

CRCWFN: coupled real Coulomb wavefunctions

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A subroutine is given to solve a set of coupled radial Schrödinger equations for real multipole potentials. The subroutine uses the piecewise analytic method and is particularly useful for long-range Coulomb excitation calculations. It is designed to be used within a conventional coupled channels code to provide coupled Coulomb wavefunctions to match to the solutions calculated for short-range nuclear couplings.

PROGRAM SUMMARY

Title of program: CRCWFN

Catalogue number: ACPT

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

Licensing provisions: none

Computer: Sun Sparcstation 2

Operating System: UNIX

Programming language used: Fortran77

Memory required to execute with typical data: 820 Kbytes for test case

No. of bits in a word: 32

Peripherals used: terminal, printer

No. of lines in distributed program, including test data, etc.: 1612

CPC Program Library subprograms used: Cat. no.: ABNK;
Title: COULFG; *Ref. in CPC:* 27 (1982) 147–166

Keywords: nuclear, coupled channels, Coulomb-excitation, Schrödinger equation, heavy-ions

Nature of physical problem

Solutions to coupled Schrödinger radial equations are calculated for real multipole potentials. The method is particularly suited to Coulomb excitation of heavy ions where multiple coupling is significant to large radii. The subroutine is designed to be used within existing conventional coupled channels codes.

Method of solution

The piecewise analytic method of Gordon [1] is used. The integration range is divided into segments. In each segment the potential is approximated by a straight line and analytic solutions for the straight line potentials (Airy functions) are calculated. First and second order corrections for the approximation of the potential are applied by analytic integrals. Matrix methods are used to find solutions that are continuous and smooth at each boundary.

Restriction on the complexity of the problem

The potentials must be real and expressed as a inverse power series of r . The method is not stable in classically forbidden regions ($E < V$). The subroutine returns the solution and derivative at the end point with no information on the behaviour within the integration region.

Typical running time

1.4 CPU seconds execution time for test case (with compiler optimisation).

Reference

[1] R.G. Gordon, J. Chem. Phys. 51 (1969) 14–25.

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LONG WRITE-UP

1. Introduction

Coupled channel calculations are performed by solving a set of coupled radial Schrödinger equations. The conventional approach [1] uses numerical integration methods (e.g. Numerov [2]), which we shall refer to as step-by-step methods, to integrate solutions outwards from the origin to a sufficiently large radius that the coupling is negligible. The solutions are then matched to solutions of the uncoupled equations (Coulomb wavefunctions) with the correct scattering boundary conditions. This matching process produces the S-matrix values.

This method is very successful when the coupling is short ranged but in many reactions (e.g. heavy-ion scattering) long-ranged Coulomb multipole couplings are significant. In such reactions the radius at which the coupling is negligible is very large and the step-by-step integration methods become very inefficient [3]. There has therefore been a long term interest in alternative methods to calculate the effect of coupling in the Coulomb excitation region [4]. In this paper we describe a method that includes coupling to all orders and which can be included within existing coupled channels codes.

The objective is to produce a complete set of solutions at a radius R_{in} which obey the asymptotic boundary conditions and which include the effects of coupling at radii greater than R_{in} . The radius R_{in} is chosen to be sufficiently large that the nuclear potentials are negligible. We call the set of solutions coupled Coulomb wavefunctions [5,6,3]. These can be matched at R_{in} to solutions integrated out from the origin by conventional methods in order to obtain the S-matrix.

Burke and Schey [4] were the first to address the problem using asymptotic expansions. Alder and Pauli [7], and Norcross and Seaton [8,9] showed how the solutions can be expressed as products of uncoupled Coulomb functions and modulating amplitudes. The modulating amplitudes obey coupled second-order differential equations [5,10] which, as the amplitudes are slowly varying functions of r , can be approximated by coupled first-order equations. Rösler [11] showed the modulating amplitudes may be expressed as an asymptotic series in inverse powers of r . If the states are degenerate (or the adiabatic approximation is used) the amplitudes can be calculated accurately using a three-term recursion relation. However, for the non-degenerate case the resulting four-term recursion relation is numerically ill-conditioned [6]. Rhoades-Brown et al. [6] solve the approximate coupled first-order equations for the modulating amplitudes using first-order Born approximation to integrate from R_{out} to R_{in} . The integrals can be expressed as an asymptotic series and can be evaluated using rapid recursion relations. This is equivalent to DWBA for Coulomb excitation in the asymptotic region and assumes multiple excitation and reorientation are negligible in this region.

