COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 377–395. NORTH-HOLLAND PUBLISHING COMPANY

COULOMB WAVE FUNCTIONS FOR ALL REAL η AND ρ *

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Received 25 July 1974

PROGRAM SUMMARY

Title of program: RCWFN

Catalogue number: ABPC

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue).

Computer:	*Installation*:
CDC 7600	University of Manchester Regional Computing Centre
IBM 370/165	Daresbury Nuclear Physics Laboratory, Warrington, Lancs.
IBM 360/195	Rutherford High Energy Laboratory, Didcot, Berks.

Operating system: UMRCC Scope V2.0

Programming language used: ASA Fortran

High-speed core required: < 1 Kwords

No. of bits in a word: 60

Overlay structure: None

No. of magnetic tapes required: None

Other peripherals used: Card reader, line printer

No. of cards in the combined program and test deck: 282

Card punching code: EBCDIC

Keywords: Nuclear, atomic, Schrodinger equation, reactions, scattering, heavy ion, wavefunction, Coulomb, potential, hypergeometric function, continued fraction, Runge–Kutta.

Nature of the physical problem
The subroutine RCWFN calculates the regular and irregular Coulomb wavefunctions, $F_l(\eta,\rho)$ and $G_l(\eta,\rho)$ and their radial derivatives for real, positive energy for all (η,ρ), $(-1000 \leqslant \eta \leqslant 1000, \rho > 0)$ rapidly and with high accuracy. It is well suited for calculations of Coulomb matrix elements for heavy-ion scattering [1] $(1 < \eta < 200, \eta < \rho < 1000)$ and for all programs which require matching to asymptotic Coulomb wavefunctions in both nuclear and atomic physics.

Method of solution
An entirely new technique, developed by Steed [2], is used, which differs greatly from standard methods [3]. The method is based on the continued-fraction expansion of the quantities F_l'/F_l and $(G_l' + F_l')/(G_l + iF_l)$ and it is applicable for all values of $\rho \geqslant \rho_{TP} = \eta + [\eta^2 + l(l+1)]^{1/2}$ without restriction. A somewhat modified method is used for values of $\rho < \rho_{TP}$. The results are given for all l-values between MINL and MAXL inclusive (MAXL ⩾ MINL ⩾ 0) and for any required ρ-value. In general results are obtained without integrating the differential equation. The subroutine is fast and compact ‡‡; the results can be obtained to any desired accuracy in the range 10^{-6}–10^{-12}.

Restriction on the complexity of the problem
Subroutine RCWFN has been programmed for real values of η and ρ: the value of η is unrestricted (positive, negative or zero) while the value of ρ cannot be zero. There is a loss of accuracy in cases when $\rho < 0.2\rho_{TP}$.

Typical running time
For the $l = 0$ functions the averaging running time (CDC 7600 CP time) is 0.005 sec for ACCUR = 10^{-7} and STEP = 100.0 (i.e. practical values), and there is no significant increase with l-value.

References
[1] A.R. Barnett, D.H. Feng and L.J.B. Goldfarb, Phys. Lett. 48B (1974) 290; and Computer Phys. Commun., to be published.
[2] J.W. Steed, PhD thesis, University of Manchester (1967) unpublished.
[3] C.E. Froberg, Rev. Mod. Phys. 27 (1955) 399;
C. Bardin et al., Computer Phys. Commun. 3 (1972) 73.

* Work supported by the United Kingdom Science Research Council.
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‡ Now with Software Sciences Limited, Park Green, Macclesfield, UK.

‡‡ When the $-separator format on the CDC card input is used the entire subroutine occupies 36 cards.

LONG WRITE-UP

1. Introduction

The Coulomb functions $F_l(\eta,\rho)$ and $G_l(\eta,\rho)$, together with their derivatives with respect to ρ, are basic to the solution of charged-particle scattering problems for both positive and negative values of η. An example taken from nuclear physics is the calculation of Coulomb excitation, in which the radial matrix elements

$$M_{ll'}^{\lambda-1} = (k^{\lambda}/kk') \times \int_0^{\infty} f_l(\eta,\rho)\, \rho^{-\lambda-1}\, f_{l'}(\eta',\rho')\mathrm{d}\rho \qquad (1)$$

are integrals over the regular solution $f_l = F_l$ if there is no nuclear distortion. Nuclear effects give rise to nuclear phase shifts δ_l different from zero for the lower partial waves and in this case

$$f_l = F_l + \tfrac{1}{2}\mathrm{i}[1 - \exp(2\mathrm{i}\delta_l)]\ (G_l + \mathrm{i}F_l)$$

in the region outside the range of nuclear interactions. For problems of this type we require the Coulomb functions in the region

$$\rho \geqslant \rho_{\mathrm{TP}} = \eta + [\eta^2 + l(l+1)]^{1/2}$$

since, otherwise, the integrand in (1) is vanishingly small. The value ρ_{TP} is the turning point of the functions which separates the monotonic region $\rho < \rho_{\mathrm{TP}}$ from the oscillatory one $\rho > \rho_{\mathrm{TP}}$.

The subroutine RCWFN calculates the Coulomb functions for the region $0.1\rho_{\mathrm{TP}} < \rho < \infty$ and the method of it uses represents a substantial break with tradition [1–4]. It relies on a continued-fraction representation and does not solve the differential equation (save in the small region $0.1\rho_{\mathrm{TP}} < \rho < \rho_{\mathrm{TP}}$). The subroutine is thus exceptionally fast, it evaluates F_l, F_l', G_l and G_l' at a given ρ-value independently of any other, it can evaluate a single l-value if desired (i.e. there is no need for recursion from $l = 0$) and the results can be obtained to any desired degree of accuracy. The second of these properties makes the evaluation of (1) by gaussian quadrature methods very attractive [5,6]. The methods of continued fractions are discussed in section 3 below.

2. General properties of the Coulomb functions

The Coulomb functions are solutions of the differential equation

$$\frac{\mathrm{d}^2U_l}{\mathrm{d}\rho^2} + \left(1 - \frac{2\eta}{\rho} - \frac{l(l+1)}{\rho^2}\right)U_l = 0, \qquad (2)$$

where the parameters ρ and η are defined as

$$\rho = kr = (2\mu E)^{1/2} r/\hbar$$

and

$$\eta = Z_1 Z_2 e^2/\hbar v = \mu Z_1 Z_2 e^2/\hbar^2 k.$$

The two charges are $Z_1 e$ and $Z_2 e$, μ is the reduced mass of the system in amu, k is the wave number and E the centre-of-mass energy. The numerical expressions obtained from the 1969 Atomic Constants [7] are

$$k\ (\mathrm{fm}^{-1}) = 0.218\,741\,0\ [\mu(\mathrm{amu}) \cdot E(\mathrm{MeV})]^{1/2}$$

and

$$\eta = (1.439\,906 \times 0.218\,741\,0/2.0) Z_1 Z_2 \times [\mu(\mathrm{amu})/E(\mathrm{MeV})]^{1/2}.$$

The regular and irregular solutions of eq. (2), $F_l(\eta,\rho)$ and $G_l(\eta,\rho)$, have boundary conditions

$$\begin{aligned} F_l(\eta,\rho) &\xrightarrow[\rho\to\infty]{} \sin\theta_{l'}, \quad F_l(\eta,0) = 0, \\ G_l(\eta,\rho) &\xrightarrow[\rho\to\infty]{} \cos\theta_{l'}, \quad G_l(\eta,0) = \infty, \end{aligned} \qquad (3)$$

where

$$\theta_l = \rho - \eta \ln 2\rho - \tfrac{1}{2}l\pi + \sigma_l.$$

The Coulomb phase shift σ_l is given by

$$\sigma_l = \arg \Gamma(l + 1 + \mathrm{i}\eta).$$

The solutions for successive l-values are connected by the following recurrence relations, with $U_l = F_l$ or G_l,

$$R_l U_{l-1} = U_l' + S_l U_l, \qquad (4)$$

$$U_{l-1}' = S_l U_{l-1} - R_l U_l, \qquad (5)$$

$$R_{l+1}U_{l+1} = T_lU_l - R_lU_{l-1}, \tag{6}$$

where the coefficients are given for $l \geqslant 1$ by

$$R_l = (l^2 + \eta^2)^{1/2}/l, \qquad S_l = l/\rho + \eta/l,$$
$$T_l = \frac{(2l+1)[l(l+1)/\rho + \eta]}{l(l+1)}. \tag{7}$$

The primes denote differentiation with respect to ρ. Further necessary relations are the wronskian

$$W = F_l'G_l - F_lG_l' = 1, \quad \text{and} \tag{8}$$

$$W_l = F_lG_{l+1} - F_{l+1}G_l = 1/R_{l+1}. \tag{9}$$

3. Continued fractions and the Coulomb functions

A continued fraction is defined as

$$h = b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2 + \cdots}},$$

which we shall write as

$$h = b_0 + \frac{a_1}{b_1+}\,\frac{a_2}{b_2+}\cdots\frac{a_n}{b_n+\ldots}. \tag{10}$$

We state two necessary theorems, whose proof can be found in ref. [8].

Theorem 1. The continued fraction h is said to converge if the nth convergent h_n (the result of terminating the fraction at b_n) is such that the sequence h_n as $n \to \infty$ tends to a limit h. The limit h is then the value of the continued fraction.

Theorem 2. Let two sequences, A_n and B_n satisfy the two-term recurrence relations (expressed in matrix form)

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = \begin{pmatrix} A_{n-1} & A_{n-2} \\ B_{n-1} & B_{n-2} \end{pmatrix} \begin{pmatrix} b_n \\ a_n \end{pmatrix}, \tag{11}$$

with the initial set of values

$$\begin{pmatrix} A_0 & A_{-1} \\ B_0 & B_{-1} \end{pmatrix} = \begin{pmatrix} b_0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Then the nth convergent of the continued fraction

$$h_n = A_n/B_n.$$

The *equivalence transformation* allows us to rewrite (10) as

$$h = b_0 + \frac{c_1a_1}{c_1b_1+}\,\frac{c_1c_2a_2}{c_2b_2+}\,\frac{c_2c_3a_3}{c_3b_3+}\cdots\frac{c_{n-1}c_na_n}{c_nb_n+\cdots} \tag{12}$$

for all $c_p \neq 0$ and it will be used in manipulating the results into their final form.

3.1. Steed's procedure for evaluating Coulomb functions

The mathematical methods and the algorithms described in this program were developed as original work by Steed [9] which is unpublished. His program has been translated into Fortran IV and extended to any arbitrary value of MINL.

We derive in sections 3.2 and 3.3 two continued fractions involving the Coulomb functions, the one being

$$f_m \equiv F_m'/F_m, \tag{13}$$

while the other is

$$p_m + iq_m \equiv (G_m' + iF_m')/(G_m + iF_m). \tag{14}$$

The use of eqs. (13) and (14) enables us to solve for F_m', G_m and G_m' in terms of F_m, thus (dropping the subscript)

$$F' = fF, \tag{15}$$
$$G = (F' - pF)/q = (f - p)F/q, \tag{16}$$
$$G' = pG - qF = p(f - p)F/q - qF, \tag{17}$$

and then the value of F itself, i.e. the scaling factor for eqs. (15) – (17) can be found by substitution in the wronskian equation (8)

$$F_m = \pm 1/(F'G - FG')^{1/2}. \tag{18}$$

The sign of F_m is obtained during the evaluation of f_m (section 3.2).

