

(2.1) Functions F(x), G(x) and Related Integrals

$$F(x) = \int_0^x \frac{\operatorname{erf}(w)}{w} dw, \quad G(x) = \int_x^\infty \frac{\operatorname{erfc}(w)}{w} dw, \quad \int_0^x e^{-a^2 w^2} \ln w \, dw, \quad \int_x^\infty e^{-a^2 w^2} \ln w \, dw$$

$$a > 0, \quad x > 0$$

Alternate Formulas

$$(2.1.1) \quad F(aX) = \int_0^X \frac{\operatorname{erf}(ax)}{x} dx, \quad G(aX) = \int_X^\infty \frac{\operatorname{erfc}(ax)}{x} dx.$$

$$(2.1.2) \quad \int_0^T e^{-a^2 w^2} \ln w \, dw = \frac{\sqrt{\pi}}{2a} [\operatorname{erf}(aT) \ln T - F(aT)]$$

$$(2.1.3) \quad \int_T^\infty e^{-a^2 w^2} \ln w \, dw = \frac{\sqrt{\pi}}{2a} [\operatorname{erfc}(aT) \ln T + G(aT)].$$

$$(2.1.4) \quad \int_0^\infty e^{-a^2 w^2} \ln w \, dw = -\frac{\sqrt{\pi}}{2a} \left[\frac{\gamma}{2} + \ln(2a) \right].$$

Functional Relationships

$$(2.1.5) \quad F(X) = \frac{\gamma}{2} + \ln(2X) + G(X) \quad (\gamma = \text{Euler Constant} = 0.5772156649015328606\dots)$$

$$(2.1.6) \quad \int_1^\infty e^{-ax} \frac{\ln x}{\sqrt{x}} dx = -\left[\frac{\partial}{\partial v} E_v(a) \right]_{v=1/2} = 2\sqrt{\frac{\pi}{a}} G(\sqrt{a}) = G_{1/2}(a)$$

where $G_v(a)$ is defined in Section (2.2) and explored fully in Chapter 3, Folder 18.

Convergent Series

$$(2.1.7) \quad F(X) = \frac{2X}{\sqrt{\pi}} \sum_{k=0}^\infty \frac{(-1)^k X^{2k}}{k!(2k+1)^2}$$

$$(2.1.8) \quad G(X) = \frac{1}{2} E_1(X^2) - \frac{1}{2\pi} \sum_{k=0}^\infty \frac{C_k}{(k+1/2)} E_{k+3/2}(X^2), \quad C_k = \frac{(1/2)_k}{k!}$$

$$(2.1.9) \quad G(X) = \frac{1}{2} E_1(X^2) - e^{-X^2} \ln 2 + \frac{X^2}{2\pi} \sum_{k=0}^\infty C_k \frac{E_{k+1/2}(X^2)}{(k+1/2)^2}$$

Accelerated Series

$$(2.1.10) \quad G(X) = \frac{1}{2} E_1(X^2) - \frac{1}{2\pi} H(X)$$

$$(2.1.11) \quad H(X) = \sum_{k=0}^\infty \frac{C_k}{(k+1/2)} E_{k+3/2}(X^2) \\ = e^{-X^2} \sum_{k=1}^n W_k (-X^2)^{k-1} + \sqrt{\pi} \operatorname{ierfc}(X) \sum_{k=1}^n S_{k,0} (-X^2)^{k-1} + (-X^2)^n \sum_{k=0}^\infty S_{n,k+1} E_{k+3/2}(X^2)$$

where

$$W_1 = \sum_{k=1}^{\infty} \frac{C_k}{(k+1/2)^2} = 2\pi \ln 2 - 4, \quad W_n = \sum_{k=1}^{\infty} S_{n,k}, \quad n \geq 1.$$

$$S_{1,k} = \frac{C_k}{(k+1/2)^2}, \quad k \geq 0. \quad S_{n+1,k} = \frac{S_{n,k+1}}{(k+1/2)}, \quad k \geq 0, \quad n \geq 1.$$

Explicitly,

$$S_{10} = \frac{C_o}{(1/2)^2} = 4, \quad S_{n,k} = \frac{(1/2)_k}{(n+k-1)!(n+k-1/2)^2}, \quad k \geq 0, \quad n \geq 1$$

and numerical values for the W sequence are found in Chapter 3, Folder 16.

Asymptotic Series

$$(2.1.12) \quad F(X) = \frac{2X}{\sqrt{\pi}} \sum_{k=0}^{\infty} \frac{(-1)^k X^{2k}}{k!(2k+1)^2} \quad \text{for } X \rightarrow 0$$

$$(2.1.13) \quad G(X) = F(X) - \frac{\gamma}{2} - \ln(2X) \quad (\text{See also (2.1.9)}) \quad \text{for } X \rightarrow 0$$

$$(2.1.14) \quad G(X) = \frac{1}{2X\sqrt{\pi}} \sum_{k=0}^N \frac{(-1)^k (1/2)_k}{X^{2k}} E_{k+3/2}(X^2) + W_N,$$

$$|W_N| \leq \frac{1}{2X\sqrt{\pi}} \frac{(1/2)_{N+1}}{X^{2N+2}} E_{N+5/2}(X^2) \quad \text{for } X \rightarrow \infty$$

$$(2.1.15) \quad F(X) = \frac{\gamma}{2} + \ln(2X) + G(X) \quad \text{for } X \rightarrow \infty$$

LaPlace Transform

$$(2.1.16) \quad \int_0^{\infty} e^{-pt} \frac{\ln t}{\sqrt{t}} dt = -\frac{\sqrt{\pi}}{\sqrt{p}} [\gamma + \ln(4p)], \quad p > 0.$$

Computer Subroutines

F(X): DOUBLE PRECISION FUNCTION DFERF(...)
G(X): DOUBLE PRECISION FUNCTION DGERFC(...)

References : Chapter 3, Folders 6, 16 and 18

(2.2) Functions $E_v(x)$, $G_v(x)$ and Related Integrals

$$E_v(x) = \int_1^\infty \frac{e^{-xt}}{t^v} dt, \quad G_v(x) = \int_1^\infty \frac{E_v(xt)}{t^v} dt = -\frac{\partial E_v(x)}{\partial v} = \int_1^\infty \frac{e^{-xt} \ln t}{t^v} dt, \quad x > 0$$

For Integer and Half Odd Integer Orders with Application to

$$I_n(b, T) = \int_T^\infty \frac{e^{-b^2 x^2} \ln x}{x^n} dx, \quad n = 0, 1, 2, \dots, \quad T > 0$$

Introduction

The relation

$$(2.2.1) \quad \int_x^\infty \frac{E_\mu(t)}{t^v} dt = \frac{1}{x^{v-1}} \frac{E_v(x) - E_\mu(x)}{\mu - v}, \text{ or equivalently } \int_1^\infty \frac{E_\mu(xt)}{t^v} dt = \frac{E_v(x) - E_\mu(x)}{\mu - v}, \quad \mu \neq v$$

can be verified by differentiation w.r.t. x . Notice that if $\mu \rightarrow v$, we get the case where $\mu = v$ on the left, and we define $G_v(x)$ by

$$(2.2.2) \quad G_v(x) \equiv \int_1^\infty \frac{E_v(xt)}{t^v} dt = \frac{-\partial E_v(x)}{\partial v} = \int_1^\infty \frac{e^{-xt} \ln t}{t^v} dt \quad \text{or} \quad \int_x^\infty \frac{E_v(t)}{t^v} dt = \frac{1}{x^{v-1}} G_v(x), \quad \mu = v$$

Basic Properties of $E_v(x)$ and $G_v(x)$, $v > 1$

Basic properties of the exponential integral

$$(2.2.3) \quad E_v(x) = \int_1^\infty \frac{e^{-xt}}{t^v} dt, \quad v \geq 0$$

can be found in most handbooks. In this section we repeat some of these properties and note the similarity of $E_v(x)$ and $G_v(x)$

$$(2.2.4) \quad E_{v+1}(x) < E_v(x)$$

$$(2.2.5) \quad G_{v+1}(x) < G_v(x), \quad v \geq 1$$

$$(2.2.6) \quad \frac{e^{-x}}{x+v} < E_v(x) \leq \frac{e^{-x}}{x+v-1}, \quad v \geq 1$$

$$(2.2.7) \quad \frac{e^{-x}}{(x+v)(x+v+1)} < \frac{E_{v+1}(x)}{x+v} < G_v(x) \leq \frac{E_v(x)}{x+v-1} \leq \frac{e^{-x}}{(x+v-1)^2}, \quad v \geq 1$$

$$(2.2.8) \quad vE_{v+1}(x) + xE_v(x) = e^{-x}$$

$$(2.2.9) \quad vG_{v+1}(x) + xG_v(x) = E_{v+1}(x) \quad v \geq 1$$

$$(2.2.10) \quad E'_v(x) = -E_{v-1}(x)$$

$$(2.2.11) \quad G'_v(x) = -G_{v-1}(x), \quad v > 1$$

$$(2.2.12) \quad E_v(0) = 1/(v-1),$$

$$(2.2.13) \quad G_v(0) = 1/(v-1)^2 \quad v > 1$$

Closed Forms

$$(2.2.14) \quad E_{1/2}(x) = \sqrt{\pi} \operatorname{erfc}(\sqrt{x}) / \sqrt{x}, \quad E_{3/2}(x) = 2\sqrt{\pi} \operatorname{ierfc}(\sqrt{x})$$

$$(2.2.15) \quad G_{1/2}(x) = 2\sqrt{\frac{\pi}{x}} G(\sqrt{x})$$

where $G(x)$ is described in Section (2.1) and Chapter 3, Folder 16.

Convergent Series

$$(2.2.16) \quad E_1(x) = -\gamma - \ln x - \sum_{n=1}^{\infty} \frac{(-x)^n}{nn!}$$

$$(2.2.17) \quad E_2(x) = x[\gamma + \ln x - 1] + 1 - \sum_{n=2}^{\infty} \frac{(-x)^n}{(n-1)n!}$$

$$(2.2.18) \quad G_1(x) = \frac{\pi^2}{12} + \frac{1}{2} E_1^2(x) - (\gamma + \ln x) \sum_{n=1}^{\infty} \frac{(-x)^n}{nn!} + \sum_{n=1}^{\infty} \frac{(-x)^n}{n^2 n!} - \sum_{k=2}^{\infty} \frac{(-x)^k}{k} A_k$$

$$(2.2.19) \quad G_2(x) = 1 - \frac{\pi^2}{12} x - \frac{x}{2} (\gamma + \ln x)^2 + x(\gamma + \ln x) - x - x \sum_{n=1}^{\infty} \frac{(-x)^n}{n^2 (n+1)n!} \\ + x \sum_{n=2}^{\infty} \frac{(-x)^n}{n(n+1)} A_n - \frac{x}{2} \sum_{n=2}^{\infty} \frac{(-x)^n}{n+1} D_n$$

where

$$A_n = \frac{1}{n!} \sum_{k=1}^{n-1} \frac{C_k^n}{n-k}, \quad D_n = \frac{1}{n!} \sum_{k=1}^{n-1} \frac{C_k^n}{k(n-k)}, \quad n \geq 2$$

and C_k^n are binomial coefficients. Two other options for $G_2(x)$ are also given in Chapter 3, Folder 18.

Application of $E_v(x)$ and $G_v(x)$ to $I_n(b, T) = \int_T^{\infty} \frac{e^{-b^2 x^2} \ln x}{x^n} dx, \quad n = 0, 1, 2, \dots, \quad T > 0$

Explicit formula

$$(2.2.20) \quad I_n(b, T) = \frac{\ln T}{2T^{n-1}} E_{(n+1)/2}(b^2 T^2) + \frac{1}{4T^{n-1}} G_{(n+1)/2}(b^2 T^2)$$

For $n = 0$ the results are computed in (2.1):

$$(2.2.21) \quad I_0(b, T) = \int_T^{\infty} e^{-b^2 x^2} \ln x dx = \frac{\sqrt{\pi}}{2b} [\operatorname{erfc}(bT) \ln T + G(bT)]$$

For even integers we get the G_v function of half-odd orders:

$$(2.2.22) \quad I_{2n}(b, T) = \frac{\ln T}{2T^{2n-1}} E_{n+1/2}(b^2 T^2) + \frac{1}{4T^{2n-1}} G_{n+1/2}(b^2 T^2) \quad n \geq 0$$

For odd integers, we get the G_v functions of integer orders,

$$(2.2.23) \quad I_{2n+1}(b, T) = \frac{\ln T}{2T^{2n}} E_{n+1}(b^2 T^2) + \frac{1}{4T^{2n}} G_{n+1}(b^2 T^2) \quad n \geq 0$$

Recurrence for $I_n(b, T)$:

$$(2.2.24) \quad \frac{(n+1)}{2b^2} I_{n+2} + I_n = \frac{\ln T}{2b^2} \cdot \frac{e^{-b^2 T^2}}{T^{n+1}} + \frac{1}{4b^2 T^{n+1}} E_{(n+3)/2}(b^2 T^2) \quad n \geq 0$$

and this shows that the even and odd sequences are de-coupled. Also, the amplification factors (for the growth and/or decay of homogeneous solutions)

$$\frac{2b^2}{n+1} \text{ or } \frac{n+1}{2b^2}$$

for forward or backward recurrence show that a stable recurrence occurs (ratios less than or equal to 1) by recursion away from $N_b = [2b^2]$ or N_b+1 since one of these is an even index and one is odd. Notice that if $T=1$ then,

$$(2.2.25) \quad I_n(b, 1) = \frac{1}{4} G_{(n+1)/2}(b^2) = -\frac{1}{4} \left[\frac{\partial}{\partial v} E_v(b^2) \right]_{v=(n+1)/2}$$

Stability of Recurrence Relations

It is known that the recurrence for $E_v(x)$ is stable if one generates $E_v(x)$ for the order closest to x and recurs away from this index with the two-term recurrence relation above. This pattern also applies to $G_v(x)$ and this is what is done to generate sequences in the subroutines for the integer and half-odd integer orders.

Computer Subroutines

The computation of $E_v(x)$ and $G_v(x)$ is described in Chapter3, Folder18. These computations result in subroutines

$E_v(x)$: SUBROUTINE DEXINT(...) for sequences of positive integer orders
SUBROUTINE DHEXINT(...) for sequences of positive half-odd integer orders
 $G_v(x)$: SUBROUTINE DGEXINT(...) for sequences of positive integer orders
SUBROUTINE DGHEXINT(...) for sequences of positive half-odd integer orders

References: Chapter 3, Folders 16 and 18

(2.3) Functions I(a,b,x), J(a,b,x), U(a,b,x), V(a,b,x) and Related Integrals

$$\begin{aligned} I(a,b,x) &= \int_x^\infty e^{-a^2w^2} \operatorname{erfc}(bw)dw, & J(a,b,x) &= \int_x^\infty e^{-a^2w^2} \operatorname{erf}(bw)dw \\ U(a,b,x) &= \int_0^x e^{-a^2w^2} \operatorname{erfc}(bw)dw, & V(a,b,x) &= \int_0^x e^{-a^2w^2} \operatorname{erf}(bw)dw \\ & a \geq 0, \quad b \geq 0 \quad x > 0 \end{aligned}$$

Other Notations

The I, J, U, V notation is commonly used to denote other integrals. Consequently, we often added a subscript 5 to these functions to distinguish them from other notations. The subscript 5 is a designation for Folder 5 in Chapter 3. Thus, I, J, U, and V can also be I_5, J_5, U_5 , and V_5 .

Convergent Series For I(a,b,x)

A series expansion is developed for

$$(2.3.1) \quad I(a,b,x) = \frac{1}{2\sqrt{\pi}\sqrt{a^2+b^2}} G(a,b,x), \quad G(a,b,x) = \sum_{k=0}^{\infty} \frac{(1/2)_k}{k!} \left(\frac{a^2}{a^2+b^2} \right)^k E_{k+3/2}(d^2x^2) \quad a \leq b$$

$$(2.3.2) \quad I(a,b,x) = \frac{be^{-a^2x^2}}{a^2+b^2} \sum_{k=1}^{\infty} \left(\frac{4a^2}{a^2+b^2} \right)^{k-1} [(k-1)! i^{2k-1} \operatorname{erfc}(bx)], \quad a \leq b$$

which converges for all a and b but the convergence is best for $a \leq b$. A companion relation

$$(2.3.3) \quad I(a,b,x) = \frac{\sqrt{\pi}}{2a} \operatorname{erfc}(ax) \operatorname{erfc}(bx) - \frac{b}{a} I(b,a,x) \quad a > b$$

is used for $a > b$ since $I(b,a,x)$ contains the factor $[b^2/(a^2+b^2)]^k$ and the convergence is best for $a > b$. $G(a,b,x)$ is further broken down into

$$(2.3.4) \quad \begin{aligned} \frac{G(a,b,x)}{\sqrt{a^2+b^2}} &= 2 \frac{e^{-d^2x^2}}{a} \tan^{-1} \frac{a}{b} - dx^2 S(a,b,x), & d^2 &= a^2+b^2 \\ S(a,b,x) &= \sum_{k=0}^{\infty} \frac{(1/2)_k}{k!(k+1/2)} \left(\frac{a^2}{a^2+b^2} \right)^k E_{k+1/2}(d^2x^2), & a &\leq b \end{aligned}$$

to break out the dominant behavior when x is small. Both of these series converge without the restrictions $a \leq b$ or $a > b$ but the restrictions ensure that the ratios

$$a^2/d^2 \quad \text{or} \quad b^2/d^2$$

do not exceed 1/2 and each series can be terminated in no more than 50 terms with errors $O(10^{-15})$.

These formulae are manipulated in Chapter 3, Folder 5 to obtain forms which are suitable for computation.

Convergent Series For J(a,b,x)

Notice that

$$(2.3.5) \quad J(a,b,x) = I(a,0,x) - I(a,b,x) = \frac{\sqrt{\pi}}{2a} \operatorname{erfc}(ax) - I(a,b,x)$$

The complete computation for numerical evaluation is given in Chapter 3, Folder 5.

Convergent Series For U(a,b,x)

Notice that

$$(2.3.6) \quad U(a,b,x) = I(a,b,0) - I(a,b,x) = \frac{1}{a\sqrt{\pi}} \tan^{-1} \frac{a}{b} - I(a,b,x)$$

Further details of computation are given in Chapter 3, Folder 5.

Convergent Series For V(a,b,x)

Notice that

$$(2.3.7) \quad V(a,b,x) = \frac{\sqrt{\pi}}{2a} \operatorname{erf}(ax) - U(a,b,x) = \frac{1}{a\sqrt{\pi}} \tan^{-1} \frac{b}{a} - J(a,b,x)$$

The details for a more robust numerical evaluation are given in Chapter 3, Folder 5.

Functional Relations

$$(2.3.8) \quad aI(a,b,x) + bI(b,a,x) = \frac{\sqrt{\pi}}{2} \operatorname{erfc}(ax) \operatorname{erfc}(bx)$$

$$(2.3.9) \quad aJ(a,b,x) + bJ(b,a,x) = \frac{\sqrt{\pi}}{2} [1 - \operatorname{erf}(ax) \operatorname{erf}(bx)] = \frac{\sqrt{\pi}}{2} [\operatorname{erfc}(ax) + \operatorname{erf}(ax) \operatorname{erfc}(bx)]$$

$$(2.3.10) \quad J(a,b,x) + I(a,b,x) = \frac{\sqrt{\pi}}{2a} \operatorname{erfc}(ax)$$

$$(2.3.11) \quad aU(a,b,x) + bU(b,a,x) = \frac{\sqrt{\pi}}{2} [1 - \operatorname{erfc}(ax) \operatorname{erfc}(bx)] = \frac{\sqrt{\pi}}{2} [\operatorname{erf}(ax) + \operatorname{erfc}(ax) \operatorname{erf}(bx)]$$

$$(2.3.12) \quad aV(a,b,x) + bV(b,a,x) = \frac{\sqrt{\pi}}{2} \operatorname{erf}(ax) \operatorname{erf}(bx)$$

$$(2.3.13) \quad U(a,b,x) + V(a,b,x) = \frac{\sqrt{\pi}}{2a} \operatorname{erf}(ax)$$

Asymptotics for $x \rightarrow +\infty$

$$(2.3.14) \quad I(a,b,x) = \frac{1}{2b\sqrt{\pi}} \sum_{k=0}^N \frac{(-1)^k (1/2)_k}{(bx)^{2k}} E_{k+1} [x^2(a^2 + b^2)] + W_N(a,b,x),$$

$$|W_N(a,b,x)| \leq \frac{1}{2b\sqrt{\pi}} \frac{(1/2)_{N+1}}{(bx)^{2N+2}} E_{N+2} [x^2(a^2 + b^2)] \quad a \leq b$$

$$(2.3.15) \quad I(a,b,x) = \frac{\sqrt{\pi}}{2a} \operatorname{erfc}(ax) \operatorname{erfc}(bx) - \frac{b}{2a^2\sqrt{\pi}} \sum_{k=0}^N \frac{(-1)^k (1/2)_k}{(ax)^{2k}} E_{k+1} [x^2(a^2 + b^2)] + R_N(a,b,x),$$

$$|R_N(a,b,x)| \leq \frac{b}{a} |W_N(b,a,x)| \quad a > b$$

Now, we use relations

$$(2.3.16) \quad J(a, b, x) = \int_x^\infty e^{-a^2 w^2} \operatorname{erf}(b w) dw = \frac{\sqrt{\pi}}{2a} \operatorname{erfc}(ax) - I(a, b, x),$$

$$(2.3.17) \quad U(a, b, x) = \int_0^x e^{-a^2 w^2} \operatorname{erfc}(b w) dw = I(a, b, 0) - I(a, b, x) = \frac{1}{a\sqrt{\pi}} \tan^{-1} \frac{a}{b} - I(a, b, x)$$

$$(2.3.18) \quad V(a, b, x) = \int_0^x e^{-a^2 w^2} \operatorname{erf}(b w) dw = \frac{\sqrt{\pi}}{2a} \operatorname{erf}(ax) - U(a, b, x) = \frac{1}{a\sqrt{\pi}} \tan^{-1} \frac{b}{a} - J(a, b, x)$$

to get the expansions for J, U, and V.

