### QUANTUM MECHANICS

VOLUME II

### ALBERT MESSIAH

Saclay, France



1966

NORTH-HOLLAND PUBLISHING COMPANY AMSTERDAM

VECTOR ADDITION COEFFICIENTS, ROTATION MATRICES

(c. § 2

# 1. Angular Momentum. Notations and Conventions

The following notations and conventions concerning the angular momentum will be adopted throughout the Appendix.

Units:  $\hbar = 1$ .

Angular momentum components: J. angular momentum operator, having cartesian coordinates  $J_x$ ,  $J_y$  and  $J_z$ .

$$J_{\pm} = J_x \pm iJ_y. \tag{C.1}$$

Commutation relations

$$[J_x, J_y] = iJ_x$$
  $[J_y, J_z] = iJ_x$   $[J_z, J_x] = iJ_y$ 

$$[J_s, J_{\pm}] = \pm J_{\pm}$$
  $[J_+, J_-] = 2J_s$ .

Basis vectors of a standard representation {PJz}: \\ \taJM \>

$$f^2|\tau JM
angle = J(J+1) |\tau JM
angle$$

(C.4)

(C.5)

$$J_{\rm c}|\tau JM\rangle = M|\tau JM\rangle$$

$$J_{\pm}|\tau JM\rangle = VJ(J+1) - M(M \pm 1)|\tau JM \pm 1\rangle$$
 (C.6)

$$\langle \tau J M | \tau' J' M' \rangle = \delta_{\tau \tau'} \delta_{J J'} \delta_{M M'}$$
 (C.7)

(J integral or half-integral > 0, M = -J, -J+1, ..., +J).

to form a complete set; in the rest of the Appendix it will be omitted au denotes the quantum numbers that must be added to J and Mwhen not needed.

### I. CLEBSCH-GORDON (C.-G.) COEFFICIENTS AND "3y" SYMBOLS

# 2. Definition and Notations

fi. fs angular momenta of quantum systems I and 2 respectively. f, angular momentum of the total system of I and 2 taken together:

$$J = J_1 + J_2. \tag{C.8}$$

The tensor product of the  $(2j_1+1)$  vectors of system 1

$$|j_1m_1\rangle$$
 (j. fixed,  $m_1=-j_1,...,+j_1$ )

by the  $(2j_1+1)$  vectors of system 2

$$|2m_2\rangle$$
 (ja fixed,  $m_2 = -j_2, ..., +j_2$ )

VECTOR ADDITION COEFFICIENTS, ROTATION MATRICES c. § 2]

1055 gives the  $(2j_1+1)(2j_2+1)$  simultaneous eigenvectors of  $j_1^2$ ,  $j_2^2$ ,  $j_{12}$ ,  $j_{21}$ , the vectors

$$|j_1j_2m_1m_2\rangle = |j_1m_1\rangle|j_2m_2\rangle$$
 (C.9)

from which we can obtain, by a unitary transformation, the  $(2j_1+1)$  $(2j_2+1)$  simultaneous eigenvectors of  $\mu^2$ ,  $j_2^2$ ,  $\beta$ ,  $J_z$ , the vectors

$$|j_1j_2JM\rangle$$
 (C.10)  $|j_1j_2JM\rangle$  (C.10)  $(J=|j_1-j_2|,...,j_1+j_2;M=-J,...,+J).$ 

(C.2)

(C.3)

The Clebsch-Gordon 1), or vector addition, coefficients

### (jijzm1m2/JII)

are the coefficients of that unitary transformation:

$$|j_1j_2JM\rangle = \sum_{m_1,m_2} |j_1j_2m_1m_2\rangle\langle j_1j_2m_1m_2|JM\rangle.$$
 (C.11)

Phase convention 2)

We complete the definition of the vectors in (C.9) and (C.10) by fixing their relative phases as follows:

- (i) the |jimi>, the |jzmz> and the |jijzJM> obey relations (C.6);
- $\langle ijiji(j_1-J)|JJ\rangle$  real > 0.

1) There are many symbols employed in the literature to denote the Clobsch Gordon coefficients. We note in particular:

(hismims|hish M) [Condon and Shortly, Theory of Atomic Spectra (University Press, Cambridge, 4th ed., 1957)].