The convergence of the continued-fraction expansion of eq. (13) is sufficiently rapid and is valid for all values of ρ, except for special cases with negative η (section 3.2). On the other hand eq. (14) can only be used for $\rho \geqslant \rho_{TP}$ since it very rapidly tends to G_m'/G_m for smaller

values of ρ. For example, at $\rho = 0.95\ \rho_{TP}$ and $m = 0$, the real and imaginary parts of eq. (14), p and q, differ by a factor of 10^{-12}, and a loss of significance results. Therefore in the region $\rho < \rho_{TP}$ the differential equation (2) for G_m and G'_m is integrated inward to the desired ρ value from the starting values of $G_m(\eta,\rho_{TP})$ and $G'_m(\eta,\rho_{TP})$ and then combined with $f_m(\eta,\rho)$ as above. The method of integration is the standard 4th-order Runge–Kutta algorithm used simultaneously for G_m and G'_m [10].

In subroutine RCWFN the Coulomb functions are calculated at a required ρ-values for a range of l-values, from l = MAXL to l = MINL, by using the recurrence relations eqs. (4)–(5) as is described in section 4.

3.2. A continued fraction for F'_l/F_l

Consider the recurrence relation (6) and let $V_n = U_{k+1}$ and also $k = n + l$ with l fixed at the desired value. Then

$$V_n = V_{n-1}b_n + V_{n-2}a_n, \tag{19}$$

where

$$b_n = T_k/R_{k+1} = \frac{(2k+1)[(k+1)/\rho + \eta/k]}{[(k+1)^2 + \eta^2]^{1/2}}$$

and

$$a_n = -R_k/R_{k+1} = -\frac{(k^2+\eta^2)^{1/2}(k+1)}{[(k+1)^2+\eta^2]^{1/2}k}$$

in the notation of eq. (7). Since V_n is a Coulomb function the sequence (19) is satisfied by the two independent solutions F_n and G_n. The most general sequences V_n are thus

$$A_n = \alpha F_n + \beta G_n \equiv \alpha F_{n+1+l} + \beta G_{n+1+l}$$

and

$$B_n = \gamma F_n + \delta G_n \equiv \gamma F_{n+1+l} + \delta G_{n+1+l}$$

from which we can find those coefficients which yield initial values of the sequences A_n, B_n in conformity with Theorem 2, namely $A_0 = b_0, A_{-1} = 1, B_0 = 1$, $B_{-1} = 0$. These coefficients are

$$\alpha = (b_0 G_l - G_{l+1})R_{l+1}, \quad \beta = (b_0 F_l - F_{l+1})R_{l+1},$$
$$\gamma = -G_l R_{l+1}, \quad \delta = F_l R_{l+1}. \tag{20}$$

The conditions of Theorem 2 are met and so the limit as $n \to \infty$ of the continued fraction defined by a_n, b_n is $\lim_{n\to\infty} A_n/B_n$ which, since $F_{n+1+l} \to 0$ and $G_{n+1+l} \to \infty$ is just the ratio β/δ. From eqs. (19), (20), this limit is both $b_0 + (a_1/b_1+)[a_2/b_2+\cdots)]$ and $b_0 - F_{l+1}/F_l$ which means that

$$\frac{F_{l+1}}{F_l} = \frac{-a_1}{b_1+}\frac{a_2}{b_2+}\frac{a_3}{b_3+\cdots} \tag{21}$$

with a_n, b_n defined as above. This continued fraction for the ratio F_{l+1}/F_l is recast into one for F'_l/F_l with the help of (5), by eliminating F_{l+1}, and we reach the penultimate result

$$\frac{F'_l}{F_l} = S_{l+1} + R_{l+1}\left(\frac{a_1}{b_1+}\ \frac{a_2}{b_2+\cdots}\right).$$

The application of the equivalence transformation equation (12), with $c_p = \rho p(p+1)R_{p+1}$ then yields the final result:

$$\frac{F'_l(\eta,\rho)}{F_l(\eta,\rho)} = \frac{l+1}{\rho} + \frac{\eta}{l+1} + \frac{H_{l+1}}{K_{l+1}+}\frac{H_{l+2}}{K_{l+2}+}\frac{H_{l+3}}{K_{l+3}+\cdots}, \tag{22}$$

with

$$H_p = -\rho^2(p^2-1)(p^2+\eta^2), \quad p = l+2, l+3, \cdots,$$

and

$$K_p = (2p+1)[p(p+1)+\eta\rho], \quad p = l+1, l+2, \cdots,$$

with

$$H_{l+1} = -\rho[(l+1)^2+\eta^2](l+2)/(l+1).$$

To obtain the sign of F_l we observe that as $n \to \infty$ the value of $B_n \to \delta G_{n+1+l} = F_l R_{l+1} G_{n+1+l}$ and $G_{n+1+l} \to \infty$ while remaining positive. The sign of F_l is hence the sign of the nth denominator when the continued fraction has converged.

3.2.1. A minor difficulty with eq. (22)

For the scattering of like charges, the value of η is positive and eq. (22) holds for all $\rho > 0$; however when η is negative, a peculiar difficulty can arise at the first step of the algorithm (section 3.4) in which $D_1 =$

$1.0/K_{p+1}$. A zero of K_{p+1} arises when

$\eta\rho = -p(p+1) = -(L+1)(L+2)$

and here L = MAXL and, if $\rho < \rho_{TP}$, also L = MINL. Elaborate methods are available to circumvent this difficulty but in our subroutine we choose to avoid this value of ρ by setting

$\rho = \rho + 10^{-6}$ (cards 37 – 39).

The accuracy of the results is reduced for values of ρ which make $F_l(\eta,\rho) = 0.0$ within the value of ACCUR For the evaluation of integrals over products of F_l-values such a reduced accuracy is not a problem.

3.3. A continued fraction for $(G_l' + iF_l')/(G_l + iF_l)$

The boundary conditions at infinity, eq. (3), suggest the substitution

$$G_l + iF_l = y_l \exp(i\theta_l) \tag{23}$$

which leads to the following differential equation for $y_l(\eta,\rho)$:

$$d^2y_l/d\rho^2 + 2i(1 - \eta/\rho)dy_l/d\rho + (i\eta - l)(i\eta + l + 1)y_l = 0.$$

After the substitution $Z = (2i\rho)^{-1}$ this equation can be recognised as that for the hypergeometric function ${}_2F_0(a,b;Z)$:

$$Z^2\,{}_2F_0'' + [(a+b+1)Z - 1]\,{}_2F_0' + ab\,{}_2F_0 = 0 \tag{24}$$

with $a = i\eta - l$ and $b = i\eta + l + 1$. Thus the solution of eq. (23) is

$$y_l(\eta,\rho) = {}_2F_0(i\eta - l, i\eta + l + 1; (2i\rho)^{-1}) \equiv 1 + \frac{ab}{1!(2i\rho)} + \frac{a(a+1)b(b+1)}{2!(2i\rho)^2} + \cdots. \tag{25}$$

The series expansion is the definition of the (specialised) hypergeometric function, and the result (25) is a known asymptotic form for $G_l + iF_l$ when ρ is large, quoted for example as eq. 12.16 of ref. [2].

The series (25) however is convergent only in an asymptotic sense. viz. only for very small Z (i.e. large ρ) and whose summation is terminated after the term with the smallest absolute magnitude. Nevertheless *the ratio* of two such hypergeometric functions has a very strong convergence property, namely that it can be expanded as a continued fraction which is convergent throughout the complex Z-plane exterior to the cut along the real axis from $Z = 1$ to $Z = \infty$, i.e. for all ρ. We can now proceed to derive such a ratio.

Since ${}_2F_0'(a,b;Z) = dF/dZ = ab\,{}_2F_0(a+1,b+1;Z)$ we find that the complex ratio

$$\frac{G_l' + iF_l'}{G_l + iF_l} = \frac{i(\rho - \eta)}{\rho} + i\frac{ab}{2\rho^2}\,\frac{{}_2F_0(a+1,b+1;(2i\rho)^{-1})}{{}_2F_0(a,b;(2i\rho)^{-1})}. \tag{26}$$

We derive a continued fraction for the ratio of F's directly from eq. (24) using the above differentiation property: eq. (24) reads on dividing by ${}_2F_0'$ and rearranging,

$$\frac{{}_2F_0(a,b;Z)}{{}_2F_0(a+1,b+1;Z)} = 1 - (a+b+1)Z - Z^2(a+1)(b+1)\,\frac{{}_2F_0(a+2,b+2;Z)}{{}_2F_0(a+1,b+1;Z)}.$$

Inverting this equation, incrementing a and b by 1 and using the equation again, and repeating, gives us immediately the required continued fraction:

$$\frac{{}_2F_0(a+1,b+1;Z)}{{}_2F_0(a,b;Z)} = \cfrac{1}{1-(a+b+1)Z - \cfrac{(a+1)(b+1)Z^2}{1-(a+b+3)Z - \cfrac{(a+2)(b+2)Z^2}{1-(a+b+5)Z-\cdots}}}. \tag{27}$$

Now $Z = (2i\rho)^{-1}$ and we can make an equivalence transformation with $c_p = 2\rho$ to reach the final result:

$$p_l + iq_l = \frac{G_l' + iF_l'}{G_l + iF_l} = \frac{1}{\rho}\left((\rho - \eta)i + \cfrac{i(i\eta - l)(i\eta + l + 1)}{2(\rho - \eta + i) + \cfrac{(i\eta - l + 1)(i\eta + l + 2)}{2(\rho - \eta + 2i) + \cdots}}\right) \tag{28}$$

The continued-fraction (28) is programmed [see eqs. (32)]:

$a_1 = -\eta^2 - l(l+1) + i\eta$, $\quad a_{k+1} - a_k = 2k + 2i\eta$,

$b_1 = 2(\rho - \eta) + 2i$, $\quad b_{k+1} - b_k = 2i$,

and

$(\Delta p)_1 + i(\Delta q)_1 = ia_1/b_1$.

We note in passing that the result for $(G_l' - iF_l')/(G_l - iF_l)$ is exactly $p_l - iq_l$; its convergence takes the same number of iterations.

We stress that (28) can only be evaluated in practice for

$$\rho \geqslant \rho_{TP} = \eta + [\eta^2 + l(l+1)]^{1/2}$$

for otherwise it tends too rapidly towards G_l'/G_l. A further point is of academic interest. If we take one of the Gauss relations [8]

$$aZ\frac{F(a+1,b+1;Z)}{F(a,b;Z)} = \frac{F(a,b+1;Z)}{F(a,b;Z)} - 1$$

we can re-express eq. (26) in terms of the ratio on the right-hand side, which itself can be developed as the *continued-fraction of Gauss*

$$\frac{F(a,b+1;Z)}{F(a,b;Z)} = \frac{1}{1-}\,\frac{aZ}{1-}\,\frac{(b+1)Z}{1-}\,\frac{(a+1)Z}{1-}\,\frac{(b+2)Z}{1-\cdots}.$$

This version of eq. (26) converges only half as rapidly as does eq. (28).