Related Functions

A generalization of I(a,b,T)

Details relating to the manipulation of

$$(2.3.19) \quad Y_n(a, b, T) = \int_T^\infty e^{-a^2 w^2} i^n \operatorname{erfc}(bw) dw, \quad n \geq -1$$

$$a > 0, \quad b \geq 0$$

are found in Chapter 3, Folder 29 for the series representations:

For Case I, $a \leq b$,

$$(2.3.20) \quad Y_n(a, b, T) = \frac{be^{-a^2 T^2}}{a^2 + b^2} \sum_{k=1}^{\infty} \left(\frac{4a^2}{a^2 + b^2} \right)^{k-1} \frac{\Gamma(n/2 + k)}{\Gamma(n/2 + 1)} i^{n+2k-1} \operatorname{erfc}(bT), \quad n \geq 0$$

and for case II, $a > b$,

$$(2.3.21) \quad Y_n(a, b, T) = \frac{\sqrt{\pi}}{2a} \sum_{k=0}^n (-1)^k \left(\frac{b}{a} \right)^k i^k \operatorname{erfc}(aT) i^{n-k} \operatorname{erfc}(bT) + (-1)^{n+1} \left(\frac{b}{a} \right)^{n+1} Y_n(b, a, T)$$

with the special case

$$(2.3.22) \quad Y_{-1}(a, b, T) = \frac{\operatorname{erfc}(T\sqrt{a^2 + b^2})}{\sqrt{a^2 + b^2}}.$$

The recurrence

$$(2.3.23) \quad Y_{n-2} = \frac{a^2}{a^2 + b^2} \left[2nY_n + \frac{b}{a^2} e^{-a^2 T^2} i^{n-1} \operatorname{erfc}(bT) \right]$$

is numerically stable on backward recurrence and is used in subroutine INTEG129 to generate even and odd sequences of Y_n .

Integral of I(a,b,T)

Integration of $Y_0(a, b, T) = I_5(a, b, T)$ for Case I, $a \leq b$, gives

$$(2.3.24) \quad \int_T^\infty I_5(a, b, w) dw = \frac{b}{a^2 + b^2} \sum_{k=1}^{\infty} \left(\frac{4a^2}{a^2 + b^2} \right)^{k-1} [(k-1)! Y_{2k-1}(a, b, T)], \quad a \leq b$$

and integration of Case II, $a > b$, in Chapter 3, Folder 5 gives

$$(2.3.25) \quad \int_T^\infty I_5(a, b, w) dw = \frac{\sqrt{\pi}}{2a} \int_T^\infty \operatorname{erfc}(aw) \operatorname{erfc}(bw) dw - \frac{b}{a} \int_T^\infty I_5(b, a, w) dw \quad a > b$$

where the $I_5(b, a, T)$ integral on the right is computed above since the first parameter is less than the second parameter. The integral

$$\int_T^\infty \operatorname{erfc}(aw)\operatorname{erfc}(bw)dw$$

is computed in Chapter3, Folder 9, but we can get an alternate form from

$$Y_1(a, b, T) = \int_T^\infty e^{-a^2 w^2} \operatorname{ierfc}(bw)dw$$

by integration by parts:

$$(2.3.26) \quad \int_T^\infty \operatorname{erfc}(aw)\operatorname{erfc}(bw)dw = \frac{1}{b} \left[\operatorname{erfc}(aT)\operatorname{ierfc}(bT) - \frac{2a}{\sqrt{\pi}} Y_1(a, b, T) \right],$$

with

$$(2.3.27) \quad Y_1(a, b, T) = \frac{be^{-a^2 T^2}}{a^2 + b^2} \sum_{k=1}^\infty \left(\frac{4a^2}{a^2 + b^2} \right)^{k-1} \frac{\Gamma(1/2 + k)}{\Gamma(3/2)} i^{2k} \operatorname{erfc}(bT), \quad \frac{\Gamma(1/2 + k)}{\Gamma(3/2)} = 2(1/2)_k, \quad a \leq b$$

For this computation we can always choose $a \leq b$ since the integral is symmetric in a and b and a can be chosen to be the smaller of the two parameters.

Representations of $i^n \operatorname{erfc}(z)$, $n = -1, 0, 1$

Take $b = 0$ in $I(a, b, x)$:

$$(2.3.28) \quad \frac{\sqrt{\pi}}{2a} \operatorname{erfc}(ax) = \frac{1}{2\sqrt{\pi}} \frac{1}{a} \sum_{k=0}^\infty C_k E_{k+3/2}(a^2 x^2), \quad C_k = (1/2)_k / k!$$

$$(2.3.29) \quad \operatorname{erfc}(z) = \frac{1}{\pi} \sum_{k=0}^\infty C_k E_{k+3/2}(z^2)$$

Differentiate wrt z to get

$$(2.3.30) \quad \frac{e^{-z^2}}{z} = \frac{1}{\sqrt{\pi}} \sum_{k=0}^\infty C_k E_{k+1/2}(z^2)$$

Integrate $\operatorname{erfc}(z)$ above

$$(2.3.31) \quad \operatorname{ierfc}(z) = \frac{1}{\sqrt{\pi}} \operatorname{erfc}(z) - \frac{z}{2\pi} \sum_{k=0}^\infty \frac{(1/2)_k}{k!(k+1)} E_{k+3/2}(z^2)$$

LaPlace Transforms

$$(2.3.32) \quad \int_0^\infty e^{-pt} \frac{\operatorname{erf}(\sqrt{\alpha t})}{\sqrt{t}} dt = \frac{2}{\sqrt{\pi p}} \tan^{-1} \sqrt{\frac{\alpha}{p}}$$

$$(2.3.33) \quad \int_0^\infty e^{-pt} \sqrt{t} \operatorname{erf}(\sqrt{\alpha t}) dt = \frac{1}{p\sqrt{\pi}} \left[\frac{1}{\sqrt{p}} \tan^{-1} \sqrt{\frac{\alpha}{p}} + \frac{\sqrt{\alpha}}{p + \alpha} \right]$$

$$(2.3.34) \quad \int_0^\infty e^{-pt} \frac{\operatorname{erfc}(\sqrt{\alpha t})}{\sqrt{t}} dt = \frac{2}{\sqrt{\pi p}} \tan^{-1} \sqrt{\frac{p}{\alpha}}$$

$$(2.3.35) \quad \int_0^\infty e^{-pt} \sqrt{t} \operatorname{erfc}(\sqrt{\alpha t}) dt = \frac{1}{p\sqrt{\pi}} \left[\frac{1}{\sqrt{p}} \tan^{-1} \sqrt{\frac{p}{\alpha}} - \frac{\sqrt{\alpha}}{p + \alpha} \right]$$

Special Cases

$$(2.3.36) \quad I(a, b, 0) = \int_0^\infty e^{-a^2 w^2} \operatorname{erfc}(bw) dw = \frac{1}{a\sqrt{\pi}} \tan^{-1} \frac{a}{b}$$

$$(2.3.37) \quad I(a, a, x) = \frac{\sqrt{\pi}}{4a} \operatorname{erfc}^2(ax)$$

$$(2.3.38) \quad J(a, b, 0) = \int_0^\infty e^{-a^2 w^2} \operatorname{erf}(bw) dw = \frac{1}{a\sqrt{\pi}} \tan^{-1} \frac{b}{a}$$

$$(2.3.39) \quad V(0, b, x) = \int_0^x \operatorname{erf}(bw) dw = x \operatorname{erf}(bx) - \frac{1}{b\sqrt{\pi}} (1 - e^{-b^2 x^2})$$

Inequalities

A restatement of (2.3.8) gives the relation

$$(2.3.40) \quad W \equiv \frac{\sqrt{\pi}}{2} \operatorname{erfc}(ax) \operatorname{erfc}(bx) = aI(a, b, x) + bI(b, a, x)$$

Divide W by $a+b$. Then the right side is a convex linear combination of $I(a, b, x)$ and $I(b, a, x)$. Therefore

$$(2.3.41) \quad \min[I(a, b, x), I(b, a, x)] \leq \frac{W}{a+b} \leq \max[I(a, b, x), I(b, a, x)]$$

Divide W by $\sqrt{a^2 + b^2}$ and we have the dot product of two vectors, one of which has length 1. By the Cauchy inequality, we have

$$(2.3.42) \quad \left(\frac{W}{\sqrt{a^2 + b^2}} \right)^2 \leq I^2(a, b, x) + I^2(b, a, x)$$

Notice that if $b = a$, then the max and min are the same and

$$(2.3.43) \quad I(a, a, x) = \frac{W}{2a} = \frac{\sqrt{\pi}}{4a} \operatorname{erfc}^2(ax).$$

We have similar results for $J(a, b, x)$:

$$(2.3.44) \quad \bar{W} \equiv \frac{\sqrt{\pi}}{2} [1 - \operatorname{erf}(ax) \operatorname{erf}(bx)] = aJ(a, b, x) + bJ(b, a, x)$$

$$(2.3.45) \quad \min[J(a, b, x), J(b, a, x)] \leq \frac{\bar{W}}{a+b} \leq \max[J(a, b, x), J(b, a, x)]$$

$$(2.3.46) \quad \left(\frac{\bar{W}}{\sqrt{a^2 + b^2}} \right)^2 \leq J^2(a, b, x) + J^2(b, a, x)$$

If $a = b$ then the max and min are equal and

$$(2.3.47) \quad J(a, a, x) = \frac{\bar{W}}{2a} = \frac{\sqrt{\pi}}{4a} [1 - \operatorname{erf}^2(ax)].$$

Because of (2.3.11) and (2.3.12), we also have similar relations for U and V .

Computer Subroutines

I(a,b,x): SUBROUTINE INTEG15(...)

J(a,b,x): SUBROUTINE INTEGJ5(...)

V(a,b,x): SUBROUTINE INTEGV5(...)

$Y_n(a,b,T)$: SUBROUTINE INTEG129(...)

References: Chapter 3, Folder 5, Chapter 3, Folder 29

(2.4) Functions $I_{20}(a,b,T)$ and $I_{20}^c(a,b,T)$

$$I_{20}(a,b,T) = \int_T^\infty e^{-a^2x^2} \operatorname{erf}(bx) \ln x dx, \quad I_{20}^c(a,b,T) = \int_T^\infty e^{-a^2x^2} \operatorname{erfc}(bx) \ln x dx,$$

$$a > 0, \quad b > 0, \quad T \geq 0$$

Series Representations

Case I, $a \leq b$

$$(2.4.1) \quad I_{20}^c(a,b,T) = I_5(a,b,T) \ln T + \frac{E_1(X)}{2a\sqrt{\pi}} \tan^{-1}\left(\frac{a}{b}\right) - \frac{S(a,b,T)}{4\sqrt{\pi}\sqrt{a^2+b^2}} \quad a \leq b$$

where $I_5(a,b,T)$ is the I function of Chapter 3, Folder 5 and

$$S(a,b,T) = \sum_{k=0}^{\infty} \frac{C_k}{(k+1/2)} \left(\frac{a^2}{a^2+b^2} \right)^k E_{k+3/2}(X), \quad X = T^2(a^2+b^2), \quad C_k = (1/2)_k/k!, \quad k \geq 0$$

Notice that $a^2/(a^2+b^2) \leq 1/2$ and the convergence of the S series is better than $O(2^{-k}k^{-3/2})$.

Case II, $a > b$ The reflexive relation

$$(2.4.2) \quad I_{19}^c(a,b,T) = -\operatorname{erfc}(aT)\operatorname{erfc}(bT)\ln T + \frac{2a}{\sqrt{\pi}} I_{20}^c(a,b,T) + \frac{2b}{\sqrt{\pi}} I_{20}^c(b,a,T)$$

is derived in Chapter 3, Folder 20 and used to compute for $a > b$:

$$(2.4.3) \quad I_{20}^c(a,b,T) = \frac{\sqrt{\pi}}{2a} [I_{19}^c(a,b,T) + \operatorname{erfc}(aT)\operatorname{erfc}(bT)\ln T] - \frac{b}{a} I_{20}^c(b,a,T) \quad a > b$$

$$= I_5(a,b,T) \ln T + \frac{\sqrt{\pi}}{2a} I_{19}^c(a,b,T) - \frac{b}{a} \left[\frac{E_1(X)}{2b\sqrt{\pi}} \tan^{-1}\left(\frac{b}{a}\right) - \frac{S(b,a,T)}{4\sqrt{\pi}\sqrt{a^2+b^2}} \right]$$

where $I_{20}^c(b,a,T)$ fits into Case I because the first parameter is smaller than the second parameter.

$I_{19}^c(a,b,T)$ is computed in Chapter 3, Folder 19. $I_{20}^c(0,b,T)$ is evaluated explicitly, and the results for $I_{20}^c(a,0,T)$ are given in Chapter 3, Folder 16. For I_{20} , we can use $\operatorname{erfc}(x)=1-\operatorname{erf}(x)$ and get a pair from

$$(2.4.4) \quad I_{20}(a,b,T) = \frac{\sqrt{\pi}}{2a} [\operatorname{erfc}(aT)\ln T + G(aT)] - I_{20}^c(a,b,T)$$

and $I_{20}^c(a,b,T)$ above where $G(x)$ is computed in Section (2.1). However another analysis yields the pair

$$(2.4.5) \quad I_{20}(a,b,T) = J_5(a,b,T) \ln T + \frac{\sqrt{\pi}}{2a} G(aT) - \left[\frac{E_1(X)}{2a\sqrt{\pi}} \tan^{-1}\left(\frac{a}{b}\right) - \frac{S(a,b,T)}{4\sqrt{\pi}\sqrt{a^2+b^2}} \right], \quad a \leq b$$

and for $a > b$, we have

$$(2.4.6) \quad I_{20}(a,b,T) = I_{20}(a,b,0) - \frac{\sqrt{\pi}}{2a} [\operatorname{erf}(aT)\operatorname{erf}(bT)\ln T - I_{19}(a,b,T)] + \frac{b}{a} [I_{20}(b,a,0) - I_{20}(b,a,T)].$$

Results for $T \rightarrow 0$ in $I_{20}(a,b,0)$ and $I_{20}(b,a,0)$ are given in Chapter 3, Folder 20.

Computer Subroutine

$I_{20}(a, b, T)$ and $I_{20}^c(a, b, T)$: SUBROUTINE INTEG120(...) on KODE=1 and KODE=2

References: Chapter 3, Folder 20

(2.5) Functions $P(a,b,T)$, $P^c(a,b,T)$ and $Q(a,b,T)$

$$P(a,b,T) = \int_T^\infty \frac{e^{-a^2 w^2} \operatorname{erf}(bw)}{w} dw, \quad P^c(a,b,T) = \int_T^\infty \frac{e^{-a^2 w^2} \operatorname{erfc}(bw)}{w} dw,$$

$$Q(a,b,T) = \int_T^\infty e^{-a^2 w^2} E_1(b^2 w^2) dw$$

$$a > 0, \quad b > 0, \quad T \geq 0$$

Series Representations

$$(2.5.1) P(a,b,T) = \begin{cases} \frac{1}{2} E_1(a^2 T^2) - G(\sqrt{X}) - \ln \left[\frac{2\sqrt{a^2 + b^2}}{b + \sqrt{a^2 + b^2}} \right] \operatorname{erfc}(\sqrt{X}) + \frac{\sqrt{X}}{2\sqrt{\pi}} S_1(a,b,X), & a \leq b \\ \frac{1}{2} E_1(a^2 T^2) \operatorname{erf}(bT) + \ln \left[\frac{b + \sqrt{a^2 + b^2}}{a} \right] \operatorname{erfc}(\sqrt{X}) - \frac{bT}{\sqrt{\pi}} S_2(b,a,X), & a > b \end{cases}$$

$$(2.5.2) Q(a,b,T) = \begin{cases} \frac{\sqrt{\pi}}{a} \ln \left[\frac{a + \sqrt{a^2 + b^2}}{b} \right] \operatorname{erfc}(\sqrt{X}) - TS_2(a,b,X) & a \leq b \\ \frac{\sqrt{\pi}}{2a} E_1(b^2 T^2) \operatorname{erfc}(aT) - \frac{\sqrt{\pi}}{a} \ln \left[\frac{2\sqrt{a^2 + b^2}}{a + \sqrt{a^2 + b^2}} \right] \operatorname{erfc}(\sqrt{X}) - \frac{\sqrt{\pi}}{a} G(\sqrt{X}) & a > b \\ + \frac{\sqrt{X}}{2a} S_1(b,a,X) & a > b \end{cases}$$

$$S_1(a,b,X) = \sum_{k=1}^{\infty} C_k \left(\frac{a^2}{a^2 + b^2} \right)^k \frac{E_{k+1/2}(X)}{k}, \quad S_2(a,b,X) = \sum_{k=0}^{\infty} \left(\frac{a^2}{a^2 + b^2} \right)^k \frac{E_{k+1}(X)}{2k+1}$$

$$X = T^2(a^2 + b^2), \quad C_k = \frac{(1/2)_k}{k!}, \quad k=1,2,\dots$$

and the computation of

$$(2.5.3) \quad G(x) = \int_x^\infty \frac{\operatorname{erfc}(v)}{v} dv$$

is described in (2.1). Notice that whenever S_1 and S_2 are used, the powers of $a^2/(a^2+b^2)$ or $b^2/(a^2+b^2)$ are less than (or equal to) $1/2^k$, making the convergence of these series quite acceptable numerically.

Special Cases

$$(2.5.4) \quad P(a,b,0) = \ln \left[\frac{b + \sqrt{a^2 + b^2}}{a} \right], \quad Q(a,b,0) = \frac{\sqrt{\pi}}{a} \ln \left[\frac{a + \sqrt{a^2 + b^2}}{b} \right]$$

$$P(a,0,T) = 0, \quad Q(0,b,T) = \frac{\sqrt{\pi}}{b} \operatorname{erfc}(bT) - TE_1(b^2 T^2)$$

Functional Relations

$$(2.5.5) \quad P(a, b, T) + P^c(a, b, T) = \frac{1}{2} E_1(a^2 T^2).$$

$$(2.5.6) \quad P(a, b, T) = \frac{1}{2} E_1(a^2 T^2) \operatorname{erf}(bT) + \frac{b}{\sqrt{\pi}} Q(b, a, T).$$

To compute $P^c(a, b, T)$ from (2.5.5) and (2.5.1), the subtractions should be done analytically to retain significant digits.

