (2.1.17) in (2.1.8). For small $|u|$, (2.1.17) is easily inverted. From expansion for the functions in $\phi_1(\theta)$ (see for instance ABRAMOWITZ & STEGUN (1964, p.75), we derive

$$\text{(2.1.18)} \qquad \phi_1(\theta) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}(2n+1)2^{2n-1}B_{2n}}{n(2n)!}\theta^{2n}$$

$$= \tfrac{1}{2}\theta^2 + \frac{1}{36}\theta^4 + \frac{1}{405}\theta^6 + \frac{1}{4200}\theta^8 + \frac{1}{42525}\theta^{10} + \ldots$$

(all coefficients are positive, B_{2n} is a Bernoulli number). Hence, on inversion we obtain

$$\text{(2.1.19)} \qquad \theta = u\left(1 - \frac{1}{36}u^2 + \frac{1}{4320}u^4 + \frac{139}{5443200}u^6 - \frac{571}{2351462400}u^8 + \ldots\right).$$

For large $|u|$, the inversion can be performed by using numerical techniques.

The function dt/du of (2.1.14) or (2.1.15) can also be computed by using the asymptotic expansion of $1/\Gamma(z)$ given in (2.1.2). If we expand dt/du in a Taylor series (which is, owing to the singularities in $u = 2\sqrt{\pi}\ e^{\pm i\pi/4}$, convergent for $|u| < 2\sqrt{\pi}$)

$$\frac{dt}{du} = a_0 + a_1 u + a_2 u^2 + \dots,$$

then we obtain by substitution in (2.1.14) and termwise integration the expansion for $1/\Gamma(z)$ of (2.1.2). Equating coefficients gives for the a_k with even k

$$a_{2k} = i(-1)^k\ c_k\ \Gamma(\tfrac{1}{2})/\Gamma(k+\tfrac{1}{2}), \qquad k = 0,1,\dots .$$

The coefficients with odd k are not obtained in this way, but they are not needed for the evaluation of dt/du since only its even part contributes to the integral in (2.1.14). The validity for this procedure for obtaining a_{2k} is verified by Theorem 1.21. Derivatives of the function dt/du can easily be obtained when a Taylor series is used, which is important for a quadrature rule including derivatives.

We reproduce the results of numerical experiments in Table III where we give for several values of z the successive values of $T_0(h)$ and $T_{\frac{1}{2}h}(h)$ for the computation of $\Gamma(z)$. The parameter h has initial value 1 and is halved in each following step. The process is finished when h is so small that

$$|T_0(h) - T_{\frac{1}{2}h}(h)| < 10^{-12}.$$

Also the number n of function values larger than 10^{-16} is shown. If we compare the results with Table II we note that for small values of z the infinite case is in favour with respect to the finite one.

By performing the transformation $u \to u/\sqrt{z}$ in (2.1.14) we obtain the integral

$$(2.1.20)\qquad 1/\Gamma(z) = \frac{z^{\frac{1}{2}-z}e^z}{2\pi i}\int_{-\infty}^{\infty} e^{-\frac{1}{2}u^2}\, g(u/\sqrt{z})du.$$

Computations based on this representation are given in Table IV. It follows that the number of function evaluations differs not much compared with those of Table III. However, the rate of convergence does not change with the z-values. The initial value of h is always 1.

TABLE III

Trapezoidal rule for (2.1.14)

	$T_0(h)$	$T_{\frac{1}{2}h}(h)$	n
z=1	0.97254347897700	1.0290513969982	8
	0.99999978786434	1.0000002121358	16
	1.00000000000000	1.0000000000000	32
z=5	13.229092791198	87.785157107740	3
	22.993151762846	25.099041617017	7
	23.999989704928	24.000010295083	15
	24.000000000001	24.000000000001	30
z=10	142628.08540651	11529351.211699	2
	281770.42598279	508354.53410949	5
	362573.72152775	363186.79635760	10
	362879.99999999	362880.00000004	21

An infinite interval for $1/\Gamma(z)$ can be obtained in several ways. We used the transformation (2.1.12) (or (2.1.17)) since it has connection with asymptotic methods. Choosing other transformations, for instance

$$\theta = \pi \tanh u, \qquad u \in \mathbb{R}$$

the representation (2.1.8) becomes

$$(2.1.21)\qquad 1/\Gamma(z) = \tfrac{1}{2}z^{1-z}e^z \int_{-\infty}^{\infty} e^{z\phi_1(\pi \tanh u)} \cosh^{-2} u\, du.$$

Via (2.1.9) we have an explicit representation of the integrand, whereas in (2.1.14) we need to invert (2.1.12). The singularities of the integrand of (2.1.21) are at the zeros of cosh u and at infinity. The results of numerical computations are given in Table V. Compared with the results of Table II we conclude that for z = 1 the above transformation is very effective. Comparing Table V with Table III we conclude that it is not advisable to use the rather complicated integrand (due to inversion) of representation (2.1.14). The simple transformation leading to (2.1.21) seems to be rather worthwhile; this conclusion can also be found in TAKAHASI & MORI (1973), STENGER (1973) and HABER (1977).

TABLE IV

Trapezoidal rule for (2.1.20)

	$T_0(h)$	$T_{\frac{1}{2}h}(h)$	n
	0.97254347897700	1.0290513969982	8
z=1	0.99999978786434	1.0000002121358	16
	1.00000000000000	1.0000000000000	32
	23.603075367063	24.410502412539	8
z=5	23.999999784886	24.000000215115	16
	24.000000000001	24.000000000001	33
	357311.91970676	368624.35956460	8
z=10	362879.99739841	362880.00260161	17
	362880.00000001	362880.00000002	34

TABLE V

Trapezoidal rule for (2.1.21)

	$T_0(h)$	$T_{\frac{1}{2}h}(h)$	
	0.98953124698326	1.0106921778034	7
z=1	0.99999977864943	1.0000002213507	14
	1.00000000000000	1.0000000000000	29
	21.731290970155	26.796140759783	6
z=5	23.999404500479	24.000595529075	13
	24.000000000000	24.000000000001	26
	306674.38913557	444130.53887048	6
z=10	362819.83941229	362940.18054196	12
	362880.00000001	362880.00000001	24

REMARK 2.4. Representation (2.1.14) can also be used for complex z with Re z > 0. In order to avoid oscillations due to the dominant exponential function it is convenient to make this function independent of arg z by transforming $u \exp(\frac{1}{2}i \arg z) \to u$ or $z^{\frac{1}{2}}u \to u$. The singularities of dt/du (in the new variable u) approach the real u-axis if $\arg z \to \pm \frac{1}{2}\pi$. Hence, the strip of analyticity of the integrand becomes narrower according as $\arg z \to \pm\frac{1}{2}\pi$, which disturbs the rate of convergence of the trapezoidal rule. For large |z| the singularities have little influence, as follows from remarks in Subsection 1.1.6. Anyhow, it is possible to compute Γ(z) for $|\arg z| < \pi/2$ in a stable way. As noticed in Remark 2.2, complex values of z are more difficult to handle in the finite case.

2.1.2. THE GAMMA FUNCTION

A representation for Γ(z) follows from (2.1.1) by writing

$$\Gamma(z) = e^{-z}z^{z} \int_0^\infty e^{-z\phi(t)}\, t^{-1} dt \tag{2.1.22}$$

where φ is given in (2.1.6). By substituting

$$\tfrac{1}{2}v^2 = \phi(t), \tag{2.1.23}$$

or

$$v = (t-1)[2(t-1-\ln t)/(t-1)^2]^{\frac{1}{2}}, \qquad t > 0 \tag{2.1.24}$$

where the square root is positive for real t, we obtain

$$\Gamma(z) = e^{-z}z^{z} \int_{-\infty}^{\infty} e^{-\frac{1}{2}zv^2}\, \frac{1}{t}\frac{dt}{dv}\, dv, \tag{2.1.25}$$

with

$$\frac{dt}{dv} = \frac{vt}{t-1}, \qquad t > 0. \tag{2.1.26}$$

Notice the strong resemblance with the representation for 1/Γ(z).

It is interesting to compare the numerical results for Γ(z) and 1/Γ(z). Applying the trapezoidal rule on (2.1.25) we obtain Table VI. The initial value of h is 1; the function values larger than 10^{-16} are counted (value of n). Remark that this number is roughly doubted compared with the results of Table III. Again, the evaluation of the integrand of (2.1.25) requires the inversion of transformation (2.1.24).

TABLE VI

Trapezoidal rule for (2.1.25)

	$T_0(h)$	$T_{\frac{1}{2}h}(h)$	n
z=1	0.99999986782879	1.0000001321712	33
	1.0000000000000	0.99999999999998	67
z=5	2.4806867975251	2.3193139243437	14
	2.4000003609344	2.3999996390656	30
	2.4000000000000	2.4000000000000	61
z=10	4.6063316290432	2.6559782040619	10
	3.6311549165525	3.6264450834481	21
	3.6288000000003	3.6288000000002	43

REMARK 2.5. The asymptotic expansion for $\Gamma(z)$ is obtained by substituting the Taylor series for dt/dv (in powers of v) in (2.1.25) and termwise integration. The similarity between (2.1.14) and (2.1.15) and (2.1.25) (with (2.1.26)) shows up in the connection between the coefficients in both asymptotic expansions given in (2.1.2)

To conclude this subsection we perform a different transformation in (2.1.22). Let us take

$$t = e^{v-e^{-v}}, \qquad v \in \mathbb{R}.$$

Then (2.1.22) becomes

$$\Gamma(z) = e^{-z}z^z \int_{-\infty}^{\infty} \exp[-z(e^{v-e^{-v}}-1-v+e^{-v})](1+e^{-v})dv. \tag{2.1.27}$$

With this transformation the behaviour of the integrand is rather symmetric

:h respect to large positive and negative values of v. The integrand
ıaves as

$$e^{-ze^{|v|}}, \qquad v \to \pm \infty.$$

reover the integrand is analytic for all $v \in \mathbb{C}$. Using the terminology of
Finition 1.1 we can say that the integrand belongs to H_a for $0 < a < \frac{1}{2}\pi$.
ıce, we expect that (2.1.27) is a good representation for the evaluation
$\Gamma(z)$ by using the trapezoidal rule, especially when z is bounded away
›m zero. In Table VII we give some numerical results. We take as finite
:erval of integration the v-interval $[-v_0, v_0]$, with v_0 a number (depend-
ʒ on z) such that the integrals over $(-\infty, -v_0]$, and (v_0, ∞) can be neglected.
≥ initial value of h is $v_0/8$. Again, n is the number of function values
rger than 10^{-16}, the computations are terminated as soons as
$_0(h) - T_{\frac{1}{2}h}(h)| < 10^{-12}$.

TABLE VII

Trapezoidal rule for (2.1.27)

	$T_0(h)$	$T_{\frac{1}{2}h}(h)$	n
	1.0000176584359	0.99998234152482	21
z=1	0.99999999998037	1.00000000000197	42
	1.0000000000000	1.00000000000000	85
	24.010704014105	23.989295980470	17
z=5	23.999999997288	24.000000002713	35
	24.000000000000	24.000000000000	70
	358324.34492922	367435.65957836	15
z=10	362880.00225379	362879.99774623	30
	362880.00000001	362880.00000001	61

2.2 THE MODIFIED BESSEL FUNCTIONS

The modified Bessel functions are the functions $I_\nu(x)$ (the function of the first kind) and $K_\nu(x)$ (the function of the third kind); x is called the argument, ν is called the order. We consider real values of x and ν, $x > 0$ and $\nu \geq 0$. For relevant properties we refer to ABRAMOWITZ & STEGUN (1964, Chapter 9).