3.4. Steed's algorithm for evaluating continued fractions

Several methods are available to compute the continued fraction

$$h_n \equiv \frac{A_n}{B_n} = b_0 + \frac{a_1}{b_1+} \cdots \frac{a_n}{b_n}$$

and hence to find its limit. One is to calculate the sequences A_n, B_n by their two-term recurrence relations, eq. (11), and to divide the results. A second is to use the algorithm

$$A_1/B_1 = b_0 + a_1/b_1, \quad \Delta_1 = a_1,$$

$$B_0 = 1, \qquad B_1 = b_1.$$

$$\Delta_k = -a_k\Delta_{k-1}, \qquad B_k = b_k B_{k-1} + a_k B_{k-2}.$$

$$\frac{A_k}{B_k} = \frac{A_{k-1}}{B_{k-1}} + \frac{\Delta_k}{B_k B_{k-1}} \quad \text{for } k = 1, 2, 3, \cdots.$$

A significant amount of labour can be bypassed by the use of an algorithm due to Steed [9] which we now establish. If we define the quantity D_n to be the ratio of denominators B_{n-1}/B_n then the relation

$$B_n = B_{n-1}\,b_n + B_{n-2}a_n$$

is equivalent to the relation

$$D_n = 1/(b_n + a_n D_{n-1}). \tag{29}$$

The identical expression results from A_{n-1}/A_n but the two sequences are different because of their different starting values, eq. (11). Now

$$h_n \equiv A_n/B_n$$

$$= \frac{A_{n-1}\,b_n + A_{n-2}\,a_n}{B_{n-1}\,b_n + B_{n-2}\,a_n}$$

$$= \frac{(A_{n-1}/B_{n-1})b_n + (A_{n-2}\,B_{n-2}/B_{n-2}\,B_{n-1})\,a_n}{b_n + (B_{n-2}/B_{n-1})\,a_n}$$

$$= (h_{n-1}\,b_n + h_{n-2}\,D_{n-1})D_n. \tag{30}$$

Furthermore, from eq. (29), $b_nD_n + a_nD_nD_{n-1} = 1$ which then yields for the difference between h_n and h_{n-1} the recurrence relation

$$\Delta h_n \equiv h_n - h_{n-1}$$

$$= (b_nD_n - 1)(h_{n-1} - h_{n-2})$$

$$= (b_nD_n - 1)\Delta h_{n-1}. \tag{31}$$

The expression (31) forms the basis of *Steed's algorithm* as follows

$$h_0 = b_0, \qquad D_1 = 1/b_1,$$

$$\Delta h_1 = a_1D_1, \qquad D_n = 1/(D_{n-1}\,a_n + b_n),$$

$$\Delta h_n = (b_nD_n - 1)\Delta h_{n-1}, \qquad h_n = h_{n-1} + \Delta h_n, \tag{32}$$

which can be iterated until $\Delta h_n/h_n$ is sufficiently small. This method is used in subroutine RCWFN.

4. Notes on the program

The calling sequence for the subroutine is CALL RCWFN (RHO, ETA, MINL, MAXL, FC, FCP, GC, GCP, ACCUR, STEP) where the arguments have the following type and meaning:

RHO — real, $\rho > 0$. Accuracy reduced if ρ such that $\rho < 0.2\,\rho_{TP}$.

ETA — real, unlimited, RCWFN has been tested for $-1000 \leqslant \eta \leqslant 1000$.

MINL integer, MAXL integer — Coulomb functions are calculated for MINL $\leqslant l \leqslant$ MAXL with MINL $\geqslant 0$

FC, FCP — real arrays of dimension at least MAXL − MINL + 1 for F_l, F_l', G_l, G_l'.

GC, GCP — Normally the dimension will be $\geqslant$ MAXL + 1.

ACCUR — real, accuracy parameter of the continued fractions. If ACCUR $< 10^{-15}$ or ACCUR $> 10^{-6}$ it is reset to 10^{-6} within RCWFN. A suitable value on the CDC 7600 is 10^{-10}.

STEP — real, number of steps in Runge–Kutta integration below the turning point. A suitable value is 100.0 and RCWFN chooses this as a minimum value, which it increases to 1000.0 when necessary.

The subroutine sets up the variables:

R — the desired RHO value

TURN — $\eta + (\eta^2 + \text{MINL(MINL} + 1))^{1/2}$, the turning point for MINL

KTR — control variables = 1 if R $\geqslant$ TURN and −1 if R < TURN

KTRP — = −1 if a second evaluation of F_l'/F_l at R = TURN is required,

and then begins the evaluation of $F'_{\text{MAXL}}/F_{\text{MAXL}}$. This is done in terms of two ratios

$$x_l = F_l/F_L \quad \text{and} \quad x_l' = F_l'/F_L$$

for L = MAXL. Starting values for these ratios are $x_L = 1$ and $x_L' = f_L$ [which is evaluated by the continued fraction eq. (22)]. Both x_l and x_l' satisfy the downward recurrence relations, eq. (4) and eq. (5), which are used to calculate (and store) values of x_l and x_l' until the value $l = m$ = MINL is reached. This procedure gives us all the values of F_l and F_l' between l = MAXL, MINL to within a common multiplier and this is determined from the wronskian at $l = m$ = MINL. The ratio x_m'/x_m gives f_m, and the continued fraction eq. (28) for $(G_m' + iF_m')/(G_m + iF_m)$ is used to evaluate $p_m + iq_m$, and hence the complete solution for the four Coulomb functions at l = MINL. The values of G_l and G_l' are then obtained by upward recurrence to l = MAXL, and the values of F_l, F_l' result by renormalising the stored values of x_l, x_l' by the quantity $(x_m' G_m - x_m G_m')^{-1/2}$.

The modification of this method of solution if $\rho <$ TURN arises after the x_l, x_l' have been obtained. The subroutine sets ρ = TURN and l = MINL = m and proceeds to evaluate F_m, F_m', G_m and G_m'. These are functions at the turning point, and now the differential equations for $G_m(\rho)$ and $G_m'(\rho)$ are integrated inwards, simultaneously, until the required ρ-value is reached. The rest of the calculation proceeds as before. The 4th-order Runge–Kutta technique [10] is employed for the integration. We found this method to be satisfactory over 6–10 orders of magnitude ($G, G' \sim 10^6 - 10^{10}$) in that 6D accuracy was maintained in the final results with 1000 steps in the integration. In extreme cases of say 50–100 orders of magnitude only 1D or 2D survived. This loss of accuracy is not merely a function of the step length but also of the truncation errors in the 4th-order algorithm. Consequently this method of extrapolation towards small ρ eventually cannot compete with approximations designed for small ρ [1, 2, 4]. The use of the logarithmic variables defined by Froberg (eqs. 6.1, 6.2) seems a more efficient procedure but in practice it offered no advantages.

The subroutine has been extensively tested on the CDC 7600 at the University of Manchester Regional Computing Centre, on the IBM 370/165 at the Daresbury Laboratory, and on the IBM 360/195 at the Rutherford High Energy Laboratory. For these latter two machines, and others of smaller word length, if accuracies exceeding 10^{-6} are desired it is important to run the routine in double word length, including the arrays FC, FCP, GC, GCP. Suitable declaration statements for IBM machines are:

```
IMPLICIT    REAL*8    (A–H, O–Z)
REAL*8   K, K1, K2, K3, K4, M1, M2, M3, M4
FLOAT(I)  = DFLOAT(I)
EXP(X)    = DEXP(X)
ALOG(X)   = DLOG(X)
ABS(X)    = DABS(X)
IFIX(X)   = X
SQRT(X)   = DSQRT(X)
```

Ensure that card 156 which defines R3 reads

```
R3        = 1.0/3.0D0
```

(as it does in our listing).

5. Test deck and accuracy checks

The Coulomb wavefunction test program CFNCHK is a short routine to call RCWFN for specified arguments and to compute two test quantities. These are the wronskian

$$W = F_l' G_l - F_l G_l' = 1 \tag{8}$$

and the relation

$$W_l = F_l G_{l+1} - F_{l+1} G_l = 1/R_{l+1}. \tag{9}$$

Two input cards are required for each case:

CARD 1
ETA, N, (L(I), I = 1, 10) FORMAT (F10.3, 11I5)

CARD 2
RHO(I), I = 1, N FORMAT (7F10.3)

where N $\leqslant$ 7 is the number of ρ-values to be found on CARD 2, and N = 0 calls EXIT. If N is made negative a heading on a new page is produced, and (−N) ρ-values are sought. Repetitions of CARD 2 can be used for 14 or 21 ρ-values. The array L contains up to 10 l-values which will be calculated for each ρ-value. The program outputs the input data, the values of F_l, F_l', G_l, G_l' and the quantities

TEST 1 = $W - 1$ and TEST 2 = $W_l - 1/R_{l+1}$

and both are expected to be zero.

The value of TEST 1 is not an independent test since the Wronskian relation is used in the subroutine. It can thus be regarded as a check on the arithmetic and it is usually less than 2×10^{-14} with single-precision arithmetic on the CDC 7600. The quantity TEST 2, on the other hand, *is* a test of the results since it is evaluated after two separate calls to RCWFN. The first has MINL = 0, MAXL = l while the second has MINL = 1, MAXL = $l + 1$ and this means that evaluations of the continued fractions for different l-values are called for. Since the definition of TEST 2 embodies all the properties of the Coulomb functions which determine their solution it does not follow that if TEST 2 is 10^{-12}, for example, that the wavefunctions themselves have this accuracy, or indeed even a related accuracy. Nevertheless our experience does suggest that its value gives a reasonable guide to the errors. We display in the test run output the test cases of Bardin et al. [4] for which $\rho > 0.2\rho_{TP}$, and some others. The results, given to 12D, are obtained with ACCUR = 10^{-14} and STEP = 999.0; the column labelled W-1 contains TEST 1 and that headed TEST contains TEST 2, as described above. The agreement in most cases is excellent having regard to the values of TEST and of the approximate errors discussed in [4], but a systematic discrepancy is evident in those cases where the asymptotic Riccati method (no. 8 of [4]) is used for the lowest values of ρ. The values of F_l, G_l agree to 9D-12D while those for F_l', G_l' in ref. [4] are seriously different from our results. An example is for $\eta = -50.0$, $\rho = 5.0$ where F_0, G_0 agree to 12D whereas F_0' differs at 7D and G_0' at 5D; the expected accuracy claimed by Bardin et al. is about 10D. This behaviour is illustrated in table 1 and it indicates presumably that the boundary line for the use of the asymptotic Riccati method was drawn somewhat too low in ρ-value. Since the two methods of solution agree for F_l, G_l, a numerical differentiation can be used to obtain the derivative independently, and this agrees with the values provided by RCWFN. It is clearly an extremely difficult task to assess the errors of all such high-accuracy calculations (except in special cases as above) and beyond about 8D it is often unclear which program is checking which.

In practice, however, such precision is irrelevant. The same test deck calculated with ACCUR = 10^{-7} and STEP = 100.0 produced results which are in agreement with those of Bardin et al. to the 6th digit (except, of course, for the cases in table 1), and very similar results were obtained on the IBM machines. For normal nuclear-reaction calculations such precision is adequate. Further comments on the range and limitations of RCWFN will be found in the last section.

6. Limitations of the method

Arising out of the considerations of accuracy in the previous section, it is natural to investigate the limits of the present approach. We will restrict ourselves to a few observations derived from extensive use and development of the subroutine. A mathematical study will appear later. For all values of $\rho \geqslant \rho_{TP}$ the algorithms are only limited by the word -size used and by the round-off errors inherent in calculating the continued fractions until convergence. A convenient feature of the algorithms is that relatively few additional iterations are necessary to obtain results to a considerably higher

Table 1

Comparison of continued fraction method with some asymptotic Riccati results. The first row is from the test run output; the second (with the same power of 10) from ref. [4].