Asymptotics

For bT large, we have

$$(2.5.7) \quad P(a, b, T) \sim \frac{1}{2} E_1(a^2 T^2) - \frac{1}{2bT\sqrt{\pi}} \sum_{k=0}^{\infty} (-1)^k \frac{(1/2)_k}{(bT)^{2k}} E_{k+3/2}(X), \quad X = T^2(a^2 + b^2)$$

$$(2.5.8) \quad P^c(a, b, T) \sim \frac{1}{2bT\sqrt{\pi}} \sum_{k=0}^{\infty} (-1)^k \frac{(1/2)_k}{(bT)^{2k}} E_{k+3/2}(X), \quad X = T^2(a^2 + b^2)$$

$$(2.5.9) \quad Q(a, b, T) \sim \frac{T}{2(bT)^2} \sum_{k=0}^{\infty} (-1)^k \frac{(k)!}{(bT)^{2k}} E_{k+3/2}(X), \quad X = T^2(a^2 + b^2)$$

For aT large, we use (2.5.5) in conjunction with (2.5.8) to compute $P(a, b, T)$

$$(2.5.10) \quad P(a, b, T) = \frac{1}{2} E_1(a^2 T^2) \operatorname{erf}(bT) + \frac{b}{\sqrt{\pi}} Q(b, a, T)$$

$$(2.5.11) \quad P(a, b, T) \sim \frac{1}{2} E_1(a^2 T^2) \operatorname{erf}(bT) + \frac{b}{\sqrt{\pi}} \left[\frac{T}{2(aT)^2} \sum_{k=0}^{\infty} (-1)^k \frac{(k)!}{(aT)^{2k}} E_{k+3/2}(X) \right], \quad X = T^2(a^2 + b^2)$$

$$(2.5.12) \quad P^c(a, b, T) \sim \frac{1}{2} E_1(a^2 T^2) \operatorname{erfc}(bT) - \frac{b}{\sqrt{\pi}} \left[\frac{T}{2(aT)^2} \sum_{k=0}^{\infty} (-1)^k \frac{(k)!}{(aT)^{2k}} E_{k+3/2}(X) \right], \quad X = T^2(a^2 + b^2)$$

For large aT in $Q(a, b, T)$, we solve for Q from (2.5.5), exchange parameters and use (2.5.6),

$$(2.5.13) \quad Q(a, b, T) = \frac{\sqrt{\pi}}{a} \left[P(b, a, T) - \frac{1}{2} E_1(b^2 T^2) \operatorname{erf}(aT) \right]$$

$$(2.5.14) \quad Q(a, b, T) \sim \frac{\sqrt{\pi}}{a} \left[\frac{1}{2} E_1(b^2 T^2) \operatorname{erfc}(aT) - \frac{1}{2aT\sqrt{\pi}} \sum_{k=0}^{\infty} (-1)^k \frac{(1/2)_k}{(aT)^{2k}} E_{k+3/2}(X) \right], \quad X = T^2(a^2 + b^2).$$

For $a \rightarrow 0$ we get

$$(2.5.15) \quad P(a, b, T) = \frac{1}{2} E_1(a^2 T^2) - G(bT) + O(a^2) = -\frac{\gamma}{2} - \ln(aT) - G(bT) + O(a^2) \quad a \rightarrow 0$$

where $G(x)$ is defined in (2.1) with its properties displayed in Chapter 3, Folders 6 and 16.

Computer Subroutines

P(a,b,T) or P^c(a,b,T): SUBROUTINE INTEG P(...) with **KODE=1** or **KODE=2**

Q(a,b,T): SUBROUTINE INTEG Q(...)

References: Chapter 3, Folders 6, 11, and 16

(2.6) Functions $I_1(a,b,T)$ and $I_1^c(a,b,T)$

$$I_1(a,b,T) = \int_T^\infty \frac{e^{-a^2 w^2} \operatorname{erf}(bw)}{w^2} dw = \frac{1}{2} \int_0^t \frac{e^{-a^2/\tau} \operatorname{erf}(b/\sqrt{\tau})}{\sqrt{\tau}} d\tau$$

$$I_1^c(a,b,T) = \int_T^\infty \frac{e^{-a^2 w^2} \operatorname{erfc}(bw)}{w^2} dw = \frac{1}{2} \int_0^t \frac{e^{-a^2/\tau} \operatorname{erfc}(b/\sqrt{\tau})}{\sqrt{\tau}} d\tau$$

$$a > 0, \quad b > 0, \quad T = \frac{1}{\sqrt{t}}, \quad t > 0$$

Other Notations

See the Preface for a detailed explanation of the notation used in the edition dated August, 2003. In that version, I_1 and I_1^c were defined by the second integral of the title lines. In order to refer to the first integral, the symbols \bar{I}_1 or \bar{I}_1^c were used. In this edition, I_1 and I_1^c are defined by the first integral of the title lines and there is no \bar{I}_1 or \bar{I}_1^c .

Representations

$$(2.6.1) \quad I_1(a,b,T) = \frac{e^{-a^2 T^2} \operatorname{erf}(bT)}{T} + \frac{b}{\sqrt{\pi}} E_1(X) - 2a^2 J_5(a,b,T), \quad X = (a^2 + b^2)T^2$$

$$(2.6.2) \quad I_1(a,b,T) = \frac{e^{-a^2 T^2} \operatorname{erf}(bT)}{T} + \frac{b}{\sqrt{\pi}} E_1(X) - a\sqrt{\pi} \operatorname{erfc}(aT) + 2a^2 I_5(a,b,T)$$

$$= -\frac{e^{-a^2 T^2} \operatorname{erfc}(bT)}{T} + \frac{b}{\sqrt{\pi}} E_1(X) + \frac{\sqrt{\pi}}{T} \operatorname{ierfc}(aT) + 2a^2 I_5(a,b,T)$$

$$(2.6.3) \quad I_1(a,b,T) = \frac{\sqrt{\pi}}{T} \operatorname{erf}(bT) \operatorname{ierfc}(aT) + \frac{b}{\sqrt{\pi}} E_1(X) - 2ab I_5(b,a,T)$$

$$(2.6.4) \quad I_1^c(a,b,T) = \frac{e^{-a^2 T^2} \operatorname{erfc}(bT)}{T} - \frac{b}{\sqrt{\pi}} E_1(X) - 2a^2 I_5(a,b,T)$$

$$(2.6.5) \quad I_1^c(a,b,T) = \frac{\sqrt{\pi}}{T} \operatorname{erfc}(bT) \operatorname{ierfc}(aT) - \frac{b}{\sqrt{\pi}} E_1(X) + 2ab I_5(b,a,T)$$

where J_5 and I_5 are the J and I integrals of Folder 5 in Chapter 3,

$$(2.6.6) \quad J_5(a,b,T) = J(a,b,T) = \int_T^\infty e^{-a^2 x^2} \operatorname{erf}(bx) dx,$$

$$I_5(a,b,T) = I(a,b,T) = \int_T^\infty e^{-a^2 x^2} \operatorname{erfc}(bx) dx$$

Functional Relations

$$(2.6.7) \quad I_1(a,b,T) + I_1^c(a,b,T) = \frac{\sqrt{\pi}}{T} \operatorname{ierfc}(aT)$$

Asymptotics for small t

$$(2.6.8) \quad I_1^c(a, b, T) \sim \frac{b}{2\sqrt{\pi}} \sum_{k=0}^N C_k \left(\frac{t}{b^2} \right)^{k+1} E_{k+2} \left(\frac{a^2 + b^2}{t} \right) + R_N, \quad T = 1/\sqrt{t}$$

$$(2.6.9) \quad I_1(a, b, T) = \sqrt{\pi t} \operatorname{ierfc}(a/\sqrt{t}) - I_1^c(a, b, T)$$

$$C_k = (-1)^k (1/2)_k, \quad k = 0, 1, \dots \quad |R_N| \leq \frac{b}{2\sqrt{\pi}} |C_{N+1}| \left(\frac{t}{b^2} \right)^{N+2} E_{N+3} \left(\frac{a^2 + b^2}{t} \right)$$

Special Cases, T>0

$$(2.6.10) \quad b=0, \quad I_1(a, 0, T) = 0$$

$$(2.6.11) \quad a=0, \quad I_1(0, b, T) = \int_T^\infty \frac{\operatorname{erf}(bw)}{w^2} dw = \frac{\operatorname{erf}(bT)}{T} + \frac{b}{\sqrt{\pi}} E_1(b^2 T^2)$$

Computer Subroutines

$I_1(a, b, T)$ or $I_1^c(a, b, T)$: SUBROUTINE INTEG11(...) with KODE=1 or KODE=2

References: Chapter 3, Folders 1, 2, and 10

(2.7) Functions $I_{13}(a,b,T)$ and $I_{13}^c(a,b,T)$

$$I_{13}(a,b,T) = \int_T^\infty \frac{e^{-a^2 w^2} \operatorname{erf}(bw)}{w^3} dw = \frac{1}{2} \int_0^t e^{-a^2/u} \operatorname{erf}(b/\sqrt{u}) du,$$

$$I_{13}^c(a,b,T) = \int_T^\infty \frac{e^{-a^2 w^2} \operatorname{erfc}(bw)}{w^3} dw = \frac{1}{2} \int_0^t e^{-a^2/u} \operatorname{erfc}(b/\sqrt{u}) du$$

$$a > 0, \quad b > 0, \quad T = \frac{1}{\sqrt{t}}, \quad t > 0$$

Representations

$$(2.7.1) \quad I_{13}(a,b,T) = \frac{e^{-a^2 T^2}}{2T^2} \operatorname{erf}(bT) + \frac{b}{T} i \operatorname{erfc}(T\sqrt{a^2 + b^2}) - a^2 P(a,b,T)$$

$$(2.7.2) \quad I_{13}(a,b,T) = \frac{\operatorname{erf}(bT)}{2T^2} E_2(a^2 T^2) + \frac{b}{2T\sqrt{\pi}} E_{3/2}[T^2(a^2 + b^2)] - \frac{a^2 b}{\sqrt{\pi}} Q(b,a,T)$$

where P and Q are the functions of Chapter 3, Folder11. For the complementary integral, we have

$$(2.7.3) \quad I_{13}^c(a,b,T) = \frac{e^{-a^2 T^2}}{2T^2} \operatorname{erfc}(bT) - \frac{a^2}{2} E_1(a^2 T^2) - \frac{b}{T} i \operatorname{erfc}(T\sqrt{a^2 + b^2}) + a^2 P(a,b,T)$$

$$(2.7.4) \quad I_{13}^c(a,b,T) = \frac{1}{2T^2} E_2(a^2 T^2) \operatorname{erfc}(bT) - \frac{b}{2T\sqrt{\pi}} E_{3/2}[T^2(a^2 + b^2)] + \frac{a^2 b}{\sqrt{\pi}} Q(b,a,T)$$

$$(2.7.5) \quad I_{13}^c(a,b,T) = \frac{1}{2T^2} E_2(a^2 T^2) - I_{13}(a,b,T)$$

where $E_{3/2}(x^2) = 2\sqrt{\pi} i \operatorname{erfc}(x)$. Significant digits in (2.7.3) can be saved if the E and P functions are combined analytically before evaluation (See (2.5.1)).

Computer Subroutine

$I_{13}(a,b,T)$ or $I_{13}^c(a,b,T)$: SUBROUTINE INTEG13(...) with KODE=1 or KODE=2

Reference: Chapter 3, Folder13

(2.8) Functions $I_2(a, b, T)$, $I_2^c(a, b, T)$, $I_9(a, b, T)$ and $I_9^c(a, b, T)$

$$I_2(a, b, T) = \int_0^T \operatorname{erf}(aw) \operatorname{erf}(bw) dw = \frac{1}{2} \int_t^\infty \frac{\operatorname{erf}(a/\sqrt{u}) \operatorname{erf}(b/\sqrt{u})}{u^{3/2}} du,$$

$$I_2^c(a, b, T) = \int_T^\infty \operatorname{erfc}(aw) \operatorname{erfc}(bw) dw = \frac{1}{2} \int_0^t \frac{\operatorname{erfc}(a/\sqrt{u}) \operatorname{erfc}(b/\sqrt{u})}{u^{3/2}} du$$

$$I_9(a, b, T) = \int_0^T w \operatorname{erf}(aw) \operatorname{erf}(bw) dw = \frac{1}{2} \int_t^\infty \frac{\operatorname{erf}(a/\sqrt{u}) \operatorname{erf}(b/\sqrt{u})}{u^2} du$$

$$I_9^c(a, b, T) = \int_T^\infty w \operatorname{erfc}(aw) \operatorname{erfc}(bw) dw = \frac{1}{2} \int_0^t \frac{\operatorname{erfc}(a/\sqrt{u}) \operatorname{erfc}(b/\sqrt{u})}{u^2} du$$

$$a > 0, \quad b > 0, \quad T = \frac{1}{\sqrt{t}}, \quad t > 0$$

Representations

$$(2.8.1) \quad I_2(a, b, T) = T \operatorname{erf}(aT) \operatorname{erf}(bT) + \frac{e^{-a^2 T^2}}{a\sqrt{\pi}} \operatorname{erf}(bT) + \frac{e^{-b^2 T^2}}{b\sqrt{\pi}} \operatorname{erf}(aT) - \frac{\sqrt{a^2 + b^2}}{ab\sqrt{\pi}} \operatorname{erf}(T\sqrt{a^2 + b^2})$$

Now from Chapter 3, Folder 7, we have

$$(2.8.2) \quad I_2^c(a, b, T) = J_3(a, b, 0, T)$$

$$= \frac{e^{-a^2 T^2} \operatorname{erfc}(bT)}{a\sqrt{\pi}} + \frac{e^{-b^2 T^2} \operatorname{erfc}(aT)}{b\sqrt{\pi}} - \operatorname{Terfc}(aT) \operatorname{erfc}(bT) - \frac{\sqrt{a^2 + b^2}}{ab\sqrt{\pi}} \operatorname{erfc}(T\sqrt{a^2 + b^2})$$

and the following expression resolves the indeterminant form for small a ,

$$(2.8.3) \quad J_3(a, b, 0, T) = \operatorname{erfc}(aT) \operatorname{ierfc}(bT) / b - S(a, b, 0, T)$$

$$S(a, b, 0, T) = \frac{a}{\pi b} \left[\frac{\sqrt{\pi} \operatorname{erfc}(TX)}{X + b} - \frac{bT}{2X} \sum_{m=0}^{\infty} \frac{(3/2)_m}{(m+1)!} \left(\frac{a^2}{a^2 + b^2} \right)^m E_{m+3/2}(T^2 X^2) \right]$$

$$X^2 = a^2 + b^2, \quad a \leq b.$$

Since $I_2^c(a, b, T)$ is symmetric in a and b , we can always take a to be the smaller of the two parameters giving rapid convergence in the series since $a^2 / (a^2 + b^2) \leq 1/2$ and the other terms are $O(1/\sqrt{m})$.

$$(2.8.4) \quad I_2^c(a, b, 0) = J_3(a, b, 0, 0) = \frac{1}{a\sqrt{\pi}} + \frac{1}{b\sqrt{\pi}} - \frac{\sqrt{a^2 + b^2}}{ab\sqrt{\pi}} = \frac{(2/\sqrt{\pi})}{a + b + \sqrt{a^2 + b^2}}$$

The power series for $I_2(a, b, T)$ is

$$(2.8.5) \quad I_2(a, b, T) = \int_0^T \operatorname{erf}(aw) \operatorname{erf}(bw) dw$$

$$= \frac{4abT^3}{\pi} \sum_{k=0}^{\infty} \frac{U_k(a^2, b^2) T^{2k}}{2k+3} = \frac{4T(aT)(bT)}{\pi} \sum_{k=0}^{\infty} \frac{U_k(a^2 T^2, b^2 T^2)}{2k+3}$$

where

$$(2.8.6) \quad U_k(a^2, b^2) = \sum_{m=0}^k C_m(a^2) C_{k-m}(b^2), \quad C_k(a^2) = \frac{(-1)^k a^{2k}}{k!(2k+1)}, \quad k \geq 0$$

and

$$(2.8.7) \quad I_2^c(a, b, T) = \frac{(2/\sqrt{\pi})}{a+b+\sqrt{a^2+b^2}} - T + \frac{2T(aT)}{\sqrt{\pi}} \sum_{k=0}^{\infty} \frac{C_k(a^2 T^2)}{2k+2} + \frac{2T(bT)}{\sqrt{\pi}} \sum_{k=0}^{\infty} \frac{C_k(b^2 T^2)}{2k+2} - \frac{4T(aT)(bT)}{\pi} \sum_{k=0}^{\infty} \frac{U_k(a^2 T^2, b^2 T^2)}{2k+3}.$$

A computational form for $I_2^c(a, b, T)$ for aT and bT bounded away from zero (larger parameters) is

$$(2.8.8) \quad I_2^c(a, b, T) = \frac{T}{(aT)(bT)} \left[\frac{\text{ierfc}(T\sqrt{a^2+b^2})}{\sqrt{\pi}} - \text{ierfc}(aT)\text{ierfc}(bT) \right]$$

From Chapter 3, Folder 29, we also have

$$(2.8.9) \quad I_2^c(a, b, T) = \int_T^{\infty} \text{erfc}(aw) \text{erfc}(bw) dw = \frac{1}{b} \left[\text{erfc}(aT) \text{ierfc}(bT) - \frac{2a}{\sqrt{\pi}} Y_1(a, b, T) \right],$$

with

$$(2.8.10) \quad Y_1(a, b, T) = \frac{be^{-a^2 T^2}}{a^2 + b^2} \sum_{k=1}^{\infty} \left(\frac{4a^2}{a^2 + b^2} \right)^{k-1} \frac{\Gamma(1/2 + k)}{\Gamma(3/2)} i^{2k} \text{erfc}(bT), \quad \frac{\Gamma(1/2 + k)}{\Gamma(3/2)} = 2(1/2)_k, \quad a \leq b$$

For this computation we can always choose $a \leq b$ since the integral is symmetric in a and b and a can be chosen to be the smaller of the two parameters. This makes the convergence of $Y_1(a, b, T)$ rapid since $a^2/(a^2 + b^2) \leq 1/2$ and the other factors are $O(1/\sqrt{k})$.

Other representations which resolve the indeterminate forms (2.8.1) and (2.8.2) for a or b to zero are

$$(2.8.11) \quad I_2(a, b, T) = T \text{erf}(aT) \text{erf}(bT) + \frac{e^{-b^2 T^2}}{b\sqrt{\pi}} \text{erf}(aT) - 2 \left(\frac{1}{a\sqrt{\pi}} + R \right) e^{-a^2 T^2/2} \sinh(a^2 T^2/2) \\ - R e^{-a^2 T^2} \text{erf}(bT) + RT \sqrt{a^2 + b^2} e^{-a^2 T^2} \sum_{n=1}^{\infty} (-2)^n i^n \text{erfc}(bT) (bT\phi)^{n-1}$$

where

$$(2.8.12) \quad R = \frac{1}{b\sqrt{\pi}} \cdot \frac{a}{b + \sqrt{a^2 + b^2}}, \quad bT\phi = \frac{a^2 T}{b + \sqrt{a^2 + b^2}}$$

and, without loss of generality we take $a \leq b$. For $I_2^c(a, b, T)$ and $a \leq b$, we have

$$(2.8.13) \quad I_2^c(a, b, T) = \text{erfc}(aT) \frac{\text{ierfc}(bT)}{b} - R e^{-a^2 T^2} \text{erfc}(bT) \\ - R T e^{-a^2 T^2} \sqrt{a^2 + b^2} \sum_{n=1}^{\infty} (-2)^n i^n \text{erfc}(bT) (bT\phi)^{n-1}$$

The powers in the series are less than one if (aT) is less than $(1 + \sqrt{2})$ with $a \leq b$ and the series converges rapidly since

$$i^n \text{erfc}(bT) \leq i^n \text{erfc}(0) = \frac{1}{2^n \Gamma(n/2 + 1)}, \quad n \geq 0.$$

For $I_9(a, b, T)$ and $I_9^c(a, b, T)$, we get

$$(2.8.14) \quad 2I_9(a, b, T) = T \cdot I_2(a, b, T) - \frac{1}{a\sqrt{\pi}} V_5(a, b, T) - \frac{1}{b\sqrt{\pi}} V_5(b, a, T) - \frac{\sqrt{a^2 + b^2}}{ab\sqrt{\pi}} \left[T \operatorname{erf}(T\sqrt{a^2 + b^2}) - \frac{1}{\sqrt{\pi}\sqrt{a^2 + b^2}} (1 - e^{-T^2(a^2 + b^2)}) \right]$$

$$(2.8.15) \quad 2I_9(a, b, T) = T^2 \operatorname{erf}(aT) \operatorname{erf}(bT) + \frac{Te^{-a^2 T^2} \operatorname{erf}(bT)}{a\sqrt{\pi}} + \frac{Te^{-b^2 T^2} \operatorname{erf}(aT)}{b\sqrt{\pi}} - \frac{1}{a\sqrt{\pi}} V_5(a, b, T) - \frac{1}{b\sqrt{\pi}} V_5(b, a, T) - \frac{1}{ab\pi} (1 - e^{-T^2(a^2 + b^2)})$$

$$(2.8.16) \quad 2I_9^c(a, b, T) = T \cdot I_2^c(a, b, T) + \frac{1}{a\sqrt{\pi}} I_5(a, b, T) + \frac{1}{b\sqrt{\pi}} I_5(b, a, T) - \frac{1}{ab\sqrt{\pi}} \operatorname{ierfc}(T\sqrt{a^2 + b^2})$$

and

$$(2.8.17) \quad 2I_9^c(a, b, T) = -T^2 \operatorname{erfc}(aT) \operatorname{erfc}(bT) + \frac{Te^{-a^2 T^2} \operatorname{erfc}(bT)}{a\sqrt{\pi}} + \frac{Te^{-b^2 T^2} \operatorname{erfc}(aT)}{b\sqrt{\pi}} + \frac{1}{a\sqrt{\pi}} I_5(a, b, T) + \frac{1}{b\sqrt{\pi}} I_5(b, a, T) - \frac{1}{ab\sqrt{\pi}} \frac{e^{-T^2(a^2 + b^2)}}{\sqrt{\pi}} = \frac{-\operatorname{ierfc}(aT) \operatorname{ierfc}(bT)}{ab} + \frac{1}{a\sqrt{\pi}} I_5(a, b, T) + \frac{1}{b\sqrt{\pi}} I_5(b, a, T)$$

The V_5 and I_5 functions are the V and I functions of Chapter3, Folder 5.