Much attention is paid in the literature to the computation of a sequence of functions of the first kind

$$I_\nu(x),\ldots,I_{\nu+n}(x)$$

for some $n \geq 0$ and $0 \leq \nu < 1$. See GAUTSCHI (1967), (1975) and AMOS, DANIEL & WESTON (1977). However, for computation of a single function value for large x and/or ν this method is not efficient.

$K_\nu(x)$ can be computed for general ν by using the recurrence relation. For this function it is sufficient to have an algorithm for $0 \leq \nu < 2$ since recursion is numerically stable for increasing order. In TEMME (1975[a]) an algorithm with an ALGOL 60 program is given. In LUKE (1969) and (1975[a]) more information can be found for the computation of this function.

In this section we give results which enable computation for a large domain of the parameters x and ν. The method of computation is not disturbed if one or both parameters are large.

The results of this section can be applied for the case of complex parameters. If ν is real, the domain of x may be chosen as Re $x > 0$. The rate of convergence of the algorithms, however, will slow down for complex variables.

As mentioned in previous sections, the integral representations we use for the trapezoidal rule, are connected with asymptotic expansions. For the modified Bessel functions the following expansions are developed in OLVER (1974, p.377)

$$(2.2.1)\qquad \begin{aligned} I_\nu(x) &\sim (t/2\pi\nu)^{\frac{1}{2}}\, e^{\nu\eta} \sum_{k=0}^{\infty} u_k\, \nu^{-k} \\ K_\nu(x) &\sim (\pi t/2\nu)^{\frac{1}{2}}\, e^{-\nu\eta} \sum_{k=0}^{\infty} (-1)^k u_k\, \nu^{-k} \end{aligned}$$

where

(2.2.2) $t = (1+z^2)^{-\frac{1}{2}},\quad z = x/\nu,\quad \eta = t^{-1} + \ln \frac{tz}{t+1}$.

The graph of the function η, as a function of z, is drawn in Figure 2.2.1. The zero of η is at $z_0 \simeq 0.6627$.

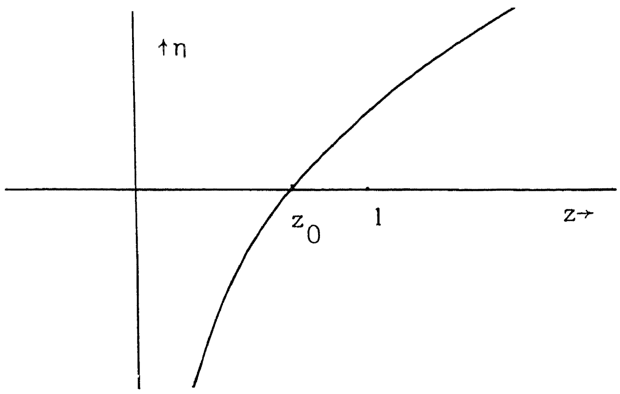

Fig. 2.2.1. The function $\eta(z)$

For fixed x, we have

(2.2.3) $\nu\eta \to x \quad \text{for} \quad \nu \to 0,$

and the well-known aymptotic expansions for large x (cf. formulas 9.7.1 and 9.7.2 in ABRAMOWITZ & STEGUN (1964, p.377)) are special cases of (2.2.1). The expansions in (2.2.1) are valid for $\nu \to \infty$, $x \geq 0$ (uniformly with respect to x) or $x \to \infty$, $\nu \geq 0$ (uniformly with respect to ν) and also for complex variables. For details the reader is referred to OLVER (1974).

The coefficients u_k in (2.2.1) are polynomials in t given in (2.2.2). They satisfy the recurrence relation

(2.2.4) $$u_{k+1}(t) = \tfrac{1}{2}t^2(1-t^2)u_k'(t) + \frac{1}{8}\int_0^t (1-5\tau^2)u_k(\tau)d\tau,$$

for $k = 0,1,\ldots$, with $u_0 = 1$. Hence, by writing

$$u_k(t) = t^k \sum_{i=0}^{k} p_i^{(k)} t^{2i}$$

an algorithm for the coefficients $p_i^{(k)}$ is easily constructed. Some of the u_k are listed in ABRAMOWITZ & STEGUN (1964, p.378). LUKE (1975[b]) gives a rearrangement of the series in (2.2.1) of the form

$$\sum_{k=0}^{\infty} c_k t^k, \quad \sum_{k=0}^{\infty} (-1)^k c_k t^k$$

respectively, with t given in (2.2.2). The c_k satisfy the difference equation

$$8\nu k c_k = -(2k-1)^2 c_{k-1} + (2k-5)(2k-1)c_{k-3}, \tag{2.2.5}$$

$c_0 = 1$, $c_k = 0$ for $k < 0$. Luke gives the c_k for $k = 1,\ldots,7$. From a numerical point of view, (2.2.5) is much simpler than (2.2.4).

2.2.1 THE MODIFIED BESSEL FUNCTION OF THE FIRST KIND

If we consider the well-known representation of the function of the first kind of integral order

$$I_n(x) = \frac{1}{\pi} \int_0^{\pi} e^{x \cos\theta} \cos n\theta \, d\theta, \tag{2.2.6}$$

we can apply the trapezoidal rule. The integrand is periodic and analytic in θ. According to Subsection 1.2.4, and as follows from KRESS (1971) the convergence is very fast. Also, an integral for the remainder can be considered, but details will not be given here. We discuss a different representation for $I_\nu(x)$. The drawback of (2.2.6) is its limitation to integer n, and, moreover, if we consider large n, a loss of accuracy owing to oscillations of the integrand. To avoid this, we use an integral which generalizes (2.2.6) to general order.

Let us consider Schläfli's integral

$$I_\nu(x) = \frac{1}{2\pi i} \int_L e^{x \cosh t - \nu t} \, dt \tag{2.2.7}$$

where the integration is taken along a contour as drawn in Figure 2.2.2.

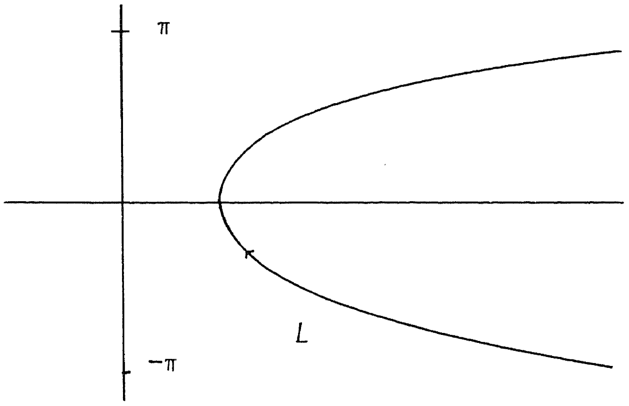

Fig. 2.2.2. Contour for (2.2.7)

The integral in (2.2.7) is an analytic function for all complex values of ν and Re $x > 0$; however, here we consider real parameters. If we take the contour to consist of three sides of a rectangle, with vertices at $\infty - \pi i$, $-\pi i$, πi and $\infty + \pi i$, (2.2.7) is easily reduced to (2.2.6) in the case of integer order.

We choose a contour so that the integrand of (2.2.7) is real and of constant sign. Saddle points of the integrand are zeros of $\phi'(t)$ where

(2.2.8) $$\phi(t) = x \cosh t - \nu t.$$

Saddle points occur at

(2.2.9) $$t_k = (-1)^k \operatorname{arc\,sinh} (\nu/x) + k\pi i, \qquad k \in \mathbb{Z},$$

but if $x > 0$ and $\nu \geq 0$ only t_0 has to be considered. The ideal contour of integration follows from Im $\phi(t)$ = Im $\phi(t_0) = 0$, which gives, by writing

(2.2.10) $$t = \sigma + i\tau, \qquad \sigma,\tau \in \mathbb{R},$$

the following relation between τ and σ

(2.2.11) $$\sinh \sigma = \frac{\nu}{x} \frac{\tau}{\sin \tau} \qquad -\pi < \tau < \pi.$$

Remark that for $\nu = 0$ the contour of integration is the interval $[-i\pi, i\pi]$, giving (2.2.6) with $n = 0$. For $\nu > 0$, the contour in Figure 2.2.2 will be taken as governed by (2.2.11). On L, $\phi(t)$ is real and $\phi(t) - \phi(t_0)$ is negative. Remark that $\phi(t_0) = \nu\eta$ (see 2.2.2). Next, we integrate with respect to τ, giving

(2.2.12) $$I_\nu(x) = \frac{e^{\nu\eta}}{2\pi} \int_{-\pi}^{\pi} e^{f(\tau)}\, d\tau$$

with

(2.2.13) $$f(\tau) = x \cosh \sigma \cos \tau - \nu\sigma - \nu\eta,$$

the relation between σ and τ being given in (2.2.11). If $\nu > 0$, the integrand can be considered as belonging to $C_c^\infty([-\pi,\pi])$. As mentioned earlier, the case $\nu = 0$ is an exception; if $\nu = 0$ (2.2.12) reduces to (2.2.6) with $n = 0$. Next we suppose $\nu > 0$.

The integrand of (2.2.12) is singular for complex τ-values at the points where

(2.2.14) $$\cosh \sigma = [1 + (\frac{\nu\tau}{x \sin \tau})^2]^{\frac{1}{2}} = 0,$$

i.e., where

(2.2.15) $$\frac{\sin \tau}{\tau} = \pm\, i\nu/x.$$

This equation has solutions in the strips $\frac{1}{2}\pi \le |\mathrm{Re}\ \tau| \le \pi$. For small ν/x an approximation is

$$\tau = \pm\, \pi \pm i\pi\nu/x,$$

which are near the endpoints of integration, where singularities have little influence. For large ν/x the singularities are far off the interval $[-\pi,\pi]$. Their imaginary parts tend to $\pm\,\infty$ if $\nu/x \to \infty$.

The behaviour of f near the endpoints of integration is given by

$$f(\tau) \sim -r - \nu \ln r, \qquad r = \frac{\pi\nu}{\pi - |\tau|}.$$

From Remark 1.12 we expect (if $\nu \neq 0$) for the trapezoidal rule convergence of order

(2.2.16) $$R_h(f) = O(\lambda^{-\frac{1}{2}(\nu+3/2)} e^{-\sqrt{2\pi\nu\lambda}}), \qquad \lambda \to \infty,$$

$\lambda = 2\pi/h = n$ (the number of function evaluations). We notice that large values of ν may speed up the rate of convergence.

