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Erratum

Erratum to "COULCC: A continued-fraction algorithm for Coulomb functions of complex order with complex arguments" [Comput. Phys. Commun. 36 (1985) 363–372]

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1. Erratum

The subroutine COULCC, published in Comput. Phys. Commun. [1] as ACDP, is corrected in one place.

1.1. Arguments very nearly but not purely real

The Coulomb functions $F_{\ell}(\eta, \rho)$, when ℓ, η, ρ are all real, may be evaluated most efficiently by the same method as used in COULFG [2]. However, if the ℓ, η, ρ are *slightly* off their real axes, the program should ensure that its case selections are consistently applied.

The modified version of the program ensures that the value of ω for the intermediate calculation of $H_{\lambda}^{\omega} = G_{\lambda} + i\omega F_{\lambda}$ is kept as $\omega = 1$ in the AXIAL case selection:

REPLACE CARD ACDP0371IF(REAL(X).GE.XNEAR) OMEGA = SIGN(ONE,IMAG(THETAM)+ACC8)ACDP0371BY THE TWO CARDSIF(REAL(X).GE.XNEAR) OMEGA = SIGN(ONE,IMAG(THETAM)+ACC8)ACDP0371IF (AXIAL)OMEGA = ONEACDP0371

2. Test run output

2.1. Input

```
(100.,+2e-15),(0,0),(10,0),1,1,-1,F, 'near axial +'
(100., 0 ),(0,0),(10,0),1,1,-1,F, 'axial'
(100.,-2e-15),(0,0),(10,0),1,1,-1,F, 'near axial -'
(0,0),(0,0),(0,0),0,0,F, '
```

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2.2. New output

1TEST OF THE CONTINUED-FRACTION COULOMB & BESSEL ROUTINES

0.0000, ETA = 0X = 100.0000 0.000 0.000, ZLMIN = 10.000 0.000 NL = 1 MODE = 1 KFN = -1near axial + COULCC :: IFAIL = 0 RERR = 1.3E-13 ITS = -12 92 5 0 0 3 0 ZL = 10.0000.000 :: FC = F= -1.956700347364D-02 -1.994110388930D-15, = -1.002577662468D+00 0.0000000000D+00 GC = GFC ' = -9.970480203629D-01 0.0000000000D+00, GC' = 1.951484195888D-02 -1.498801083244D-14 0X = 100.0000 0.0000, ETA =0.000 0.000, ZLMIN = 10.0000.000 NL = 1 MODE = 1 KFN = -1axial RERR = 5 COULCC :: IFAIL = 0 1.3E-13 ITS = -12 92 0 0 3 0 ZL = 10.0000.000 :: FC = F= -1.956700347364D-02 0.0000000000D+00, GC = G= -1.002577662468D+00 0.0000000000D+00 FC' =-9.970480203629D-01 0.0000000000D+00, GC ' = 1.951484195888D-02 -1.698641227676D-14 0.0000, ETA =0X = 100.0000 0.000 0.000, ZLMIN = 10.000 0.000 1 MODE = NL = 1 KFN = -1near axial -COULCC :: IFAIL = 0 RERR = 1.3E-13 ITS = -12 92 5 0 0 3 0 ZL = 10.0000.000 :: FC = F= -1.956700347364D-02 1.994110388930D-15, GC = G= -1.002577662468D+00 0.0000000000D+00 FC ' = -9.970480203629D-01 0.0000000000D+00, GC′ = 1.951484195888D-02 -1.898481372109D-14

References

[1] I.J. Thompson, A.R. Barnett, Comput. Phys. Commun. 36 (1985) 363.

[2] A.R. Barnett, Comput. Phys. Commun. 27 (1982) 147.

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