The corresponding expressions for $I_9(a, b, T)$ and $I_9^c(a, b, T)$ for $a \leq b$ which remove the indeterminacies for a to zero are

$$(2.8.18) \quad 2I_9(a, b, T) = T^2 \operatorname{erf}(aT) \operatorname{erf}(bT) + \frac{Te^{-b^2 T^2} \operatorname{erf}(aT)}{b\sqrt{\pi}} - \frac{1}{b\sqrt{\pi}} V_5(b, a, T) + U(a, b, T)$$

$$U(a, b, T) = H_1(a, b, T) + H_2(a, b, T) - W(a, b, T), \quad a \leq b$$

and

$$(2.8.19) \quad 2I_9^c(a, b, T) = \frac{\operatorname{Terfc}(aT)}{b} \operatorname{ierfc}(bT) + \frac{1}{b\sqrt{\pi}} I_5(b, a, T) + W(a, b, T), \quad a \leq b$$

where

$$H_1(a, b, T) = \frac{1}{a\sqrt{\pi}} \left[Te^{-a^2 T^2} - \frac{\sqrt{\pi}}{2a} \operatorname{erf}(aT) \right], \quad H_2(a, b, T) = \left[\frac{1}{a^2 \pi} \tan^{-1} \left(\frac{a}{b} \right) - \frac{1}{ab\pi} \right]$$

$$W(a, b, T) = -\frac{e^{-a^2 T^2} \operatorname{ierfc}(bT)}{ab\sqrt{\pi}} + \frac{1}{a\sqrt{\pi}} I_5(a, b, T) = \frac{1}{a\sqrt{\pi}} \left[-\frac{e^{-a^2 T^2} \operatorname{ierfc}(bT)}{b} + \frac{\operatorname{ierfc}(T\sqrt{a^2 + b^2})}{d} \right] + G_9(a, b, T)$$

$$G_9(a, b, T) = \frac{1}{2\pi d^2} \sum_{k=1}^{\infty} \frac{(1/2)_k}{k!} \left(\frac{a}{d} \right)^{2k-1} E_{k+3/2}(d^2 T^2), \quad d^2 = a^2 + b^2.$$

and the representations which remove the indeterminacies for a to zero are

$$H_1(a, b, T) = \frac{2T^2}{\sqrt{\pi}} \sum_{k=1}^{\infty} \frac{(-1)^k (aT)^{2k-1}}{(k-1)!(2k+1)}, \quad H_2(a, b, T) = \frac{1}{b^2 \pi} \sum_{k=1}^{\infty} \frac{(-1)^k (a/b)^{2k-1}}{(2k+1)}, \quad \frac{a}{b} < 1$$

$$W(a, b, T) = \frac{(a/b)e^{-a^2 T^2}}{\sqrt{\pi}\sqrt{a^2 + b^2} (b + \sqrt{a^2 + b^2})} \left[-\operatorname{ierfc}(bT) + bT \sum_{n=2}^{\infty} (-2)^{n-1} n! \operatorname{erfc}(bT) (bT)^{n-2} \right] + G_9(a, b, T)$$

Asymptotics for small and large T

For $I_2^c(a, b, T)$, (2.8.4) gives the case for $T \rightarrow 0$. For $I_2(a, b, T)$, (2.8.1) gives

$$(2.8.20) \quad I_2(a, b, T) \sim T - \frac{\sqrt{a^2 + b^2}}{ab\sqrt{\pi}} \text{ for } T \rightarrow \infty.$$

For $I_9^c(a, b, T)$ we have

$$(2.8.21) \quad I_9^c(a, b, 0) = \frac{1}{2ab\pi} \left[\frac{b}{a} \tan^{-1} \left(\frac{a}{b} \right) + \frac{a}{b} \tan^{-1} \left(\frac{b}{a} \right) - 1 \right].$$

For $I_9(a, b, T)$ and $T \rightarrow \infty$,

$$(2.8.22) \quad I_9(a, b, T) \approx \frac{1}{2} \left[T^2 - \frac{1}{a^2\pi} \tan^{-1} \left(\frac{b}{a} \right) - \frac{1}{b^2\pi} \tan^{-1} \left(\frac{a}{b} \right) - \frac{1}{ab\pi} \right], \quad T \rightarrow \infty$$

follows from (2.8.15) with

$$V_5(a, b, T) \approx \frac{1}{a\sqrt{\pi}} \tan^{-1} \left(\frac{b}{a} \right), \quad T \rightarrow \infty.$$

Computer Subroutines

$I_2(a, b, T)$ or $I_2^c(a, b, T)$: SUBROUTINE INTEG12(...) with KODE=1 or KODE=2

$I_9(a, b, T)$ or $I_9^c(a, b, T)$: SUBROUTINE INTEG19(...) with KODE=1 or KODE=2

References: Chapter 3, Folders 7, 9, and 29

(2.9) Function $I_{19}(a,b,T)$ and $I_{19}^c(a,b,T)$

$$I_{19}(a,b,T) = \int_0^T \frac{\operatorname{erf}(aw)\operatorname{erf}(bw)}{w} dw = \frac{1}{2} \int_t^\infty \frac{\operatorname{erf}(a/\sqrt{\tau})\operatorname{erf}(b/\sqrt{\tau})}{\tau} d\tau$$

$$I_{19}^c(a,b,T) = \int_T^\infty \frac{\operatorname{erfc}(aw)\operatorname{erfc}(bw)}{w} dw = \frac{1}{2} \int_0^t \frac{\operatorname{erfc}(a/\sqrt{\tau})\operatorname{erfc}(b/\sqrt{\tau})}{\tau} d\tau$$

$$a > 0, \quad b > 0, \quad T = 1/\sqrt{t}, \quad t > 0$$

Representations

$$(2.9.1) \quad I_{19}^c(a,b,T) = G(bT)\operatorname{erfc}(aT) - \frac{a}{2\pi\sqrt{a^2+b^2}} \sum_{k=0}^{\infty} C_k \left(\frac{a^2}{a^2+b^2} \right)^k G_{k+3/2}(X)$$

$$+ \frac{a}{\sqrt{\pi}} \ln \left[\frac{b^2}{a^2+b^2} \right] I_5(a,b,T) \quad a \leq b$$

$$+ \frac{a}{2\pi\sqrt{a^2+b^2}} \sum_{k=1}^{\infty} \left(\frac{a^2}{a^2+b^2} \right)^k E_{k+3/2}(X) \sum_{m=1}^k \frac{C_{k-m}}{m}, \quad X = T^2(a^2+b^2).$$

where $G(X)$ is the function of Chapter 3, Folder 16; $I_5(a,b,T)$ is the I function of Chapter 3, Folder 5, $C_k = (1/2)_k/k!$, $k \geq 0$, and $G_{k+3/2}(X)$ and $E_{k+3/2}(X)$ are the functions of Chapter 3, Folder 18. The convergence of the series is rapid since $a^2/(a^2+b^2)$ is at most $1/2$.

The representation for $a > b$ is obtained by exchanging a and b since $I_{19}^c(a,b,T)$ is symmetric in a and b . For $I_{19}(a,b,T)$ we get

$$(2.9.2) \quad I_{19}(a,b,T) = F(aT) - [G(bT) - I_{19}^c(a,b,T)]_{T \rightarrow 0} + [G(bT) - I_{19}^c(a,b,T)], \quad a \leq b$$

$$(2.9.3) \quad I_{19}(a,b,T) = F(bT) - [G(aT) - I_{19}^c(b,a,T)]_{T \rightarrow 0} + [G(aT) - I_{19}^c(b,a,T)], \quad a > b$$

and the limit for $T \rightarrow 0$ is computable from I_{19}^c above:

$$(2.9.4) \quad G(bT) - I_{19}^c(a,b,T) = G(bT) - G(bT)\operatorname{erfc}(aT) - R(a,b,T) = G(bT)\operatorname{erf}(aT) - R(a,b,T)$$

where R is the regular part of I_{19}^c ,

$$(2.9.5) \quad R(a,b,T) = \frac{a}{\sqrt{\pi}} \ln \left[\frac{b^2}{a^2+b^2} \right] I_5(a,b,T) - \frac{a}{2\pi\sqrt{a^2+b^2}} \sum_{k=0}^{\infty} C_k \left(\frac{a^2}{a^2+b^2} \right)^k G_{k+3/2}(X)$$

$$+ \frac{a}{2\pi\sqrt{a^2+b^2}} \sum_{n=1}^{\infty} \left(\frac{a^2}{a^2+b^2} \right)^n E_{n+3/2}(X) \sum_{m=1}^n \frac{C_{n-m}}{m}, \quad X = T^2(a^2+b^2)$$

$$a \leq b$$

$$\text{with } C_k = (1/2)_k/k!, \quad G_{k+3/2}(0) = \frac{1}{(k+1/2)^2}, \quad E_{n+3/2}(0) = \frac{1}{(n+1/2)}, \quad I_5(a,b,0) = \frac{1}{a\sqrt{\pi}} \tan^{-1} \frac{a}{b}$$

Then the difference is

$$(2.9.6) \quad \left[G(bT) - I_{19}^c(a, b, T) \right]_{T \rightarrow 0} = -R(a, b, 0), \quad a \leq b$$

since from Chapter 3, Folder18,

$$(2.9.7) \quad G(bT) \operatorname{erf}(aT) = \operatorname{erf}(aT) \left[F(bT) - \frac{\gamma}{2} - \ln(2bT) \right] \rightarrow 0 \quad \text{as } T \rightarrow 0.$$

For $a > b$ we simply exchange a and b in the formulas since both I_{19} and I_{19}^c are symmetric in a and b .

Computer Subroutine

$I_{19}(a, b, T)$ or $I_{19}^c(a, b, T)$: SUBROUTINE INTEG19(...) with KODE=1 or KODE=2

References: Chapter 3, Folders 5, 16, 18 and 19

(2.10) Functions $I_6(a,b,T)$ and $I_6^c(a,b,T)$ and Related Integrals

$$I_6(a,b,T) = \int_T^\infty \frac{\text{erf}(aw)\text{erf}(bw)}{w^2} dw = \frac{1}{2} \int_0^t \frac{1}{\sqrt{u}} \text{erf}\left(\frac{a}{\sqrt{u}}\right) \text{erf}\left(\frac{b}{\sqrt{u}}\right) du,$$

$$I_6^c(a,b,T) = \int_T^\infty \frac{\text{erfc}(aw)\text{erfc}(bw)}{w^2} dw = \frac{1}{2} \int_0^t \frac{1}{\sqrt{u}} \text{erfc}\left(\frac{a}{\sqrt{u}}\right) \text{erfc}\left(\frac{b}{\sqrt{u}}\right) du$$

$$a > 0, \quad b > 0, \quad T = \frac{1}{\sqrt{t}}, \quad t > 0$$

Other Notations

The symbol $I(a,b,T)$ is a common symbol for integrals and is used in Folder 6 where the development occurs. We chose to define this integral for this part of the presentation as $I_6(a,b,T)$ to make it unique.

Representations

Symmetric Form

$$(2.10.1) \quad I_6(a,b,T) = \frac{\text{erf}(aT)\text{erf}(bT)}{T} + \frac{aE_1(a^2T^2)}{\sqrt{\pi}} \text{erf}(bT)$$

$$+ \frac{bE_1(b^2T^2)}{\sqrt{\pi}} \text{erf}(aT) + \frac{2}{\sqrt{\pi}} \left[a \ln\left(\frac{b + \sqrt{a^2 + b^2}}{a}\right) + b \ln\left(\frac{a + \sqrt{a^2 + b^2}}{b}\right) \right] \text{erfc}(\sqrt{X})$$

$$- \frac{2abT}{\pi} \left[\sum_{k=0}^{\infty} \left(\frac{a^2}{a^2 + b^2} \right)^k \frac{E_{k+1}(X)}{2k+1} + \sum_{k=0}^{\infty} \left(\frac{b^2}{a^2 + b^2} \right)^k \frac{E_{k+1}(X)}{2k+1} \right],$$

$$T = 1/\sqrt{t}, \quad X = (a^2 + b^2)/t = T^2(a^2 + b^2).$$

Non-symmetric form for $a \leq b$ is

$$(2.10.2) \quad I_6(a,b,T) = \text{erf}(aT) \left[\frac{\text{erf}(bT)}{T} + \frac{b}{\sqrt{\pi}} E_1(b^2T^2) \right] + \frac{a}{\sqrt{\pi}} E_1(a^2T^2)$$

$$- \frac{2a}{\sqrt{\pi}} G(\sqrt{X}) + \frac{2}{\sqrt{\pi}} \left[-a \ln\left(\frac{2\sqrt{a^2 + b^2}}{b + \sqrt{a^2 + b^2}}\right) + b \ln\left(\frac{a + \sqrt{a^2 + b^2}}{b}\right) \right] \text{erfc}(\sqrt{X})$$

$$- \frac{2abT}{\pi} E_1(X) + \frac{a\sqrt{X}}{\pi} \sum_{k=1}^{\infty} \frac{(1/2)_k}{k!} \left(\frac{a^2}{a^2 + b^2} \right)^k \frac{E_{k+1/2}(X)}{k}$$

$$- \frac{2abT}{\pi} \sum_{k=1}^{\infty} \left(\frac{a^2}{a^2 + b^2} \right)^k \frac{E_{k+1}(X)}{2k+1}, \quad T = 1/\sqrt{t}, \quad X = (a^2 + b^2)/t = T^2(a^2 + b^2)$$

Non-symmetric form for $a \geq b$

Since $I_6(a,b,T)$ is symmetric in a and b , we exchange a and b above for the case $a \geq b$.

The symmetric form is computationally efficient for a and b relatively close together. When a and b are widely separated, one of the series in $a^2/(a^2 + b^2)$ or $b^2/(a^2 + b^2)$ can be slowly convergent. Therefore the non-symmetric form was developed for overall computational use. In the non-symmetric forms, the series in $a^2/(a^2 + b^2)$ or $b^2/(a^2 + b^2)$ are rapidly convergent since each ratio is at most $1/2$. The G function is addressed in Chapter 3, Folders 6 and 16.

From Chapter 3, Folder 15, we have $I_6(a,b,T)$ in terms of the basic functions P and Q of Folder 11,

$$(2.10.3) \quad I_6(a, b, T) = \frac{\operatorname{erf}(aT)\operatorname{erf}(bT)}{T} + \frac{2a}{\sqrt{\pi}}P(a, b, T) + \frac{2b}{\sqrt{\pi}}P(b, a, T)$$

$$(2.10.4) \quad I_6(a, b, T) = \operatorname{erf}(aT) \left[\frac{\operatorname{erf}(bT)}{T} + \frac{b}{\sqrt{\pi}}E_1(b^2T^2) \right] + \frac{2a}{\sqrt{\pi}}P(a, b, T) + \frac{2ab}{\pi}Q(a, b, T)$$

$$(2.10.5) \quad P(a, b, T) + P^c(a, b, T) = \frac{1}{2}E_1(a^2T^2)$$

$$(2.10.6) \quad P(a, b, T) = \frac{1}{2}E_1(a^2T^2)\operatorname{erf}(bT) + \frac{b}{\sqrt{\pi}}Q(b, a, T)$$

$$(2.10.7) \quad I_6(a, b, T) = \frac{\operatorname{erf}(aT)\operatorname{erf}(bT)}{T} + \frac{1}{\sqrt{\pi}} \left[aE_1(a^2T^2)\operatorname{erf}(bT) + bE_1(b^2T^2)\operatorname{erf}(aT) \right] \\ + \frac{2ab}{\pi}[Q(a, b, T) + Q(b, a, T)]$$

$$(2.10.8) \quad I_6^c(a, b, T) = \frac{\operatorname{erfc}(aT)\operatorname{erfc}(bT)}{T} - \frac{2a}{\sqrt{\pi}}P^c(a, b, T) - \frac{2b}{\sqrt{\pi}}P^c(b, a, T)$$

$$(2.10.9) \quad I_6^c(a, b, T) = \operatorname{erfc}(aT) \left[\frac{\operatorname{erfc}(bT)}{T} - \frac{b}{\sqrt{\pi}}E_1(b^2T^2) \right] - \frac{2a}{\sqrt{\pi}}P^c(a, b, T) + \frac{2ab}{\pi}Q(a, b, T)$$

$$(2.10.10) \quad I_6^c(a, b, T) = \frac{\operatorname{erfc}(aT)\operatorname{erfc}(bT)}{T} - \frac{1}{\sqrt{\pi}} \left[aE_1(a^2T^2)\operatorname{erfc}(bT) + bE_1(b^2T^2)\operatorname{erfc}(aT) \right] \\ + \frac{2ab}{\pi}[Q(a, b, T) + Q(b, a, T)]$$

Special Cases

$$(2.10.11) \quad I_6(a, b, 0) = \int_0^\infty \frac{\operatorname{erf}(aw)\operatorname{erf}(bw)}{w^2} dw = \frac{2}{\sqrt{\pi}} \left[a \ln \left(\frac{b + \sqrt{a^2 + b^2}}{a} \right) + b \ln \left(\frac{a + \sqrt{a^2 + b^2}}{b} \right) \right]$$

Quadrature

In Chapter 3, Folder 3, a special quadrature procedure was developed. to overcome the slow convergence of the tail of $I(a, b, T)$. This involves using the approximation $\operatorname{erf}(x) = 1 + O(10^{-16})$ for $x \geq 6$. The procedure is as follows:

$$\text{Let } W_m = \min\left(\frac{6}{a}, \frac{6}{b}\right), \quad W_M = \max\left(\frac{6}{a}, \frac{6}{b}\right), \quad X = \min(a, b), \quad T = 1/\sqrt{t}.$$

Then,

$$\text{Case I:} \quad T \leq W_m, \quad I = \int_T^{W_m} \frac{\operatorname{erf}(aw)\operatorname{erf}(bw)}{w^2} dw + P(X, W_m, W_M) + \frac{1}{W_M}$$

$$\text{Case II:} \quad W_m < T \leq W_M, \quad I = P(X, T, W_M) + \frac{1}{W_M}$$

$$\text{Case III:} \quad W_M < T < \infty, \quad I = 1/T = \sqrt{t}$$

where
$$\frac{1}{W_M} + P(X, L, W_M) = \frac{\text{erf}(XL)}{L} + \frac{\text{erfc}(XW_M)}{W_M} + \frac{X}{\sqrt{\pi}} \left[E_1(X^2 L^2) - E_1(X^2 W_M^2) \right]$$
 and the integral on $T \leq W_m$ is the quadrature part. For computation, the SLATEC library code DGAUS8 is a suitable, high accuracy quadrature code.

Computer Subroutines

$I_6(a, b, T)$ or $I_6^c(a, b, T)$: SUBROUTINE INTEG16(...) with $KODE=1$ or $KODE=2$
SUBROUTINE I6QUAD(...)