Numerical computation of $I_\nu(x)$ for large values of ν or x may cause underflow or overflow. For $x \to \infty$ and ν fixed the function behaves as

$$(2.2.17) \qquad I_\nu(x) = (2\pi x)^{-\frac{1}{2}} e^x[1 + O(1/x)]$$

and for $\nu \to \infty$, x fixed, we have

$$(2.2.18) \qquad I_\nu(x) = (\tfrac{1}{2}x)^\nu/\Gamma(\nu+1)[1 + O(1/\nu)].$$

These aymptotic formulas can be obtained from (2.2.1) by some limiting processes. In physical problems often combinations of Bessel functions arise, or Bessel function in combination with exponential functions. If these combinations must be computed for large (or small) values of the parameters the individual members in the combination may be so large or small that overflow or underflow may occur. Therefore, it is of practical interest to have a suitable normalization of $I_\nu(x)$. Formulas (2.2.17) and (2.2.18) suggest a normalization but owing to the non-uniformity with respect to x or ν it is better to choose a normalization containing both forms. This is achieved when using the variable η defined in (2.2.2) and appearing in the uniform expansion (2.2.1). The function $e^{-\nu\eta} I_\nu(x)$ behaves quietly for $\nu \geq 0$, $x \geq 0$. In (2.2.12) the factor $e^{\nu\eta}$ appears explicitly in the representation. Since in (2.2.12) $f(0) = 0$, a suitable normalization for the integrand is obtained, which is important for applying the trapezoidal rule as mentioned in Remarks 1.20, (vi). Since small τ-values contribute significantly to the integral in (2.2.12), it is necessary to compute $f(\tau)$ for small τ with satisfactorily small relative accuracy. In a straightforward computation of $f(\tau)$ cancellation of significant digits may occur. Writing f as, for instance,

$$f(\tau) = x \cosh \sigma(\cos \tau - 1) + 2x \sinh \tfrac{1}{2}(\sigma + t_0) \sinh \tfrac{1}{2}(\sigma - t_0) + \nu(t_0 - \sigma)$$

it turns out that the cancellation of digits can be controlled by computing $t_0 - \sigma$ within the required accuracy. We can write it as follows

$$(2.2.19)\qquad t_0 - \sigma = \text{arc sinh}(\nu/x) - \text{arc sinh}\,\frac{\nu}{x}\frac{\tau}{\sin\tau} =$$

$$= \text{arc sinh}\left[\frac{\nu}{x}\,\frac{1-\tau^2/\sin^2\tau}{\frac{\tau}{\sin\tau}\sqrt{1+\nu^2/x^2}+\sqrt{1+\left(\frac{\nu}{x}\frac{\tau}{\sin\tau}\right)^2}}\right].$$

Hence the problem is reduced to the computation of $1 - \tau/\sin\tau$ within the required accuracy, but this is a trivial matter.

The integral in (2.2.12) may be used for obtaining the uniform asymptotic expansion of $I_\nu(x)$ given in (2.2.1). If we substitute

$$(2.2.20)\qquad f(\tau) = u^2, \qquad u \in \mathbb{R}, \qquad \text{sign}(u) = \text{sign}(\tau),$$

we obtain

$$(2.2.21)\qquad I_\nu(x) = \frac{e^{\nu\eta}}{2\pi i}\int_{-\infty}^{\infty} e^{-u^2}\,\frac{d\tau}{du}\,du,$$

where $d\tau/du$ follows from the relation in (2.2.20). Expanding $d\tau/du$ in powers of u and termwise integration gives eventually the first of (2.2.1).

The integral in (2.2.21) is of the type discussed in Chapter I in the connection with trapezoidal rules for the infinite interval. The usefulness of (2.2.21) is limited owing to the inversion of the mapping in (2.2.20). It is not possible to give an explicit relation for τ as function of u; the inversion has to be carried out numerically. However, we can use a Taylor series for $d\tau/du$; the coefficients of this series can be expressed in terms of the coefficients of the asymptotic expansion of $I_\nu(x)$ given in (2.2.1). In order to obtain more insight in this method we need to know where the singularities of $d\tau/du$ in (2.2.21) are located in the u-plane. For this purpose we do not use transformation (2.2.20) but instead we start from (2.2.7) where L follows the saddle point contour described by (2.2.10) and (2.2.11). Let us define a mapping of the t-plane into the u-plane by the equation

$$(2.2.22)\qquad -u^2 = \phi(t) - \phi(t_0)$$

with the condition that $t \in L$ corresponds with $u \in \mathbb{R}$ and $\text{sign}(\tau) = \text{sign}(u)$.

The result is (we know that $\phi(t_0) = \nu\eta$)

(2.2.23) $$I_\nu(x) = e^{\nu\eta} \int_{-\infty}^{\infty} e^{-u^2} g(u)du$$

with

(2.2.24) $$g(u) = \frac{1}{2\pi i} \frac{dt}{du}$$

and the relation between t and u given in (2.2.22). An explicit formula for g as a function of u cannot be given since (2.2.22) cannot be inverted explicitly, except if $\nu = 0$. Of course numerical techniques can be used for this inversion problem followed by the evaluation of

(2.2.25) $$g(u) = \frac{1}{2\pi i} \frac{dt}{d} = \frac{1}{\pi} \frac{u}{x \sinh t - \nu} .$$

REMARK 2.6. For a numerical algorithm, the inversion of (2.2.22), i.e., the computation of t(u), may be facilitated by using (2.2.20) with (2.2.11) and (2.2.13). The equation (2.2.22) can be written as

$$-u^2 = x \cosh \sigma \cos \tau - \nu\sigma - \nu\eta$$

and σ can be eliminated by using (2.2.11). Then real variables appear in the inversion process. If $\tau(u)$ is computed, t(u) follows from $t(u) = \sigma(u)+i\tau(u)$.

Expanding g of (2.2.23) in a Taylor series, we write

(2.2.26) $$g(u) = a_0 + a_1 u + a_2 u^2 + \ldots$$

and substituting this in (2.2.23) we obtain an expansion that may be identified with the first of (2.2.1). Theorem 1.21 gives the validity of this procedure. Equating coefficients gives the relation

(2.2.27) $$a_{2k} = (2\pi\nu)^{-\frac{1}{2}}(1+z^2)^{-\frac{1}{4}} u_k \, \nu^{-k}/\Gamma(k+\tfrac{1}{2}), \qquad k = 0,1,\ldots, \qquad z = x/\nu.$$

The coefficients with odd index are not obtained in this way. However, for the integration of (2.2.23) only the even part of g is relevant.

REMARK 2.7. Application of the above mentioned theorem is not straightforward, since the exponential function in (2.2.23) does not depend on a large parameter. Considering ν as a large parameter and performing the transformation $u \to \nu^{\frac{1}{2}}u$ and the substitution $z = \nu^{-1}x$ the new function g does not depend explicitly on ν, as is easily verified. After these preparations the theorem can be applied.

For the evaluation of the even part of g by using (2.2.26) it is important to know the domain of convergence of the Taylor series. This domain is characterized by the singularities of g nearest to the origin. The singularities of g also influence the rate of convergence of the trapezoidal rule. Hence it is worthwhile to pay attention to these points.

The singularities of g are given by the zeros of the dominator in the right-hand side of (2.2.25), except for t_0 since $u(t_0) = 0$. The remaining zeros are given in (2.2.9) for $k \neq 0$, and the corresponding u-values follow from (2.2.22), giving

$$(2.2.28) \qquad u^2(t_k) = [(-1)^{k+1}+1]\nu\eta + \nu k\pi i, \qquad k = \pm 1, \pm 2, \ldots .$$

Not all of the k-values need to be considered, however. In fact, the function t(u), defined implicitly in (2.2.22), is not single-valued. Of course we confine us to the principal branch, which maps the real u-axis on the contour L. This branch of t(u) has singular points at $u(t_k)$ for $k = +1$ and $k = -1$, while the remaining k-values give singularities for other branches of t(u). This follows from a further analysis of the mapping defined in (2.2.22). Details will not be given here, but the above assertions can be made plausible by observing that for $\nu = 0$ ϕ of (2.2.28) is a periodic function in the τ-direction. For small ν the right-hand side of (2.2.28) is

$$2x + O(\nu) \qquad \text{for} \qquad k = \pm 1, \pm 3, \ldots,$$

$$O(\nu) \qquad \text{for} \qquad k = \pm 2 \ \ \pm 4, \ldots .$$

Since small ν-values do not disturb the qualitative aspects of the mapping at $u = 0$, the condensation of singular points in the neighborhood of $u = 0$ is not possible. For the same reason the k-values $\pm 3, \pm 5$ may excluded.

It follows that the radius of convergence of the Taylor series of g is given by

$$R = (\nu^2\pi^2 + 4\eta^2\nu^2)^{\frac{1}{4}}$$

which reduces to $R = \sqrt{2x}$ if $\nu = 0$ (see (2.2.3)).

The distance from the singularities to the real u-axis is given by

$$a = \begin{cases} R \sin[\frac{1}{2} \arctan (\pi/2\eta)] & \text{als} \quad \eta \geq 0 \\ R \cos[\frac{1}{2} \arctan (\pi/2\eta)] & \text{als} \quad \eta < 0 \end{cases}$$

which defines the strip of analyticity of g, and hence the rate of convergence of the trapezoidal rule. The width of this strip indeed tends to 0 if $\eta \to 0$. As mentioned earlier, for $\nu = 0$ the interval of integration is $[-\sqrt{2x}, \sqrt{2x}]$ and for $\nu = 0$ the singularities are located at the endpoints of this interval. In Figure 2.2.3 the location of the singularities of g is sketched for fixed x and variable $\nu \geq 0$.

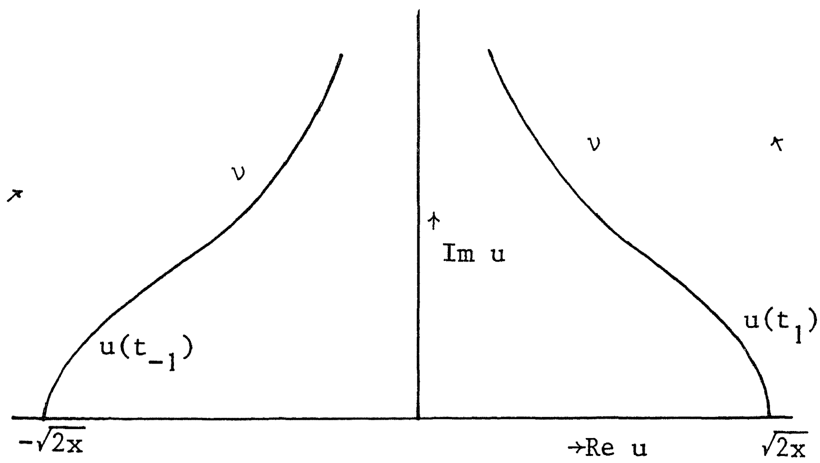

Fig. 2.2.3. Location of singularities of the integrand of (2.2.23)

It follows that for small ν-values the discretization error in the trapezoidal rule is not small enough for an efficient use of this rule. However, if x is large and ν is small the real parts of $u(t_{\pm 1})$ are of order $O(\sqrt{2x})$ for $x \to \infty$. In that case the singularities have no influence, as mentioned earlier in Subsection 1.1.6.3. If $\nu = 0$, (2.2.12) reduces to (2.2.6) with $n = 0$, and transformation (2.2.22) is not appropriate.