In this paper the coupled Coulomb wavefunctions are calculated using the piecewise analytic method [12]. The integration range is divided into segments in which the potential can be approximated by a straight line. The solution in each segment can then be expressed as a product of Airy functions and slowly varying coefficients. The coefficients can be calculated from analytic integrals so the solution is only evaluated at each segment boundary. This method was first described by Gordon [12] for atomic scattering and has been used for heavy-ion Coulomb excitation by Tolsma [13,14].

In the piecewise method the segment size is dependent on the smoothness of the potential and the oscillatory nature of the solutions is provided by the basis Airy functions. This allows for much larger step sizes than conventional methods such as Numerov. Although the calculation per step is more complicated, time savings of several orders of magnitude are typical.

The piecewise method is preferable to the Alder–Pauli factorisation methods because it solves the coupled equations to all orders of coupling. Multi-step contributions and reorientation effects are treated fully. However the piecewise method is slower than the Alder–Pauli based methods.

For a general derivation of the piecewise method and an analysis of the errors see Gordon [12,15].

Tolsma [14] describes improvements to the method including diagonalising the coupled potentials in each step, re-orthogonalising the solutions, and using Coulomb functions instead of Airy functions as reference solutions. Our comparatively simple implementation achieves an acceptable performance without employing these features. The subroutine CRCWFN can be included in existing coupled channels codes. It has been added as an option in recent versions of FRESKO [1].

2. Piecewise analytic method

In this section we briefly describe the piecewise method. To illustrate the method we first describe a one channel application before generalising for coupled channels.

2.1. One channel problem

We seek a solution to the one-channel radial equation

$$\frac{d^2 u}{dr^2}(r) + [k^2 - U(r)]u(r) = 0 \tag{1}$$

in the range $R_{in} \leq r \leq R_{out}$ where k is the asymptotic wave number and $U(r)$ is the potential:

$$U(r) = \frac{2\mu}{\hbar^2} V(r) + \frac{l(l+1)}{r^2}. \tag{2}$$

The integration range is divided into segments. We will discuss the method of choosing the segment length later.

Initially consider one segment from r_0 to r_1 . We approximate the potential $U(r)$ in the segment by a straight line $U^0(r)$

$$U^0(r) = U_{BAR} + (r - \bar{r}) \left. \frac{dU}{dr} \right|_{r=\bar{r}}, \tag{3}$$

where U_{BAR} is the average of the potential in the segment and dU/dr is evaluated at the mid point \bar{r} . The general solution of the radial equation with the approximate potential

$$\frac{d^2 w}{dr^2}(r) + [k^2 - U^0(r)]w(r) = 0 \tag{4}$$

can be written as a linear combination of Airy functions

$$w(r) = a A(r) + b B(r), \tag{5}$$

where

$$A(r) = Ai(\alpha(\beta + r)), \quad B(r) = Bi(\alpha(\beta + r)). \tag{6}$$

The Airy functions obey the equation $d^2 Ai(z)/dz^2 = z Ai(z)$, so the constants α and β can be shown to be

$$\alpha = [dU/dr|_{r=\bar{r}}]^{1/3}, \quad \beta = \frac{U_{\text{BAR}} - k^2}{dU/dr|_{r=\bar{r}}} - \bar{r}. \quad (7)$$

The solution of the original radial eq. (1) can be written as a product of the Airy functions $A(r)$, $B(r)$ and coefficients $a(r)$, $b(r)$ that vary slowly with r :

$$u(r) = a(r) A(r) + b(r) B(r). \quad (8)$$

The radial dependence of the coefficients can be shown [12] to be proportional to the error in the linear approximation for the potential

$$a'(r) = -\pi B(r)[U(r) - U^0(r)]u(r), \quad b'(r) = \pi A(r)[U(r) - U^0(r)]u(r). \quad (9)$$

Assuming we know the solution and derivative at $r = r_0$ then the values of the coefficients at r_0 are uniquely determined (as the solution and derivative must be continuous)

$$u(r_0) = a(r_0) A(r_0) + b(r_0) B(r_0), \quad u'(r_0) = a(r_0) A'(r_0) + b(r_0) B'(r_0). \quad (10)$$

(Terms including $a'(r_0)$ and $b'(r_0)$ can be shown to cancel [12]).

