# Chebyshev Expansions for Integrals of the Error Function

By Van E. Wood

**1. Introduction.** The repeated integrals of the error function [1, Chapter 7] are defined by

$$\text{(1a)} \qquad i^n \operatorname{erfc} z = \int_z^\infty i^{n-1} \operatorname{erfc} t \, dt, \qquad (n = 0, 1, 2, \cdots),$$

$$\text{(1b)} \qquad i^0 \operatorname{erfc} z = \operatorname{erfc} z, \qquad i^{-1} \operatorname{erfc} z = 2\pi^{-1/2} e^{-z^2}.$$

From the recurrence relation

$$\text{(2)} \qquad i^n \operatorname{erfc} z = -zn^{-1} i^{n-2} \operatorname{erfc} z + (2n)^{-1} i^{n-2} \operatorname{erfc} z, \qquad (n = 1, 2, 3, \cdots),$$

the integrals may be calculated for small $z$, although with considerable loss of accuracy. For large $z$, backward recurrence may be used [2]; this is certainly the best method if one needs several of these functions for fairly large arguments, but if one wants values of a single function for a large range of arguments, it is very convenient to use Chebyshev expansions. In this note we present such expansions for the cases $n = 1$ and $n = 2$, $z$ real and nonnegative.

**2. General Remarks.** The integrals of the error function may be expressed in terms of generalized hypergeometric functions as follows:

$$\text{(3a)} \qquad i^n \operatorname{erfc} z = 2^{-n} \sum_{k=0}^{n-2} \frac{(-2z)^k}{k!\,\Gamma\left(1 + \frac{n-k}{2}\right)} + \frac{(-z)^n}{n!} + \frac{(-z)^{n-1}}{\pi^{1/2}\Gamma(n)} \times {}_2F_2\left(-\frac{1}{2}, 1; \frac{n}{2}, \frac{n+1}{2}; -z^2\right)$$

$$\text{(3b)} \qquad = \frac{e^{-z^2}}{\pi^{1/2} 2^n z^{n+1}} \, {}_2F_0\left(\frac{n+1}{2}, \frac{n+2}{2}; -z^{-2}\right).$$

The first expression is closely related to the recurrence relation (2) and also suffers from cancellation of terms, but for the cases of interest here can be used for $z < 1$, as explained further below. In the cases $n = 1, 2$, the ${}_2F_2$ reduces to a confluent hypergeometric function. All we wish to do in this case is to give Chebyshev expansions for these hypergeometric functions, thus making the evaluation of the series a little more efficient. The expression (3b) is just the usual asymptotic expansion for the integrals of the error function [1], [3]; by expanding the ${}_2F_0$ in Chebyshev polynomials, this asymptotic series is converted to a rapidly convergent, easily evaluated form, as discussed by Clenshaw [4]. The coefficients occurring in the expansions of the hypergeometric functions in terms of Chebyshev polynomials may be expressed in terms of generalized hypergeometric functions of higher order,

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as discussed by Fields, Wimp, and Luke [5], [6], [7], but for numerical calculation of these coefficients it is somewhat easier in the present case to use the solution of the differential equation to obtain a recurrence relation for the coefficients [4]. The recurrence relations for the confluent functions are easily found; for the asymptotic expansion the appropriate differential equation is

$$v^3 f'' + 2(k^2 + (n+2)v^2)f' + (n+1)(n+2)f = 0 \tag{4}$$

where

$$\pi^{1/2} 2^n f = {}_2F_0(\tfrac{1}{2}(n+1), \tfrac{1}{2}(n+2); -z^{-2}) = \tfrac{1}{2} \sum_{r=0}^{\infty} \epsilon_r a_{2r} T_{2r}(v) ;$$

$$v = kz^{-1} ; \epsilon_r = 2 - \delta_{r_0} .$$

The $a$'s are then found to satisfy the relations

$$\begin{aligned}(r+n)(r+n-1)a_{r-2} = (r-n)(r-n+1)a_{r+2} - 2((2k)^2 + 2n + 1)\, ra_r \\ - 2r(a'_{r-1} + a'_{r+1}) ;\end{aligned} \tag{5a}$$