2.2.2 THE MODIFIED BESSEL FUNCTION OF THE THIRD KIND

In connection with the trapezoidal rule, the function $K_\nu(z)$ is discussed by several authors. We mention HUNTER (1964) for $\nu = 0,1$ and complex z, $|\arg z| < \frac{1}{2}\pi$, MECHEL (1966) for $\nu = 0,1$ and $|\arg z| \leq \pi$ and LUKE (1969, II, p.221) for repeated integrals of $K_\nu(x)$ with $|\arg z| < \frac{1}{2}\pi$.

In this subsection we give integral representations resulting from asymptotic analysis. We start with an integral for the infinite interval which resembles (2.2.7). Also, a finite interval will be considered.

In (2.2.1) the asymptotic expansions of $I_\nu(x)$ and $K_\nu(x)$ are given. There is a strong resemblance between both expansions. The same phenomenon occurs in the expansions of $\Gamma(z)$ and $1/\Gamma(z)$, as noticed in Remark 2.5. The integrals for $\Gamma(z)$ and $1/\Gamma(z)$ in (2.1.14) and (2.1.25) respectively are also very similar. The integrals for the Bessel functions used in this chapter are in the same way related to each other.

We use the well-known representation

$$(2.2.29) \qquad K_\nu(x) = \frac{1}{2}\int_{-\infty}^{\infty} e^{-x\cosh t + \nu t}\, dt$$

with real x and ν, $x > 0$. (The integral defines an analytic function for all complex ν and Re $x > 0$).

LUKE (1969) uses a generalization of (2.2.29) for the repeated integrals of $K_\nu(x)$. He claims that the discretization error increases if x increases. That is correct, but for large x the method is still applicable, since then a small part of the interval of integration contributes to the integration. As outlined in Chapter 1, a small discretization error does not necessarily result in a large number of relevant function evaluations.

The maximum of the integrand of (2.2.29) occurs at the zero of the derivative of ϕ given in (2.2.8). A real zero is

$$(2.2.30) \qquad t_0 = \text{arc sinh}(\nu/x).$$

This maximum corresponds to a saddle point of ϕ if complex values of t are considered. Since

(2.2.31) $\phi(t_0) = x \cosh t_0 - \nu t_0 = \nu\eta,$

with η defined in (2.2.2), the integral (2.2.29) can be written as

(2.2.32) $$K_\nu(x) = \tfrac{1}{2}e^{-\nu\eta} \int_{-\infty}^{\infty} e^{-[\phi(t)-\phi(t_0)]}\, dt.$$

The exponential term before the integral is the dominant term in the asymptotic expansion of $K_\nu(x)$, cf. (2.2.21). In the terminology of Definition 1.1 we can say that the integrand belongs to H_a with $0 < a < \frac{1}{2}\pi$. If x is bounded away from zero the integrand decreases very fast according as $|t|$ increases. From these aspects it follows that (2.2.25) is a suitable starting point for the trapezoidal rule.

When we apply the trapezoidal rule to (2.2.25) it is possible to give more information concerning the discretization error. According to the results given in Subsection 1.1.2 we have

$$K_\nu(x) = \tfrac{1}{2}e^{-\nu\eta} h \sum_{n=-\infty}^{\infty} e^{-[\phi(nh)-\phi(t_0)]} + R_0(h),$$

with

$$R_0(h) = -\sum_{\substack{m=-\infty \\ m\neq 0}}^{\infty} K_{\nu+2\pi im/h}(x).$$

Approximating this series by its terms with $m = \pm 1$ and using known asymptotic expansions for Bessel functions with large orders, it is possible to estimate $R_0(h)$ for $h \to 0$. For instance, if $|\nu \pm 2\pi i/h|$ is much larger than x we have

$$R_0(h) \sim -2 \operatorname{Re} K_{\nu+2\pi i/h}(x) \sim -2 \operatorname{Re}[(\tfrac{1}{2}x)^{-\nu-2\pi i/h}\, \Gamma(\nu+2\pi i/h)]$$

$$\sim -2\sqrt{2\pi}\, (\tfrac{1}{2}x)^{-\nu} e^{-\nu} \operatorname{Re}[e^{-2\pi i/h}\, (\nu+2\pi i/h)^{\nu+2\pi i/h-\frac{1}{2}}]$$

for $h \to 0$ and/or $\nu \to \infty$. Hence

$$|R_0(h)| \sim 2\sqrt{2\pi}\, (\tfrac{1}{2}xe)^{-\nu} (\nu^2+4\pi^2/h^2)^{(\nu-\frac{1}{2})/2} e^{-2\pi/h \arg(\nu+2\pi i/h)}.$$

If $h\nu$ is small if h is small, we have

$$|R_0(h)| \sim 2\sqrt{2\pi}\ (\tfrac{1}{2}xe)^{-\nu}(\tfrac{2\pi}{h})^{\nu-\frac{1}{2}}\ e^{-\pi^2/h}.$$

It follows that for moderate x and ν the discretization error can be estimated by using $\exp(-\pi^2/h)$. In order to obtain an absolute accuracy of, say, 10^{-12} we should take h = 0.36. Hence, we expect that for x=ν=1 about 25 function evaluations are needed for the computation of the integral in (2.2.22) by using the trapezoidal rule (within absolute precision of 10^{-12}).

For large values of x and ν the estimation of $|R_0(h)|$ can be based on other, more complicated, asymptotic expansions of $K_{\nu+2\pi i/h}(x)$.

Next we discuss the analogue of (2.2.23). If we substitute (cf. (2.2.22))

(2.2.33) $\quad \phi(t) - \phi(t_0) = u^2,\ \mathrm{sign}(u) = \mathrm{sign}(t-t_0),$

(2.2.32) becomes

(2.2.34) $\quad K_\nu(x) = e^{-\nu\eta} \int_{-\infty}^{\infty} e^{-u^2} k(u)du$

with

$$k(u) = \tfrac{1}{2}\frac{dt}{du}.$$

Writing

(2.2.35) $\quad k(u) = b_0 + b_1u + b_2u^2 + \ldots$

and comparing this with the expansion (2.2.26), we obtain

$$b_{2k} = (-1)^k \pi a_{2k}, \qquad k = 0,1,2,\ldots,$$

with a_{2k} given in (2.2.27). The validity of this follows from Theorem 1.21 and Remark 2.7.

Consequently if the u_k of (2.2.1) are available, the even part of k(u) can be computed by the even part of the right-hand side of (2.2.35) (if |u| is small enough). The domain of convergence of (2.2.35) follows from that of the function g discussed in the previous subsection. The singularities of k are located along the curves as drawn in Figure 2.2.3 after having rotated them clockwise with an angle of $\frac{1}{2}\pi$. For large ν the singularities of k approach the interval of integration of the integral in (2.2.34), with real parts of the singularities of order $O(\nu \ln \nu)^{\frac{1}{2}}$. Consequently, their influence is not important in that case.

We conclude this subsection with another integral representation for $K_\nu(x)$. It enables us to give an integral as (2.2.12), which resulted in a natural way from a saddle point contour in the complex plane. The starting point is

$$(2.2.36) \qquad K_\nu(x) = \frac{\pi^{\frac{1}{2}}(2/x)^\nu \Gamma(\nu+\frac{1}{2})}{2\pi i} \int_L e^{xs} \frac{ds}{(1-s^2)^{\nu+\frac{1}{2}}}$$

where L is sketched in Figure 2.2.4. The many-valued function $(1-s^2)^{-\nu-\frac{1}{2}}$ has branch-cuts from -1 to $-\infty$ and from 1 to $+\infty$ and it is real for $-1 < s < 1$.

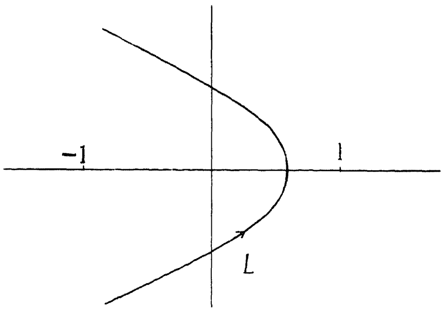

Fig. 2.2.4. Contour for (2.2.36)

The relation (2.2.36) follows from other well-known integrals for $K_\nu(x)$. It can also be derived from results for confluent hypergeometric functions in TEMME (1975^b) and the relation

$$(2.2.37) \qquad K_\nu(x) = \pi^{\frac{1}{2}} e^{-x}(2x)^\nu \, U(\nu+\tfrac{1}{2},\ 2\nu+1,\ 2x).$$

A suitable contour of integration follows from a saddle point analysis. For convenience we write

$$(2.2.38) \qquad \lambda = \nu+\tfrac{1}{2}.$$

The integrand of (2.2.36) has a saddle point at $s_0 \in (-1,1)$ given by

$$(2.2.39) \qquad s_0 = [\lambda-(\lambda^2+x^2)^{\frac{1}{2}}]/x.$$

The steepest descent path through s_0 is given by

$$\mathrm{Im}[xs - \lambda \ln(1-s^2)] = 0,$$

which yields writing $s = \frac{\lambda}{x}(\sigma + i\tau)$,

(2.2.40) $$\sigma = \tau \operatorname{cotg} \tau - (\tau^2/\sin^2\tau + x^2/\lambda^2)^{\frac{1}{2}}, \qquad -\pi < \tau < \pi.$$

Integration with respect to τ gives eventually the analogue of (2.2.12)

(2.2.41) $$K_\nu(x) = \tfrac{1}{4}\pi^{-\frac{1}{2}}(2/x)^{\nu+1}\Gamma(\nu+3/2)e^{\lambda(\sigma_0 - \ln \frac{2\lambda^2|\sigma_0|}{x^2})} \int_{-\pi}^{\pi} e^{f(\tau)}d\tau,$$

with

(2.2.42) $$f(\tau) = \lambda[\sigma - \sigma_0 - \ln(\frac{\sigma}{\sigma_0} \cdot \frac{\tau}{\sin\tau})], \qquad -\pi < \tau < \pi, \quad \sigma_0 = xs_0/\lambda.$$

The integrand of (3.46) can be defined outside the interval $(-\pi,\pi)$ by prescribing it equal to zero. Hence, it can be considered as an element of $C_c^\infty([-\pi,\pi])$ and the integral can be computed by the methods of Subsection 1.2. Singularities in the complex τ-plane occur at the points where

$$\frac{\sin \tau}{\tau} = \pm i\lambda/x.$$

A similar equation was found for the integral representation for $I_\nu(x)$ in (2.2.12) and, consequently, the same remarks made there are appropriate here.

Again we arrive at a representation with an explicit representation for the function f of the integrand, in constrast with (2.2.34), where the function k(u) is implicitly defined.

The dominant factor for large ν and or x in (2.2.41) is

(2.2.43) $$(2/x)^{\nu+1}\Gamma(\nu+3/2)e^{\lambda(\sigma_0 - \ln \frac{2\lambda^2|\sigma_0|}{x^2})}$$

and it can be used for a normalization of $K_\nu(x)$. By using the Stirling approximation for the gamma function this expression can be compared with the scaling factor $e^{-\nu\eta}$ in (2.2.1), (2.2.32) and (2.2.34). As is easily verified

$$(2.2.44)\qquad \left(\frac{2}{x}\right)^{\lambda} e^{-\lambda} \lambda^{\lambda} e^{\lambda(\sigma_0 - \ln \frac{2\lambda^2|\sigma_0|}{x^2})} = e^{-\lambda\zeta},$$

with cf. (2.2.2)

$$(2.2.45)\qquad \zeta = \sqrt{1+z^2} + \ln [z/(1 + \sqrt{1+z^2})], \qquad z = x/\lambda.$$

Some of the above representations for $I_\nu(x)$ and $K_\nu(x)$ will be used for numerical computations. The results are given in the following subsection.