Integrating eqs. (9) from r_0 to r_1 we obtain an expression for the solution at $r = r_1$:

$$u(r_1) = a(r_1) A(r_1) + b(r_1) B(r_1), \quad (11)$$

with

$$\begin{aligned} a(r_1) &= a(r_0) - \pi \int_{r_0}^{r_1} dr B(r) [U(r) - U^0(r)] u(r), \\ b(r_1) &= b(r_0) + \pi \int_{r_0}^{r_1} dr A(r) [U(r) - U^0(r)] u(r). \end{aligned} \quad (12)$$

This expression is exact but requires knowledge of the solution $u(r)$. We use it as the basis for approximations:

(i) As the coefficients are slow varying we can approximate $u(r)$ on the right hand side by the approximate solution

$$u^0(r) = a(r_0) A(r) + b(r_0) B(r). \quad (13)$$

(ii) $U(r) - U^0(r)$ is approximated in the segment by a quadratic $\Delta U(r)$ so that the integrals may be solve analytically.

An approximate form of the solution at r_1 is therefore

$$\begin{aligned} u(r_1) &\approx a^{(1)}(r_1) A(r_1) + b^{(1)}(r_1) B(r_1) \\ a^{(1)}(r_1) &= a(r_0) - \pi \int_{r_0}^{r_1} dr B(r) \Delta U(r) u^0(r), \end{aligned} \quad (14)$$

$$b^{(1)}(r_1) = b(r_0) + \pi \int_{r_0}^{r_1} dr A(r) \Delta U(r) u^0(r).$$

It is easier to apply the boundary conditions if we reformulate the problem so the coefficients remain constant over the segment but corrections are made to the functions $A(r_1)$ and $B(r_1)$:

$$\begin{aligned} u(r_1) &\approx a^{(1)}(r_1) A(r_1) + b^{(1)}(r_1) B(r_1) \\ &= a(r_0) A^C(r_1) + b(r_0) B^C(r_1), \end{aligned} \quad (15)$$

where

$$\begin{aligned} A^C(r_1) &= [(1 + D^{AA})A(r_1) + D^{BA} B(r_1)], \\ B^C(r_1) &= [(1 + D^{BB})B(r_1) + D^{AB} A(r_1)], \end{aligned} \quad (16)$$

$$\begin{aligned} D^{AA} &= \pi \int_{r_0}^{r_1} dr B(r) \Delta U(r) A(r), & D^{BB} &= -\pi \int_{r_0}^{r_1} dr A(r) \Delta U(r) B(r), \\ D^{AB} &= -\pi \int_{r_0}^{r_1} dr B(r) \Delta U(r) B(r), & D^{BA} &= \pi \int_{r_0}^{r_1} dr A(r) \Delta U(r) A(r). \end{aligned}$$

Analytical expressions exist for these integrals [12,14]. (Precautions must be taken to avoid cancellation errors when evaluating the analytic expressions on the computer.)

We now have expressions for the solutions at $r = r_0$ and $r = r_1$,

$$\begin{aligned} u(r_0) &= a(r_0) A(r_0) + b(r_0) B(r_0), & u'(r_0) &= a(r_0) A'(r_0) + b(r_0) B'(r_0), \\ u(r_1) &= a(r_0) A^C(r_1) + b(r_0) B^C(r_1), & u'(r_1) &= a(r_0) A^C'(r_1) + b(r_0) B^C'(r_1), \end{aligned} \quad (17)$$

where there are two unknowns ($a(r_0)$ and $b(r_0)$), and all other terms are determined by the energy and potential within the segment.