References: Chapter 3, Folders 3, 6, 11, 15

(2.11) Functions $W_3(a,b,T)$ and $W_3^c(a,b,T)$ and Related Integrals

$$W_3(a,b,T) = \int_T^\infty \frac{\text{erf}(aw)\text{erf}(bw)}{w^3} dw = \frac{1}{2} \int_0^t \text{erf}(a/\sqrt{\tau})\text{erf}(b/\sqrt{\tau}) d\tau$$

$$W_3^c(a,b,T) = \int_T^\infty \frac{\text{erfc}(aw)\text{erfc}(bw)}{w^3} dw = \frac{1}{2} \int_0^t \text{erfc}(a/\sqrt{\tau})\text{erfc}(b/\sqrt{\tau}) d\tau$$

$$J_\nu(a,T) = \int_T^\infty \frac{\text{erf}(aw)}{w^\nu} dw, \nu > 1, \quad J_\nu^c(a,T) = \int_T^\infty \frac{\text{erfc}(aw)}{w^\nu} dw, \nu \neq 1$$

$$a > 0, \quad b > 0, \quad T = \frac{1}{\sqrt{t}}, \quad t > 0$$

Explicit Representations

$$(2.11.1) \quad W_3(a,b,T) = \frac{\text{erf}(aT)\text{erf}(bT)}{2T^2} + \frac{1}{\sqrt{\pi}}[aI_1(a,b,T) + bI_1(b,a,T)]$$

$$(2.11.2) \quad W_3^c(a,b,T) = \frac{\text{erfc}(aT)\text{erfc}(bT)}{2T^2} - \frac{1}{\sqrt{\pi}}[aI_1^c(a,b,T) + bI_1^c(b,a,T)]$$

$$(2.11.3) \quad J_\nu(a,T) = \int_T^\infty \frac{\text{erf}(aw)}{w^\nu} dw = \frac{1}{(\nu-1)T^{\nu-1}} \left[\text{erf}(aT) + \frac{aT}{\sqrt{\pi}} E_{\nu/2}(a^2T^2) \right], \quad \nu > 1$$

$$(2.11.4) \quad J_\nu^c(a,T) = \int_T^\infty \frac{\text{erfc}(aw)}{w^\nu} dw = \frac{1}{(\nu-1)T^{\nu-1}} \left[\text{erfc}(aT) - \frac{aT}{\sqrt{\pi}} E_{\nu/2}(a^2T^2) \right], \quad \nu \neq 1$$

$$(2.11.5) \quad J_2(a,T) = \int_T^\infty \frac{\text{erf}(aw)}{w^2} dw = \frac{\text{erf}(aT)}{T} + \frac{a}{\sqrt{\pi}} E_1(a^2T^2), \quad \nu = 2$$

$$(2.11.6) \quad J_2^c(a,T) = \int_T^\infty \frac{\text{erfc}(aw)}{w^2} dw = \frac{\text{erfc}(aT)}{T} - \frac{a}{\sqrt{\pi}} E_1(a^2T^2), \quad \nu = 2$$

$$(2.11.7) \quad J_3(a,T) = \frac{\text{erf}(aT)}{2T^2} + \frac{a}{T} \text{ierfc}(aT) \quad \nu = 3$$

$$(2.11.8) \quad J_3^c(a,T) = \frac{\text{erfc}(aT)}{2T^2} - \frac{a}{T} \text{ierfc}(aT) = \frac{2i^2 \text{erfc}(aT)}{T^2} \quad \nu = 3$$

Functional Relations

$$(2.11.9) \quad W_3^c(a,b,T) - W_3(a,b,T) = \frac{1}{2T^2} - J_3(a,T) - J_3(b,T) = J_3^c(a,T) - J_3(b,T)$$

$$(2.11.10) \quad J_3(a,T) + J_3^c(a,T) = \frac{1}{2T^2}$$

$$(2.11.11) \quad J_\nu(a,T) + J_\nu^c(a,T) = \frac{1}{(\nu-1)T^{\nu-1}} \quad \nu > 1.$$

Computer Subroutines

$W_3(a,b,T)$ or $W_3^c(a,b,T)$: SUBROUTINE INTEGW3(...) with KODE=1 or KODE=2

References Chapter 3, Folder 10

(2.12) Functions $I_3(a, b, c, T)$ and $I_3^c(a, b, c, T) = J_3(a, b, c, T)$

$$I_3(a, b, c, T) = \int_T^\infty e^{-c^2 w^2} \operatorname{erf}(aw) \operatorname{erf}(bw) dw = \frac{1}{2} \int_0^t \frac{e^{-c^2/u}}{u^{3/2}} \operatorname{erf}\left(\frac{a}{\sqrt{u}}\right) \operatorname{erf}\left(\frac{b}{\sqrt{u}}\right) du,$$

$$I_3^c(a, b, c, T) = J_3(a, b, c, T) = \int_T^\infty e^{-c^2 w^2} \operatorname{erfc}(aw) \operatorname{erfc}(bw) dw = \frac{1}{2} \int_0^t \frac{e^{-c^2/u}}{u^{3/2}} \operatorname{erfc}\left(\frac{a}{\sqrt{u}}\right) \operatorname{erfc}\left(\frac{b}{\sqrt{u}}\right) du$$

$$a \geq 0, b \geq 0, c > 0, T = \frac{1}{\sqrt{t}}, t > 0$$

Series Representations

$$(2.12.1) \quad I_3(a, b, c, T) = \frac{\sqrt{\pi}}{2c} \operatorname{erfc}(cT) - I_5(c, a, T) - I_5(c, b, T) + J_3(a, b, c, T)$$

$$(2.12.2) \quad J_3(a, b, c, T) = \int_T^\infty e^{-c^2 w^2} \operatorname{erfc}(aw) \operatorname{erfc}(bw) dw$$

CASE I ($a, c \leq b$) ($c \leq a \leq b$ or $a \leq c \leq b$)

$$(2.12.3) \quad J_3(a, b, c, T) = \operatorname{erfc}(aT) I_5(c, b, T) - \frac{2a}{\sqrt{\pi}} \int_T^\infty e^{-a^2 w^2} I_5(c, b, w) dw = \operatorname{erfc}(aT) I_5(c, b, T) - S(a, b, c, T)$$

$$S(a, b, c, T) = \frac{a}{\pi d} \left[\frac{\sqrt{\pi} \operatorname{erfc}(TX)}{X + d} \sum_{k=0}^{\infty} \frac{(1/2)_k}{(k+1)!} \left(\frac{c^2}{d^2} \right)^k P_k(y) \right. \\ \left. - \frac{(TX)d}{2X^2} \sum_{m=0}^{\infty} \frac{(3/2)_m}{(m+1)!} E_{m+3/2}(T^2 X^2) \sum_{k=0}^m \binom{m}{k} \frac{(a^2/X^2)^{m-k} (c^2/X^2)^k}{2k+1} \right]$$

$$d^2(b, c) = b^2 + c^2, \quad X^2 = a^2 + b^2 + c^2, \quad y = a^2/(X+d)^2, \quad P_0(y) = 1$$

$$P_k(y) = F(-k, 1, k+2, y), \quad k \geq 1 \quad a, c \leq b.$$

Here $F(-k, 1, k+2, y)$ is the Gauss hypergeometric function, which for this application, can be computed with the series

$$(2.12.4) \quad F(a, b, c, z) = \sum_{m=0}^{\infty} \frac{(a)_m (b)_m}{m! (c)_m} z^m, \quad (a)_0 = 1, \quad (a)_m = (a)(a+1)\dots(a+m-1), \quad m \geq 1$$

With the first parameter a negative integer(-k), this F function is a polynomial of degree k since $(-k)_m = (-k)(-k+1)\dots(-k+m-1)$ is zero for $m=k+1$ and higher indices. I_5 is the I function of Chapter 3, Folder5.

An alternate formulation of this case is presented in Chapter 3, Folder 28 where $S(a, b, c, T)$ is computed by the series

$$(2.12.5) \quad S(a, b, c, T) = \frac{2a}{\sqrt{\pi}} \int_T^\infty e^{-a^2 w^2} I_5(c, b, w) dw = \frac{a}{\pi d} \sum_{k=0}^{\infty} C_k \left(\frac{c^2}{d^2} \right)^k R_k(a, d, T),$$

where

$$R_k(a, d, T) = \int_T^\infty e^{-a^2 w^2} E_{k+3/2}(d^2 w^2) dw, \quad k \geq 0,$$

$$d^2 = b^2 + c^2 \quad C_k = (1/2)_k / k!.$$

Here $R_k(a, d, T)$ is expanded in the form

$$R_k(a, d, T) = \sqrt{\pi} \sum_{m=1}^{k+1} A(k+1, m) Y_{2m-1}(a, d, T)$$

where $Y_{2m-1}(a, d, T)$ is computed by backward recurrence on the two term relation

$$Y_{n-2} = \frac{a^2}{a^2 + d^2} \left[2nY_n + \frac{d}{a^2} e^{-a^2 T^2} i^{n-1} \operatorname{erfc}(dT) \right]$$

starting at some large *odd* index N . The details of computation as well as the coefficients $A(k+1, m)$ are given in Chapter 3, Folder 28. Another more desirable form for S is presented in Chapter 3, Folder 29:

$$(2.12.6) \quad S(a, b, c, T) = \frac{2ab}{\sqrt{\pi} \sqrt{b^2 + c^2}} \sum_{k=1}^{\infty} \left(\frac{4c^2}{b^2 + c^2} \right)^{k-1} [(k-1)! Y_{2k-1}(\sqrt{a^2 + c^2}, b, T)], \quad a, c \leq b$$

where sequences of the integral

$$Y_n(a, b, T) = \int_T^{\infty} e^{-a^2 w^2} i^n \operatorname{erfc}(bw) dw, \quad a > 0, \quad b \geq 0, \quad n \geq -1$$

are computed by a series in conjunction with the recurrence above in subroutine INTEG129.

CASE II ($a \leq b \leq c$)

$$(2.12.7) \quad J_3(a, b, c, T) = \frac{\sqrt{\pi}}{2c} \operatorname{erfc}(aT) \operatorname{erfc}(bT) \operatorname{erfc}(cT) - \frac{a}{c} J_3(b, c, a, T) - \frac{b}{c} J_3(a, c, b, T)$$

Notice that c is larger than a and b . This is precisely the criteria to compute $J_3(b, c, a, T)$ and $J_3(a, c, b, T)$ by Case I. This relation is analogous to

$$(2.12.8) \quad I_5(a, b, T) = \frac{\sqrt{\pi}}{2a} \operatorname{erfc}(aT) \operatorname{erfc}(bT) - \frac{b}{a} I_5(b, a, T)$$

in Chapter 3, Folder 5 when $a \geq b$.

Power Series for small aT , bT , cT

$$(2.12.9) \quad I_3(a, b, c, T) = I_3(a, b, c, 0) - \int_0^T e^{-c^2 w^2} \operatorname{erf}(aw) \operatorname{erf}(bw) dw$$

And using the power series for each erf function, we get

Case I, $a, c \leq b$

$$(2.12.10) \quad I_3(a, b, c, 0) = \frac{1}{c\sqrt{\pi}} \tan^{-1} \frac{a}{c} - S(a, b, c, 0)$$

$$S(a, b, c, 0) = \frac{a}{d\sqrt{\pi}} \cdot \frac{1}{X+d} \sum_{k=0}^{\infty} \frac{(1/2)_k}{(k+1)!} \left(\frac{c^2}{d^2} \right)^k P_k(y)$$

where $d^2 = b^2 + c^2$, $X^2 = a^2 + b^2 + c^2$, $y = a^2/(X+d)^2$, $P_0(y) = 1$, $P_k(y) = F(-k, 1, k+2, y)$, $k \geq 1$ for $a, c \leq b$ and $a = \min(a, b)$, $b = \max(a, b)$. In Case II, c takes the place of b as the dominant parameter.

Case II, $a \leq b \leq c$

$$(2.12.11) \quad I_3(a, b, c, 0) = \frac{a}{c} S(b, c, a, 0) + \frac{b}{c} S(a, c, b, 0)$$

Now the power series for the integral is

$$(2.12.12) \quad \int_0^T e^{-c^2 w^2} \operatorname{erf}(aw) \operatorname{erf}(bw) dw = \frac{4abT^3}{\pi} \sum_{k=0}^{\infty} \frac{V_k T^{2k}}{2k+3}$$

$$V_k T^{2k} = \sum_{n=0}^k D_n (c^2 T^2) U_{k-n}(a^2 T^2, b^2 T^2), \quad U_k(a^2 T^2, b^2 T^2) = \sum_{m=0}^k C_m (a^2 T^2) C_{k-m}(b^2 T^2)$$

$$C_k(x^2) = \frac{(-1)^k x^{2k}}{k!(2k+1)}, \quad D_k(x^2) = \frac{(-1)^k x^{2k}}{k!}$$

Series Expansion for Large c

(2.12.13)

$$\int_T^{\infty} e^{-c^2 w^2} \operatorname{erf}(aw) \operatorname{erf}(bw) dw = \frac{2ab}{\pi c^3} \sum_{k=0}^{\infty} (-1)^k Y_{k+1}(c^2 T^2) \frac{\Gamma(k+3/2)}{\Gamma(k+1)} \sum_{m=0}^k \binom{k}{m} \frac{(a^2/c^2)^m}{2m+1} \cdot \frac{(b^2/c^2)^{k-m}}{2(k-m)+1}$$

where

$$(2.12.14) \quad Y_k(x) = \Gamma(k+1/2, x)/\Gamma(k+1/2).$$

Then

$$(2.12.15) \quad Y_{k+1} = Y_k + \frac{e^{-x} x^{k+1/2}}{\Gamma(k+3/2)} = Y_k + T_k, \quad k = 0, 1, \dots$$

where $T_{k+1} = T_k \cdot \frac{x}{(k+3/2)}$ with $T_0 = \frac{e^{-x} \sqrt{x}}{(\sqrt{\pi}/2)}$ and $Y_0 = \operatorname{erfc}(\sqrt{x})$

Because of the way in which the terms interact, the condition

$$(2.12.16) \quad \frac{a^2 + b^2}{c^2} \leq \frac{1}{2p} \quad \text{with} \quad p = \begin{cases} 1 & \text{for } c^2 T^2 \leq 5 \\ c^2 T^2 - 4 & \text{for } c^2 T^2 > 5 \end{cases}$$

was determined experimentally to give accurate results. Notice also that the binomial coefficients can be generated very rapidly and efficiently by additions using the Pascal triangle relation

$$B_{k+1,m} = B_{k,m} + B_{k,m-1}, \quad m = 1, k.$$

Quadrature for $I_3(a, b, c, T)$

For the quadrature, we follow the procedure of Chapter 3, Folder 3 by replacing the erf functions with 1 when the arguments exceed 6. As noted, the error is uniformly $O(10^{-15})$ for $\operatorname{erf}(x) = 1$ when $x \geq 6$. Then, we have the same cases as in Folder 3:

Let $W_m = \min\left(\frac{6}{a}, \frac{6}{b}\right), \quad W_M = \max\left(\frac{6}{a}, \frac{6}{b}\right), \quad X = \min(a, b), \quad \text{and} \quad T = \frac{1}{\sqrt{t}} :$

Case I: $1/\sqrt{t} = T \leq W_m$

$$(2.12.17) \quad I_3(a, b, c, T) = \int_T^{W_m} e^{-c^2 w^2} \operatorname{erf}(aw) \operatorname{erf}(bw) dw + J_5(c, X, W_m) + I_5(c, X, W_M)$$

Case II: $W_m < T \leq W_M$

$$(2.12.18) \quad I_3(a, b, c, T) = J_5(c, X, T) + I_5(c, X, W_M)$$

Case III: $W_M < T < \infty$

$$(2.12.19) \quad I_3(a, b, c, T) = \frac{\sqrt{\pi}}{2c} \operatorname{erfc}(cT)$$

where $J_5(a, b, x)$ and $I_5(a, b, x)$ are the I functions of Chapter 3, Folder 5.

Special Cases

$c = 0$ (Chapter 3, Folder 9 for $\int_0^T \operatorname{erf}(aw) \operatorname{erf}(bw) dw$)

$$(2.12.20) \quad J_3(a, b, 0, T) = \int_T^\infty \operatorname{erfc}(aw) \operatorname{erfc}(bw) dw \\ = \frac{\operatorname{erfc}(aT) \operatorname{ierfc}(bT)}{b} + \frac{e^{-a^2 T^2} \operatorname{erfc}(bT)}{a\sqrt{\pi}} - \frac{\sqrt{a^2 + b^2}}{ab\sqrt{\pi}} \operatorname{erfc}(T\sqrt{a^2 + b^2})$$

$a=0$ and $c=0$

$$(2.12.21) \quad J_3(0, b, 0, T) = \int_T^\infty \operatorname{erfc}(bw) dw = \frac{\operatorname{ierfc}(bT)}{b}$$

$c=0$ and $T=0$

$$(2.12.22) \quad J_3(a, b, 0, 0) = \int_0^\infty \operatorname{erfc}(aw) \operatorname{erfc}(bw) dw = \frac{(2/\sqrt{\pi})}{a + b + \sqrt{a^2 + b^2}}$$

$a=0, c=0, T=0$

$$(2.12.23) \quad J_3(0, b, 0, 0) = \frac{1}{b\sqrt{\pi}} \text{ since } \operatorname{ierfc}(0) = 1/\sqrt{\pi}$$

Inequalities

We derived the relation

$$(2.12.24) \quad W \equiv \frac{\sqrt{\pi}}{2} \operatorname{erfc}(aT) \operatorname{erfc}(bT) \operatorname{erfc}(cT) = aJ_3(b, c, a, T) + bJ_3(a, c, b, T) + cJ_3(a, b, c, T)$$

Following the derivation in the APPENDIX of Chapter 3, Folder 5, divide both sides by $a+b+c$ and we get a convex linear combination of the J_3 's. Then

$$(2.12.25) \min[J_3(b,c,a,T), J_3(a,c,b,T), J_3(a,b,c,T)] \leq \frac{W}{a+b+c} \leq \max[J_3(b,c,a,T), J_3(a,c,b,T), J_3(a,b,c,T)]$$

Also, if we divide by $\sqrt{a^2 + b^2 + c^2}$ we have the dot product of two vectors on the right, one of which has length 1. By the Cauchy Inequality, we get

$$(2.12.26) \left(\frac{W}{\sqrt{a^2 + b^2 + c^2}} \right)^2 \leq J_3^2(b,c,a,T) + J_3^2(a,c,b,T) + J_3^2(a,b,c,T)$$

Notice that if $c = b = a$, then the max and min are the same and $J_3(a,a,a,T) = \frac{W}{3a} = \frac{\sqrt{\pi}}{6a} \operatorname{erfc}^3(aT)$ as it

should be: $\int_T^\infty e^{-a^2 w^2} \operatorname{erfc}^2(aw) dw = \frac{\sqrt{\pi}}{6a} \operatorname{erfc}^3(aT)$ since $-\frac{2ae^{-a^2 w^2}}{\sqrt{\pi}} dw$ is the differential of $\operatorname{erfc}(aw)$.

Numerical Considerations

In Chapter 3, Folder 7f, leading terms of each expression are combined to reduce losses of significance by small differences of large numbers. These are implemented in the computer subroutine INTEG13.

Computer Subroutine

$I_3(a,b,c,T)$ or $I_3^c(a,b,c,T)$: SUBROUTINE INTEG13(...) with KODE=1 or KODE=2

References: Chapter 3, Folder 7, Folder 28, Folder 29

(2.13) Functions $I_4(a,b,c,T)$, $I_4^c(a,b,c,T)$, $J_4(a,b,c,T)$ and $J_4^c(a,b,c,T)$

$$I_4(a,b,c,T) = \int_T^\infty w^2 e^{-c^2 w^2} \operatorname{erf}(aw) \operatorname{erf}(bw) dw = \frac{1}{2} \int_0^t \frac{e^{-c^2/u}}{u^{5/2}} \operatorname{erf}\left(\frac{a}{\sqrt{u}}\right) \operatorname{erf}\left(\frac{b}{\sqrt{u}}\right) du,$$

$$I_4^c(a,b,c,T) = \int_T^\infty w^2 e^{-c^2 w^2} \operatorname{erfc}(aw) \operatorname{erfc}(bw) dw = \frac{1}{2} \int_0^t \frac{e^{-c^2/u}}{u^{5/2}} \operatorname{erfc}\left(\frac{a}{\sqrt{u}}\right) \operatorname{erfc}\left(\frac{b}{\sqrt{u}}\right) du$$

$$J_4(a,b,c,T) = \int_T^\infty w e^{-c^2 w^2} \operatorname{erf}(aw) \operatorname{erf}(bw) dw = \frac{1}{2} \int_0^t \frac{e^{-c^2/u}}{u^2} \operatorname{erf}\left(\frac{a}{\sqrt{u}}\right) \operatorname{erf}\left(\frac{b}{\sqrt{u}}\right) du$$

$$J_4^c(a,b,c,T) = \int_T^\infty w e^{-c^2 w^2} \operatorname{erfc}(aw) \operatorname{erfc}(bw) dw = \frac{1}{2} \int_0^t \frac{e^{-c^2/u}}{u^2} \operatorname{erfc}\left(\frac{a}{\sqrt{u}}\right) \operatorname{erfc}\left(\frac{b}{\sqrt{u}}\right) du$$

$$a \geq 0, \quad b \geq 0, \quad c > 0, \quad T = \frac{1}{\sqrt{t}}, \quad t > 0$$

Series Representations

For $I_4(a,b,c,T)$ and $I_4^c(a,b,c,T)$ we have

$$(2.13.1) \quad I_4(a,b,c,T) = \frac{T e^{-c^2 T^2} \operatorname{erf}(aT) \operatorname{erf}(bT)}{2c^2} + \frac{1}{2c^2 \sqrt{\pi}} \left\{ \frac{a e^{-(a^2+c^2)T^2} \operatorname{erf}(bT)}{(a^2+c^2)} + \frac{b e^{-(b^2+c^2)T^2} \operatorname{erf}(aT)}{(b^2+c^2)} \right\} \\ + \frac{ab}{2c^2 \sqrt{\pi}} \left\{ \frac{1}{a^2+c^2} + \frac{1}{b^2+c^2} \right\} \frac{\operatorname{erfc}(TX)}{X} + \frac{1}{2c^2} I_3(a,b,c,T)$$

$$(2.13.2) \quad I_4^c(a,b,c,T) = \frac{T e^{-c^2 T^2} \operatorname{erfc}(aT) \operatorname{erfc}(bT)}{2c^2} - \frac{1}{2c^2 \sqrt{\pi}} \left\{ \frac{a e^{-(a^2+c^2)T^2} \operatorname{erfc}(bT)}{(a^2+c^2)} + \frac{b e^{-(b^2+c^2)T^2} \operatorname{erfc}(aT)}{(b^2+c^2)} \right\} \\ + \frac{ab}{2c^2 \sqrt{\pi}} \left\{ \frac{1}{a^2+c^2} + \frac{1}{b^2+c^2} \right\} \frac{\operatorname{erfc}(TX)}{X} + \frac{1}{2c^2} I_3^c(a,b,c,T)$$

where $X^2 = a^2 + b^2 + c^2$ and $I_3(a,b,c,T)$ and $I_3^c(a,b,c,T)$ are the functions of (2.12) and Chapter 3, Folder 7. For $b \rightarrow \infty$ and $b=0$,

$$(2.13.3) \quad I_4(a, \infty, c, T) = \int_T^\infty w^2 e^{-c^2 w^2} \operatorname{erf}(aw) dw = \frac{1}{2c^2} \left[T e^{-c^2 T^2} \operatorname{erf}(aT) + \frac{a}{a^2+c^2} \frac{e^{-(a^2+c^2)T^2}}{\sqrt{\pi}} + J_5(c, a, T) \right]$$

$$(2.13.4) \quad I_4^c(a, 0, c, T) = \int_T^\infty w^2 e^{-c^2 w^2} \operatorname{erfc}(aw) dw = \frac{1}{2c^2} \left[T e^{-c^2 T^2} \operatorname{erfc}(aT) - \frac{a}{a^2+c^2} \frac{e^{-(a^2+c^2)T^2}}{\sqrt{\pi}} + I_5(c, a, T) \right]$$

where the J_5 and I_5 functions are the functions of (2.3) which are computed in Chapter 3, Folder5.