2.2.3 NUMERICAL RESULTS AND COMPUTER PROGRAMS

The computer programs discussed here are based on the integral representations (2.2.12) and (2.2.41). We give them as ALGOL 60 procedures. The numerical results may be compared with existing tables of the modified Bessel functions. However here we use when testing the programs the Wronskian

$$(2.2.46)\qquad I_\nu(x)K_{\nu+1}(x) + I_{\nu+1}(x)K_\nu(x) = 1/x.$$

As mentioned in the previous subsections, if large values of x and ν are considered it is advisable to normalize the functions $I_\nu(x)$ and $K_\nu(x)$. When using the ALGOL 60 procedures given below one can choose a suitable normalization by assigning specific values to the variable *norm*, which appears as an integer variable in the heading of the procedures for $I_\nu(x)$ and $K_\nu(x)$. The following normalizations are possible.

value of *norm*	computed function	
1	$I_\nu(x)$	$K_\nu(x)$
2	$e^{-x}I_\nu(x)$	$e^{x}K_\nu(x)$
3	$e^{-\nu\eta}I_\nu(x)$	$e^{\nu\eta}K_\nu(x)$
4	$(x/2)^{-\nu}\Gamma(\nu+1)I_\nu(x)$	$(x/2)^{\nu}\Gamma(\nu)^{-1}K_\nu(x)$

These normalizations all correspond with the asymptotic behaviour of the functions $I_\nu(x)$, $K_\nu(x)$. For large values of x and/or ν the computed functions are normalized such that overflow or underflow may be prevented. The following indications for the use of *norm* can be made

values of *norm*	values of x and ν
1	both moderate
2	x large with respect to ν
3	both large
4	ν large with respect to x.

The third case contains the remaining ones; it is based on the uniform asymptotic expansion of the modified Bessel functions. That is, it can also be used if $x \gg \nu$ or $x \ll \nu$.

When testing the procedure for the normalized functions with the Wronskian (2.2.46), this formula must be adapted for the cases where *norm* is 3 or 4. Denoting the computed functions by

$$\text{(2.2.47)}\qquad I_\nu^{(n)}(x),\ K_\nu^{(n)}(x) \quad \text{when} \quad norm = n = 2,3 \text{ or } 4,$$

we have

$$\text{(2.2.48)}\qquad I_\nu^{(3)}(x)\ K_{\nu+1}^{(3)}(x)e^{\mu} + I_{\nu+1}^{(3)}(x)\ K_\nu^{(3)}(x)e^{-\mu} = 1/x$$

with

$$\text{(2.2.49)}\qquad \mu = -\frac{(2\nu+1)}{[x^2+\nu^2]^{\frac12}+[x^2+(\nu+1)^2]^{\frac12}} + \text{arc sinh}\left(\frac{\nu+1}{x}\right) +$$

$$+\ \nu \text{ arc sinh} \frac{2\nu+1}{(\nu+1)[x^2+\nu^2]^{\frac12}+\nu[x^2+(\nu+1)^2]^{\frac12}}$$

and

$$\text{(2.2.50)}\qquad I_\nu^{(4)}(x)\ K_{\nu+1}^{(4)}(x) + \frac{x^2}{4\nu(\nu+1)}\ I_{\nu+1}^{(4)}(x)\ K_\nu^{(4)}(x) = 1/2.$$

The functions $I_\nu(x)$, $K_\nu(x)$ or their normalizations $I_\nu^{(n)}(x)$, $K_\nu^{(n)}(x)$, $n = 2,3,4$ can be computed by the procedures *inux*, *knux*. These procedures call for the nonlocal procedures *log one plus x*, *sin x min x*, *arcsinh* and *non exp gam*. A description of these procedures, including tne source texts will be given.

1. The procedures *inux*, *knux*.

The heading of the procedures reads as follows:

<u>real</u> <u>procedure</u> *inux(x,nu,d,norm)*; <u>value</u> *x,nu,d,norm*; <u>real</u> *x,nu*;
<u>integer</u> *d,norm*;

<u>real</u> <u>procedure</u> *knux(x,nu,d,norm)*; <u>value</u> *x,nu,d,norm*; <u>real</u> *x,nu*;
<u>integer</u> *d,norm*;

The meaning of the formal parameters is

x: <arithmetic expression>;
the argument of the Bessel functions;
$x \geq 0$ for $I_\nu(x)$, $x > 0$ for $K_\nu(x)$;

nu: <arithmetic expression>;
the order of the Bessel functions; $nu \geq 0$;

d: <arithmetic expression>;
the desired number of significant digits in the computed values;

norm: <arithmetic expression>;
the choice of *norm* determines the normalization of the Bessel functions (see page 31).

2. The procedure *log one plus x*.

It computes $\ln(1+x)$ for $x > -1$. For small $|x|$ a polynomial approximation given in HART (1968, code 2665) is used, for the remaining values of x the standard computer function ln is used.

3. The procedure *sin x min x*.

It computes $[\sin(x)-x]/x^3$ for real values of x. For $|x| \leq 2$ a Chebyshev expansion is used, the coefficients of which are obtained by telescoping the Taylor series of sin(x). For $|x| > 2$ (where the subtraction sin(x)-x is harmless with respect to cancellation of digits) the standard computer function sin is used.

4. The procedure *arcsinh*.

Here we use the formula

$$\operatorname{arcsinh}(x) = \ln[x+(x^2+1)^{\frac{1}{2}}].$$

For small x we use the procedure *log one plus x* by writing

$$\operatorname{arcsinh}(x) = \ln\{1+x+x^2/[1+(x^2+1)^{\frac{1}{2}}]\}.$$

5. The procedure *non exp gam*.

It computes the function g(x) defined by

$$g(x) = e^x x^{-x}\Gamma(x), \qquad x > 0.$$

For $x > 1000$ we use the Stirling approximation, for $8 \le x \le 1000$ we use a polynomial of best approximation given in HART (1968, code 5403), for $0 < x < 8$ we use recursion based on $\Gamma(x+1) = x\Gamma(x)$.

The above procedures in 2,3,4 and 5 are designed for using them on a CDC computer with floating point arithmetic and machine accuracy of 2^{-47}. The relative precision is slightly greater than (or about) 10^{-14}. This imposes limitations upon the accuracy obtainable by the procedures *inux* and *knux*. However they are designed such that only the auxiliarly procedures in 2,3, 4 and 5 should be revised if higher accuracy is wanted.

The trapezoidal rules used in the procedures have as initial value of the stepsize, denoted by h, a quantity depending on x and ν. This initial value of h is chosen on the basis of the following considerations. The function f in the integrands of (2.2.12) and (2.2.41) has for small values of $|\tau|$ the expansion

$$f(\tau) = -\tfrac{1}{2}a\tau^2 + O(\tau^4)$$

where

$$a = \begin{cases} (\nu^2+x^2)^{\frac{1}{2}} & \text{for (2.2.12)} \\ \lambda w x^{-2}(\lambda+w) & \text{for (2.2.41)} \end{cases}$$

where $\lambda = \nu+\frac{1}{2}$, $w = (x^2+\lambda^2)^{\frac{1}{2}}$. As initial value of h we take

$$h = \pi/(1 + [a^{\frac{1}{2}}])$$

where [.] is the entier function. If this value is larger than $\pi/4$ we take $h = \pi/4$.

In this way we have an h-value for which $\exp(-\frac{1}{2}ah^2)$ is not extremely small. If we should start with a fixed value of h, say $\pi/4$, then very much iterations may be needed, especially if x and ν are large. A remarkable effect of this choice of h is that for large x and ν the number of iterations for obtaining a given accuracy, say 10^{-10}, is constant. Also the number of relevant function evaluations is constant considered as a function of ν and x (if they are large). For more information we refer to Table VIII.

During the computations the interval of integration (originally $[0,\pi]$, since f is even) reduces to an interval $[0,b]$, $b \le \pi$, if values of the integrand are met that are smaller than 10^{-d-1}. In this way a rather efficient algorithm is constructed. We can use such a device because $\exp[f(\tau)]$ is monotone on $[0,\pi]$.

Table VIII contains results of the verification of the Wronskians (2.2.46), (2.2.48) and (2.2.50). The accuracy parameter d is 10. The iterations in the trapezoidal rule in *inux* and *knux* are continued until successive approximations agree within relative accuracy of 10^{-6}. Under the heading "wronski" we give the computed value of

$$|x[I_{\nu+1}(x)K_\nu(x) + I_\nu(x)K_{\nu+1}(x)] - 1|$$

or analogue expressions for *norm* = 3 or 4. Under the heading "iterations" we give the number of iterations needed in the trapezoidal rule for the four functions $I_{\nu+1}$, K_ν, I_ν, $K_{\nu+1}$. Under "function evaluation" we give the number of *relevant* function evaluations of the integrand, i.e., the number of those values of $\exp[f(\tau)]$ in the computations that are not smaller than 10^{-11}.

Next we give the numerical results and the ALGOL 60 texts of the procedures.