It is a simple problem in linear algebra to solve for the coefficients a, b in each segment to give a smooth, continuous solution across the integration region R_{in} to R_{out} . This can be solved efficiently using the LU decomposition method [16]. This method has the advantage that once the matrix has been decomposed, the backsubstitution stage can be repeated easily for a range of different solutions. One disadvantage of the method described is we only obtain the solution at the end points and have no information on the behaviour of the solution within the integration region.

The segment sizes must be chosen to allow the integration to proceed quickly within a known degree of accuracy. This is done by ensuring the error in approximating the potential $U(r) - U^0(r)$ is within a user determined tolerance. As we use a linear approximation, the error is proportional to the second derivative of the potential. In the subroutine CRCWFN the step size h is determined from the user set tolerance ACC by

$$h = 4 \left[\text{ACC} / (d^2 U / dr^2) |_{r=r_0} \right]^{1/2}. \quad (18)$$

For example, if the potential is $U(r) = 100/r$ and $\text{ACC} = 0.0001$ then the stepsize is $h = 0.25$ fm for $r_0 = 20$ fm, and $h = 8$ fm for $r_0 = 200$ fm.

For very large r (more than 1000 fm) it is more efficient to use constant potential approximations instead of linear approximations. The reference solutions are sines and cosines rather than Airy functions. The subroutine CRCWFN allows the user to specify a radius RSWITCH at which this change from linear to constant approximations takes place.

2.2. Coupled channels problem

The coupled channels form of the piecewise method uses generalised forms of eqs. (1)–(18) with the solutions and potentials represented by vectors and matrices. In the following description bold type indicates a column vector or matrix.

In a coupled channels calculation we must solve a set of N coupled radial Schrödinger equations for each total angular momentum J and parity:

$$\left(\frac{d^2}{dr^2} + k_m^2 - U_{mm}^J(r) \right) u_m^J(r) = \sum_{n \neq m} U_{mn}^J(r) u_n^J(r), \quad (19)$$

where k_m is the asymptotic wave number for channel m , $u_m^J(r)$ is the m th element of the radial solution vector $\mathbf{u}^J(r)$ and U_{mn}^J is an element of the potential matrix $\mathbf{U}^J(r)$ that couples channels m and n ,

$$[\mathbf{U}(r)]_{mn} = U_{mn}(r) = \frac{2\mu_m}{\hbar^2} V_{mn}(r) + \delta_{mn} \frac{l_m(l_m + 1)}{r^2}. \quad (20)$$

(We will omit the J superscripts in the following discussion.)

The integration range is divided into segments and in each segment a reference potential matrix \mathbf{U}° is constructed from linear approximations to the diagonal elements of \mathbf{U} ,

$$[\mathbf{U}^\circ(r)]_{mn} = \delta_{mn} \left(\bar{U}_{mm} + (r - \bar{r}) \frac{dU_{mm}}{dr} \Big|_{r=\bar{r}} \right), \quad (21)$$

where \bar{U}_{mm} is the average of $U_{mm}(r)$ over the segment.

The reference potential \mathbf{U}° is diagonal so the reference solutions of the approximate radial equation

$$\left(\frac{d^2}{dr^2} + k_m^2 - U_{mm}^\circ(r) \right) w_m(r) = 0 \quad (22)$$

can be expressed as products of diagonal matrices of Airy functions \mathbf{A} and \mathbf{B} and coefficient vectors \mathbf{a} , \mathbf{b}

$$\mathbf{w}(r) = \mathbf{A}(r) \mathbf{a} + \mathbf{B}(r) \mathbf{b}, \quad (23)$$

where

$$[\mathbf{A}(r)]_{mn} = \delta_{mn} \text{Ai}(\alpha_m(\beta_m + r)), \quad [\mathbf{B}(r)]_{mn} = \delta_{mn} \text{Bi}(\alpha_m(\beta_m + r)), \quad (24)$$

$$\alpha_m = \left(\frac{dU_{mm}}{dr} \Big|_{r=\bar{r}} \right)^{1/3}, \quad \beta_m = \frac{\bar{U}_{mm} - k_m^2}{dU_{mm}/dr|_{r=\bar{r}}} - \bar{r}.$$