Using the symmetry in a and b we can relate these functions by

$$(2.13.5) \quad I_4(a,b,c,T) = \int_T^\infty w^2 e^{-c^2 w^2} dw - I_4^c(a,0,c,T) - I_4^c(0,b,c,T) + I_4^c(a,b,c,T)$$

$$(2.13.6) \quad I_4^c(a,b,c,T) = \int_T^\infty w^2 e^{-c^2 w^2} dw - I_4(a,\infty,c,T) - I_4(\infty,b,c,T) + I_4(a,b,c,T)$$

where

$$\int_T^\infty w^2 e^{-c^2 w^2} dw = \frac{1}{2c^2} \left[T e^{-c^2 T^2} + \frac{\sqrt{\pi}}{2c} \operatorname{erfc}(cT) \right].$$

For $J_4(a, b, c, T)$ and $J_4^c(a, b, c, T)$ we have

$$(2.13.7) \quad J_4(a, b, c, T) = \frac{e^{-c^2 T^2}}{2c^2} \operatorname{erf}(aT) \operatorname{erf}(bT) + \frac{1}{c^2 \sqrt{\pi}} \left[b J_5(\sqrt{b^2 + c^2}, a, T) + a J_5(\sqrt{a^2 + c^2}, b, T) \right]$$

$$(2.13.8) \quad J_4^c(a, b, c, T) = \frac{e^{-c^2 T^2}}{2c^2} \operatorname{erfc}(aT) \operatorname{erfc}(bT) - \frac{1}{c^2 \sqrt{\pi}} \left[b I_5(\sqrt{b^2 + c^2}, a, T) + a I_5(\sqrt{a^2 + c^2}, b, T) \right]$$

where $J_5(a, b, T)$ and $I_5(a, b, T)$ are the functions of (2.3) and Chapter 3, Folder 5. For $b \rightarrow \infty$ and $b=0$,

$$(2.13.9) \quad J_4(a, \infty, c, T) = \frac{1}{2c^2} \left[e^{-c^2 T^2} \operatorname{erf}(aT) + \frac{a}{\sqrt{a^2 + c^2}} \operatorname{erfc}(T\sqrt{a^2 + c^2}) \right]$$

$$(2.13.10) \quad J_4^c(a, 0, c, T) = \frac{1}{2c^2} \left[e^{-c^2 T^2} \operatorname{erfc}(aT) - \frac{a}{\sqrt{a^2 + c^2}} \operatorname{erfc}(T\sqrt{a^2 + c^2}) \right]$$

and again using the symmetry in a and b we have the relations

$$(2.13.11) \quad J_4(a, b, c, T) = \frac{1}{2c^2} e^{-c^2 T^2} - J_4^c(a, 0, c, T) - J_4^c(0, b, c, T) + J_4^c(a, b, c, T)$$

$$(2.13.12) \quad J_4^c(a, b, c, T) = \frac{1}{2c^2} e^{-c^2 T^2} - J_4(a, \infty, c, T) - J_4(\infty, b, c, T) + J_4(a, b, c, T) .$$

Quadrature for $I_4(a, b, c, T)$

The outline for this procedure is set in Chapter 3, Folder3 where we replace $\operatorname{erf}(x)$ function with 1 when $x \geq 6$ according to the estimate $\operatorname{erf}(x) = 1 + O(10^{-16})$ and integrate analytically to estimate the tail when c is small. Then the procedure is:

$$\text{Let } W_m = \min\left(\frac{6}{a}, \frac{6}{b}\right), \quad W_M = \max\left(\frac{6}{a}, \frac{6}{b}\right), \quad X = \min(a, b), \quad T = \frac{1}{\sqrt{t}}$$

Case I: $T \leq W_m$

$$(2.13.13) \quad I_4(a, b, c, T) = \int_T^{W_m} w^2 e^{-c^2 w^2} \operatorname{erf}(aw) \operatorname{erf}(bw) dw + P(c, X, W_m, W_M)$$

Case II: $W_m < T \leq W_M$

$$(2.13.14) \quad I_4(a, b, c, T) = P(c, X, T, W_M)$$

Case III: $W_M < T < \infty$

$$(2.13.15) \quad I_4(a, b, c, T) = \frac{1}{2c^2} \left[T e^{-c^2 T^2} + \frac{\sqrt{\pi}}{2c} \operatorname{erfc}(cT) \right]$$

where

$$(2.13.16) \quad P(c, X, L, U) = \frac{1}{2c^2} \left\{ L e^{-c^2 L^2} \operatorname{erf}(XL) + U e^{-c^2 U^2} \operatorname{erfc}(XU) + \frac{\sqrt{\pi}}{2c} \operatorname{erfc}(cL) \right. \\ \left. + \frac{(X/\sqrt{\pi})}{X^2 + c^2} \left[e^{-(X^2 + c^2)L^2} - e^{-(X^2 + c^2)U^2} \right] - [I_5(c, X, L) - I_5(c, X, U)] \right\}$$

and I_5 is the integral I in Folder 5.

Quadrature for $J_4(a,b,c,T)$

The outline for this procedure is set in Chapter 3, Folder 3 where we replace $\text{erf}(x)$ function with 1 when $x \geq 6$ according to the estimate $\text{erf}(x)=1 + O(10^{-16})$. Then the procedure is:

$$\text{Let } W_m = \min\left(\frac{6}{a}, \frac{6}{b}\right), \quad W_M = \max\left(\frac{6}{a}, \frac{6}{b}\right) \quad X = \min(a, b), \quad T = \frac{1}{\sqrt{t}}$$

Then,

Case I, $T \leq W_m$

$$(2.13.17) \quad J_4(a, b, c, T) = \int_T^{W_m} w e^{-c^2 w^2} \text{erf}(aw) \text{erf}(bw) dw + S(c, X, W_m, W_M) + \frac{1}{2c^2} e^{-c^2 W_M^2}$$

Case II, $W_m < T \leq W_M$

$$(2.13.18) \quad J_4(a, b, c, T) = S(c, X, T, W_M) + \frac{1}{2c^2} e^{-c^2 W_M^2}$$

Case III, $W_M < T < \infty$

$$(2.13.19) \quad J_4(a, b, c, T) = \frac{1}{2c^2} e^{-c^2 T^2}$$

where

$$(2.13.20) \quad \begin{aligned} \frac{1}{2c^2} e^{-c^2 W_M^2} + S(c, X, L, W_M) &= \frac{1}{2c^2} \left[e^{-c^2 L^2} \text{erf}(XL) + e^{-c^2 W_M^2} \text{erfc}(XW_M) \right] \\ &+ \frac{X}{2c^2 \sqrt{c^2 + X^2}} \left[\text{erfc}(L\sqrt{c^2 + X^2}) - \text{erfc}(W_M\sqrt{c^2 + X^2}) \right] \end{aligned}$$

Computer Subroutines

$I_4(a,b,c,T)$: SUBROUTINE I4QUAD(...)

SUBROUTINE I4SER(...)

$J_4(a,b,c,T)$: SUBROUTINE J4QUAD(...)

SUBROUTINE J4SER(...)

References: Chapter 3, Folder 8

(2.14) Functions $I_{14}(a,b,c,T)$ and $I_{14}^c(a,b,c,T)$

$$I_{14}(a,b,c,T) = \int_T^\infty e^{-c^2 w^2} \frac{\operatorname{erf}(aw)\operatorname{erf}(bw)}{w^2} dw = \frac{1}{2} \int_0^t e^{-c^2/u} \frac{\operatorname{erf}(a/\sqrt{u})\operatorname{erf}(b/\sqrt{u})}{\sqrt{u}} du,$$

$$I_{14}^c(a,b,c,T) = \int_T^\infty e^{-c^2 w^2} \frac{\operatorname{erfc}(aw)\operatorname{erfc}(bw)}{w^2} dw = \frac{1}{2} \int_0^t e^{-c^2/u} \frac{\operatorname{erfc}(a/\sqrt{u})\operatorname{erfc}(b/\sqrt{u})}{\sqrt{u}} du$$

$$a > 0, \quad b > 0, \quad T = \frac{1}{\sqrt{t}} \quad t > 0$$

Series Representation

$$(2.14.1) \quad I_{14}(a,b,c,T) = \frac{I_2(a,b,T) e^{-c^2 T^2}}{T^2} +$$

$$-2c^2 \left[I_3(a,b,c,T) + \frac{1}{a\sqrt{\pi}} P(\sqrt{a^2+c^2}, b, T) + \frac{1}{b\sqrt{\pi}} P(\sqrt{b^2+c^2}, a, T) - \frac{\sqrt{a^2+b^2}}{ab\sqrt{\pi}} P(c, \sqrt{a^2+b^2}, T) \right]$$

$$-2 \left[\frac{1}{a\sqrt{\pi}} I_{13}(\sqrt{a^2+c^2}, b, T) + \frac{1}{b\sqrt{\pi}} I_{13}(\sqrt{b^2+c^2}, a, T) - \frac{\sqrt{a^2+b^2}}{ab\sqrt{\pi}} I_{13}(c, \sqrt{a^2+b^2}, T) \right]$$

where from Chapter 3, Folder 9

$$(2.14.2) \quad I_2(a,b,T) = T \operatorname{erf}(aT) \operatorname{erf}(bT) + \frac{e^{-a^2 T^2}}{a\sqrt{\pi}} \operatorname{erf}(bT) + \frac{e^{-b^2 T^2}}{b\sqrt{\pi}} \operatorname{erf}(aT) - \frac{\sqrt{a^2+b^2}}{ab\sqrt{\pi}} \operatorname{erf}(T\sqrt{a^2+b^2}),$$

$I_{13}(a,b,T)$ is computed in Chapter 3, Folder 13, $P(a,b,T)$ is computed in Chapter 3, Folder 11, and $I_3(a,b,c,T)$ is computed in Chapter 3, Folder 7. Similarly for $I_{14}^c(a,b,c,T)$,

$$(2.14.3) \quad I_{14}^c(a,b,c,T) = -\frac{I_2^c(a,b,T) e^{-c^2 T^2}}{T^2} +$$

$$+2c^2 \left[-I_3^c(a,b,c,T) + \frac{1}{a\sqrt{\pi}} P^c(\sqrt{a^2+c^2}, b, T) + \frac{1}{b\sqrt{\pi}} P^c(\sqrt{b^2+c^2}, a, T) - \frac{\sqrt{a^2+b^2}}{ab\sqrt{\pi}} P^c(c, \sqrt{a^2+b^2}, T) \right]$$

$$+2 \left[\frac{1}{a\sqrt{\pi}} I_{13}^c(\sqrt{a^2+c^2}, b, T) + \frac{1}{b\sqrt{\pi}} I_{13}^c(\sqrt{b^2+c^2}, a, T) - \frac{\sqrt{a^2+b^2}}{ab\sqrt{\pi}} I_{13}^c(c, \sqrt{a^2+b^2}, T) \right]$$

where from Chapter 3, Folder 9

$$(2.14.4) \quad I_2^c(a,b,w) = -\operatorname{werfc}(aw)\operatorname{erfc}(bw) + \frac{e^{-a^2 w^2}}{a\sqrt{\pi}} \operatorname{erfc}(bw) + \frac{e^{-b^2 w^2}}{b\sqrt{\pi}} \operatorname{erfc}(aw) - \frac{\sqrt{a^2+b^2}}{ab\sqrt{\pi}} \operatorname{erfc}(w\sqrt{a^2+b^2})$$

$$= \frac{T}{(aT)(bT)} \left[\frac{\operatorname{ierfc}(T\sqrt{a^2+b^2})}{\sqrt{\pi}} - \operatorname{ierfc}(aT)\operatorname{ierfc}(bT) \right]$$

and the other complementary functions are treated in the Folders cited above for $I_{14}(a,b,c,T)$.

Using the relation $\operatorname{erfc}(x)=1-\operatorname{erf}(x)$ we also have

$$(2.14.5) \quad I_{14}^c(a,b,c,T) = \frac{\sqrt{\pi}}{T} \operatorname{ierfc}(cT) - I_1(c,a,T) - I_1(c,b,T) + I_{14}(a,b,c,T)$$

$$(2.14.6) \quad I_{14}(a, b, c, T) = \frac{\sqrt{\pi}}{T} \operatorname{ierfc}(cT) - I_1^c(c, a, T) - I_1^c(c, b, T) + I_{14}^c(a, b, c, T)$$

where $I_1(c, a, T)$, $I_1(c, b, T)$, $I_1^c(c, a, T)$ and $I_1^c(c, b, T)$ are computed in Chapter 3, Folder10 and displayed in Section (2.6).

Computer Subroutines

$I_{14}(a, b, c, T)$ or $I_{14}^c(a, b, c, T)$: SUBROUTINE INTEG14(...) with KODE=1 or KODE=2

References Chapter 3, Folders14 and 10

(2.15) Functions $U(a,b,t)$, $V(a,b,t)$, $I_{21}(a,b,c,t)$, $I_{21}^c(a,b,c,t)$, $J_{21}(a,b,c,t)$, $G_n(a,b,T)$

$$U(a,b,t) = e^{a^2t+2ab} \operatorname{erfc}(a\sqrt{t} + b/\sqrt{t})$$

$$V(a,b,t) = \int_0^t U(a,b,\tau) d\tau, \quad I_{21}(a,b,c,t) = \int_0^t U(a,b,\tau) \operatorname{erf}(c/\sqrt{\tau}) d\tau$$

$$I_{21}^c(a,b,c,t) = \int_0^t U(a,b,\tau) \operatorname{erfc}(c/\sqrt{\tau}) d\tau \quad J_{21}(a,b,c,t) = \int_0^t \frac{U(a,b,\tau) e^{-c^2/\tau}}{\tau^{3/2}} d\tau$$

$$a > 0, \quad b > 0, \quad c > 0, \quad t > 0$$

$$G_n(a,b,T) = \int_T^\infty \frac{e^{-a^2w^2} i^n \operatorname{erfc}(bw)}{w^n} dw, \quad a > 0, \quad b \geq 0, \quad T > 0, \quad n \geq 0$$

Representations

$$(2.15.1) \quad V(a,b,t) = \frac{2}{a} \sqrt{\frac{t}{\pi}} e^{-b^2/t} - \left(\frac{1}{a^2} + \frac{2b}{a} \right) \operatorname{erfc}\left(\frac{b}{\sqrt{t}}\right) + \frac{U(t)}{a^2}$$

$$V(a,b,t) = \frac{2\sqrt{t}}{a} \operatorname{ierfc}\left(\frac{b}{\sqrt{t}}\right) + \frac{1}{a^2} \left[U(a,b,t) - \operatorname{erfc}\left(\frac{b}{\sqrt{t}}\right) \right]$$

$$(2.15.2) \quad I_{21}(a,b,c,t) = V(t) \operatorname{erf}(c/\sqrt{t}) + \frac{c}{\sqrt{\pi}} \left[\frac{2}{a\sqrt{\pi}} E_1(X) - 2 \left(\frac{1}{a^2} + \frac{2b}{a} \right) I_5(c,b,T) + \frac{2\sqrt{t}}{a^2\sqrt{\pi}} S_1(a,b,c,t) \right]$$

$$(2.15.3) \quad I_{21}^c(a,b,c,t) = V(t) \operatorname{erfc}(c/\sqrt{t}) - \frac{c}{\sqrt{\pi}} \left[\frac{2}{a\sqrt{\pi}} E_1(X) - 2 \left(\frac{1}{a^2} + \frac{2b}{a} \right) I_5(c,b,T) + \frac{2\sqrt{t}}{a^2\sqrt{\pi}} S_1(a,b,c,t) \right]$$

where $X = (b^2 + c^2)/t$, I_5 is the I function of Folder 5 and $S_1(a,b,c,t)$ in computational form suitable for a quadrature is

$$(2.15.4) \quad S_1(a,b,c,t) = e^{-X} \int_0^\infty \frac{e^{-2Bw-w^2}}{c^2 + (b + w\sqrt{t})^2} dw, \quad B = a\sqrt{t} + b/\sqrt{t}.$$

For J_{21} , we get

$$(2.15.5) \quad J_{21}(a,b,c,t) = \frac{2\sqrt{t}}{\sqrt{\pi}} S_1(a,b,c,t).$$

A series for large parameter L ($L \geq 2$) is

$$X = (b^2 + c^2)/t, \quad B = a\sqrt{t} + b/\sqrt{t},$$

$$(2.15.6) \quad S_1(a,b,c,t) = \frac{e^{-X}}{2tB} \sum_{k=0}^\infty \frac{U_k(x)}{L^k} [e^{B^2} E_{(k+3)/2}(B^2)],$$

$$L = \frac{B}{\sqrt{a^2t + c^2/t}}, \quad x = \frac{a\sqrt{t}}{\sqrt{a^2t + c^2/t}},$$

and $U_k(x)$, $k \geq 0$, are Chebyshev polynomials of the second kind which can be generated by forward recurrence on their three-term recurrence relation.

The expressions for $V(t)$, I_{21} and I_{21}^c above contain reciprocal powers of a , but the integrals are analytic functions of a . Therefore, to avoid losses of significance by small differences of large numbers when a is small, we develop the power series in the parameter a . The results are:

$$(2.15.7) \quad U(t) = e^{a^2 t + 2ab} \operatorname{erfc}(a\sqrt{t} + b/\sqrt{t}) = \sum_{n=0}^{\infty} i^n \operatorname{erfc}\left(\frac{b}{\sqrt{t}}\right) (-2a\sqrt{t})^n$$

$$(2.15.8) \quad V(t) = 4t \sum_{n=2}^{\infty} i^n \operatorname{erfc}\left(\frac{b}{\sqrt{t}}\right) (-2a\sqrt{t})^{n-2}$$

$$(2.15.9) \quad I_{21}(a, b, c, t) = V(t) \operatorname{erf}\left(\frac{c}{\sqrt{t}}\right) + \frac{4c\sqrt{t}}{\sqrt{\pi}} e^{-X} \sum_{n=2}^{\infty} (-2a\sqrt{t})^{n-2} y_n, \quad 0 \leq a\sqrt{t} \leq 1$$

$$(2.15.10) \quad I_{21}^c(a, b, c, t) = V(t) \operatorname{erfc}\left(\frac{c}{\sqrt{t}}\right) - \frac{4c\sqrt{t}}{\sqrt{\pi}} e^{-X} \sum_{n=2}^{\infty} (-2a\sqrt{t})^{n-2} y_n$$

$$(2.15.11) \quad J_{21}(a, b, c, t) = \frac{e^{-X}}{\sqrt{t}} \sum_{n=0}^{\infty} (-2a\sqrt{t})^n y_n \quad X = (b^2 + c^2)/t,$$

where

$$(2.15.12) \quad y_n = 2T^{n-1} e^X G_n(c, b, T), \quad G_n(c, b, T) = \int_T^{\infty} e^{-c^2 w^2} \frac{i^n \operatorname{erfc}(bw)}{w^n} dw \quad T = \frac{1}{\sqrt{t}}.$$

An extensive stability analysis on the 3-term recurrence for y_n shows that the recurrence must be started with two (quadrature) values near the index $[2X]$.

Recurrence for $y_n = 2T^{n-1} e^X G_n(c, b, T)$

y_n is scaled to avoid extremes in values from exponentials:

$$(2.15.13) \quad y_n = 2T^{n-1} e^X G_n(c, b, T), \quad X = (b^2 + c^2)/t = (b^2 + c^2)T^2$$

$$(2.15.14) \quad n(n+1)y_{n+1} + 2n(bT)y_n + Xy_{n-1} = e^{b^2 T^2} i^{n-1} \operatorname{erfc}(bT)$$

$$(2.15.15) \quad y_0 = \frac{2e^X}{T} \int_T^{\infty} e^{-c^2 w^2} \operatorname{erfc}(bw) = \frac{2e^X}{T} I_5(c, b, T), \quad X = (b^2 + c^2)/t, \quad T = \frac{1}{\sqrt{t}},$$

$$(2.15.16) \quad y_1 = -bTy_0 + \frac{1}{\sqrt{\pi}} [e^X E_1(X)],$$

Here $I_5(c, b, T)$ is the I function of Folder 5. A stability analysis indicates that the recurrence must be carried out by recurring away from the index $N=[2X]$ to keep homogeneous solutions of the difference equation from amplifying rounding errors.