[Blatt and Weisskopf, Theoretical Nuclear Physics (Wiley, New York, 1952)]. Cys (JM; mime)

[E. P. Wigner, Group Theory and its Application to the Quantum Mechanics of Atomic Spectra (English translation; Academic Press, New York, 1958)]. 1) This convention is adopted by most authors, in particular by Wigner, Condon and Shortly, Blatt and Weisskopf, op. cit. note 1 of this page, and by Racah, Phys. Rev. 62 (1942) 437.

"3j" symbol (Wigner) 1):

$$\binom{j_1 \quad j_2 \quad J}{m_1 \quad m_2 - M} \equiv \frac{(-)^{j_1 - j_3 + M}}{\sqrt{2J + 1}} \langle j_1 j_2 m_1 m_2 | JM \rangle. \tag{C.12}$$

### 3. Principal Properties

Reality. They are all real:

$$\langle j_1 j_2 m_1 m_2 | JM \rangle^{\bullet} = \langle j_1 j_2 m_1 m_2 | JM \rangle$$
.

Selection rules

- (i)  $m_1 + m_2 = M$ ;
- (ii)  $|j_1-j_2| < J < j_1+j_2$  ("triangular inequalities").

If these two conditions are not met,  $\langle j_1 j_2 m_1 m_2 | JM \rangle = 0$ .

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \quad \text{is:}$$

- (i) invariant in a circular permutation of the three columns;
  - (ii) multiplied by (-)4.44 in a permutation of two columns;
- (iii) multiplied by (-)'1+4+4 when we simultaneously change the signs of m1, m2, and ms.

$$\langle i_1 j_2 m_1 m_2 | JM \rangle = (-)^{i_1+i_2-J} \langle j_2 j_1 m_2 m_1 | JM \rangle \tag{C.1}$$

$$= (-)^{i_1 - J + m_1} \sqrt{\frac{2J + 1}{2j_1 + 1}} \langle J_{j1} M - m_2 | j_1 m_1 \rangle$$
 (C.13b)

$$= (-)^{i_1-J-m_1} \sqrt{\frac{2J+1}{2j_2+1}} \langle j_1 J - m_1 M | j_2 m_2 \rangle \quad (C.13c)$$

$$= (-)^{i+h-J} \langle j_1 j_2 - m_1 - m_2 | J - M \rangle.$$
 (C.13d)

 $V(abc, \alpha\beta\gamma) \equiv (-)^{a \to -c} \binom{abc}{\alpha\beta\gamma} \equiv \frac{(-)^{a \to r}}{\sqrt{2c+1}} \langle ab\alpha\beta|c - \gamma \rangle.$ 1) Receh, op. cit., note 2, p. 1055, employs the symbol:

$$\sum_{m_1 = -j_1}^{+j_1} \sum_{m_2 = -j_3}^{+j_2} \langle j_1 j_2 m_1 m_2 | J'M' \rangle = \delta_{JJ'} \delta_{MM'} \qquad (C.14a)$$

$$||f_1 - f_2|| < J < f_1 + f_2; \quad -J < M < J)$$

$$\sum_{j_1-j_1|M-j_2} \sum_{\langle j_1j_2m_1m_2|JM\rangle \langle j_1j_2m_1'm_2'|JM\rangle = \delta_{m_1m_1} \delta_{m_2m_2}} (C.14b)$$

$$(-j_1 < m_1 < +j_1; -j_2 < m_2 < +j_2)$$

$$\sum_{m_1 = -f_1}^{+f_1} \sum_{m_2 = -f_3}^{+f_3} \left( j_1 j_2 j_3 \right) \left( j_1 j_2 j_3' \right) = \frac{1}{2j_3 + 1} \delta_{h, h} \delta_{m_3 m_1}$$
(C.15)

$$\sum_{\mathbf{n}_1 = -f_1} \sum_{\mathbf{n}_2 = -f_3} \left( m_1 m_2 m_3 \right) \left( \frac{f_1 f_2 f_3}{m_1 m_2 m_3} \right) = \frac{1}{2j_3 + 1} \delta_{j_1 j_1} \delta_{j_2 j_3} \delta_{m_3 m_3}$$
(C.15a)
$$\sum_{f_1 + f_1} \sum_{\mathbf{n}_2 = -f_3} \left( 2j_3 + 1 \right) \left( \frac{j_1 f_2 f_3}{m_1 m_2 m_3} \right) \left( \frac{j_1 f_2 f_3}{m_1 m_2 m_3} \right) = \delta_{m_1 m_1} \delta_{m_3 m_3}$$
(C.15b)