The solution vector to the coupled equations (19) can be written as a product of the reference solution matrices and coefficients vectors $\mathbf{a}(r)$, $\mathbf{b}(r)$ which vary slowly with r . The solution at the beginning of a segment is

$$\mathbf{u}(r_0) = \mathbf{A}(r_0) \mathbf{a}(r_0) + \mathbf{B}(r_0) \mathbf{b}(r_0) . \quad (25)$$

If the solution at r_0 is known then $\mathbf{a}(r_0)$ and $\mathbf{b}(r_0)$ are uniquely determined. The solution at r_1 can be obtained by the same procedure as for the one channel case

$$\mathbf{u}(r_1) \approx \mathbf{A}^c(r_1) \mathbf{a}(r_0) + \mathbf{B}^c(r_1) \mathbf{b}(r_0) . \quad (26)$$

The matrices \mathbf{A}^c and \mathbf{B}^c are obtained using a generalised form of eq. (16) involving matrix multiplications. For example

$$\mathbf{D}^{AA} = \pi \int_{r_0}^{r_1} dr \mathbf{B}(r) \Delta U(r) \mathbf{A}(r) , \quad (27)$$

where $\Delta U(r)$ is a matrix of quadratic fits to $U(r) - U^0(r)$. As the reference potential U^0 is diagonal, effects of coupling appear only in these correction integrals.

Evaluation of the off-diagonal terms of these integrals is likely to be sensitive to cancellation errors if the solutions in two channels are very similar. The subroutine CRCWFN checks for loss of accuracy and if more than six digits are lost the subroutine repeats the integral assuming the basis functions in the two channels are identical. This is important for nearly degenerate states of the same orbital angular momentum.

We use the LU decomposition technique [16] to solve the boundary conditions and obtain a continuous solution across the integration range. For an N channel problem the matrix of solutions has a $(2N \times 2N)$ matrix on the diagonal corresponding to each segment boundary. As there may be typically a hundred segments, the resulting matrix can be very large but sparse, with all the non-zero elements within a band extending $2N$ either side of the diagonal. The subroutine CRCWFN uses a system of pointers to avoid storage and manipulation of zero elements. Once the matrix of reference solutions is decomposed into lower and upper triangular form we can use backsubstitution [16] repeatedly to propagate solution vectors from R_{out} to R_{in} .

The piecewise method is applicable to any smooth potential. Our implementation (CRCWFN) has been designed for Coulomb excitation. The potentials must be real and expressed as an expansion in inverse powers of r . These constraints increase the efficiency of the subroutine as all the arithmetic is real, and the approximations to the potential can be calculated analytically.

Care must be taken when integrating into classically forbidden regions. If $V > E$ then the Airy functions are exponential in behaviour. If the integration is continued into the classically forbidden region, the most rapidly increasing component will dominate and the linear independence of the solution is lost. This problem is common in solving coupled equations but is particularly serious in this case as we specify the asymptotic boundary conditions and therefore do not obtain a regular solution. The Numerov integration region should therefore be chosen such that R_{in} is a few fm inside the classical turning point of the largest partial wave.

For very high partial waves the classical turning point is at a sufficiently large radius that only Coulomb forces act. It has proved acceptable in these cases to omit the Numerov integration completely and match the coupled Coulomb wavefunctions to zero a few fm inside the classical turning point. This

technique is included as an option in FRESKO [1] and, although simplified, can produce acceptable results for high partial waves very quickly.

3. Coupled Coulomb wavefunctions

In this section we define coupled Coulomb wavefunctions, describe how they can be calculated using the piecewise integration method, and show how they can be used to obtain the S-matrix.

We use the overline notation to indicate a coupled Coulomb wavefunction (e.g. $\overline{F}^{(n)}(r)$). The coupled Coulomb wavefunction $\overline{F}^{(n)}(R_{\text{in}})$ is the solution vector at R_{in} that, when integrated out to R_{out} , has the form of a Coulomb function $F_{l_n}(R_{\text{out}})$ in channel n and zero in all other channels.