TABLE VIII

Test of *inux* and *knux*

	x	ν	wronski	function evaluations $I_{\nu+1}(x)$	function evaluations $K_\nu(x)$	function evaluations $I_\nu(x)$	function evaluations $K_{\nu+1}(x)$	iterations $I_{\nu+1}(x)$	iterations $K_\nu(x)$	iterations $I_\nu(x)$	iterations $K_{\nu+1}(x)$
norm = 1	1	0	3.0(−11)	30	30	16	27	3	3	2	3
	1	5	4.2(−12)	11	53	12	49	2	3	2	3
	1	10	1.3(−12)	19	36	19	34	3	3	3	3
	5	0	4.7(−10)	15	61	16	14	2	4	2	2
	5	5	8.5(−14)	23	22	24	24	3	3	3	3
	5	10	2.7(−13)	18	27	19	26	3	3	3	3
	10	0	1.5(−12)	29	61	32	28	3	4	3	3
	10	5	4.3(−14)	21	20	22	18	3	3	3	3
	10	10	2.1(−14)	18	23	18	21	3	3	3	3
norm = 2	10^3	0	1.3(−11)	18	62	18	29	3	4	3	3
	10^5	5	7.1(−14)	18	11	18	11	3	2	3	2
	10^{10}	10	2.1(−14)	18	19	18	18	3	3	3	3
	10^3	0	1.3(−11)	18	62	18	29	3	4	3	3
	10^5	5	6.4(−14)	18	12	18	11	3	2	3	2
	10^{10}	10	2.1(−14)	18	19	18	18	3	3	3	3
	10^3	0	1.3(−11)	18	62	18	29	3	4	3	4
	10^5	5	7.1(−14)	18	12	18	11	3	2	3	2
	10^{10}	10	1.4(−14)	18	19	18	18	3	3	3	3
norm = 3	10^3	10^3	4.3(−14)	18	18	18	18	3	3	3	3
	10^3	10^5	3.6(−14)	18	18	18	18	3	3	3	3
	10^3	10^{10}	5.7(−14)	18	18	18	18	3	3	3	3
	10^5	10^3	4.3(−14)	18	18	18	18	3	3	3	3
	10^5	10^5	2.8(−14)	18	18	18	18	3	3	3	3
	10^5	10^{10}	9.2(−14)	18	18	18	18	3	3	3	3
	10^{10}	10^3	4.3(−14)	18	18	18	18	3	3	3	3
	10^{10}	10^5	4.3(−14)	18	18	18	18	3	3	3	3
	10^{10}	10^{10}	4.3(−14)	18	18	18	18	3	3	3	3
norm = 4	1	10^3	3.6(−14)	18	18	18	18	3	3	3	3
	1	10^5	3.6(−14)	18	18	18	18	3	3	3	3
	1	10^{10}	3.6(−14)	18	18	18	18	3	3	3	3
	5	10^3	1.4(−14)	18	18	18	18	3	3	3	3
	5	10^5	2.1(−14)	18	18	18	18	3	3	3	3
	5	10^{10}	2.8(−14)	18	18	18	18	3	3	3	3
	10	10^3	1.4(−14)	18	18	18	18	3	3	3	3
	10	10^5	1.4(−14)	18	18	18	18	3	3	3	3
	10	10^{10}	2.8(−14)	18	18	18	18	3	3	3	3

```
real  procedure  inux(x,nu,d,norm);  value  x,nu,d,norm;  real  x,nu;
                                     integer  d,norm;
begin  real  a,b,c,e,eps,g,h,nu2,p,q,pi,t,ts,v,w,xx,x2,y,z;
   real  procedure  f(t);  value  t;  real  t;
   if  t = 0  then  f:= 1  else  if  t > b  then  f:= 0  else
   begin  if  nu = 0  then  y:= exp(-2×x×sin(t/2)↑2)  else
      begin  if  t > 2  then
         begin  ts:= sin(t);  if  ts > 0  then
            begin  ts:= t/ts;  p:= ts×ts-1;  y:= 1/ts-1  end
         end  else
         begin  y:= sin x min x(t)×t×t;  ts:= 1/(1+y);
            p:= -y×ts×(1+ts)
         end ;
         if  ts > 0  then
         begin  z:= sqrt(x2+nu2×(1+p));  c:= cos(t);
            a:= 2×sin(t/2)↑2;
            y:= exp(-nu×arcsinh(nu×p/(ts×w+z))
            ( if  c > 0  then  (sin(t)↑2×x2+nu2×ts×(c×ts+1)×(y+a))/
               (c×z+w)  else  w-c×z))
         end  else  y:= 0;
      end ;
      if  y < e  then  b:= t;  f:= y
   end  f;
   x2:= x×x;  nu2:= nu×nu;  e:= 10↑(-d-1);  b:= pi:= 4×arctan(1);
   w:= sqrt(x2+nu2);  g:= .5;  eps:= 10↑(-.6×d);
   h:= pi/(1+entier(sqrt(w)));  if  h > .785  then  h:= pi/4;
   for  t:= h, h+t  while  t < b  do  g:= g+f(t);
   g:= h×(g+( if  nu > 0  then  0  else  f(pi)/2));
   for  h:= h, h/2  while  v > eps  do
   begin  q:= 0;
      for  t:= h/2, t+h  while  t < b  do  q:= q+f(t);
      q:= q×h;  q:= (g+q)/2;  v:= abs((g-q)/q);  g:= q
   end ;  g:= g/pi;
   if  norm = 1  then  inux:= g× exp(w-nu×arcsinh(nu/x))  else
   if  norm = 2  then  inux:= g× exp(nu×(nu/(x+w)-arcsinh(nu/x)))  else
   if  norm = 3  then  inux:= g  else
   if  norm = 4  then
   begin  if  nu = 0  then  inux:= g  else
      begin  p:= x2/(nu+w);  inux:= non exp gam(nu)×nu×g×
         exp(p-nu×log one plus x(p/nu/2))
      end
   end
end  inux;
```

```
real  procedure  knux(x,nu,d,norm);  value  x,nu,d,norm;  real  x,nu;
                                     integer  d,norm;
begin  real  a,b,c,e,eps,g,h,nu2,p,q,pi,t,ts,v,w,xx,x2,y,z;
   real  procedure  f(t);  value  t;  real  t;
   if  t = 0  then  f:= 1  else  if  t > b  then  f:= 0  else
   begin  if  t > 2  then
      begin  ts:= sin(t);  if  ts > 0  then
         begin  ts:= t/ts; p:= ts×ts-1; y:= 1/ts-1  end
      end  else
      begin  y:= sin x min x(t)×t×t; ts:= 1/(1+y);
         p:= -y×ts×(1+ts)
      end ;
      z:= sqrt(x2+ nu2× (1+p)); c:= -p×nu/(w+z)+( if  t < 1.57  then
       -t×sin(t/2)/cos(t/2)-y×ts  else  ts×cos(t)-1);
      p:= -c×nu×(nu+w)/x2;
      y:=  if  ts > 0  then  exp(nu×(c-
           log one plus x(ts×(p-y))))  else  0;
      if  y < e  then  b:= t; f:= y
   end  f;
   x2:= x×x; a:= nu; nu:= nu+.5; nu2:= nu×nu; e:= 10↑(-d-1); eps:=n×e;
   b:= pi:= 4×arctan(1); w:= sqrt(x2+nu2); m:= 0;  tt:= 0;
   h:= pi/(1+entier(sqrt(w×nu×(nu+w)/x2))); if h > .785 then h:= pi/4;
   for  t:= h, h+t  while  t < b  do  g:= g+f(t); g:= h×g;
   for  h:= h, h/2  while  v > eps  do
   begin  q:= 0;
      for  t:= h/2, t+h  while  t < b  do q:= q+f(t);
      q:= q×h; q:= (g+q)/2; v:= abs((g-q)/q); g:= q
   end ;
   g:= .5×nu×sqrt(2/(pi×x))×non exp gam(nu)×g;
   if  norm = 1  then  knux:= g×exp(-w+nu×arcsinh(nu/x))  else
   if  norm = 2  then  inux:= g× exp(nu×(nu/(x+w)-arcsinh(nu/x)))  else
   if  norm = 3  then
   begin  z:= sqrt(x2+a×a); knux:= sqrt((nu+w)/x)×
     exp(-(a+.25)/(w+z)+a×arcsinh((a+.25)/(nu×z+a×w)))×g
   end  else
   if  norm = 4  then
   begin  if  a = 0  then  knux:= 0  else
      begin  p:= x2/(nu+w); knux:= sqrt(2×a/x)/nonexp gam(a)×
         exp(-.5-p+nu×log one plus x((p+1)/2/a))×g
      end
   end
end  knux;
```

```
real  procedure  log one plus x(x);  value  x;  real  x;
comment  computes ln(1+x) for x > -1;
if  x = 0  then  log one plus x:= 0  else
if  x < -0.2928 ∨ x > 0.4142  then  log one plus x:= ln(1+x)  else
begin  real  y,z;
   z:= x/(x+2); y:= z×z;
   log one plus x:= z×(2+ y×
   ( .66666 66666 63366 + y×
   ( .40000 00012 06045 + y×
   ( .28571 40915 90488 + y×
   ( .22223 82333 2791  + y×
   ( .18111 36267 967   + y×
     .16948 21248 8))))))
end  log one plus x;

real  procedure  non exp gam(x);  value  x;  real  x;
comment  computes the euler gamma function multiplied
   by exp(x - x×ln(x));
if  x ≥ 1000  then
non exp gam:= sqrt(8×arctan(1)/x) × exp((30-1/x/x)/x/360)
else  if  x ≥ 8  then
begin  real  xx; xx:= 1/x/x;
   non exp gam:= sqrt(8×arctan(1)/x)×exp((
    .83333 33333 3317E-1 + xx×(
   -.27777 77756 577 E-2 + xx×(
    .79364 31104 8   E-3 + xx×(
   -.59409 56105     E-3 + xx×
    .76634 5188      E-3 ))))/x)
end  else
begin  integer  n;  real  g,z;
   n:= entier(8-x); z:= x+n+1;
   g:= non exp gam(z)×exp(-z+ z×ln(z));
   for  n:= n  step  -1  until  0  do  g:= g/(x+n);
   non exp gam:= g × exp(x-x×ln(x))
end  non exp gam;

real  procedure  sin x min x(x);  value  x;  real  x;
comment  computes (sin(x)-x)/x↑3 for real x;
if  x = 0  then  sin x min x:=-1/6  else
if  abs(x) > 2  then  sin x min x:= (sin(x)-x)/(x×x×x)  else
begin  real  a,b,c,y;
   y:= x×x/2; a:= .5E-14; b:= 0;  for  c:=
   -.00000 00000 01453, .00000 00003 03330,
   -.00000 00469 91333, .00000 51247 52332,
   -.00036 51217 36064, .01515 92974 54270  do
    begin  b:= -2×a-b; a:= -y×b-a+c  end ;
    sin x min x:= (a+b/2)×y-a-.15113 70754 27879
end  sin x min x;

real  procedure  arc sinh(x);  value  x;  real  x;
if  x = 0  then  arc sinh:= 0  else
begin  real  y; y:= abs(x);
     arc sinh:= sign(x) × ( if  y > E+8  then  ln(2×y)  else
     if  y > .36  then  ln(y+ sqrt(1+x×x))  else
     log one plus x(y×(1+y/(1+sqrt(1+x×x)))))
end  arcsinh;
```

2.3. PARABOLIC CYLINDER FUNCTIONS

In this chapter we consider functions that are solutions of the differential equation

$$\frac{d^2y}{dx^2} - (\tfrac{1}{4}x^2 + a)y = 0. \tag{2.3.1}$$

The solutions are called parabolic cylinder functions since they are encountered as solutions of the wave equation by the method of separation of variables in parabolic cylinder coordinates. Also the name Weber-Hermite functions is used. The solutions of (2.3.1) are entire functions of x and a. Practical applications appear to be confined to real solutions of real equations; therefore attention is confined to such solutions. Especially we consider

$$a \geq -\tfrac{1}{2} \quad \text{and} \quad x \in \mathbb{R}, \tag{2.3.2}$$

whereas the case $a < -\frac{1}{2}$ is considered in a later paper.

Following J.C.P. MILLER (1955) (see also ABRAMOWITZ & STEGUN (1964, Chapter 19)), linearly independent solutions of (2.3.1) are denoted by U(a,x) and V(a,x), with Wronskian

$$UV' - U'V = (2/\pi)^{\frac{1}{2}}. \tag{2.3.3}$$

The function U(a,x) can be represented by the integral

$$U(a,x) = \frac{e^{-\frac{1}{4}x^2}}{\Gamma(a+\frac{1}{2})} \int_0^\infty t^{a-\frac{1}{2}} e^{-\frac{1}{2}t^2 - xt}\, dt, \qquad \operatorname{Re} a > -\tfrac{1}{2}. \tag{2.3.4}$$

The function V(a,x) is defined in terms of U(a,x) by

$$V(a,x) = \pi^{-1}\Gamma(a+\tfrac{1}{2})[\sin \pi a\, U(a,x) + U(a,-x)]. \tag{2.3.5}$$

An integral representation which is valid for all complex values of a is

$$U(a,x) = -\tfrac{1}{2}(2\pi)^{-\frac{1}{2}} e^{\frac{1}{4}x^2} \int_L e^{-xs+\frac{1}{2}s^2} s^{-a-\frac{1}{2}}\, ds, \tag{2.3.6}$$

where L is shown in Figure 2.3.1. For large s we have on L, in order to ensure convergence of the integral, $\frac{1}{4}\pi < |\arg s| < \frac{3}{4}\pi$. The many valued function $s^{-a-\frac{1}{2}}$ is real for $s > 0$; its branch-cut can be taken from 0 to $-\infty$.