$$a'_{r-1} = a'_{r+1} + 2ra_r ; \qquad r = 2, 4, 6, \cdots . \tag{5b}$$

**3. Results and Discussion.** We obtain for the first two integrals of the error function

$$\pi^{1/2} i \operatorname{erfc} z = -\pi^{1/2} z + \tfrac{1}{2} \sum \epsilon_r b_r T_{2r}(z) = \tfrac{1}{4} z^{-2} e^{-z^2} \sum \epsilon_r c_r T_{2r}(z^{-1}) ; \tag{6a}$$

$$4i^2 \operatorname{erfc} z = 1 + 2z^2 - 2\pi^{-1/2} z \sum \epsilon_r d_r T_{2r}(z) = \tfrac{1}{2} \pi^{-1/2} z^{-3} e^{-z^2} \sum \epsilon_r e_r T_{2r}(z^{-1}) ; \tag{6b}$$

where the coefficients $b$, $c$, $d$, $e$, are given to 7 decimal places in Table I. Using the expansions in $T_{2r}(z)$ for $z < 1$ and those in $T_{2r}(z^{-1})$ for $z > 1$, one can calculate

TABLE I

*Numerical values of expansion coefficients occurring in Eq.* 6

| $r$ | $b_r$ | $c_r$ | $d_r$ | $e_r$ |
|---|---|---|---|---|
| 0 | 2.8929827 | 1.3618413 | 2.3109853 | 1.0388528 |
| 1 | .4300235 | −.2409343 | .1519739 | −.3229885 |
| 2 | −.0156956 | .0560098 | −. 34009 | .1028703 |
| 3 | . 7391 | −.0152168 | . 1139 | −.0347257 |
| 4 | −. 319 | . 45926 | −. 38 | .0123637 |
| 5 | . 12 | −. 14980 | . 1 | −. 46072 |
| 6 | | . 5192 | | . 17850 |
| 7 | | −. 1890 | | −. 7152 |
| 8 | | . 717 | | . 2951 |
| 9 | | −. 282 | | −. 1249 |
| 10 | | . 114 | | . 541 |
| 11 | | −. 48 | | −. 239 |
| 12 | | . 21 | | . 108 |
| 13 | | −. 9 | | −. 49 |
| 14 | | . 4 | | . 23 |
| 15 | | −. 1 | | −. 11 |
| 16 | | | | . 5 |
| 17 | | | | −. 3 |
| 18 | | | | . 1 |

$i$ erfc $z$ and $i^2$ erfc $z$ correct to 6 significant figures (7 s.f. for $z > 1$) using single precision on a computer with word length of 8 decimal places, for all $z$ for which $e^{-z^2}$ can be calculated correctly. To obtain greater accuracy, it is necessary either to use double precision or to use more than two different expansions for each function. From Gautschi's formula [2] for the number of terms required for calculation by backward recurrence, we see that that method will be better (for 7 s.f. accuracy) if all the $z$'s of interest are greater than about 2.5. The advantage accruing from the use of Chebyshev approximations would be still greater for multiple-precision calculations of very high accuracy.

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# An Integral Representation for the Modified Bessel Function of the Third Kind, Computable for Large, Imaginary Order

**By James D. Lear and James E. Sturm**

The one-dimensional Schroedinger equation describing the quantum-mechanical motion of a particle of total energy $E$ and mass $\mu$ in a potential field of the form:

$$V = B \exp(-r/a) \quad \text{for } r > 0$$
$$V = \infty \quad \text{for } r \leq 0$$

has, as time-independent solutions, the functions

$$\left(\frac{\nu \sinh \pi\nu}{\pi}\right)^{1/2} K_{i\nu}(z)$$

where $\nu = 2a(2\mu E/\hbar^2)^{1/2}$, $z = 2aBe^{-r/2a}$, $K_{i\nu}(z)$ is the modified Bessel function of the third kind, and the normalization is to unit amplitude of the asymptotic ($r$ increasing) solution [1]. In attempting to compute values for $K_{i\nu}(z)$ through use of the representation:

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