Coupled Coulomb functions are obtained by integrating uncoupled Coulomb functions evaluated at R_{out} inwards to R_{in} . We construct solution vectors at $r = R_{\text{out}}$ with an uncoupled Coulomb function F_l or G_l in one channel and zero in all other channels. For example the m th element of vector $\overline{F}^{(n)}(R_{\text{out}})$ is

$$F_m^{(n)}(R_{\text{out}}) = \delta_{mn} F_{l_n}(R_{\text{out}}). \quad (28)$$

The bracketed superscript refers to the non-zero element at R_{out} . With the corresponding $\overline{G}^{(n)}$ vectors this gives $2N$ linearly independent vectors. These solutions are integrated using the piecewise method to give the corresponding coupled Coulomb wavefunctions at R_{in} , $\overline{F}^{(n)}(R_{\text{in}})$ and $\overline{G}^{(n)}(R_{\text{in}})$.

The m th channel component of the solution of the coupled radial Schrödinger equation (19) satisfies the asymptotic boundary condition

$$u_m(R_{\text{out}}) = \frac{1}{2}i \left[\delta_{ma} H_{l_a}^-(R_{\text{out}}) - S_{ma} H_{l_m}^+(R_{\text{out}}) \right], \quad (29)$$

where a is the incident channel and R_{out} is a radius beyond which all coupling is assumed negligible. The outgoing and ingoing Coulomb functions are defined $H_{l_m}^+ = G_{l_m} + iF_{l_m}$ and $H_{l_a}^- = G_{l_a} - iF_{l_a}$.

As the coupled Coulomb wavefunctions include the effects of coupling in the region $R_{\text{in}} < r < R_{\text{out}}$, an equivalent expression for the boundary condition (29) is

$$u_m(R_{\text{in}}) = \frac{1}{2}i \left(\overline{H}_m^{-(a)}(R_{\text{in}}) - \sum_n S_{na} \overline{H}_m^{+(n)}(R_{\text{in}}) \right), \quad (30)$$

where

$$\overline{H}_m^{-(a)}(R_{\text{in}}) = \overline{G}_m^{(a)}(R_{\text{in}}) - i\overline{F}_m^{(a)}(R_{\text{in}}), \quad \overline{H}_m^{+(n)}(R_{\text{in}}) = \overline{G}_m^{(n)}(R_{\text{in}}) + i\overline{F}_m^{(n)}(R_{\text{in}}). \quad (31)$$

In this equation $\overline{H}_m^{-(a)}(R_{\text{in}})$ is the m th channel contribution of an incoming wave in channel a and $\overline{H}_m^{+(n)}(R_{\text{in}})$ is the m th channel contribution to an outgoing wave in channel n . The S-matrix can therefore be obtained by matching, at R_{in} , the coupled Coulomb wavefunctions to solutions integrated out from the origin.

4. Description of input

The calling sequence is:

CALL CRCWFN (NCH, AK2, KMAX, COUPL, RIN, ROUT, ACCRCY,
V, FCC, GCC, MCH, MAXV, CORREC, DERIV, CFG, SWITCH)

The variables have the following type and meaning (all real variables are declared to be double precision):

NCH (integer) Number of channels used.

AK2(MCH) (real array) Asymptotic wave number squared k_m^2 for each channel.

KMAX (integer) Maximum inverse power of r in expansion of potential.

COUPL(MCH,MCH,KMAX) (real array) Magnitude of coupling potential for each multipolarity (see below).

RIN(2) (real) RIN(1) $\equiv R_{in}$ is the inner radius at which the solutions are calculated. If DERIV is FALSE the solutions are also calculated at RIN(2).

ROUT (real) Outer radius of the integration.

ACCRCY (real) Tolerance used in choosing segment size (typically 0.01).

V(MAXV) (real array) Large work array.

FCC(MCH,MCH,2) (real array) This array, along with GCC, contains the solution vectors:

- On input FCC(m,n,1) is the m th element of the n th solution vector at R_{out} . It is normally set to: $FCC(m,n,1) = \delta_{mn} F_l(k_m R_{out}, \eta_m)$. FCC(m,n,2) is the derivative with respect to r . These initial conditions are calculated internally if CFG is TRUE.