η	ρ	$F_0(\eta,\rho)$	$F'_0(\eta,\rho)$	$G_0(\eta,\rho)$	$G'_0(\eta,\rho)$	TEST
-500	0.61	-1.56747 426448 E-1	-5.16358 838507 E-1	-1.11662 577817 E-2	6.34290 607911 E+0	1E-14
		-1.56747 426448	-5.16398 330790	-1.11662 577815	6.34290 326579	4E-13
-200	0.155	9.26335 589426 E-2	-5.20338 827163 E+0	-1.05498 227730 E-1	-4.86920 468457 E+0	2E-15
		9.26335 591744	-5.20248 460204	-1.05498 227893	-4.87023 387696	4E-9
-50	5	1.52236 975714 E-1	2.03091 041166 E+0	4.41680 690236 E-1	-6.76485 374767 E-1	1E-14
		1.52236 975714	2.03091 614165	4.41680 690236	-6.76468 750507	9E-13
-50	50	5.81412 475321 E-1	8.49247 350399 E-1	4.89200 660675 E-1	-1.00539 231599 E+0	-4E-13
		5.81412 475320	8.49247 565739	4.89200 660676	-1.00539 213480	-4E-14
-10	3.1	1.92806 827635 E-1	-1.55175 356287 E+0	-5.74163 450399 E-1	-5.65539 205794 E-1	-8E-15
		1.92806 828167	-1.55165 779834	-5.74163 451255	-5.65824 394424	3E-9
34	116.4	-1.22893 716648 E+0	1.33208 933613 E-1	2.00811 761092 E-1	7.91944 540370 E-1	-3E-12
		-1.22893 716643	1.33217 506068	2.00811 761083	7.91943 139574	-8E-11
50	153.3	-1.29566 554688 E+0	-7.28583 466960 E-2	-1.30262 077773 E-1	7.64479 168841 E-1	-2E-12
		-1.29566 554683	-7.28495 928556	-1.30262 077755	7.64480 048891	-8E-11
100	1000	-1.65581 311974 E-1	-9.34063 273097 E-1	-1.04432 596295 E+0	1.48165 711328 E-1	-1E-13
		-1.65581 311968	-9.34063 273043	-1.04432 596295	1.48165 711669	-4E-14
200	476	4.20046 440799 E-1	-6.10636 723020 E-1	-1.52505 808348 E+0	-1.63656 974114 E-1	6E-13
		4.20046 440740	-6.10639 246490	-1.52505 808337	-1.63647 811979	-2E-10
500	1095	1.46929 027367 E+0	3.23944 539005 E-1	1.11156 684610 E+0	-4.35525 914746 E-1	-2E-12
		1.46929 027350	3.23935 776975	1.11156 684581	-4.35532 543385	-4E-10

Table 2

A sample calculation to 18D of Coulomb functions with $\rho = 2\eta$ and L = 0 [11]. The parameter ACCUR was set at 10^{-21} in the double precision version of RCWFN.

TEST OF THE MANCHESTER COULOMB WAVEFUNCTION PROGRAM - RCWFN

ETA	RHO	L	F	FP	G	GP
.25	.5	0	.348512502280354298	.725140251049386111	1.148208486965474131	-.480292122691679932
.50	1.0	0	.516601500314181575	.592924555360720776	1.197486970798485546	-.561323515538948353
.75	1.5	0	.606541989014514342	.523229033995603027	1.237932738932948680	-.580796804239306086
1.00	2.0	0	.661781613832681298	.481557455709949203	1.275778784768276589	-.582728813097184743
1.25	2.5	0	.700411103046531477	.453547031343177808	1.310604085222607841	-.579059078471091182
1.50	3.0	0	.730129112311153282	.433000424831788472	1.342290560734846743	-.573580220118165108
1.75	3.5	0	.754460672412615498	.416997407026594634	1.371121194810441860	-.567618741047685957
2.00	4.0	0	.775197191073771120	.404007816494934739	1.397483426793015884	-.561670987933261970
2.25	4.5	0	.793351758259822650	.393147580377034250	1.421741252870013592	-.555927256629963202
2.50	5.0	0	.809551965068304961	.383864008546991053	1.444202721094029777	-.550455774990027672
2.75	5.5	0	.824215134429597640	.375789975554407382	1.465120421468198788	-.545273210668750535
3.00	6.0	0	.837634064540468182	.368669959985817686	1.484700303049553169	-.540373914869506708
3.25	6.5	0	.850022806838043657	.362319457588325567	1.503111000288887515	-.535742845976427728
3.50	7.0	0	.861542985630724314	.356601224972436893	1.520491689156036555	-.531361532415477779
3.75	7.5	0	.872319866950039350	.351410632362223010	1.536958272808690755	-.527210876264827421
4.00	8.0	0	.882452654489153772	.346666242351198408	1.552608151535213074	-.523272454238079663
4.25	8.5	0	.892021351143997427	.342303533886405391	1.567523889484354348	-.519529081432638804
4.50	9.0	0	.901091483333817700	.338270595896988515	1.581776045432882446	-.515965008142906423
4.75	9.5	0	.909717444651540790	.334525096436583609	1.595425374507632458	-.512565935144917499
5.00	10.0	0	.917944918945897700	.331032101931063326	1.608524555599835509	-.509318942457823266
5.25	10.5	0	.925812672729550718	.327762477354522733	1.621119558954193636	-.506212380834634570
5.50	11.0	0	.933353905198317896	.324691692217860823	1.633250738609044811	-.503235751464668172
5.75	11.5	0	.940597281426529682	.321798915631097252	1.644953712609229450	-.500379586793187456
6.00	12.0	0	.947567734446372403	.319066320910719973	1.656260078075885120	-.497635338641548594
6.25	12.5	0	.954287095934420434	.316478544490719144	1.667197998651929992	-.494995276216347290
6.50	13.0	0	.960774597898490051	.314022260088792310	1.677792677345653551	-.492452394697346902
6.75	13.5	0	.967047275962114927	.311685840084069795	1.688066777506918472	-.490000334123593851
7.00	14.0	0	.973120296666177565	.309459083672891084	1.698040737979436540	-.487633307835965076
7.25	14.5	0	.979007225442517074	.307332996715905967	1.707733064943878743	-.485346039550612073
7.50	15.0	0	.984720247788432251	.305299612001220344	1.717160568290292703	-.483133708102033583
7.75	15.5	0	.990270353176653246	.303351841401840432	1.726338564312094101	-.480991848934439717
8.00	16.0	0	.995667489034255634	.301483353419602548	1.735281048937165334	-.478916561495292902
8.25	16.5	0	1.000920690486788669	.299688471097679328	1.744000846487446741	-.476903971773195223
8.50	17.0	0	1.006038190332746411	.297962086397732744	1.752509738001118190	-.474950699311727625
8.75	17.5	0	1.011027512778279866	.296299587978959090	1.760818572397683218	-.473053578115389050
9.00	18.0	0	1.015895553744867882	.294696799957335341	1.768937363168798799	-.471209680940693404
9.25	18.5	0	1.020648650007829034	.293149929716171825	1.776875372801137583	-.469416296533851127
9.50	19.0	0	1.025292638990764838	.291655523220975984	1.784641186755169267	-.467670909436361035
9.75	19.5	0	1.029832910700812731	.290210426589853536	1.792242778515140158	-.465971182031829076
10.00	20.0	0	1.034274453020203063	.288811752905226998	1.799687566975111865	-.464314938552189343
11.00	22.0	0	1.051141102578809651	.283631381712959554	1.828030344913430501	-.458086194401178475
12.00	24.0	0	1.066745825490252472	.279015514826064592	1.854343697745818603	-.452412680675066787
13.00	26.0	0	1.081280026096515860	.274861048424339390	1.878921290712321990	-.447208597641140071
14.00	28.0	0	1.094893552080730428	.271090091115407894	1.901996020021938888	-.442406227263446124
15.00	30.0	0	1.107706056074175111	.267642463576946072	1.923755848790880422	-.437951244059142786
16.00	32.0	0	1.119814695678222311	.264470773751189782	1.944354775729600062	-.433799440113401204
17.00	34.0	0	1.131299508700884521	.261537079600348111	1.963920632728151733	-.429914385544036685
18.00	36.0	0	1.142227261840811469	.258810565539925006	1.982560754520918599	-.426265723268157505
19.00	38.0	0	1.152654267553005929	.256265886101158525	2.000366183406406425	-.422827903563157789
20.00	40.0	0	1.162628485736277329	.253881960578569601	2.017414842373797009	-.419579229738988896
21.00	42.0	0	1.172191118653625588	.251641079694132620	2.033773967174558210	-.416501127910900059
22.00	44.0	0	1.181377839682654270	.249528232643018539	2.049501996475792945	-.413577580862956136
23.00	46.0	0	1.190219752840324810	.247530592699566542	2.064650059335835526	-.410794683862887565
24.00	48.0	0	1.198744151244637430	.245637118813482713	2.079263159118716626	-.408140292347680451
25.00	50.0	0	1.206975123287461823	.243838243337522006	2.093381125553251018	-.405603739682524577

order of accuracy. As an example we give in table 2 a short list of $l = 0$ wavefunctions to 18D for selected values of $\rho = 2\eta$ which can be compared with the calculations of Abramowitz and Rabinowitz [11] in 1954. The agreement is complete to within 1 unit in the seventh decimal place, as was indeed claimed by them. A double-precision version of the subroutine was used for table 2 and each derivative was checked by numerical differention. The value of the parameter ACCUR when $\rho \geqslant \rho_{TP}$ approximately determines the final accuracy of the results; it was taken as 10^{-21}.

For large values of ρ the limitation on the efficiency of RCWFN is the calculation of $f_l = F'_l/F_l$ which requires about $\rho + 50$ iterations. Thus a practical upper limit to ρ is perhaps 20 000. For small ρ, say 0.001, the limit is in the calculation of

$$p_l + iq_l = (G'_l + iF'_l)/(G_l + iF_l)$$

which may require 50 000 iterations. Clearly these are inefficient methods if many results are required. The calculation in RCWFN will cease if more than 20 000 iterations for f_l, or 23 000 for $p_l + iq_l$, are required or if $|G'_l|$ approaches the computer word size during the integration, and zeros are returned for the functions.

In calculations involving high partial waves, $l \sim$ 500–1000, errors may propagate by successive iterations from the $l = 0$ wavefunctions. We have run some checks on this point, examples of which appear at the end of the test run output. For an η-value of 50.0 and a ρ-value of 600.0, which exceeds the turning point for $l = 500$ ($\rho_{TP} = 552.99$), we evaluate the Coulomb functions for MINL = 0, 100, 200, 300, 400, 500 and MAXL = 500 and hence show that rounding errors are of minor importance. Similar conclusions are evident for $\eta = 50.0$, $\rho = 1200.0$, MINL = 0(200) 1000 and MAXL = 1000. It is to be noted that in our method we do not calculate the $l = 0$ (or, in general, $l =$ MINL) wavefunctions directly but combine the claculation of e.g. F'_{1000}/F_{1000}, after downward recurrence to F'_0/F_0 with the value of $(G'_0 + iF'_0)/(G_0 + iF_0)$. The method thus differs from the classical one [1–4].

Acknowledgements

The authors wish to acknowledge the expert advice and willing assistance of M.G. James in all computing matters. Useful discussions with Drs. P.J.A. Buttle and M. Vallieres are acknowledged. One of us (DHF) wishes to thank the Science Research Council for the provision of a Postdoctoral Fellowship.

