NAG Fortran Library Routine Document

S21CCF

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details.

1 Purpose

S21CCF returns the value of one of the Jacobian theta functions $\theta_0(x,q)$, $\theta_1(x,q)$, $\theta_2(x,q)$, $\theta_3(x,q)$ or $\theta_4(x,q)$ for a real argument x and non-negative $q \leq 1$, via the routine name.

2 Specification

```
real FUNCTION S21CCF(K, X, Q, IFAIL)
INTEGER              K, IFAIL
real                 X, Q
```

3 Description

This routine evaluates an approximation to the Jacobian theta functions $\theta_0(x,q)$, $\theta_1(x,q)$, $\theta_2(x,q)$, $\theta_3(x,q)$ and $\theta_4(x,q)$ given by

$$\begin{aligned}
\theta_0(x,q) &= 1 + 2\textstyle\sum_{n=1}^{\infty}(-1)^n q^{n^2}\cos(2n\pi x),\\
\theta_1(x,q) &= 2\textstyle\sum_{n=0}^{\infty}(-1)^n q^{(n+\frac{1}{2})^2}\sin\{(2n+1)\pi x\},\\
\theta_2(x,q) &= 2\textstyle\sum_{n=0}^{\infty} q^{(n+\frac{1}{2})^2}\cos\{(2n+1)\pi x\},\\
\theta_3(x,q) &= 1 + 2\textstyle\sum_{n=1}^{\infty} q^{n^2}\cos(2n\pi x),\\
\theta_4(x,q) &= \theta_0(x,q),
\end{aligned}$$

where x and q (the *nome*) are real with $0 \leq q \leq 1$. Note that $\theta_1(x-\frac{1}{2},1)$ is undefined if $(x-\frac{1}{2})$ is an integer, as is $\theta_2(x,1)$ if x is an integer; otherwise, $\theta_i(x,1) = 0$ for $i = 0,1,\ldots,4$.

These functions are important in practice because every one of the Jacobian elliptic functions (see S21CBF) can be expressed as the ratio of two Jacobian theta functions (see Whittaker and Watson (1990)). There is also a bewildering variety of notations used in the literature to define them. Some authors (e.g., Section 16.27 in Abramowitz and Stegun (1972)) define the argument in the trigonometric terms to be x instead of πx. This can often lead to confusion, so great care must therefore be exercised when consulting the literature. Further details (including various relations and identities) can be found in the references.

S21CCF is based on a truncated series approach. If t differs from x or $-x$ by an integer when $0 \leq t \leq \frac{1}{2}$, it follows from the periodicity and symmetry properties of the functions that $\theta_1(x,q) = \pm\theta_1(t,q)$ and $\theta_3(x,q) = \pm\theta_3(t,q)$. In a region for which the approximation is sufficiently accurate, θ_1 is set equal to the first term ($n = 0$) of the transformed series

$$\theta_1(t,q) = 2\sqrt{\frac{\lambda}{\pi}}e^{-\lambda t^2}\sum_{n=0}^{\infty}(-1)^n e^{-\lambda(n+\frac{1}{2})^2}\sinh\{(2n+1)\lambda t\}$$

and θ_3 is set equal to the first two terms (i.e., $n \leq 1$) of

$$\theta_3(t,q) = \sqrt{\frac{\lambda}{\pi}}e^{-\lambda t^2}\left\{1 + 2\sum_{n=1}^{\infty} e^{-\lambda n^2}\cosh(2n\lambda t)\right\},$$

where $\lambda = \pi^2/|\log_e q|$. Otherwise, the trigonometric series for $\theta_1(t,q)$ and $\theta_3(t,q)$ are used. For all values of x, θ_0 and θ_2 are computed from the relations $\theta_0(x,q) = \theta_3(\frac{1}{2} - |x|, q)$ and $\theta_2(x,q) = \theta_1(\frac{1}{2} - |x|, q)$.

4 References

Abramowitz M and Stegun I A (1972) *Handbook of Mathematical Functions* (3rd Edition) Dover Publications

Byrd P F and Friedman M D (1971) *Handbook of Elliptic Integrals for Engineers and Scientists* pp. 315–320 (2nd Edition) Springer-Verlag

Magnus W, Oberhettinger F and Soni R P (1966) *Formulas and Theorems for the Special Functions of Mathematical Physics* 371–377 Springer-Verlag

Tølke F (1966) *Praktische Funktionenlehre (Bd. II)* 1–38 Springer-Verlag

Whittaker E T and Watson G N (1990) *A Course in Modern Analysis* (4th Edition) Cambridge University Press

5 Parameters

1: K – INTEGER *Input*

On entry: the function $\theta_K(x,q)$ to be evaluated. Note that K = 4 is equivalent to K = 0.

Constraint: $0 \leq K \leq 4$.

2: X – ***real*** *Input*

On entry: the argument x of the function.

Constraints:

X must not be an integer when Q = 1.0 and K = 2,
(X − 0.5) must not be an integer when Q = 1.0 and K = 1.

3: Q – ***real*** *Input*

On entry: the argument q of the function.

Constraint: $0.0 \leq Q \leq 1.0$.

4: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, −1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 for details.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

For environments where it might be inappropriate to halt program execution when an error is detected, the value −1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, for users not familiar with this parameter the recommended value is 0. **When the value −1 or 1 is used it is essential to test the value of IFAIL on exit.**

6 Error Indicators and Warnings

If on entry IFAIL = 0 or −1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL = 1

On entry, K < 0,
or K > 4,
or Q < 0.0,

or Q > 1.0,
or (X – 0.5) is an integer when Q = 1.0 and K = 1,
or X is an integer when Q = 1.0 and K = 2.

IFAIL = 2

The evaluation has been abandoned because the function value is infinite. The result is returned as the largest machine representable number (see X02ALF).

7 Accuracy

In principle the routine is capable of achieving full relative precision in the computed values. However, the accuracy obtainable in practice depends on the accuracy of the Fortran intrinsic functions for elementary functions such as SIN and COS.

8 Further Comments

None.

9 Example

The example program evaluates $\theta_2(x, q)$ at $x = 0.7$ when $q = 0.4$, and prints the results.

9.1 Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S21CCF Example Program Text.
*     Mark 20 Release. NAG Copyright 2001.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             Q, X, Y
      INTEGER          IFAIL, K
*     .. External Functions ..
      real             S21CCF
      EXTERNAL         S21CCF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S21CCF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) ' K    X     Q         Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) K, X, Q
      IFAIL = 0
*
      Y = S21CCF(K,X,Q,IFAIL)
*
      WRITE (NOUT,99999) K, X, Q, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,I2,2X,F4.1,2X,F4.1,2X,1P,E12.4,I6)
      END
```

9.2 Program Data

```
S21CCF Example Program Data
 2  0.7  0.4  : Values of K, X and Q
```

9.3 Program Results

```
 S21CCF Example Program Results

   K     X      Q          Y         IFAIL

   2    0.7    0.4   -6.9289E-01      0
```