- On output FCC(m,n,1) is the m th element of the n th solution vector at R_{in} : If DERIV is TRUE then FCC(m,n,2) is the derivative with respect to r . If DERIV is FALSE then FCC(m,n,2) is the solution at RIN(2). GCC(MCH,MCH,2) (real array) As for FCC for Coulomb functions G_l .

MCH (integer) Maximum number of channels.

MAXV (integer) Size of work array V. This must be $> 10 \cdot NCH \cdot NCH \cdot NSTEPS$. Unfortunately NSTEPS (the number of segments required) is not known initially. NSTEPS = ROUT-RIN may be acceptable as a first estimate. The subroutine will print an error message to stream 6 if this parameter is too small.

CORREC (logical) If FALSE the correction calculations are omitted and the uncoupled basis functions are used. This should only be used for a quick check of array sizes and will not give accurate values for the solutions.

DERIV (logical) If TRUE the subroutine returns the coupled Coulomb wavefunctions and derivatives evaluated at one radius, RIN(1). If FALSE the subroutine returns the values of the coupled Coulomb wavefunctions at two radii, RIN(1) and RIN(2).

CFG (logical) If TRUE the subroutine calls COULFG [17] to calculate uncoupled Coulomb wavefunctions at ROUT (see below) and construct the initial values for FCC and GCC.

SWITCH (real) Radius to change from linear approximations to constant approximations (with sines and cosines as reference solutions). Constant approximations are more efficient for large radii (typically more than 1000 fm).

CRCWFN must be called separately for each total angular momentum and parity. The potentials must be real and expressed in inverse powers of r . The array of coefficients COUPL must be assigned so the potential between channels m and n is

$$U_{mn}(r) = \sum_{k=1}^{\text{KMAX}} \frac{\text{COUPL}(m, n, k)}{r^k} = \frac{2\mu_m}{\hbar^2} V_{mn}(r). \quad (32)$$

For example the Coulomb monopole and centrifugal barrier should be entered as

$$\text{COUPL}(m, n, 1) = \delta_{mn} 2\eta_m k_m, \quad \text{COUPL}(m, n, 2) = \delta_{mn} l_m(l_m + 1), \quad (33)$$

where η_m , k_m and l_m are the Sommerfeld parameter, asymptotic wavenumber and orbital angular momentum for channel m .

If the flag $\text{CFG} = \text{TRUE}$ the subroutine will calculate the uncoupled Coulomb wavefunctions at R_{out} and construct the arrays FCC and GCC. The Coulomb wavefunctions are evaluated using COULFG [17] with the values of η_m and l_m extracted from the array elements of COUPL. This facility is very inefficient in a full coupled channels calculation since COULFG has to be called separately for each total angular momentum. It is far more efficient to calculate the Coulomb functions in the calling program, and construct the matrices FCC and GCC prior to calling CRCWFN with $\text{CFG} = \text{FALSE}$.

5. Test run

The test run example is for $^{16}\text{O} + ^{58}\text{Ni}$ with incident energy $E_{\text{LAB}} = 50$ MeV with total angular momentum $J = 20\hbar$ and positive parity. The 2^+ state of ^{58}Ni at 2.15 MeV is included which gives four channels for each parity.

The coupling matrix elements have been calculated using the rotational model with quadrupole deformation parameter $\beta_2 = 0.15$ [1]. The test run output is produced using the test program supplied with the code.

The output includes the input information and three sets of solutions evaluated at $R_{\text{in}} = 25$ fm:

- (1) The uncoupled Coulomb functions evaluated at R_{in} using COULFG.
- (2) The uncoupled Coulomb functions at R_{in} calculated by integrating uncoupled Coulomb functions inwards from $R_{\text{out}} = 200$ fm using CRCWFN with no coupling.
- (3) The coupled Coulomb wavefunctions at R_{in} integrated in from $R_{\text{out}} = 200$ fm using CRCWFN.

Comparing (1) and (2) indicates the accuracy of the method in the uncoupled case. Comparing (1) and (3) shows the effect of Coulomb excitation in the region $R_{\text{in}} \leq r \leq R_{\text{out}}$.

