1 SUMMARY

To compute the various **vector coupling coefficients** (3–*j*, 6–*j*, 9–*j* and their kindred) of the theory of **angular momentum** in **quantum mechanics,** i.e. the Wigner 3–*j*, 6–*j* and 9–*j* symbols, the Clebsch-Gordan and Wigner coefficient, the Racah coefficient and Jahn's U-function.

ATTRIBUTES — Version: 1.0.0. **Types:** FG01A; FG01AD. **Original date:** August 1969. **Origin:** J.Soper*, Harwell.

2 HOW TO USE THE PACKAGE

2.1 The entry points

There are eight different entry points (main entry is called FG01B) and the present version of the routine is an amalgamation of several old separate versions, hence the the non-uniform use of the name roots FG01, FG02 and FG03.

2.2 The argument lists and calling sequences

All the arguments for all entries must be REAL (DOUBLE PRECISION in the D version) variables and must be set by the user to integer, or half-odd-integer values. The nearest exact value will be assumed, and the argument values must be within ±0.05 of the intended values otherwise errors will occur.

The Wigner 3-j symbol

To compute the Wigner 3-j symbol $\begin{pmatrix} A & B & C \\ X & Y & Z \end{pmatrix}$

The single precision version

```
W=FG01A(A,B,C,X,Y,Z)
```

The double precision version

```
W=FG01AD(A,B,C,X,Y,Z)
```

where A, B, and C are the three angular momenta, and X, Y, and Z are the corresponding magnetic quantum numbers.

The Clebsch-Gordan or Wigner coefficient

To compute the Clebsch-Gordan or Wigner coefficient $(ABXY|ABCZ)$

The single precision version

```
W=FG01B(A,B,C,X,Y,Z)
```

The double precision version

```
W=FG01BD(A,B,C,X,Y,Z)
```

where A, B, and C are the three angular momenta, and X, Y, and Z are the corresponding magnetic quantum numbers.

The Wigner 3-j symbol (special case)

To compute the Wigner 3-j symbol (special case) $\begin{pmatrix} A & B & C \\ 0 & 0 & 0 \end{pmatrix}$

The single precision version

```
W=FG01C(A,B,C)
```

The double precision version

```
W=FG01CD(A,B,C)
```

where `A, B,` and `C` are the three angular momenta.

The Clebsch-Gordan or Wigner coefficient (special case)

To compute the Clebsch-Gordan or Wigner coefficient (special case) $(AB00|ABC0)$

The single precision version

```
W=FG01D(A,B,C)
```

The double precision version

```
W=FG01DD(A,B,C)
```

where `A, B,` and `C` are the three angular momenta.

The Wigner 6-j symbol

To compute the Wigner 6-j symbol $\begin{pmatrix} U & V & W \\ X & Y & Z \end{pmatrix}$

The single precision version

```
W=FG02A(U,V,W,X,Y,Z)
```

The double precision version

```
W=FG02AD(U,V,W,X,Y,Z)
```

The Racah coefficient

To compute the Racah coefficient $W(ABCD;EF)$

The single precision version

```
W=FG02B(A,B,C,D,E,F)
```

The double precision version

```
W=FG02BD(A,B,C,D,E,F)
```

The Jahn's U-function

To compute Jahn's U-function $U(ABCD;EF)$

The single precision version

```
W=FG02C(A,B,C,D,E,F)
```

The double precision version

```
W=FG02CD(A,B,C,D,E,F)
```

The Wigner 9-j symbol

To compute the Wigner 9-j symbol $\begin{pmatrix} A1 & A2 & A3 \\ A4 & A5 & A6 \\ A7 & A8 & A9 \end{pmatrix}$

The single precision version

```
W=FG03A(A1,A2,A3,A4,A5,A6,A7,A8,A9)
```

The double precision version

```
W=FG03AD(A1,A2,A3,A4,A5,A6,A7,A8,A9)
```

2.3 Restrictions

The sum of the three angular momenta appearing in any ‘‘triangular condition’’ must not exceed 100. This limit can be raised if necessary by recompiling with larger dimensions for the arrays `H` and `J` in labelled `COMMON,` see § 2.4.

The following ‘‘geometrical’’ conditions are tested by the routines and the correct value of zero returned in case of violation:

(a) all triangular conditions satisfied

(b) all angular momenta non-negative

(c) in `FG01A/AD` and `FG01B/BD,` the sums `A+X`, `B+Y` and `C+Z` must be all integral

(d) in `FG01A/AD`, `X+Y+Z = 0;` and in `FG01B/BD`, `X+Y = Z`

(e) in `FG01C/CD` and `FG01D/DD,` must be all integral with the sum `A+B+C` even.

Violation of these restrictions will be flagged by the error code `IERR` returned in common, see §2.4

2.4 The common areas.

The routine uses three named common areas which the user may reference.

The single precision version.

```
COMMON/FG01E/H(101)

COMMON/FG01F/J(101),LHJ
COMMON/FG01X/ IERR,IERCT
```

The double precision version.

```
COMMON/FG01ED/H(101)

COMMON/FG01FD/J(101),LHJ
COMMON/FG01XD/ IERR,IERCT
```

`H` is a `REAL` (`DOUBLE PRECISION` in the D version) array of length 101 which will be used by the subroutine for storing a table.

`J` is an `INTEGER` array of length 101 which is used in conjunction with array `H.`

`LHJ` is an `INTEGER` variable set to 101 the lengths of the arrays `H` and `J.`

`IERR` is an `INTEGER` variable which is set by the routine to indicate if errors have occurred. The possible values are

0 successful calculation

1 errors have occurred (one or more restrictions in §2.3 have been violated)

`IERCT` is an `INTEGER` variable which is used by the routine as an error count. It is zero initially and each time the routine detects an error it is updated by one. It can be used to check at the end of the job whether any errors have occurred.

3 GENERAL INFORMATION

Use of common: uses a common areas FG01E/ED, FG01F/FD, FG01X/XD see §2.4.

Workspace: none.

Other routines: none.

Input/Output: none.

Restrictions: see §2.3.