References

[1] C.E. Froberg, Rev. Mod. Phys. 27 (1955) 399.
[2] M.H. Hull and G. Breit, Encyclopedia of Physics, ed. S. Flugge (Springer Verlag, Berlin 1959) vol. 41/1, p. 408.
[3] B. Buck, R.N. Maddison and P.E. Hodgson, Phil. Mag. 5 (1960) 118.
[4] C. Bardin et al., Computer Phys. Commun. 3 (1972) 73.
[5] A.R. Barnett, D.H. Feng and L.J.B. Goldfarb, Phys. Lett. 48B (1974) 290.
[6] A.R. Barnett, D.H. Feng and L.J.B. Goldfarb, Computer Phys. Commun., to be published.
[7] B.N. Taylor, W.H. Parker and D.N. Langenberg, Rev, Mod. Phys. 41 (1969) 378.
[8] S. Wall, *The Analytic Theory of Continued Fractions*, (Van Nostrand, New York, 1948).
[9] J.W. Steed, PhD thesis (University of Manchester 1967) unpublished.
[10] L. Fox and D.F. Mayers, *Computing Methods for Scientists and Engineers*, (Clarendon Press, Oxford 1968) p. 202.
[11] M. Abramowitz and P. Rabinowitz, Phys. Rev. 96 (1954) 77.
[12] K.S. Kölbig, Computer Phys. Commun. 4 (1972) 214.

Note added in proof

A complete review of recent methods of computing Coulomb wavefunctions is that of Kölbig [12], which has only just come to our attention.

TEST RUN OUTPUT

TEST OF THE MANCHESTER COULOMB WAVEFUNCTION PROGRAM - RCWFN

ETA	RHO	L	F	FP	G	GP	W=1	TEST
50,0	120,000	0	2,00259933341E-01	6,32274340306E-01	1,55059921647E+00	-9,78523412082E-02	-3,E-15	-9,E-14
50,0	80,000	0	1,20366249591E-03	6,19770431959E-04	8,32243179902E+02	-4,02272469687E+02	-4,E-15	-9,E-11
9,0	50,000	0	9,35708567798E-01	-4,92126155892E-01	-6,11801989696E-01	-7,46937949161E-01	-4,E-15	5,E-12
5,0	20,000	0	-2,29347373002E-01	8,28679340870E-01	1,16571667134E+00	1,48223529679E-01	-1,E-14	-3,E-13
4,0	10,000	0	1,39920928925E+00	7,39287333242E-02	3,56558327881E-01	-6,95850221937E-01	-1,E-14	-1,E-13
-1000,0	1,000	0	9,68222518991E-02	5,12063396274E+00	1,13936784380E-01	-4,30243486522E+00	-4,E-15	9,E-15
-1000,0	10,000	0	-1,15322332817E-01	3,38892408671E+00	2,39239735828E-01	1,64091977791E+00	0,	-4,E-14
-1000,0	100,000	0	2,62318102583E-01	-1,77068805220F+00	-3,86532279941E-01	-1,20301232363F+00	-5,E-15	-3,E-13
-1000,0	1000,000	0	5,84941362837E-01	8,40086552103E-01	4,84967926715E-01	-1,01306729907E+00	-1,E-14	-3,E-12
-500,0	,590	0	-9,83596748553E-02	-5,01886992919E+00	-1,20880038910E-01	3,99878108841E+00	-7,E-15	8,E-15
-500,0	,610	0	-1,56747426448E-01	-5,16358838507E-01	-1,11662577817E-02	6,34290607911E+00	-7,E-15	1,E-14
-500,0	100,000	0	5,06441621224E-01	7,04935480214E-01	2,12199193856E-01	-1,67919306735E+00	-7,E-15	4,E-13
-500,0	1000,000	0	8,33639868856E-01	1,55997827391F-01	1,10233300886E-01	-1,17893097885E+00	-1,E-14	9,E-11
-200,0	,145	0	1,30429892607E-01	-2,15329440026E+00	-4,53284624318E-02	-6,91861702588E+00	-1,E-14	1,E-14
-200,0	,155	0	9,26335589426E-02	-5,20338827163E+00	-1,05498227730E-01	-4,88920468457E+00	-9,E-15	2,E-15
-200,0	100,000	0	3,86835282992E-01	1,22055184960F+00	5,45502478229E-01	-8,63897260489E-01	-1,E-14	-1,E-13
-200,0	1000,000	0	3,56540148972E-01	1,00264538165E+00	8,47368522143E-01	-4,21803449477E-01	-5,E-15	-3,E-12
-50,0	5,000	0	1,52236975714E-01	2,03091041166F+00	4,41680690236E-01	-6,76485374767E-01	-1,E-14	1,E-14
-50,0	5,000	1	-1,92207798328E-01	-1,95857735349E+00	-4,26299008702E-01	8,58760243738E-01	-5,E-15	-2,E-14
-50,0	5,000	2	2,67261843675E-01	1,76560377667E+00	3,84820081792E-01	-1,19942377798E+00	0,	-4,E-15
-50,0	5,000	3	-3,62923967642E-01	-1,36860370000F+00	-2,98464378931E-01	1,62987457269E+00	4,E-15	1,E-14
-50,0	5,000	5	-4,69406488262E-01	2,75219646325E-01	6,65491186260E-02	2,09133107372F+00	2,E-14	-2,E-14
-50,0	5,000	10	-3,68114360219E-01	1,33846751032E+00	3,31588324611E-01	1,51088862814E+00	1,E-14	5,E-14
-50,0	5,000	20	5,72508610339E-01	-8,88099281094F-01	-3,86487539249E-01	-1,14716299874E+00	2,E-14	1,E-14
-50,0	5,000	30	1,17551067129E-04	4,92521055485F-04	1,05772803735E+03	-4,07522179361E+03	-5,E-14	-3,E-14
-50,0	5,000	50	4,20266913301E-23	3,83028028856E-22	1,32186136031E+21	-1,17470596213E+22	4,E-15	1,E-14
-50,0	5,000	100	1,86693584349E-91	3,67291554441E-90	1,36847205283E+89	-2,66410746916E+90	1,E-14	-4,E-14
-50,0	50,000	0	5,81412475321E-01	8,49247350399E-01	4,89200660675E-01	-1,00539231599E+00	0,	-4,E-13
-50,0	50,000	1	-5,98045260245E-01	-8,13864797554E-01	-4,68803382789E-01	1,03413147948E+00	0,	4,E-13
-50,0	50,000	2	6,29139869000E-01	7,40243499434E-01	4,26347096842E-01	-1,08783352788E+00	4,E-14	3,E-13
-50,0	50,000	3	-6,70084506913E-01	-6,23348321659E-01	-3,58896812233E-01	1,15848414109E+00	1,E-13	-6,E-13
-50,0	50,000	5	-7,48260826432E-01	-2,38355261214E-01	-1,36461036469E-01	1,29296330882E+00	6,E-14	-3,E-13
-50,0	50,000	10	2,77129451057E-01	-1,22068610371E+00	-7,10519441453E-01	-4,78761065985E-01	-2,E-13	1,E-13
-50,0	50,000	20	7,55876294799E-01	-2,52360602573E-01	-1,51281009646E-01	-1,27246037462E+00	9,E-14	6,E-12
-50,0	50,000	30	-5,88392849287E-01	-8,44781662655E-01	-5,20249371722E-01	9,52599732372E-01	-4,E-14	7,E-13
-50,0	50,000	50	-8,37683933712E-01	1,33099205321F-01	9,45277610412E-02	1,17874820130E+00	-3,E-13	-3,E-13
-50,0	50,000	100	2,23304593604E-04	2,34028371225E-04	2,19814428489E+03	-2,17448224174E+03	2,E-13	-2,E-13
-10,0	2,900	0	4,58985850692E-01	-1,03668985836E+00	-3,81736647052E-01	-1,31650570171E+00	-1,E-14	3,E-14
-10,0	3,100	0	1,92806827635E-01	-1,55175356287E+00	-5,74163450399E-01	-5,65539205794E-01	-9,E-16	8,E-15
-10,0	100,000	0	9,45619474305E-01	1,50103536499E-01	1,36665938802E-01	-1,03581407356E+00	-7,E-15	2,E-13
-10,0	1000,000	0	3,85247881197E-01	9,26590385003E-01	9,17459327551E-01	-3,89076788674F-01	-9,E-16	2,E-12
-6,0	6,900	0	1,57079204316E-01	1,26309965681E+00	7,61568011342E-01	-2,42321740803E-01	-3,E-15	2,E-13
-6,0	7,100	0	3,96676536014E-01	1,11161020211E+00	6,72881591082E-01	-6,35323583974E-01	-1,E-14	0,
-6,0	17,400	0	4,09228090574E-01	-1,00596660393E+00	-7,75858032295E-01	-5,36406798978E-01	-4,E-15	2,E-14
-6,0	17,600	0	1,96558034259E-01	-1,10869089826F+00	-8,55906713933E-01	-2,59791041854E-01	3,E-15	2,E-14
-6,0	100,000	0	6,83030680099E-01	7,32156892237E-01	6,91651921576E-01	-7,22664871390E-01	-1,E-14	9,E-13
-6,0	1000,000	0	-2,31316696922E-01	-9,75619771912E-01	-9,69817536563E-01	2,32697582573E-01	4,E-15	2,E-12
-4,0	5,000	0	4,07862723006E-01	1,09821233636E+00	6,74327035383E-01	-6,36110427280E-01	-2,E-14	4,E-15
-4,0	5,000	1	-6,42256329143E-01	-7,58912963040E-01	-4,67204210149E-01	1,00494559453E+00	-2,E-14	-1,E-13
-4,0	5,000	5	2,83657834139E-01	-1,04544995379F+00	-8,70189296614E-01	-3,18202528554E-01	-2,E-14	3,E-14
-4,0	5,000	10	7,21985521560E-02	1,10084353023E-01	5,28003488054E+00	-5,79998855560E+00	-4,E-14	-6,E-14
-4,0	5,000	20	3,72990728263E-09	1,44783804452E-08	3,55670502218E+07	-1,30042852498E+08	-5,E-15	-4,E-14
-4,0	5,000	30	4,60279973470E-19	2,75619476973E-18	1,84653754219E+17	-1,06686868149E+18	-3,E-14	-6,E-14
-4,0	5,000	50	4,40630855659E-43	4,43813906512E-42	1,13810237178E+41	-1,12314953439E+42	-4,E-14	-3,E-14
-4,0	5,000	100	1,12267597835-116	2,26058262062-115	2,22290834565+114	-4,43131600080+115	-7,E-14	-8,E-14