Special Cases

$c = 0$

$$(2.15.17) \quad I_{21}(a, b, 0, t) = 0, \quad I_{21}^c(a, b, 0, t) = V(t)$$

$a = 0$ for $I_{21}(0, b, c, t)$ Using $\text{erf}(x) = 1 - \text{erfc}(x)$, we have

$$(2.15.18) \quad I_{21}(0, b, c, t) = 2J_3^c(b, T) - 2W_3^c(b, c, T) = \frac{\text{erfc}(bT)}{T^2} - \frac{2b}{T} \text{ierfc}(bT) - 2W_3^c(b, c, T).$$

We chose this form because the computational results are much better than the results in terms of J_3 and W_3 . Then, using the formula for W_3^c from Chapter 3, Folder 10

$$I_{21}(0, b, c, t) = \frac{\text{erf}(cT) \text{erfc}(bT)}{T^2} - \frac{2b}{T} \text{ierfc}(bT) + \frac{2}{\sqrt{\pi}} \left[bI_1^c(b, c, T) + I_1^c(c, b, T) \right]$$

Combining the iterated coerror functions using the formula from Folder 10,

$$I_1^c(b, c, T) = \frac{\sqrt{\pi}}{T} \text{erfc}(cT) \text{ierfc}(bT) - \frac{c}{\sqrt{\pi}} E_1(X) + 2bcI_5(c, b, T),$$

improves the computation somewhat by minimizing losses of significance

$$(2.15.19) \quad I_{21}(0, b, c, t) = \frac{4}{T^2} i^2 \text{erfc}(bT) \text{erf}(cT) + \frac{2c}{\sqrt{\pi}} \left[-\frac{b}{\sqrt{\pi}} E_1(X) + 2b^2 I_5(c, b, T) + I_1^c(c, b, T) \right]$$

The series for $0 \leq a\sqrt{t} \leq 1$ with $a=0$ gives

$$(2.15.20) \quad I_{21}(0, b, c, t) = 4ti^2 \text{erfc}\left(\frac{b}{\sqrt{t}}\right) \text{erf}\left(\frac{c}{\sqrt{t}}\right) + \frac{4c\sqrt{t}}{\sqrt{\pi}} e^{-x} y_2(c, b, T), \quad T = 1/\sqrt{t}.$$

$a = 0$ for $I_{21}^c(0, b, c, t)$

For $I_{21}^c(0, b, c, t)$, we have

$$(2.15.21) \quad I_{21}^c(0, b, c, t) = \int_0^t \text{erfc}\left(\frac{b}{\sqrt{\tau}}\right) \text{erfc}\left(\frac{c}{\sqrt{\tau}}\right) d\tau = 2W_3^c(b, c, T), \quad T = 1/\sqrt{t}$$

where W_3^c is computed in Chapter 3, Folder 10b. From above, we also have

$$(2.15.22) \quad I_{21}^c(0, b, c, t) = 4ti^2 \text{erfc}\left(\frac{b}{\sqrt{t}}\right) \text{erfc}\left(\frac{c}{\sqrt{t}}\right) - \frac{4c\sqrt{t}e^{-x}}{\sqrt{\pi}} y_2(c, b, T), \quad T = 1/\sqrt{t}.$$

$a = 0$ for $J_{21}(0, b, c, t)$

$$(2.15.23) \quad J_{21}(0, b, c, t) = \int_0^t \text{erfc}\left(\frac{b}{\sqrt{\tau}}\right) \frac{e^{-c^2/\tau}}{\tau^{3/2}} d\tau, \quad \tau = \frac{1}{w^2}$$

$$= 2 \int_T^\infty e^{-c^2 w^2} \text{erfc}(bw) dw = 2I_5(c, b, T), \quad T = \frac{1}{\sqrt{t}}.$$

$a = 0, c = 0$ for $J_{21}(0, b, 0, t)$

$$(2.15.24) \quad J_{21}(0, b, 0, t) = 2I_5(0, b, T) = 2 \int_T^\infty \operatorname{erfc}(bw) dw = \frac{2}{b} i \operatorname{erfc}(bT)$$

$a = 0, b = 0$ for $I_{21}(0, 0, c, t)$

$$(2.15.25) \quad I_{21}(0, 0, c, t) = \int_0^t \operatorname{erf}\left(\frac{c}{\sqrt{\tau}}\right) d\tau \quad (\text{see case for } a = 0)$$

$$= \frac{\operatorname{erf}(cT)}{T^2} + \frac{2c}{T} i \operatorname{erfc}(cT)$$

$a = 0$ for $S_1(0, b, c, t)$ (see also case for $a = 0$ for $J_{21}(0, b, c, t)$)

$$(2.15.26) \quad S_1(0, b, c, t) = \frac{\sqrt{\pi}}{\sqrt{t}} I_5(c, b, T), \quad T = \frac{1}{\sqrt{t}}.$$

$a = 0, b = 0$ for $S_1(0, 0, c, t)$

From above,

$$(2.15.27) \quad S_1(0, 0, c, t) = \frac{\sqrt{\pi}}{\sqrt{t}} I_5(c, 0, T) = \sqrt{\frac{\pi}{t}} \int_T^\infty e^{-c^2 w^2} dw = \frac{\pi}{2c} T \operatorname{erfc}(cT), \quad T = \frac{1}{\sqrt{t}}$$

$b=0$ for $I_{21}(a, 0, c, t)$

$$(2.15.28) \quad I_{21}(a, 0, c, t) = V(a, 0, t) \operatorname{erf}\left(\frac{c}{\sqrt{t}}\right) + \frac{c\sqrt{t}}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-a\sqrt{t})^n}{\Gamma(\frac{n}{2} + 2)} E_{\frac{n+3}{2}}\left(\frac{c^2}{t}\right)$$

Notice also that

$$V(a, 0, t) = 2 I_{23}(a\sqrt{t}) / a^2, \quad a \neq 0$$

$$(2.15.29) \quad I_{23}(x) = (e^{x^2} \operatorname{erfc}(x) - 1) / 2 + x / \sqrt{\pi} = x^2 \sum_{n=0}^{\infty} \frac{(-x)^n}{\Gamma(\frac{n}{2} + 1)(n + 2)} = \frac{x^2}{2} \sum_{n=0}^{\infty} \frac{(-x)^n}{\Gamma(\frac{n}{2} + 2)}$$

where I_{23} and related functions are found in Folder 23.

Computer Subroutines

V(a,b,t): DOUBLE PRECISION FUNCTION DVOFT(...)

$I_{21}(a, b, c, t)$ or $I_{21}^c(a, b, c, t)$: SUBROUTINE INTEG121(...) with **KODE=1** or **KODE=2**

$J_{21}^c(a, b, c, t)$: SUBROUTINE INTEGJ21(...)

$S_1(a, b, c, t)$: SUBROUTINE INTEGS1(...)

$y_n = 2T^{n-1}e^x G_n(c, b, T)$: SUBROUTINE GNSEQ(...)

References: Chapter 3, Folder 21

(2.16) Functions $I_{22}(a,b,c,t)$ and $J_{22}(a,b,c,t)$

$$I_{22}(a,b,c,t) = \int_0^t U(a,b,\tau) \frac{e^{-c^2/\tau}}{\sqrt{\tau}} d\tau$$

$$J_{22}(a,b,c,t) = \int_0^t U(a,b,\tau) \sqrt{\tau} e^{-c^2/\tau} d\tau$$

$$U(a,b,t) = e^{a^2t+2ab} \operatorname{erfc}(a\sqrt{t} + b/\sqrt{t})$$

$$a \geq 0, \quad b \geq 0, \quad c \geq 0, \quad t > 0$$

Representations

$$(2.16.1) \quad I_{22}(a,b,c,t) = \frac{1}{a\sqrt{\pi}} E_1(X) - \frac{2\sqrt{t}}{a\sqrt{\pi}} S_2(a,b,c,t)$$

$$(2.16.2) \quad J_{22}(a,b,c,t) = \frac{t}{a\sqrt{\pi}} E_2(X) - \frac{1}{a^2\sqrt{\pi}} \left(b + \frac{1}{2a} \right) E_1(X) + \frac{\sqrt{t}}{a^2} e^{-X} [e^{B^2} \operatorname{erfc}(B)]$$

$$- \frac{2c^2\sqrt{t}}{a^2\sqrt{\pi}} S_1(a,b,c,t) + \frac{\sqrt{t}}{a^3\sqrt{\pi}} S_2(a,b,c,t)$$

where $S_1(a,b,c,t)$ was defined in Chapter 3, Folder 21,

$$(2.16.3) \quad S_1(a,b,c,t) = e^{-X} \int_0^\infty \frac{e^{-2Bw-w^2}}{c^2 + (b + w\sqrt{t})^2} dw, \quad B = a\sqrt{t} + b/\sqrt{t}$$

$$X = (b^2 + c^2)/t$$

and

$$(2.16.4) \quad S_2(a,b,c,t) = e^{-X} \int_0^\infty \frac{e^{-2Bw-w^2} (b + w\sqrt{t})}{c^2 + (b + w\sqrt{t})^2} dw.$$

We also have for $L = B/\sqrt{a^2t + c^2/t} \geq 2$,

$$(2.16.5) \quad S_1(a,b,c,t) = \frac{e^{-X}}{2Bt} \sum_{k=0}^\infty \frac{U_k(x)}{L^k} [e^{B^2} E_{(k+3)/2}(B^2)], \quad B = a\sqrt{t} + b/\sqrt{t}$$

$$X = (b^2 + c^2)/t$$

$$(2.16.6) \quad S_2(a,b,c,t) = \frac{e^{-X}}{2\sqrt{t}} \sum_{k=0}^\infty \frac{T_k(x)}{L^k} [e^{B^2} E_{(k+2)/2}(B^2)], \quad x = \frac{a\sqrt{t}}{\sqrt{a^2t + c^2/t}}$$

where $T_k(x)$ and $U_k(x)$ are Chebyshev polynomials of the first and second kinds. Both polynomials can be generated by forward recurrence on their three-term recurrence relations. While each series converges for $L > 1$, we apply the series for $L \geq 2$ to obtain rapid convergence in a numerical evaluation. If $L \geq 2$ is not satisfied, then $S_1(a,b,c,t)$ and $S_2(a,b,c,t)$ are computed by quadrature according to the procedure in the APPENDIX of Chapter 3, Folder 21.

The forms developed above have numerical problems for small a because of small differences of large numbers (an indeterminate form for $a \rightarrow 0$). Therefore we develop the power series for small a , ($a\sqrt{t} \leq 1$),

$$(2.16.7) \quad I_{22}(a, b, c, t) = 2e^{-X} \left[b \sum_{n=0}^{\infty} y_n (-2a\sqrt{t})^n + \sqrt{t} \sum_{n=0}^{\infty} (n+2) y_{n+2} (-2a\sqrt{t})^n \right]$$

$$(2.16.8) \quad J_{22}(a, b, c, t) = 4\sqrt{t}e^{-X} \left[b^2 \sum_{n=0}^{\infty} y_{n+2} (-2a\sqrt{t})^n + b\sqrt{t} \sum_{n=0}^{\infty} (2n+5) y_{n+3} (-2a\sqrt{t})^n \right. \\ \left. + t \sum_{n=0}^{\infty} (n+2)(n+4) y_{n+5} (-2a\sqrt{t})^n \right]$$

where

$$(2.16.9) \quad y_n = 2T^{n-1} e^X G_n(c, b, t) = 2T^{n-1} e^X \int_T^{\infty} e^{-c^2 w^2} \frac{i^n \operatorname{erfc}(bw)}{w^n} dw, \quad T = 1/\sqrt{t},$$

is computed in (2.15) or Chapter 3, Folder 21.

Special Cases

$a = 0$ for

$$(2.16.10) \quad I_{22}(0, b, c, t) = \int_0^t \operatorname{erfc}\left(\frac{b}{\sqrt{\tau}}\right) \frac{e^{-c^2/\tau}}{\sqrt{\tau}} d\tau \\ = \frac{1}{T} E_{3/2}(c^2 T^2) - 2I_1(c, b, T)$$

where $T = 1/\sqrt{t}$ and I_1 is computed in Folder 10a. We also have

$$(2.16.11) \quad I_{22}(0, b, c, t) = 2\sqrt{t}e^{-c^2/t} \operatorname{erfc}(c/\sqrt{t}) - \frac{2b}{\sqrt{\pi}} E_1(X) - 4c^2 I_5(c, b, T)$$

where I_5 is the I function of Folder 5. Notice also that the series for small a at $a = 0$ gives

$$(2.16.12) \quad I_{22}(0, b, c, t) = 2e^{-X} [by_1(c, b, T) + 2\sqrt{t}y_2(c, b, T)]$$

$a = 0$ for

$$(2.16.13) \quad J_{22}(0, b, c, t) = \int_0^t \operatorname{erfc}\left(\frac{b}{\sqrt{\tau}}\right) \sqrt{\tau} e^{-c^2/\tau} d\tau, \\ J_{22}(0, b, c, t) = 2 \left[\frac{e^{-c^2 T^2} \operatorname{erfc}(bT)}{3T^3} - \frac{b}{3T^2 \sqrt{\pi}} E_2(X) - \frac{2c^2}{3} I_1^c(c, b, T) \right]$$

where I_1^c is defined and computed in Chapter 3, Folder 10b(also = I_1^c of (2.6)),

$$(2.16.14) \quad I_1^c(c, b, T) = \frac{\sqrt{\pi}}{T} i \operatorname{erfc}(cT) - I_1(c, b, T)$$

in terms of I_1 of Folder 10a,

$$(2.16.15) \quad I_1(c, b, T) = \frac{e^{-c^2 T^2} \operatorname{erf}(bT)}{T} + \frac{b}{\sqrt{\pi}} E_1(X) - c\sqrt{\pi} \operatorname{erfc}(cT) + 2c^2 I_5(c, b, T)$$

where I_5 is the I function of Chapter 3, Folder 5. Also,

$$(2.16.16) \quad J_{22}(0, b, c, t) = \frac{2}{3} \left[\sqrt{t}(t - 2c^2) e^{-c^2/t} \operatorname{erfc}(bT) - \frac{b}{T^2 \sqrt{\pi}} E_2(X) + \frac{2bc^2}{\sqrt{\pi}} E_1(X) + 4c^4 I_5(c, b, T) \right] \quad X = (b^2 + c^2)/t, \quad T = \frac{1}{\sqrt{t}}$$

We also have from the small a expression for $a = 0$,

$$(2.16.17) \quad J_{22}(0, b, c, t) = 4\sqrt{t} e^{-X} [b^2 y_2(c, b, T) + 5b\sqrt{t} y_3(c, b, T) + 8ty_4(c, b, T)]$$

$a = 0, b = 0$ for

$$(2.16.18) \quad I_{22}(0, 0, c, t) = \int_0^t \frac{e^{-c^2/\tau} d\tau}{\sqrt{\tau}}, \\ = 2\sqrt{\pi} i \operatorname{erfc}(cT), \quad T = \frac{1}{\sqrt{t}}$$

$a = 0, b = 0$ for

$$(2.16.19) \quad J_{22}(0, 0, c, t) = \int_0^t \sqrt{\tau} e^{-c^2/\tau} d\tau, \\ = t^{3/2} E_{5/2}(c^2 T^2), \quad T = \frac{1}{\sqrt{t}}.$$

$a = 0, c = 0$ for

$$(2.16.20) \quad I_{22}(0, b, 0, t) = \int_0^t \frac{\operatorname{erfc}(b/\sqrt{\tau})}{\sqrt{\tau}} d\tau \\ = \frac{2 \operatorname{erfc}(bT)}{T} - \frac{2b}{\sqrt{\pi}} E_1(b^2 T^2), \quad T = \frac{1}{\sqrt{t}}$$

$b=0$ for $I_{22}(a, 0, c, t)$

$$(2.16.21) \quad I_{22}(a, 0, c, t) = \sqrt{t} \sum_{n=0}^{\infty} \frac{(-a\sqrt{t})^n}{\Gamma(\frac{n}{2} + 1)} E_{\frac{n+3}{2}}\left(\frac{c^2}{t}\right)$$

Relationship Between $I_{22}(a,b,0,t)$ and $J_{22}(a,b,0,t)$

$$(2.16.22) \quad I_{22}(a,b,0,t) = 2U(a,b,t)\sqrt{t} + \frac{2at}{\sqrt{\pi}} E_2\left(\frac{b^2}{t}\right) - \frac{2b}{\sqrt{\pi}} E_1\left(\frac{b^2}{t}\right) - 2a^2 J_{22}(a,b,0,t).$$

Asymptotic Expansion For $I_{22}(a,0,c,t)$ For Large a

$$(2.16.23) \quad I_{22}(a,0,c,t) \approx \frac{e^{-c^2/t}}{a\sqrt{\pi}} \sum_{k=0}^N \frac{(-1)^k (1/2)_k}{(ac)^{2k}} [e^{c^2/t} \Gamma(k, \frac{c^2}{t})] + G_N$$

where

$$|G_N| \leq \frac{(1/2)_{N+1}}{a\sqrt{\pi} (a^2 c^2)^{N+1}} \Gamma(N+1, \frac{c^2}{t})$$

and for $k=0$ and $k=1$ we have

$$\Gamma(0,x) = \int_x^\infty \frac{e^{-w}}{w} dw = \int_1^\infty \frac{e^{-xv}}{v} dv = E_1(x), \quad \Gamma(1,x) = \int_x^\infty e^{-w} dw = e^{-x}.$$

Forward recurrence on

$$[e^x \Gamma(k+1, x)] = k[e^x \Gamma(k, x)] + x^k, \quad k = 1, 2, \dots \quad x = c^2 / t$$

is numerically stable.

Computer Subroutines

$I_{22}(a,b,c,t)$: SUBROUTINE INTEG122(...)

$J_{22}(a,b,c,t)$: SUBROUTINE INTEGJ22(...)

$S_2(a,b,c,t)$: SUBROUTINE INTEGS2(...)

References: Chapter 3, Folder 10, Folder 22

(2.17) Function $I_{24}(a,b,c,t)$, $I_{24}^c(a,b,c,t)$ and Related Integrals

$$I_{24}(a,b,c,t) = \int_0^t \tau U(\tau) \operatorname{erf}\left(\frac{c}{\sqrt{\tau}}\right) d\tau, \quad I_{24}^c(a,b,c,t) = \int_0^t \tau U(\tau) \operatorname{erfc}\left(\frac{c}{\sqrt{\tau}}\right) d\tau$$

$$J_{24}(a,b,t) = \int_0^t \tau U(\tau) d\tau \quad V_{24}(a,b,t) = \int_0^t V(\tau) d\tau$$

where

$$U(t) = e^{a^2 t + 2ab} \operatorname{erfc}(a\sqrt{t} + b/\sqrt{t})$$

$$V(t) = \int_0^t U(\tau) d\tau = \frac{2}{a} \sqrt{\frac{t}{\pi}} e^{-b^2/t} - \left(\frac{1}{a^2} + \frac{2b}{a}\right) \operatorname{erfc}\left(\frac{b}{\sqrt{t}}\right) + \frac{U(t)}{a^2}$$

$$a > 0, \quad b > 0, \quad c > 0, \quad t > 0$$

Representations

For $I_{24}(a,b,c,t)$ we have

$$(2.17.1) \quad I_{24}(a,b,c,t) = tV(t) \operatorname{erf}\left(\frac{c}{\sqrt{t}}\right) + \frac{c}{\sqrt{\pi}} T_0 - [T_1 - T_2 - T_3]$$

where $V(t)$ is computed in Folder 21 and

$$T_0(a,b,c,t) = \frac{2t}{a\sqrt{\pi}} E_2(X) - 2\left(\frac{1}{a} + \frac{2b}{a}\right) I_1^c(c,b,T) + \frac{1}{a^2} I_{22}(a,b,c,t)$$

$$T_1(a,b,c,t) = \frac{4}{3a\sqrt{\pi}} \left[\frac{e^{-b^2 T^2} \operatorname{erf}(cT)}{T^3} + \frac{c}{T^2 \sqrt{\pi}} E_2(X) - 2b^2 I_1(b,c,T) \right]$$

$$T_2(a,b,c,t) = 2\left(\frac{1}{a^2} + \frac{2b}{a}\right) [J_3(c,T) - W_3(b,c,T)] = 2\left(\frac{1}{a^2} + \frac{2b}{a}\right) [J_3^c(b,T) - W_3^c(b,c,T)]$$

$$T_3(a,b,c,t) = \frac{1}{a^2} I_{21}(a,b,c,t), \quad T = \frac{1}{\sqrt{t}}, \quad X = (b^2 + c^2)T^2$$

with I_1 , J_3 , J_3^c , W_3 , W_3^c and I_{22} computed in Folders 10 and 22 of Chapter 3.