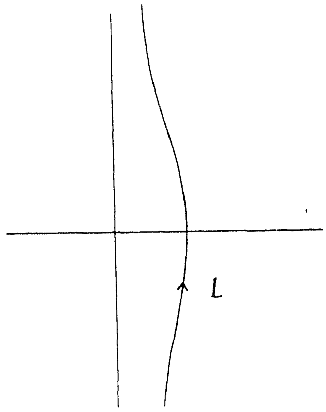

Fig. 2.3.1. Contour for (2.3.6)

The integral in (2.3.6) will be used in a later paper when negative values of a are considered.

REMARK 2.8. If $a = -n-\frac{1}{2}$ then $U(-n-\frac{1}{2},x) = (-1)^n U(-n-\frac{1}{2},-x)$, $n \in \mathbb{Z}$. This easily follows from changing the integration variable $s \to -s$ in (2.3.6). Hence, if $a = -n-\frac{1}{2}$, $n = 0,1,2,\ldots$, the right-hand side of (2.3.5) appears in indeterminate form. However, the limit of this form as $a \to -n-\frac{1}{2}$ exists and may be taken as the definition of the function $V(a,x)$ for negative half-integer order. Computational aspects of this phenomenon will not be discussed in this paper. The limiting value of $V(a,x)$ for $a \to -\frac{1}{2}$ is obtained as follows. Combining (2.3.4) with the formula obtained by replacing $x \to -x$ we obtain by using (2.3.5)

$$V(a,x) = \frac{2}{\pi} e^{-\frac{1}{2}x^2} \int_0^\infty e^{-\frac{1}{2}t^2} \frac{\sinh xt}{t}\, dt + O(1), \qquad a \to -\tfrac{1}{2}.$$

The integral can be expressed as an error function. The result is

$$V(-\tfrac{1}{2},x) = e^{-\frac{1}{4}x^2} \operatorname{erf}(ix/\sqrt{2}).$$

In terms of the familiar function $D_\nu(x)$ of Whittaker, we can write

$$(2.3.7) \qquad U(a,x) = D_{-a-\frac{1}{2}}(x).$$

We proceed with the D_ν function since it gives simpler formulas. For $x = 0$ we have

$$(2.3.8) \qquad D_\nu(0) = \pi^{\frac{1}{2}}\, 2^{\nu/2}/\Gamma(\tfrac{1-\nu}{2}).$$

For special values of ν we have

$$D_0(x) = e^{-\frac{1}{2}x^2}$$

$$(2.3.9) \qquad D_{-1}(x) = (\pi/2)^{\frac{1}{2}} e^{\frac{1}{4}x^2}\ \mathrm{erfc}(x/\sqrt{2}),$$

$$D_{-n-1}(x) = (\pi/2)^{\frac{1}{2}} e^{-\frac{1}{4}x^2}\ \frac{(-1)^n}{n!}\ \frac{d^n}{dx^n}\,[e^{\frac{1}{2}x^2}\ \mathrm{erfc}(x/\sqrt{2})],$$

where erfc is the complementary error function given by

$$(2.3.10) \qquad \mathrm{erfc}(x) = 2\pi^{-\frac{1}{2}} \int_x^\infty e^{-t^2} dt.$$

Also, there is a relation with repeated integrals of the error function

$$(2.3.11) \qquad \begin{aligned} &i^n \mathrm{erfc}(x) = \int_x^\infty i^{n-1}\ \mathrm{erfc}(t)dt, \qquad n = 0,1,2,\ldots, \\ &i^{-1}\ \mathrm{erfc}(x) = 2\pi^{-\frac{1}{2}} e^{-x^2}, \quad i^0\ \mathrm{erfc}(x) = \mathrm{erfc}(x). \end{aligned}$$

The relation is

$$(2.3.12) \qquad i^n\ \mathrm{erfc}(x) = (2^{n-1}\pi)^{-\frac{1}{2}} e^{-\frac{1}{2}x^2}\ D_{-n-1}(x\sqrt{2}).$$

Indeed, the derivatives and repeated integrals of erfc can be expressed into each other as follows

$$(2.3.13)\qquad \frac{d^n}{dx^n}[e^{x^2}\operatorname{erfc}(x)] = (-1)^n 2^{n/2} n!\; e^{\frac{1}{2}x^2} i^n \operatorname{erfc}(x/\sqrt{2}).$$

The connection with Hermite polynomials is described by

$$(2.3.14)\qquad D_n(x) = 2^{-\frac{1}{2}n} e^{-\frac{1}{4}x^2} H_n(x/\sqrt{2}).$$

Apart from their importance in mathematical physics, we mention the role of the parabolic cylinder functions in turning point problems in the study of asymptotic behaviour of differential equations.

The asymptotic behaviour of $D_\nu(x)$ for large $|x|$ is given by

$$(2.3.15)\qquad \begin{aligned} D_\nu(x) &= x^\nu e^{-\frac{1}{4}x^2}[1 + O(x^{-2})], && x \to \infty \\ D_\nu(x) &= x^\nu e^{-\frac{1}{4}x^2}[1 + O(x^{-2})] + \\ &\quad + \frac{\sqrt{2\pi}}{\Gamma(-\nu)}(-x)^{-\nu-1} e^{\frac{1}{4}x^2}[1 + O(x^{-2})], && x \to -\infty. \end{aligned}$$

If $\nu \neq 0,1,2,\ldots$, the second term in the formula for $x \to -\infty$ is dominant. If $\nu = 0,1,2,\ldots$, the function $D_\nu(x)$ degenerates to an elementary function (Hermite polynomial), as mentioned in (2.3.14). For large values of $|\nu|$ also results are available. The behaviour is quite different for positive and negative values of ν. If $\nu \to -\infty$ we have uniformly in x

$$(2.3.16)\qquad D_\nu(x) = e^{\nu\zeta}(1+e^{-2\mu})^{-\frac{1}{2}}[1 + O(|\nu^{-1}|)],$$

with μ and ζ given in (2.3.19) and (2.3.21) below. Further information on the asymptotic behaviour of the parabolic cylinder function can be found in ABRAMOWITZ & STEGUN (1964) and in OLVER (1959).

LATHAM & REDDING (1974) consider the computation of U(a,x) by Gaussian quadrature. For each a weights and positions of interpolation must be computed, which disturbs the flexibility of their method. Moreover, negative x-values are not allowed. In LATHAM & REDDING (1976), the function V(a,x) is treated by a Simpson quadrature rule for a standard integral. They reported the need of 5000 integration points, which is extremely high compared with our results if the same accuracy is considered.

Special cases of the parabolic cylinder functions are considered by several authors. We mention AMOS (1973) and GAUTSCHI (1976) for the computation of i^nerfc.

In this chapter we give integral representations which enable computation of U(a,x) and V(a,x) for $a \geq -\frac{1}{2}$ and real x and the representations give the dominant factor of the behaviour of these functions if one or both parameters a and |x| are large.

2.3.1. THE FUNCTION $D_\nu(x)$ FOR $\nu \leq 0$

The starting point is (2.3.4), which for $D_\nu(x)$ is written as

$$(2.3.17)\qquad D_\nu(x) = \frac{e^{-\frac{1}{4}x^2}}{\Gamma(-\nu)} \int_0^\infty t^{-\nu-1} e^{-\frac{1}{2}t^2 - xt} dt.$$

We suppose that in this representation

$$\nu < 0, \qquad x \in \mathbb{R}.$$

For $\nu = 0$ we have the elementary case given in (2.3.9). The maximum of the function $\exp[-\nu \ln t - \frac{1}{2}t^2 - xt]$ lies at

$$(2.3.18)\qquad t_0 = \frac{-x+\sqrt{x^2-4\nu}}{2}$$

and is positive for all (finite) values of x and ν considered. Next we make the transformation $t \to \sqrt{-\nu}\, e^t$ and we introduce the real variable μ defined by

$$(2.3.19)\qquad \sinh \mu = \frac{x}{2\sqrt{-\nu}}\,.$$

Then we have the maximum of the integrand at $t = -\mu$ and the integral becomes after shifting this maximum to the origin

$$(2.3.20)\qquad D_\nu(x) = \frac{e^{\nu\zeta}}{e^{-\nu}(-\nu)^\nu\Gamma(-\nu)} \int_{-\infty}^{\infty} e^{\nu[-t+\frac{1}{2}e^{-2\mu}(e^{2t}-1)+(1-e^{-2\mu})(e^t-1)]} dt$$

with

(2.3.21) $\quad \zeta = \frac{1}{2}[\sinh 2\mu + 2\mu - 1 + \ln(-\nu)]$.

The asymptotic expansion of $D_\nu(x)$ for $\nu \to -\infty$, of which the dominant term is given in (2.3.16) follows from the transformation of variables

(2.3.22) $\quad -t+\frac{1}{2}e^{-2\mu}(e^{2t}-1) + (1-e^{-2\mu})(e^{t}-1) = u^2$,

with sign(t) = sign(u). This gives

(2.3.23) $$D_\nu(x) = \frac{e^{\nu\zeta}}{e^{-\nu}(-\nu)^\nu\Gamma(-\nu)} \int_{-\infty}^{\infty} e^{\nu u^2} \frac{dt}{du}\, du.$$

By expanding dt/du in powers of u and interchanging the order of summation and integration the asymptotic expansion is obtained. As in the Bessel function cases (see (2.2.21) and (2.2.34)), the integrand function dt/du cannot be given explicitly as a function of u. This aspects disturbs the use of (2.3.23) as starting point for the numerical computations. Singularities of the integrand in (2.3.23) follow from the zeros of du/dt. From (2.3.22) it follows that in the u-plane singularities occur at $(\pm i\pi - 2\mu - \sinh 2\mu)^{\frac{1}{2}}$.

The computer program, which will be given in the next subsection will be based upon representation (2.3.20). First we perform a transformation $t = v-e^{-v}$ in order to speed up the convergence of the integral at negative values of the integration variable.

2.3.2. NUMERICAL RESULTS AND A COMPUTER PROGRAM FOR $D_\nu(x)$

As for the modified Bessel functions we give ALGOL 60 procedures for the computation of $D_\nu(x)$. For testing the algorithm we use a Wronskian for solutions of (2.3.1). Using (2.3.3), (2.3.5), (2.3.7) and the well-known recursion

(2.3.24) $\quad D'_\nu(x) = \nu D_{\nu-1}(x) - \frac{1}{2}xD_\nu(x)$

(which is readily verified with (2.3.17)) we obtain

(2.3.25) $$D_\nu(x)D_{\nu-1}(-x) + D_{\nu-1}(x)D_\nu(-x) = (2\pi)^{\frac{1}{2}}/\Gamma(1-\nu).$$

In order to allow large values of $|\nu|$ and $|x|$ we give normalizations in order to prevent underflow or overflow. We choose the normalization by assigning specific values to the variable *norm* appearing in the heading of the procedure for $D_\nu(x)$. The following normalizations are possible.

value of *norm*	computed function $\nu < 0$	$\nu = 0$
1	$D_\nu(x)$	$e^{-\frac{1}{4}x^2}$
2	$e^{\mathrm{sign}(x)\ x^2/4}D_\nu(x)$	1
3	$e^{-\nu\zeta}\ D_\nu(x)$	1
4	$2^{-\frac{1}{2}\nu}\Gamma(1-\frac{1}{2}\nu)e^{x\sqrt{-\nu}}\ D_\nu(x)$	$e^{-\frac{1}{4}x^2}$.