TEST OF THE MANCHESTER COULOMB WAVEFUNCTION PROGRAM - RCWFN

ETA	RHO	L	F	FP	G	GP	W=1	TEST
-4.0	50.000	0	-2.77250198046E-01	-9.94100934435E-01	-9.22832107813E-01	2.97968188586E-01	-3.E-15	6.E-14
-4.0	50.000	1	5.08732230779E-01	8.81622427233E-01	8.18834354187E-01	-5.47167525560E-01	2.E-15	-7.E-14
-4.0	50.000	2	-8.40196996900E-01	-5.09226263557E-01	-4.72776239043E-01	9.03657029357E-01	-4.E-15	-5.E-14
-4.0	50.000	3	9.47446263766E-01	-1.93913418972E-01	-1.80993170986E-01	-1.01842503613E+00	0.	-1.E-13
-4.0	50.000	5	-4.40046636665E-01	-9.21749731522E-01	-8.60048697449E-01	4.70973589530E-01	-9.E-16	3.E-12
-4.0	50.000	10	4.21084204243E-01	9.26703490800E-01	8.77093831067E-01	-4.44553277267E-01	8.E-15	-3.E-14
-4.0	50.000	20	-7.67805341241E-01	-6.40550934806E-01	-6.43787347661E-01	7.65326028717E-01	7.E-15	7.E-13
-4.0	50.000	30	-1.01812491622E+00	-2.62178848644E-01	-2.99525470558E-01	9.05066502455E-01	7.E-15	-3.E-14
-4.0	50.000	50	1.59533986051E+00	-8.64299712691E-02	-5.15310138681E-03	-6.26546507323E-01	-4.E-15	2.E-13
-4.0	50.000	100	3.14179162347E-19	5.37489508885E-19	9.37788817810E+17	-1.57855264866E+18	-1.E-14	-2.E-15
-.3	7.900	0	4.94136409096E-01	-8.78940011638E-01	-8.48600513729E-01	-5.14293320446E-01	-7.E-15	-4.E-15
-.3	8.100	0	3.09016485748E-01	-9.65595782501E-01	-9.32538631326E-01	-3.22133721542E-01	-2.E-14	4.E-14
-.3	100.000	0	9.38314793063E-01	3.42473282788E-01	3.41436566803E-01	-9.41120298466E-01	-7.E-15	-3.E-13
-.3	1000.000	0	-2.71583185525E-01	-9.62547844082E-01	-9.62259169051E-01	2.71664503970E-01	-1.E-14	-5.E-12
0.0	.001	0	9.99999833333E-04	9.99999500000E-01	9.99999500000E-01	-9.99999833333E-04	-1.E-14	-1.E-10
0.0	.010	0	9.99983333417E-03	9.99950000417E-01	9.99950000417E-01	-9.99983333417E-03	-8.E-15	5.E-11
0.0	.100	0	9.98334166468E-02	9.95004165278E-01	9.95004165278E-01	-9.98334166468E-02	-1.E-14	9.E-15
0.0	1.000	0	8.41470984808E-01	5.40302305868E-01	5.40302305868E-01	-8.41470984808E-01	-7.E-15	-2.E-15
0.0	10.000	0	-5.44021110889E-01	-8.39071529076E-01	-8.39071529076E-01	5.44021110889E-01	-4.E-15	1.E-14
0.0	100.000	0	-5.06365641110E-01	8.62318872287E-01	8.62318872287E-01	5.06365641110E-01	-1.E-14	-3.E-14
0.0	1000.000	0	8.26879540536E-01	5.62379076286E-01	5.62379076286E-01	-8.26879540536E-01	0.	5.E-15
1.0	2.000	0	6.61781613833E-01	4.81557455710E-01	1.27577878477E+00	-5.82728813097E-01	-2.E-14	-4.E-12
1.0	7.900	0	-1.05570358181E+00	1.84709582985E-01	2.00796384274E-01	9.12103548935E-01	-4.E-15	1.E-13
1.0	8.100	0	-1.00317229511E+00	3.39504302422E-01	3.79306166870E-01	8.68468884820E-01	-1.E-14	-8.E-12
1.0	9.100	0	-3.46718446657E-01	8.91613091252E-01	1.00525965799E+00	2.99082237544E-01	9.E-15	2.E-14
1.0	9.200	0	-2.56320123198E-01	9.15187922867E-01	1.03120585919E+00	2.19463267175E-01	-1.E-14	4.E-14
1.0	100.000	0	1.57407746175E-01	9.82676220296E-01	9.92660472446E-01	-1.55876438714E-01	1.E-15	8.E-13
1.0	1000.000	0	-6.01756274039E-01	7.98507100149E-01	7.99306504825E-01	6.01153816434E-01	-7.E-15	-3.E-12
8.0	1.050	0	9.88270778102E-09	4.00516771647E-08	1.33312774446E+07	-4.71591379533E+07	0.	-2.E-08
8.0	2.010	0	2.38960314934E-07	6.66457750754E-07	7.90791808745E+05	-1.97928543055E+06	-5.E-15	-3.E-09
8.0	16.000	0	9.95667489034E-01	3.01483353420E-01	1.73528104894E+00	-4.78916561495E-01	-4.E-15	-7.E-12
8.0	20.800	0	1.00861490379E+00	-5.31608367267E-01	-1.01290851251E+00	-4.57588870202E-01	-1.E-14	-3.E-13
8.0	20.900	0	9.54304912831E-01	-5.54441105976E-01	-1.05747192361E+00	-4.33503057118E-01	-1.E-14	-3.E-13
8.0	100.000	0	-1.02637831226E+00	-1.77302473353F-01	-1.93984775563E-01	9.40789578233E-01	4.E-15	5.E-10
8.0	1000.000	0	-1.25742178869E-01	9.88134928826E-01	9.96135632546E-01	1.24728136368E-01	-1.E-14	-2.E-13
10.0	5.000	0	1.72074542808E-06	3.09759950467E-06	1.67637564193E+05	-2.79370763593E+05	-4.E-15	-6.E-10
10.0	5.000	1	1.43822713899E-06	2.62336071014E-06	1.97940153028E+05	-3.34252891322E+05	-2.E-14	-6.E-10
10.0	5.000	2	1.00863819538E-06	1.88690199163E-06	2.75176377328E+05	-4.76651734756E+05	1.E-14	-6.E-10
10.0	5.000	3	5.97800909895E-07	1.15881372654E-06	4.47978845520E+05	-8.04408217941E+05	-9.E-15	-6.E-10
10.0	5.000	5	1.31826036427E-07	2.80453363740F-07	1.84915797796E+06	-3.65176286902E+06	2.E-14	-7.E-10
10.0	5.000	10	3.28278064114E-10	9.21968559646E-10	5.59559146826E+08	-1.47467884346E+09	3.E-14	-8.E-10
10.0	5.000	20	4.04283871422E-18	1.83778759676E-17	2.77870711499E+16	-1.21036896966E+17	2.E-14	-9.E-10
10.0	5.000	30	3.18942998567E-28	2.05356149068E-27	2.47223679219E+26	-1.54357040281E+27	1.E-14	-9.E-10
10.0	5.000	50	2.13937218584E-52	2.21349851593E-51	2.28070092910E+50	-2.31454436406E+51	3.E-14	-9.E-10
10.0	5.000	100	4.16264130910-126	8.43944020525-125	5.95385803310+123	-1.19522119358+125	-2.E-14	-1.E-09
10.0	50.000	0	2.37518766416E-02	8.79909263353E-01	1.13688213569E+00	-2.21787413752E-02	-2.E-15	2.E-14
10.0	50.000	1	-6.38729755079E-02	8.78710620605E-01	1.13471232589E+00	4.86566784785E-02	-2.E-14	3.E-13
10.0	50.000	2	-2.35462997144E-01	8.61043957098E-01	1.11262436375E+00	1.78293397961E-01	3.E-15	-3.E-13
10.0	50.000	3	-4.77011395975E-01	7.99223383111E-01	1.03365126526E+00	3.64523238412E-01	8.E-15	-2.E-13
10.0	50.000	5	-1.00346497670E+00	4.21525638376E-01	5.44907634434E-01	7.67647580562E-01	-4.E-15	8.E-13
10.0	50.000	10	4.16672475541E-01	-8.07592601896E-01	-1.08034461290E+00	-3.06047727789E-01	2.E-14	1.E-13
10.0	50.000	20	4.28928799671E-01	-7.64035879316E-01	-1.15590992567E+00	-2.72407317071E-01	5.E-14	4.E-13
10.0	50.000	30	-3.52635436429E-01	-6.64436751932E-01	-1.39731750175E+00	2.02960027068E-01	-5.E-14	-1.E-12
10.0	50.000	50	5.76729101128E-03	3.89565495430E-03	1.34226818062E+02	-8.27249102369E+01	1.E-14	-1.E-14
10.0	50.000	100	7.69173185691E-26	1.43607814052E-25	3.50484367333E+24	-6.45728516259E+24	-9.E-14	-9.E-14