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TEST RUN OUTPUT

TEST RUN OUTPUT: CRCWFN

```
rin(1)= 25.00 fm rin(2)= 25.50 fm rout= 200.00 fm
accrcy= 0.001 switch= 1000.0 fm maxv= 100000
nch= 4 mch= 4 kmax= 4
correc= T deriv= T cfg= T
```

Channel	L (hbar)	Eta	k**2
1	20	19.95000	23.50000
2	18	20.33000	22.64000
3	20	20.33000	22.64000
4	22	20.33000	22.64000

COUPL ARRAY:

Multipolarity (k-1) = 0	1	2	3	
coupl(1,1,k)=	193.422	420.000	0.000	0.000
coupl(2,2,k)=	193.466	342.000	0.000	0.000
coupl(3,3,k)=	193.466	420.000	0.000	0.000
coupl(4,4,k)=	193.466	506.000	0.000	0.000

All off-diagonal elements zero

(1) standard Coulomb functions evaluated at Rin

	F	dF/dr	G	dG/dr
ch1	0.4309886	-4.0062192	-1.0305832	-1.6681128
ch2	1.1037517	0.7277381	0.1938691	-4.1830650
ch3	0.2587391	4.1210217	1.0928862	-0.9830095
ch4	-0.9422517	2.3193083	0.6161566	3.5331259

(2) Coulomb wavefunctions integrated in from Rout with no coupling

ch1	0.4309893	-4.0062213	-1.0305829	-1.6681079
ch2	1.1037543	0.7277394	0.1938684	-4.1830559
ch3	0.2587400	4.1210098	1.0928893	-0.9830087
ch4	-0.9422556	2.3193076	0.6161572	3.5331109

All off-diagonal elements zero

COUPL ARRAY:

Multipolarity (k-1) = 0	1	2	3	
coupl(1,1,k)=	193.422	420.000	0.000	0.000
coupl(1,2,k)=	0.000	0.000	1755.000	0.000
coupl(1,3,k)=	0.000	0.000	-1471.000	0.000
coupl(1,4,k)=	0.000	0.000	1842.000	0.000
coupl(2,1,k)=	0.000	0.000	1755.000	0.000
coupl(2,2,k)=	193.466	342.000	-725.200	0.000

coupl(2,3,k)=	0.000	0.000	1009.000	0.000
coupl(2,4,k)=	0.000	0.000	0.000	0.000
coupl(3,1,k)=	0.000	0.000	-1471.000	0.000
coupl(3,2,k)=	0.000	0.000	1009.000	0.000
coupl(3,3,k)=	193.466	420.000	780.000	0.000
coupl(3,4,k)=	0.000	0.000	915.600	0.000
coupl(4,1,k)=	0.000	0.000	1842.000	0.000
coupl(4,2,k)=	0.000	0.000	0.000	0.000
coupl(4,3,k)=	0.000	0.000	915.600	0.000
coupl(4,4,k)=	193.466	506.000	-840.400	0.000

(3) coupled Coulomb wavefunctions integrated in from Rout

channel 1

0.4400292	-3.9318441	-1.0102250	-1.7060747
-0.0995963	0.1510136	0.0355063	0.3851530
0.0780784	-0.1385298	-0.0328094	-0.3009696
-0.0899193	0.1874776	0.0453236	0.3456246

channel 2

0.0939876	-0.1985389	-0.0496467	-0.3490727
1.0791236	0.9847477	0.2608582	-4.0966443
0.0199875	-0.3387672	-0.0891717	-0.0654668
-0.0086101	-0.0282005	-0.0078945	0.0325675

channel 3

-0.0636895	-0.2058291	-0.0567675	0.2455941
0.0895621	-0.0694513	-0.0157061	-0.3372511
0.3421038	3.9882566	1.0595084	-1.2935918
0.0824131	-0.0464794	-0.0101457	-0.3082081

channel 4

-0.0457349	0.3498873	0.0919090	0.1612075
0.0098792	0.0071870	0.0021551	-0.0366804
0.0440502	0.2558744	0.0688819	-0.1736349
-0.9774891	2.0327657	0.5390461	3.6737999