For $I_{24}^c(a,b,c,t)$ we have

$$(2.17.2) \quad I_{24}^c(a,b,c,t) = tV(t) \operatorname{erfc}\left(\frac{c}{\sqrt{t}}\right) - \frac{c}{\sqrt{\pi}} T_0^c - [T_1^c - T_2^c + T_3^c]$$

where

$$T_0^c = T_0$$

$$T_1^c = \frac{4}{3a\sqrt{\pi}} \left[\frac{e^{-b^2 T^2} \operatorname{erfc}(cT)}{T^3} - \frac{c}{T^2 \sqrt{\pi}} E_2(X) - 2b^2 I_1^c(b,c,T) \right]$$

$$T_2^c = 2\left(\frac{1}{a^2} + \frac{2b}{a}\right)W_3^c(b, c, T)$$

$$T_3^c = \frac{1}{a^2} I_{21}^c(a, b, c, t), \quad T = \frac{1}{\sqrt{t}}, \quad X = (b^2 + c^2)T^2$$

with I_1^c , J_3 , J_3^c , W_3 , W_3^c and I_{22}^c computed in Folders 10 and 22 of Chapter 3.

For $J_{24}(a, b, t)$ we have

$$(2.17.3) \quad J_{24}(a, b, t) = \int_0^t \tau U(\tau) d\tau = \lim_{c \rightarrow \infty} I_{24}(a, b, c, t) = tV(t) - \int_0^t V(\tau) d\tau$$

and

$$(2.17.4) \quad J_{24}(a, b, t) = \left(t - \frac{1}{a^2}\right)V(t) - \frac{2}{aT^3\sqrt{\pi}}E_{5/2}(b^2T^2) + \frac{4}{T^2}\left(\frac{1}{a^2} + \frac{2b}{a}\right)i^2 \operatorname{erfc}(bT)$$

$$J_{24}(a, b, t) = \left(t - \frac{1}{a^2}\right)V(t) - \frac{8}{aT^3}i^3 \operatorname{erfc}(bT) + \frac{4}{a^2T^2}i^2 \operatorname{erfc}(bT)$$

It follows that

$$(2.17.5) \quad V_{24}(a, b, t) = \int_0^t V(\tau) d\tau = \frac{1}{a^2}V(a, b, t) + \frac{2}{aT^3\sqrt{\pi}}E_{5/2}(b^2T^2) - \frac{4}{T^2}\left(\frac{1}{a^2} + \frac{2b}{a}\right)i^2 \operatorname{erfc}(bT)$$

$$= \frac{1}{a^2}V(a, b, t) + \frac{8}{aT^3}i^3 \operatorname{erfc}(bT) - \frac{4}{a^2T^2}i^2 \operatorname{erfc}(bT)$$

In all of these, computation for small a results in losses of significance by small differences of large numbers or an indeterminate form for $a \rightarrow 0$ since each integral is analytic in the parameter a .

Resolution of these forms for $a \rightarrow 0$ yields the power series in $a\sqrt{t}$ which converges best for $a\sqrt{t} < 1$:

$$(2.17.6) \quad I_{24}(a, b, c, t) = J_{24}(a, b, t) \operatorname{erf}\left(\frac{c}{\sqrt{t}}\right) + \frac{8cte^{-X}}{\sqrt{\pi}} \left[b \sum_{n=0}^{\infty} (-2a\sqrt{t})^n y_{n+3} + \sqrt{t} \sum_{n=0}^{\infty} (n+2)(-2a\sqrt{t})^n y_{n+4} \right]$$

$$(2.17.7) \quad I_{24}^c(a, b, c, t) = J_{24}(a, b, t) \operatorname{erfc}\left(\frac{c}{\sqrt{t}}\right) - \frac{8cte^{-X}}{\sqrt{\pi}} \left[b \sum_{n=0}^{\infty} (-2a\sqrt{t})^n y_{n+3} + \sqrt{t} \sum_{n=0}^{\infty} (n+2)(-2a\sqrt{t})^n y_{n+4} \right]$$

$$(2.17.8) \quad J_{24}(a, b, t) = tV(t) - V_{24}(a, b, t)$$

$$(2.17.9) \quad V_{24}(a, b, t) = 16t^2 \sum_{n=0}^{\infty} (-2a\sqrt{t})^n i^{n+4} \operatorname{erfc}(bT)$$

where $V(t)$ and the $y_n(c, b, T)$ sequence are computed in Chapter 3, Folder 21,

$$(2.17.10) \quad V(t) = 4t \sum_{n=0}^{\infty} (-2a\sqrt{t})^n i^{n+2} \operatorname{erfc}(bT) \quad T = \frac{1}{\sqrt{t}}, \quad X = (b^2 + c^2)T^2$$

$$(2.17.11) \quad y_n(c, b, T) = 2T^{n-1} e^X \int_T^{\infty} e^{-c^2 w^2} \frac{i^n \operatorname{erfc}(bw)}{w^n} dw.$$

The iterated coerror functions are generated in subroutine DINERFC and the $y_n(c,b,T)$ sequence is generated in subroutine GNSEQ.

Computer Subroutines

$I_{24}(a,b,c,t)$ or $I_{24}^c(a,b,c,t)$: SUBROUTINE INTEG124(...) with KODE=1 or KODE=2

$J_{24}(a,b,t)$: SUBROUTINE INTEGJ24(...)

$V_{24}(a,b,t)$: SUBROUTINE INTEGV24(...)

References: Chapter 3, Folders 10, 21, 22, 24

(2.18) Function $I_{25}(a,b,c,d,t)$

$$I_{25}(a,b,c,d,t) = \int_0^t U(a,b,\tau) U(c,d,\tau) d\tau$$

$$U(a,b,t) = e^{a^2 t + 2ab} \operatorname{erfc}(a\sqrt{t} + b/\sqrt{t})$$

$$a \geq 0, \quad b \geq 0, \quad c \geq 0, \quad d \geq 0, \quad t > 0$$

Representation

$$(2.18.1) \quad I_{25}(a,b,c,d,t) = \frac{1}{(a^2 + c^2)} \left\{ a^2 U(c,d,t) V(a,b,t) + \frac{c}{\sqrt{\pi}} R_1(a,b,d,t) - \frac{d}{\sqrt{\pi}} R_2(a,b,d,t) \right. \\ \left. - \frac{2ac^2}{\sqrt{\pi}} J_{22}(c,d,b,t) + c^2(1+2ab)I_{21}^c(c,d,b,t) + \frac{c}{\sqrt{\pi}} I_{22}(a,b,d,t) - \frac{d}{\sqrt{\pi}} J_{21}(a,b,d,t) \right\}$$

where

$$V(a,b,t) = \frac{2}{a} \sqrt{\frac{t}{\pi}} e^{-b^2/t} - \frac{(1+2ab)}{a^2} \operatorname{erfc}\left(\frac{b}{\sqrt{t}}\right) + \frac{1}{a^2} U(a,b,t) \\ = \frac{2\sqrt{t}}{a} \operatorname{ierfc}\left(\frac{b}{\sqrt{t}}\right) + \frac{1}{a^2} \left[U(a,b,t) - \operatorname{erfc}\left(\frac{b}{\sqrt{t}}\right) \right]$$

$$R_1(a,b,d,t) = \frac{2at}{\sqrt{\pi}} E_2(X) - 2(1+2ab)I_1^c(d,b,T)$$

$$R_2(a,b,d,t) = \frac{2a}{\sqrt{\pi}} E_1(X) - 2(1+2ab)I_5(d,b,T)$$

$$T = \frac{1}{\sqrt{t}}, \quad X = (b^2 + d^2)/t.$$

Here, I_5 and I_1^c are computed in Folders 5 and 10. V , J_{21} , I_{21}^c , I_{22} and J_{22} are the principal results of Folders 21 and 22. Notice also that I_{25} is symmetric in the pairs (a,b) and (c,d) and exchanging these pairs on the right yields an alternate form. In fact, any convex linear combination of these forms gives I_{25} ; in particular, adding and dividing by 2 gives the symmetric form.

Computer Subroutine

$I_{25}(a,b,c,d,t)$: SUBROUTINE INTEG125(...)

Reference Chapter 3, Folder 25

(2.19) Function $I_{26}(a,b,c,d,t)$

$$I_{26}(a,b,c,d,t) = \int_0^t \tau U(a,b,\tau) U(c,d,\tau) d\tau$$

$$U(a,b,t) = e^{a^2 t + 2ab} \operatorname{erfc}(a\sqrt{t} + b/\sqrt{t})$$

$$a \geq 0, \quad b \geq 0, \quad c \geq 0, \quad d \geq 0, \quad t > 0$$

Series Representations

Symmetric form

$$(2.19.1) \quad I_{26}(a,b,c,d,t) = \frac{1}{(a^2 + c^2)} \left\{ t U(a,b,t) U(c,d,t) - I_{25}(a,b,c,d,t) \right. \\ \left. + \frac{a}{\sqrt{\pi}} J_{22}(c,d,b,t) - \frac{b}{\sqrt{\pi}} I_{22}(c,d,b,t) \right. \\ \left. + \frac{c}{\sqrt{\pi}} J_{22}(a,b,d,t) - \frac{d}{\sqrt{\pi}} I_{22}(a,b,d,t) \right\}$$

where I_{22} , J_{22} and I_{25} are defined in Chapter 3, Folders 22 and 25. A more efficient computational form is also presented in terms of more fundamental integrals which eliminates redundant computation.

An alternate, non-symmetric, more complicated form is also derived in Chapter 3, Folder 26.

Computer Subroutine

$I_{26}(a,b,c,d,t)$: SUBROUTINE INTEG126(...)

Reference: Chapter 3, Folder 26

(2.20) Indefinite Integrals

$$J = \int e^{(a^2-b^2)x} \operatorname{erfc}\left(a\sqrt{x} + \frac{c}{\sqrt{x}}\right) dx$$

$$I = \int x e^{(a^2-b^2)x} \operatorname{erfc}\left(a\sqrt{x} + \frac{c}{\sqrt{x}}\right) dx$$

Representations

$$(2.20.1) \quad J \equiv \int e^{(a^2-b^2)x} \operatorname{erfc}\left(a\sqrt{x} + \frac{c}{\sqrt{x}}\right) dx$$
$$= \frac{e^{(a^2-b^2)x}}{a^2-b^2} \operatorname{erfc}\left(a\sqrt{x} + \frac{c}{\sqrt{x}}\right) + \frac{e^{-2ac}}{2} \left[-f(\sqrt{x}, a, b, c) + f(\sqrt{x}, -a, b, -c) \right]$$

$$\text{where } f(\sqrt{x}, a, b, c) = \frac{e^{2bc}}{(a^2-b^2)} \left(1 + \frac{a}{b}\right) \operatorname{erfc}\left(b\sqrt{x} + \frac{c}{\sqrt{x}}\right)$$

$$(2.20.2) \quad I = -\frac{e^{(a^2-b^2)x}}{a^2-b^2} \left[-x + \frac{1}{a^2-b^2} \right] \operatorname{erfc}[X(\sqrt{x}, a, c)]$$
$$+ \frac{e^{-2ac}}{2} [F(\sqrt{x}, a, b, c) - F(\sqrt{x}, -a, b, -c)]$$

$$F(\sqrt{x}, a, b, c) = \frac{e^{2bc}}{a^2-b^2} \left\{ \frac{-\sqrt{x}}{b\sqrt{\pi}} e^{-X^2(\sqrt{x}, b, c)} \left(1 + \frac{a}{b}\right) \right.$$
$$\left. + \left[\left(\frac{c}{b} + \frac{1}{a^2-b^2} \right) \left(1 + \frac{a}{b}\right) - \frac{a}{2b^3} \right] \operatorname{erfc}[X(\sqrt{x}, b, c)] \right\}$$

$$X(\sqrt{x}, a, c) = a\sqrt{x} + c/\sqrt{x}$$

Computer Subroutines

I: SUBROUTINE ERFINT(...)

References: Chapter 3, Folder 12

(2.21) Functions $H_{23}(x)$, $I_{23}(x)$ and $J_{23}(x)$

$$H_{23}(x) = \int_0^x e^{w^2} \operatorname{erfc}(w) dw = \frac{1}{2} \int_0^{x^2} e^v \operatorname{erfc}(\sqrt{v}) \frac{dv}{\sqrt{v}}$$

$$I_{23}(x) = \int_0^x e^{w^2} \operatorname{erfc}(w) w dw = \frac{1}{2} \int_0^{x^2} e^v \operatorname{erfc}(\sqrt{v}) dv$$

$$J_{23}(x) = \int_0^x e^{w^2} \operatorname{erfc}(w) w^2 dw = \frac{1}{2} \int_0^{x^2} e^v \operatorname{erfc}(\sqrt{v}) \sqrt{v} dv$$

$$x \geq 0$$

Representations

H_{23} is evaluated from the relations

$$(2.21.1) \quad H_{23}(x) = \begin{cases} S(x,0) & 0 \leq x \leq 1 \\ S_2 + S(x,2) & 1 < x \leq 3 \\ S_4 + S(x,4) & 3 < x \leq 4 \\ S_4 + V(x,4) & 4 < x < \infty \end{cases}$$

where $S(x, x_0)$ is the Taylor expansion about x_0 ,

$$(2.21.2) \quad S(x, x_0) = \sum_{n=0}^{\infty} (-2)^n [e^{x_0^2} i^n \operatorname{erfc}(x_0)] \frac{(x - x_0)^{n+1}}{n+1},$$

$$(2.21.3) \quad S_2 = \int_0^2 e^{v^2} \operatorname{erfc}(v) dv, \quad S_4 = \int_0^4 e^{v^2} \operatorname{erfc}(v) dv,$$

$$(2.21.4) \quad S_2 = 0.9753620874841564 \quad S_4 = 1.344468257503159.$$

and $V(x,4)$ is the integral

$$(2.21.5) \quad V(x,4) = \int_4^x y(v) dv \quad y(v) = e^{v^2} \operatorname{erfc}(v) = \frac{1}{v\sqrt{\pi}} \sum_{n=0}^{\infty} ' a_{2r} T_{2r} \left(\frac{4}{v} \right), \quad v \geq 4,$$

where $y(v)$ is a Chebyshev sum with coefficients a_{2r} (see Chapter 3, Folder 23 for numerical values).

The result for $V(x,4)$ is

$$(2.21.6) \quad V(x,4) = \frac{1}{\sqrt{\pi}} \left[\sum_{r=0}^{\infty} ' a_{2r} A_{2r}(x) + \ln \left(\frac{x}{4} \right) \right]$$

where $A_{2r}(x)$ is computed from the recurrence

$$A_0(x) = 0, \quad A_2(x) = 1 - \left(\frac{4}{x} \right)^2$$

(2.21.7)

$$A_{2r+2}(x) + A_{2r}(x) = -\frac{1}{2r(r+1)} - \left[\frac{T_{2r+2}(4/x)}{2r+2} - \frac{T_{2r}(4/x)}{2r} \right], \quad r \geq 1.$$

Truncation of $V(x,4)$ at 18 terms suffices for errors $O(10^{-16})$. Here, the prime on the sum means to halve the first term.

$I_{23}(x)$ can be evaluated explicitly,

$$(2.21.8) \quad I_{23}(x) = \frac{e^{x^2} \operatorname{erfc}(x) - 1}{2} + \frac{x}{\sqrt{\pi}}$$

and $J_{23}(x)$ can be expressed in terms of $H_{23}(x)$,

$$(2.21.9) \quad J_{23}(x) = \frac{1}{2} \left[x e^{x^2} \operatorname{erfc}(x) + \frac{x^2}{\sqrt{\pi}} - H_{23}(x) \right]$$

Reduction Formula

Let

$$(2.21.10) \quad I_{\alpha}(x) = \int_0^x e^{w^2} \operatorname{erfc}(w) w^{\alpha} dw, \quad \alpha = 2n \text{ or } 2n+1, \quad n = 1, 2, \dots$$

Then

$$(2.21.11) \quad I_{\alpha}(x) = \frac{1}{2} x^{\alpha-1} \operatorname{erfc}(x) + \frac{1}{\sqrt{\pi}} \int_0^x w^{\alpha-1} dw - \frac{(\alpha-1)}{2} \int_0^x e^{w^2} \operatorname{erfc}(w) w^{\alpha-2} dw$$

$$(2.21.12) \quad I_{\alpha}(x) = \frac{1}{2} x^{\alpha-1} \operatorname{erfc}(x) + \frac{1}{\alpha\sqrt{\pi}} x^{\alpha} - \frac{(\alpha-1)}{2} I_{\alpha-2}(x).$$

Notice that for $\alpha = 2$ we get the formula for $J_{23}(x)(=I_2(x))$ since $I_0(x) = H_{23}(x)$. Since $\alpha = 2n$ or $2n+1$, a repeated application of this formula ends up with $I_0(x)$ or $I_1(x)$ which translate to $H_{23}(x)$ or $I_{23}(x)$ respectively.

Numerically, all of the formulas derived so far suffer from high cancellation of significant digits when x is small which results in a loss of relative error. Consequently the power series is valuable in numerical evaluation.

Power Series

$$(2.21.13) \quad I_{\alpha}(x) = \int_0^x e^{w^2} \operatorname{erfc}(w) w^{\alpha} dw = x^{\alpha+1} \sum_{n=0}^{\infty} \frac{(-x)^n}{\Gamma\left(\frac{n}{2} + 1\right)(n + \alpha + 1)}, \quad \alpha = 0, 1, 2, \dots$$

where $I_0(x) = H_{23}(x)$, $I_1(x) = I_{23}(x)$ and $I_2(x) = J_{23}(x)$

Asymptotic Expansion for $H_{23}(x)$ for $x \rightarrow \infty$

$$(2.21.14) \quad H_{23}(x) = \int_0^x e^{w^2} \operatorname{erfc}(w) dw = \frac{1}{2} \int_0^{x^2} \frac{e^{\tau} \operatorname{erfc}(\sqrt{\tau})}{\sqrt{\tau}} d\tau \approx \frac{1}{2\sqrt{\pi}} \left[\gamma + 2 \ln(2x) - \sum_{n=1}^{\infty} \frac{A_n}{x^{2n}} \right]$$

where γ is the Euler constant

$$\gamma = 0.5772156649015328606 \quad \text{and} \quad A_n = \frac{(-1)^n (1/2)_n}{n}.$$

Computer Subroutines

$H_{23}(x)$: DOUBLE PRECISION FUNCTION DHERFC(...)

References: Chapter 3, Folder 23

(2.22) Incomplete Bessel Function

$$I(a, b, X) = \int_X^\infty e^{-at-b/t} dt,$$

$$a > 0, \quad b > 0, \quad X > 0$$

Representations

Small b/X expansion

$$(2.22.1) \quad I = \frac{e^{-aX}}{a} + X \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \left(\frac{b}{X} \right)^k E_k(aX)$$

Small aX expansion

$$(2.22.2) \quad I = 2\sqrt{\frac{b}{a}} K_1(2\sqrt{ab}) - X \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} (aX)^k E_{k+2}\left(\frac{b}{X}\right)$$

A representation in terms of analytic functions suitable for a quadrature,

$$(2.22.3) \quad I(a, b, X) = \sqrt{\frac{b}{a}} \int_{\ln(X\sqrt{a/b})}^{\infty} e^{-2\sqrt{ab} \cosh v + v} dv$$

The incomplete Gamma functions are explored in Chaudhry and Zubair where Equation 2.163 expresses I in terms of

$$(2.22.4) \quad \Gamma(\alpha, x : b) = \int_x^\infty t^{\alpha-1} \exp(-t - b/t) dt = \frac{1}{2\pi i} \sum_{n=0}^{\infty} \frac{(-b)^n}{n!} \int_{c-j\infty}^{c+j\infty} \frac{\Gamma(s) x^{\alpha-n-s}}{s + n - \alpha} ds,$$

which for $\alpha = 1$ is $I(1, b, x)$. Evaluation of the residues in the complex integral results in the small b/X expansion. Notice that a change of variables $t=v/a$ in $I(a, b, X)$ produces

$$(2.22.5) \quad I(a, b, X) = \frac{1}{a} I(1, ab, aX) = \frac{1}{a} \Gamma(1, aX : ab)$$

Special Cases

$X=0$ gives the Bessel Function of order 1

$$(2.22.6) \quad I(a, b, 0) = \int_0^\infty e^{-at-b/t} dt = 2\sqrt{\frac{b}{a}} K_1(2\sqrt{ab})$$

$a=0$ gives

$$(2.22.7) \quad I(0, b, X) = \int_X^\infty e^{-b/t} dt = X E_2(b/X).$$

$b=0$ gives

$$(2.22.8) \quad I(a, 0, X) = \int_X^\infty e^{-at} dt = \frac{e^{-aX}}{a}$$

References: Chapter 3, Folder17;

Chaudhry, M. A. and Zubair, S. M. "On A Class of Incomplete Gamma Functions with Applications" Chapman & Hall/CRC, Boca Raton, 2001