TEST OF THE MANCHESTER COULOMB WAVEFUNCTION PROGRAM - RCWFN

ETA	RHO	L	F	FP	G	GP	W=1	TEST
26.0	24.300	0	2.97292502747E-08	3.23118014790E-08	1.57544174746E+07	-1.68139176268E+07	4.E-15	-4.E-10
26.0	24.500	0	3.69173028846E-08	3.98202058427E-08	1.27853537642E+07	-1.32968701118E+07	0.	-4.E-10
26.0	50.700	0	9.07720563067E-01	2.25471559616E-01	2.64808995466E+00	-4.43893246791E-01	2.E-15	5.E-12
26.0	50.900	0	9.53263074069E-01	2.29864424951E-01	2.56058413409E+00	-4.31583695698E-01	0.	-1.E-11
26.0	52.000	0	1.21493404198E+00	2.42125624592E-01	2.10703938758E+00	-4.03175608979E-01	-2.E-14	-2.E-11
26.0	100.000	0	6.33002441304E-01	7.05759809379E-01	1.02105209693E+00	-4.41360804438E-01	-7.E-15	-4.E-13
26.0	1000.000	0	1.00121809253E+00	1.52767131867E-01	1.56915115128E+01	-9.74841081281E-01	-7.E-15	-8.E-12
34.0	40.200	0	5.85829750847E-07	4.95952376883E-07	1.02663827256E+06	-8.37850579753E+05	-2.E-15	-1.E-10
34.0	40.500	0	7.54363068649E-07	6.32953581764E-07	8.04606710722E+05	-6.50510769855E+05	-7.E-15	-2.E-10
34.0	67.900	0	1.24766281927E+00	2.30713705592E-01	2.24185682521E+00	-3.86978789245E-01	-5.E-15	-5.E-12
34.0	68.000	0	1.27074034088E+00	2.30806101527E-01	2.20296989948E+00	-3.86814748778E-01	-2.E-15	-2.E-11
34.0	68.100	0	1.29381781050E+00	2.30711626177E-01	2.16428307650E+00	-3.86974679008E-01	-1.E-14	-2.E-12
34.0	100.000	0	1.23024654105E+00	2.78457249564E-01	5.03570986464E-01	-6.98866617145E-01	-4.E-15	-4.E-11
34.0	116.200	0	-1.24530758487E+00	3.03100736722E-02	4.11946933130E+02	8.02011806516E-01	4.E-15	2.E-12
34.0	116.400	0	-1.22893716648E+00	1.33208933613E-01	2.00811761092E+01	7.91944540370E-01	4.E-15	-3.E-12
34.0	1000.000	0	-5.26610693682E-01	8.40807046852E-01	8.70930332566E-01	5.08374862631E-01	-7.E-15	-4.E-12
50.0	67.600	0	6.34872031775E-07	4.46639955061E-07	1.13796294833E+06	-7.74550232622E+05	0.	-7.E-13
50.0	67.800	0	7.30561336690E-07	5.11675235419E-07	9.93452150841E+05	-6.73010070679E+05	0.	2.E-12
50.0	99.900	0	1.33379109294E+00	2.15575177151E-01	2.38521990283E+00	-3.64229300580E-01	2.E-15	-9.E-12
50.0	100.000	0	1.35535307794E+00	2.15642270714E-01	2.34880489911E+00	-3.64110567292E-01	-9.E-15	-3.E-11
50.0	100.100	0	1.37691502927E+00	2.15573829979F-01	2.31238995999E+00	-3.64226716433E-01	-1.E-14	-8.E-12
50.0	153.100	0	-1.27213570977E+00	-1.62131094239E-01	-2.81900180075E+01	7.50182053754E-01	-7.E-15	7.E-14
50.0	153.300	0	-1.29566554688E+00	-7.28583466960E-02	-1.30262077773E+01	7.64479188841E+01	-7.E-15	-2.E-12
50.0	1000.000	0	9.02460923791E-01	4.64400827350E-01	4.89547545830E-01	-8.56163232319E-01	-1.E-14	-1.E-11
100.0	1000.000	0	-1.65581311974E-01	-9.34063273097E-01	-1.04432596295E+00	1.48165711328E-01	-7.E-15	-1.E-13
100.0	1000.000	1	-1.56234523525E-01	-9.35350496214E-01	-1.04576577634E+00	1.39805605618E-01	6.E-15	-4.E-13
100.0	1000.000	2	-1.37506264479E-01	-9.37700128836E-01	-1.04839406123E+00	1.23054420658E-01	-1.E-13	4.E-14
100.0	1000.000	3	-1.09338444943E-01	-9.40661432623E-01	-1.05170688765E+00	9.78602939247E-02	-4.E-14	2.E-12
100.0	1000.000	5	-2.44816942225E-02	-9.45477732181E-01	-1.05709767669E+00	2.19627751248E-02	-1.E-13	3.E-11
100.0	1000.000	10	3.46330582628E-01	-8.93566890370E-01	-9.99082523040E-01	-3.09683701194E-01	-6.E-14	3.E-12
100.0	1000.000	20	1.04777556029E+00	1.27943911132E-01	1.43156773333E-01	-9.36921989521E-01	6.E-14	-9.E-12
100.0	1000.000	30	-7.51833277569E-01	6.65051404114E-01	7.43929454387E-01	6.72022224704E-01	3.E-14	-1.E-11
100.0	1000.000	50	-1.02728883766E+00	2.26855983258F-01	2.53963904196E-01	9.17353264491F-01	-4.E-14	-1.E-11
100.0	1000.000	100	9.36270607960F-01	-4.43161964617F-01	-4.98554253144E-01	-8.32088192329E-01	-8.E-14	-1.E-11
200.0	343.000	0	2.36175579822E-07	9.74581592360E-08	5.19490430979E+06	-2.09045401279E+06	-2.E-15	2.E-10
200.0	344.000	0	3.56086598724E-07	1.45478647461E-07	3.48128926522E+06	-1.38604965934E+06	-5.E-15	2.E-10
200.0	399.000	0	1.53885091324E+00	1.67860189723E-01	3.25118563457E+00	-2.95191274637E-01	-7.E-15	-1.E-10
200.0	400.000	0	1.70803104755E+00	1.69857322090E-01	2.95864746041E+00	-2.91242987695E-01	-5.E-15	-1.E-10
200.0	401.000	0	1.87714230558E+00	1.67584921532E-01	2.66623392522E+00	-2.94692307136E-01	-1.E-14	8.E-12
200.0	475.000	0	9.81681975837E-01	-4.97941021547F-01	-1.24599573540E+00	-3.86650279840E-01	-2.E-15	-4.E-12
200.0	476.000	0	4.20046440799E-01	-6.10636723020F-01	-1.52505808348E+00	-1.63656974114E-01	-2.E-15	6.E-13
200.0	1000.000	0	-1.12173949248E+00	-1.39872626368F-01	-1.80816071552E-01	8.66926152391E-01	-4.E-15	-6.E-11
500.0	918.000	0	9.67977017096E-08	2.92443068049E-08	1.72876744622E+07	-5.10790995398E+06	4.E-15	3.E-10
500.0	920.000	0	1.76434005999E-07	5.26126912167E-08	9.61309194998E+06	-2.80121373882F+06	2.E-15	3.E-10
500.0	999.000	0	1.84475784730E+00	1.44518879335E-01	3.69787284737E+00	-2.52384106054E-01	4.E-15	-1.E-09
500.0	1000.000	0	1.98990418398E+00	1.45466034536E-01	3.44670129710E+00	-2.50575899128E-01	4.E-15	-1.E-09
500.0	1001.000	0	2.13502662979E+00	1.44423361185F-01	3.19557212237E+00	-2.52214527754E-01	-1.E-14	-6.E-10
500.0	1094.000	0	1.08691119464E+00	4.35124353444E-01	1.49313335619E+00	-3.22290648502E-01	-2.E-14	-3.E-11
500.0	1095.000	0	1.46929027367E+00	3.23944539005E-01	1.11156684610E+00	-4.35525914746E-01	-1.E-14	-2.E-12
500.0	10000.000	0	-5.31450210236E-01	-8.33357932907E-01	-8.78437947200E+01	5.04180378468E-01	2.E-15	1.E-11
1000.0	1920.000	0	2.24933066403E-05	4.66213784110F-06	1.08964346775E+05	-2.18728710472E+04	2.E-15	2.E-10
1000.0	1999.000	0	2.10432530931E+00	1.28927279390E-01	4.09255913389E+00	-2.24469801810E-01	-5.E-15	-8.E-09
1000.0	2000.000	0	2.23360882198E+00	1.29464300506E-01	3.86876233956E+00	-2.23464997529E-01	-2.E-14	-1.E-08
1000.0	2001.000	0	2.36288164524E+00	1.28884534129F-01	3.64498433934E+00	-2.24394604184E-01	-7.E-15	-7.E-10
1000.0	10000.000	0	7.55288842589E-01	6.61854934048E-01	7.39981588961E-01	-6.75555503365E-01	-1.E-14	-3.E-11

TEST OF THE MANCHESTER COULOMB WAVEFUNCTION PROGRAM - RCWFN

ETA	RHO	L	F	FP	G	GP	W=1	TEST
50.0	600.000	500	1.73798850811E-01	6.04848225640E-01	1.63257196022E+00	-7.21624255451E-02	-2.E-13	6.E-13
50.0	600.000	500	1.73798850811E-01	6.04848225639E-01	1.63257196022E+00	-7.21624255448E-02	-2.E-13	7.E-13
50.0	600.000	500	1.73798850811E-01	6.04848225639E-01	1.63257196022E+00	-7.21624255448E-02	-9.E-14	7.E-13
50.0	600.000	500	1.73798850811E-01	6.04848225639E-01	1.63257196022E+00	-7.21624255449E-02	-9.E-14	7.E-13
50.0	600.000	500	1.73798850810E-01	6.04848225638E-01	1.63257196022E+00	-7.21624255449E-02	-7.E-14	7.E-13
50.0	600.000	500	1.73798850810E-01	6.04848225638E-01	1.63257196023E+00	-7.21624255450E-02	3.E-15	8.E-13
50.0	1200.000	1000	-1.35051870473E+00	2.59965760156E-01	5.48342608435E-01	6.34903977241E-01	-3.E-13	-4.E-12
50.0	1200.000	1000	-1.35051870473E+00	2.59965760156E-01	5.48342608437E-01	6.34903977242E-01	-2.E-13	-3.E-12
50.0	1200.000	1000	-1.35051870473E+00	2.59965760156E-01	5.48342608438E-01	6.34903977242E-01	-3.E-13	-3.E-12
50.0	1200.000	1000	-1.35051870473E+00	2.59965760156E-01	5.48342608439E-01	6.34903977243E-01	-3.E-13	-3.E-12
50.0	1200.000	1000	-1.35051870472E+00	2.59965760155E-01	5.48342608439E-01	6.34903977243E-01	-2.E-13	-3.E-12
50.0	1200.000	1000	-1.35051870472E+00	2.59965760155E-01	5.48342608440E-01	6.34903977244E-01	-7.E-15	-2.E-12

PROGRAM LISTING

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ABPCRCWFN. COULOMB WAVE FUNCTIONS FOR ALL REAL ETA AND RHO.                    0
1   BARNETT, A.R., FENG, D.H., STEED, J.W., GOLDFARB, L.J.B.                   0
JOB ARBFF,:MBCNP,CP76(T36,P2000)                                               1
CONVERT,INPUT,FILE,IBM360.                                                     2
REWIND,FILE.                                                                   3
FTN,I=FILE,R=1,LX.                                                             4
LDSET,MAP=B/ZZZZMP,PRESET=NGINF.                                               5
LGO,FILE,PL=1500.                                                              6
#####S                                                                         7
      PROGRAM CFNCHK(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)                    8
C *** MAIN PROGRAM TO TEST COULOMB WAVEFUNCTIONS  MANCHESTER MAY 1974           9
      DIMENSION FC(1200),FCP(1200),GC(1200),GCP(1200),RHO(21),LLL(10)         10
      WRITE(6,1)                                                              11
100   READ(5,2) ETA,N,(LLL(I),I=1,10),M                                       12
      IF(N.EQ.0) CALL EXIT                                                    13
      IF(N.LT.0) WRITE(6,1)                                                   14
      IF(N.LT.0) N = -N                                                       15
      READ(5,3) (RHO(I),I=1,N)                                                16
      ACCUR = 1.0E-14                                                         17
      STEP  = 999.0                                                           18
      DO 10 I = 1,N                                                           19
      DO 10 J = 1,10                                                          20
      IF(LLL(J).EQ.0.AND.J.GT.1) GO TO 10                                     21
      L  = LLL(J)                                                             22
      CALL RCWFN(RHO(I),ETA,M  ,L  ,FC,FCP,GC,GCP,ACCUR,STEP)                 23
      F  = FC (L+1)                                                           24
      FP = FCP(L+1)                                                           25
      G  = GC (L+1)                                                           26
      GP = GCP(L+1)                                                           27
      RLP1 = FLOAT(L+1)/SQRT(ETA*ETA + FLOAT((L+1)**2))                       28
C *** MINL = M + 1  MAXL = L + 1 IN THIS CALL TO CHECK RESULTS ***            29
      CALL RCWFN(RHO(I),ETA,M+1,L+1,FC,FCP,GC,GCP,ACCUR,STEP)                 30
      TEST1 = FP*G - F*GP - 1.00                                              31
      TEST2 = F*GC(L+2) - G*FC(L+2) - RLP1                                    32
      WRITE(6,4) ETA,RHO(I),L,F,FP,G,GP,TEST1,TEST2                           33
10    CONTINUE                                                                34
      GO TO 100                                                               35
1     FORMAT(1H1,30X,61H TEST OF THE MANCHESTER COULOMB WAVEFUNCTION PRO       36
     1GRAM - RCWFN //,4X,4H ETA,6X,4H RHO,5X,2H L,8X,2H F,17X,2HFP,           37
     117X,2H G,19X,2HGP,10X,4H W-1,5X,4HTEST,/)                               38
2     FORMAT(F10.3,12I5)                                                      39
3     FORMAT(7F10.3)                                                          40
4     FORMAT(F10.1,F10.3,I5,4(1X,1PE18.11),2(2X,E7.0))                        41
      END                                                                     42
      SUBROUTINE RCWFN(RHO,ETA,MINL,MAXL,FC,FCP,GC,GCP,ACCUR,STEP)            43
      REAL   K,K1,K2,K3,K4,M1,M2,M3,M4                                        44
      DIMENSION FC(1),FCP(1),GC(1),GCP(1)                                     45
C *** COULOMB WAVEFUNCTIONS CALCULATED AT R = RHO BY THE                       46
C *** CONTINUED-FRACTION METHOD OF STEED  MINL,MAXL ARE ACTUAL L-VALUES        47
C *** SEE BARNETT FENG STEED AND GOLDFARB COMPUTER PHYSICS COMMUN 1974         48
      PACE = STEP                                                             49
      ACC  = ACCUR                                                            50
      IF(PACE.LT.100.0) PACE = 100.0                                          51
      IF(ACC.LT.1.0E-15.OR.ACC.GT.1.0E-6) ACC = 1.0E-6                        52
      R    = RHO                                                              53
      KTR  = 1                                                                54
      LMAX = MAXL                                                             55
      LMIN1= MINL + 1                                                         56
      XLL1 = FLOAT(MINL*LMIN1)                                                57
      ETA2 = ETA*ETA                                                          58
      TURN = ETA + SQRT(ETA2 + XLL1)                                          59
      IF(R.LT.TURN.AND.ABS(ETA).GE.1.0E-6) KTR = -1                           60
      KTRP = KTR                                                              61
      GO TO 2                                                                 62
```