We recall that ν is non-positive and x is real. As follows from (2.3.15) and (2.3.16), the values of *norm* correspond with the asymptotic behaviour of $D_\nu(x)$.

We give the following indications for the use of *norm*.

value of *norm*	values of x and ν
1	both $|x|$ and $-\nu$ moderate
2	$|x|$ large with respect to $-\nu$
3	both $|x|$ and $-\nu$ large
4	$-\nu$ large with respect to $|x|$.

The third case contains the remaining ones. It can also be used if $|x| \gg -\nu$ or $|x| \ll -\nu$.

The function $D_\nu(x)$, or its normalization, can be computed by the procedure *dnux*. It calls for some nonlocal procedures, which are also used in the modified Bessel function case. For the computation of e^t-1 for small

TABLE IX

Test of *dnux*

	x	$-\nu$	wronski	function evaluations				iterations			
				$D_\nu(x)$	$D_{\nu-1}(-x)$	$D_{\nu-1}(x)$	$D_\nu(-x)$	$D_\nu(x)$	$D_{\nu-1}(-x)$	$D_{\nu-1}(x)$	$D_\nu(-x)$
norm = 1	0	0	2.8(-14)	0	53	53	0	0	3	3	0
	0	5	4.3(-14)	48	47	47	48	3	3	3	3
	0	10	2.2(-13)	48	48	48	48	3	3	3	3
	5	0	3.0(-13)	0	104	50	0	0	3	3	0
	5	5	2.4(-13)	43	58	43	61	3	3	3	3
	5	10	1.4(-13)	44	51	44	52	3	3	3	3
	10	0	0.0(+00)	0	52	46	0	0	3	3	0
	10	5	1.4(-14)	43	49	43	50	3	3	3	3
	10	10	4.5(-13)	44	48	44	48	3	3	3	3
norm = 2	10^{3}	1	6.4(-14)	35	44	40	44	3	3	3	3
	10^{3}	5	1.7(-13)	43	44	43	44	3	3	3	3
	10^{3}	10	1.7(-13)	44	44	44	44	3	3	3	3
	10^{5}	1	1.4(-13)	35	44	40	44	3	3	3	3
	10^{5}	5	9.2(-14)	43	44	43	44	3	3	3	3
	10^{5}	10	1.5(-13)	44	44	44	44	3	3	3	3
	10^{10}	1	1.1(-13)	35	44	40	44	3	3	3	3
	10^{10}	5	3.1(-13)	43	44	43	44	3	3	3	3
	10^{10}	10	1.2(-12)	44	44	44	44	3	3	3	3
norm = 3	10^{3}	10^{3}	2.8(-14)	45	44	45	44	3	3	3	3
	10^{3}	10^{5}	1.8(-13)	44	44	44	44	3	3	3	3
	10^{3}	10^{10}	3.9(-12)	44	44	44	44	3	3	3	3
	10^{5}	10^{3}	7.1(-15)	45	44	45	44	3	3	3	3
	10^{5}	10^{5}	7.7(-13)	44	44	44	44	3	3	3	3
	10^{5}	10^{10}	4.8(-11)	44	44	44	44	3	3	3	3
	10^{10}	10^{3}	7.1(-14)	45	44	45	44	3	3	3	3
	10^{10}	10^{5}	5.0(-13)	44	44	44	44	3	3	3	3
	10^{10}	10^{10}	3.4(-11)	44	44	44	44	3	3	3	3
norm = 4	1	10^{3}	1.1(-13)	45	45	45	45	3	3	3	3
	1	10^{5}	6.5(-13)	44	44	44	44	3	3	3	3
	1	10^{10}	2.3(-10)	44	44	44	44	3	3	3	3
	10	10^{3}	3.7(-13)	45	45	45	45	3	3	3	3
	10	10^{5}	1.6(-11)	44	44	44	44	3	3	3	3
	10	10^{10}	9.4(-10)	44	44	44	44	3	3	3	3
	50	10^{3}	7.8(-12)	45	45	45	45	3	3	3	3
	50	10^{5}	1.7(-11)	44	44	44	44	3	3	3	3
	50	10^{10}	4.5(-11)	44	44	44	44	3	3	3	3

values of |t| we use a procedure for the hyperbolic sine function, called *sinh*. For a description of the procedure *dnux* we refer to the description of *inux* and *knux*.

We tested the procedure *dnux* be verifying the Wronskian (2.3.25) or its analogue for the case where *norm* is 3 or 4. The results are given in Table IX. For the interpretation of the results with headings "function evaluations" and "iterations" we refer to the description of Table VIII.

Next we give the ALGOL 60 texts of the procedures *sinh* and *dnux*.

```
real  procedure  sinh(x);  value  x;  real  x;
begin  real  ax,y;
    ax:= abs(x);
    if  ax < .3  then
    begin  y:=  if  ax < .1  then  x×x  else  x×x/9;
      x:= (((1/5040×y+1/120)×y+1/6)×y+1)×x;
      sinh:=  if  ax < .1  then  x  else  x×(1+4×x×x/27)
    end  else
    begin  ax:= exp(ax); sinh:= sign(x)×.5×(ax-1/ax)  end
end  sinh;

real  procedure  dnux(x,nu,d,norm);  value  x,nu,d,norm;  real  x,nu;
                                                    integer  d,norm;
if  nu = 0  then
begin  dnux:=  if  norm = 2  ∨  norm = 3  then  1  else  exp(-x×x/4)
end  else
begin  real  a,b,c,e,eps,h,p,q,r,s,w,sh,y,mu,v,shmu,t;
    real  procedure  g(t);  value  t;  real  t;
    g:=  if  t = 0  then  0  else  if  t<-.7  ∨  t>.4  then  exp(t)-1
    else  2 × sinh(t/2) × exp(t/2);

    real  procedure  f(v);  value  v;  real  v;
    if  v = 0  then  f:= 2  else
    if  v < a  ∨  v > b  then  f:= 0  else
    begin  y:= g(-v); t:= v-y; y:= 2+y; c:= g(t);
        c:= ((2×c-t×(c+2))+t×c)/2;
        f:= y:= y×exp(nu×(c×(1+p×(c+t))+p×t×(c+t)));
        if  y ≤ e  then
        begin if v < 0 then a:= v else b:= v end
    end  f;
    shmu:= x/2/sqrt(-nu); mu:= arcsinh(shmu);
    if  mu < -.35  ∨  mu > .2  then
    begin  p:= exp(-2×mu); q:= 1-p; p:= p/2  end  else
    begin  p:= g(-mu); q:= -p×(p+2); p:= (1-q)/2  end ;
    e:= 10↑(-d-1); c:= ((d+1)×2.3+.69)/(-nu);
    b:= log one plus x(sqrt(c/p)); c:= c+( if  x ≥ 0  then  2-p
```

```
    else  1+1/(4×p));  if  c < 1  then  c:= 1; a:= 1+1/nu;
    a:=  if  a ≥ 0  then  -ln(c)  else  -2×ln(-a+sqrt(a×(a+2)+c));
    c:= (b-a)/8; r:= 2; v:= 0;
    h:= sqrt(-1.6/nu/(1+2×p));  if  h > c  then  h:= c;
    for  v:= v+h  while  v < b  do  r:= r+f(v); v:= 0;
    for  v:= v-h  while  v > a  do  r:= r+f(v);
    r:= r×h; eps:= 10↑(-.6×d);
    for  h:= h,h/2  while  w > eps  do
    begin  s:= 0; tt:= tt+1;
        for  v:= h/2,v+h  while  v < b  do  s:= s+f(v);
        for  v:=-h/2,v-h  while  v > a  do  s:= s+f(v);
        s:= s×h; s:= (r+s)/2; w:= abs((s-r)/s); r:= s;
    end ; y:= r/non exp gam(-nu);
    if  norm = 1  then  dnux:= y×exp(nu×(q×(1+1/p/2)/2+2×mu-1
                                              +ln(-nu))/2)  else
    if  norm = 2  then  dnux:= y×exp(nu×(q/
        ( if  x ≥ 0  then  1  else  p×2)+2×mu-1+ln(-nu))/2)  else
    if  norm = 3  then  dnux:= y  else
    if  norm = 4  then  dnux:= -.5×nu×non exp gam(-.5×nu)×y×
                        exp(nu×(mu-2×shmu+q×(1+1/p/2)/4))
end  dnux;
```

2.4. A FINAL EXAMPLE

In this section we give another example for the application of the trapezoidal quadrature rule on a Laplace type integral. In investigations of the energy loss of fast particles by ionization, LANDAU (1944) used the function

$$\Phi(\lambda) = \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} e^{u \ln u + \lambda u}\, du,$$

λ real, $\sigma > 0$, in order to describe the transformation of the spectral distribution of energy. From a computational point of view the function is discussed by BÖRSCH - SUPAN (1961), who derived asymptotic expansions with error terms for large $|\lambda|$ and used them for the computation of Φ. For values of λ in the remaining interval Simpson's rule was applied after a suitable transformations of the path of integration and restriction to finite portion of this path. Also a table of the function is given by Börsch-Supan.

In this chapter we apply our methods to the function Φ defined above. It will turn out that the representation for Φ based on the saddle point contour enables computation for all values of λ. It is not necessary to choose several λ-intervals with different methods for computation as in the cited reference.

Let us write

$$u = \omega t, \qquad \omega = e^{-\lambda}$$

Then

$$\Phi(\lambda) = \frac{\omega}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} e^{\omega\, t \ln t}\, dt, \quad \omega > 0, \quad \sigma > 0.$$

The saddle point of the integrand occurs at $t = e^{-1}$ and, writing $t = \rho e^{i\theta}$ the ideal contour of integration is given by

$$\rho(\theta) = \exp(-\theta \operatorname{cotg} \theta), \qquad -\pi < \theta < \pi.$$

If we integrate with respect to θ the integral becomes

$$\phi(\lambda) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-f(\theta)} f(\theta) d\theta$$

with

$$f(\theta) = \frac{\omega\theta}{\sin \theta} \;\; \rho(\theta).$$

For $\theta \to \pm\, \pi$ we have

$$f(\theta) \sim \frac{\omega\pi}{\pi-|\theta|} \exp \frac{\pi}{\pi-|\theta|}$$

which is different from the asymptotic behaviour considered in Remark 1.12. A suitable normalization of $\phi(\lambda)$ is obtained by writing

$$\Phi(\lambda) = \frac{f(0)e^{-f(0)}}{2\pi} \int_{\pi}^{\pi} e^{-f(\theta)+f(0)} f(\theta)/f(0) d\theta$$

with $f(0) = \omega/e$.

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