```
1     R    = TURN                                                          63
      TF   = F                                                             64
      TFP  = FP                                                            65
      LMAX = MINL                                                          66
      KTRP = 1                                                             67
2     ETAR = ETA*R                                                         68
      RHO2 =   R*R                                                         69
      PL   = FLOAT(LMAX + 1)                                               70
      PMX  = PL + 0.5                                                      71
C *** CONTINUED FRACTION FOR FP(MAXL)/F(MAXL)  XL IS F  XLPRIME IS FP **   72
      FP   = ETA/PL + PL/R                                                 73
      DK   = ETAR*2.0                                                      74
      DEL  = 0.0                                                           75
      D    = 0.0                                                           76
      F    = 1.0                                                           77
      K    = (PL*PL - PL + ETAR)*(2.0*PL - 1.0)                            78
      IF(PL*PL+PL+ETAR.NE.0.0) GO TO 3                                     79
      R    = R + 1.0E-6                                                    80
      GO TO 2                                                              81
3     H    = (PL*PL + ETA2)*(1.0 - PL*PL)*RHO2                             82
      K    = K + DK + PL*PL*6.0                                            83
      D    =  1.0/(D*H + K)                                                84
      DEL  =  DEL*(D*K - 1.0)                                              85
      IF(PL.LT.PMX) DEL = -R*(PL*PL + ETA2)*(PL + 1.0)*D/PL                86
      PL   = PL + 1.0                                                      87
      FP   = FP + DEL                                                      88
      IF(D.LT.0.0) F = -F                                                  89
      IF(PL.GT.20000.) GO TO 11                                            90
      IF(ABS(DEL/FP).GE.ACC) GO TO 3                                       91
      FP   = F*FP                                                          92
      IF( LMAX.EQ.MINL) GO TO 5                                            93
      FC (LMAX+1) = F                                                      94
      FCP(LMAX+1) = FP                                                     95
C *** DOWNWARD RECURSION TO MINL FOR F AND FP, ARRAYS GC,GCP ARE STORAGE   96
      L  = LMAX                                                            97
      DO 4 LP  = LMIN1,LMAX                                                98
      PL = FLOAT(L)                                                        99
      GC (L+1) = ETA/PL + PL/R                                            100
      GCP(L+1) = SQRT(ETA2 + PL*PL)/PL                                    101
      FC (L)   = (GC(L+1)*FC(L+1) + FCP(L+1))/GCP(L+1)                    102
      FCP(L)   =  GC(L+1)*FC(L)   - GCP(L+1)*FC(L+1)                      103
4     L  = L - 1                                                          104
      F  = FC (LMIN1)                                                     105
      FP = FCP(LMIN1)                                                     106
5     IF(KTRP.EQ.-1) GO TO 1                                              107
C *** REPEAT FOR R = TURN IF RHO LT TURN                                  108
C *** NOW OBTAIN P + I.Q FOR MINL FROM CONTINUED FRACTION (32)            109
C *** REAL ARITHMETIC TO FACILITATE CONVERSION TO IBM USING REAL*8         110
      P  = 0.0                                                            111
      Q  = R - ETA                                                        112
      PL = 0.0                                                            113
      AR = -(ETA2 + XLL1)                                                 114
      AI =   ETA                                                          115
      BR = 2.0*Q                                                          116
      BI = 2.0                                                            117
      WI = 2.0*ETA                                                        118
      DR =   BR/(BR*BR + BI*BI)                                           119
      DI =  -BI/(BR*BR + BI*BI)                                           120
      DP = -(AR*DI + AI*DR)                                               121
      DQ =  (AR*DR - AI*DI)                                               122
6     P  =  P + DP                                                        123
      Q  =  Q + DQ                                                        124
      PL = PL + 2.0                                                       125
      AR = AR + PL                                                        126
      AI = AI + WI                                                        127
      BI = BI + 2.0                                                       128
      D  = AR*DR - AI*DI + BR                                             129
      DI = AI*DR + AR*DI + BI                                             130
```

```
      T  = 1.0/(D*D + DI*DI)                                              131
      DR =  T*D                                                           132
      DI = -T*DI                                                          133
      H  = BR*DR - BI*DI - 1.0                                            134
      K  = BI*DR + BR*DI                                                  135
      T  = DP*H  - DQ*K                                                   136
      DQ = DP*K  + DQ*H                                                   137
      DP = T                                                              138
      IF(PL.GT.46000.) GO TO 11                                           139
      IF(ABS(DP)+ABS(DQ).GE.(ABS(P)+ABS(Q))*ACC) GO TO 6                  140
      P  = P/R                                                            141
      Q  = Q/R                                                            142
C *** SOLVE FOR FP,G,GP AND NORMALISE F  AT L=MINL                        143
      G  = (FP - P*F)/Q                                                   144
      GP = P*G - Q*F                                                      145
      W  = 1.0/SQRT(FP*G - F*GP)                                          146
      G  = W*G                                                            147
      GP = W*GP                                                           148
      IF(KTR.EQ.1) GO TO 8                                                149
      F  = TF                                                             150
      FP = TFP                                                            151
      LMAX = MAXL                                                         152
C *** RUNGE-KUTTA INTEGRATION OF G(MINL) AND GP(MINL) INWARDS FROM TURN   153
C ***              SEE FOX AND MAYERS 1968 PG 202                         154
      IF(RHO.LT.0.2*TURN) PACE = 999.0                                    155
      R3 = 1.0/3.0D0                                                      156
      H  = (RHO - TURN)/(PACE + 1.0)                                      157
      H2 = 0.5*H                                                          158
      I2 = IFIX(PACE + 0.001)                                             159
      ETAH = ETA*H                                                        160
      H2LL = H2*XLL1                                                      161
      S  = (ETAH + H2LL/R  )/R   - H2                                     162
7     RH2= R + H2                                                         163
      T  = (ETAH + H2LL/RH2)/RH2 - H2                                     164
      K1 = H2*GP                                                          165
      M1 =  S*G                                                           166
      K2 = H2*(GP + M1)                                                   167
      M2 =  T*(G  + K1)                                                   168
      K3 =  H*(GP + M2)                                                   169
      M3 =  T*(G  + K2)                                                   170
      M3 =     M3 + M3                                                    171
      K4 = H2*(GP + M3)                                                   172
      RH = R + H                                                          173
      S  = (ETAH + H2LL/RH )/RH  - H2                                     174
      M4 =  S*(G + K3)                                                    175
      G  = G  + (K1 + K2 + K2 + K3 + K4)*R3                               176
      GP = GP + (M1 + M2 + M2 + M3 + M4)*R3                               177
      R  = RH                                                             178
      I2 = I2 - 1                                                         179
      IF(ABS(GP).GT.1.0E300) GO TO 11                                     180
      IF(I2.GE.0) GO TO 7                                                 181
      W  = 1.0/(FP*G - F*GP)                                              182
C *** UPWARD RECURSION FROM GC(MINL) AND GCP(MINL),STORED VALUES ARE R,S   183
C *** RENORMALISE FC,FCP FOR EACH L-VALUE                                 184
8     GC (LMIN1) = G                                                      185
      GCP(LMIN1) = GP                                                     186
      IF(LMAX.EQ.MINL) GO TO 10                                           187
      DO  9  L = LMIN1,LMAX                                               188
      T        = GC(L+1)                                                  189
      GC (L+1) = (GC(L)*GC (L+1) - GCP(L))/GCP(L+1)                       190
      GCP(L+1) =  GC(L)*GCP(L+1) - GC(L+1)*T                              191
      FC (L+1) = W*FC (L+1)                                               192
9     FCP(L+1) = W*FCP(L+1)                                               193
      FC (LMIN1) = FC (LMIN1)*W                                           194
      FCP(LMIN1) = FCP(LMIN1)*W                                           195
      RETURN                                                              196
10    FC (LMIN1) = W*F                                                    197
      FCP(LMIN1) = W*FP                                                   198
      RETURN                                                              199
11    W  = 0.0                                                            200
      G  = 0.0                                                            201
      GP = 0.0                                                            202
      GO TO 8                                                             203
      END                                                                 204
```

RCG → FJ
FC → F
GCP → GP
GC → G

```
#####S                                                                    205
50.0          2     0                                                    206
120.0     80.0                                                           207
9.0           1     0                                                    208
50.0                                                                     209
5.0           1     0                                                    210
20.0                                                                     211
4.0           1     0                                                    212
10.0                                                                     213
-1000.0       4     0                                                    214
1.0       10.0        100.0       1000.0                                 215
-500.0        4     0                                                    216
0.59      0.61        100.0       1000.0                                 217
-200.0        4     0                                                    218
0.145     0.155       100.0       1000.0                                 219
-50.0         2     0    1    2     3    5   10   20   30   50  100      220
5.0       50.0                                                           221
-10.0         4     0                                                    222
2.9       3.1         100.0       1000.0                                 223
-6.0          6     0                                                    224
6.9       7.1         17.4        17.6        100.0       1000.0         225
-4.0          1     0    1    5   10   20   30   50  100                  226
5.0                                                                      227
-4.0         -1     0    1    2    3    5   10   20   30   50  100      228
50.0                                                                     229
-0.3          4     0                                                    230
7.9       8.1         100.0       1000.0                                 231
0.0           7     0                                                    232
0.001     0.01        0.1         1.0         10.0        100.0       1000.0  233
1.0           7     0                                                    234
2.0       7.9         8.1         9.1         9.2         100.0       1000.0  235
8.0           7     0                                                    236
1.05      2.01        16.0        20.8        20.9        100.0       1000.0  237
10.0          2     0    1    2     3    5   10   20   30   50  100      238
5.0       50.0                                                           239
26.0         -7     0                                                    240
24.3      24.5        50.7        50.9        52.0        100.0       1000.0  241
34.0          9     0                                                    242
40.2      40.5        67.9        68.0        68.1        100.0       116.2   243
116.4     1000.0                                                         244
50.0          8     0                                                    245
67.6      67.8        99.9        100.0       100.1       153.1       153.3   246
1000.0                                                                   247
100.0         1     0    1    2     3    5   10   20   30   50  100      248
1000.0                                                                   249
200.0         8     0                                                    250
343.0     344.0       399.0       400.0       401.0       475.0       476.0   251
1000.0                                                                   252
500.0         8     0                                                    253
918.0     920.0       999.0       1000.0      1001.0      1094.0      1095.0  254
10000.0                                                                  255
1000.0        5     0                                                    256
1920.0    1999.0      2000.0      2001.0      10000.0                        257
50.0         -1   500                                                000  258
600.0                                                                    259
50.0          1   500                                                100  260
600.0                                                                    261
50.0          1   500                                                200  262
600.0                                                                    263
50.0          1   500                                                300  264
600.0                                                                    265
50.0          1   500                                                400  266
600.0                                                                    267
50.0          1   500                                                500  268
600.0                                                                    269
50.0          1  1000                                             0000    270
1200.0                                                                   271
50.0          1  1000                                                200  272
1200.0                                                                   273
50.0          1  1000                                                400  274
1200.0                                                                   275
50.0          1  1000                                                600  276
1200.0                                                                   277
50.0          1  1000                                                800  278
1200.0                                                                   279
50.0          1  1000                                               1000  280
1200.0                                                                   281
                                                                         282
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