Composition relation for the spherical harmonics

$$V_{\pi^*}(\Omega) Y_{\pi^*}(\Omega)$$

$$= \sum_{L=L, -L_1 \mid M = -L}^{L_1+L_2} \left[ \frac{(2l_1+1)(2l_2+1)}{4\pi(2L+1)} \right]^{\frac{1}{2}} \langle l_1 l_2 0 0 | L 0 \rangle \langle l_1 l_2 m_1 m_2 | L M \rangle Y_L^M(\Omega)$$
 (C.17a)

$$\sum_{L=|L_1-L_1|}^{L_1+L_2} \sum_{M=-L}^{L} (-)^M \left[ \frac{(2l_1+1)(2l_2+1)(2L+1)}{4\pi} \right]^{\frac{1}{2}} \binom{l_1 l_2 L}{0 0 0} \binom{l_1 l_2 L}{m_1 m_2 M} Y_L^{-M}(\Omega). (C.17b)$$

## 4. Methods of Calculation

Recursion relations

Relating the C.-G. whose arguments differ at most by:

(i) 
$$\Delta J = 0$$
  $\Delta M = +1$ 

$$VJ(J+1) - M(M+1) \langle j_1 j_2 m_1 m_2 | JM \rangle$$

$$= Vj_1(j_1+1) - m_1(j_2 + 1) \langle j_1 j_2 m_1 + 1 m_2 | JM + 1 \rangle$$

$$+ Vj_2(j_2+1) - m_2(m_2+1) \langle j_1 j_2 m_1 m_2 + 1 | JM + 1 \rangle$$
(C

(ii) 
$$\Delta J = 0$$
  $\Delta M = -1$ 

$$\sqrt{J(J+1) - M(M-1)} \langle j_1 j_2 m_1 m_2 | JM \rangle 
= \sqrt{j_1(j_1+1) - m_1(m_1-1)} \langle j_1 j_2 m_1 - 1 m_2 | JM - 1 \rangle 
+ \sqrt{j_2(j_2+1) - m_2(m_2-1)} \langle j_1 j_2 m_1 m_2 - 1 | JM - 1 \rangle$$
(C.19)

VECTOR ADDITION CORPTICIENTS, ROTATION MATRICES

j.

(iii) 
$$\Delta J = \pm 1$$
  $\Delta M = 0$ 

(C.20) $Ao\langle j_1 j_2 m_1 m_2 | JM \rangle = A + \langle j_1 j_2 m_1 m_2 | J+1 M \rangle + A - \langle j_1 j_2 m_1 m_2 | J-1 M \rangle$ 

$$A_0 = m_1 - m_2 + M \frac{j_2(j_2 + 1) - j_1(j_1 + 1)}{J(J+1)} \qquad (M = m_1 + m_2)$$

$$A_+ = f(J+1)$$

$$A_- = f(J)$$

 $f(x) = \sqrt{x^2 - M^2} \left[ \frac{[(j_1 + j_2 + 1)^2 - x^2][x^3 - (j_1 - j_2)^2]}{4x^2(2x - 1)(2x + 1)} \right]^{\frac{1}{2}}$ 

$$\begin{pmatrix} abc \\ \alpha\beta\gamma \end{pmatrix} = (-)^{s-b-\gamma} \sqrt{A(abc)} \sqrt{(a+\alpha)!} (a-\alpha)! (b+\beta)! (b-\beta)! (c+\gamma)! (c-\gamma)!$$

$$\times \sum (-)^{s} [t! (c-b+t+\alpha)! (c-a+t-\beta)! (a+b-c-t)! (a-t-\alpha)! (b-t+\beta)!]^{-1}$$
C.21

with

or null (01 == 1). The number of terms in this sum is v+1, where v S extends over all integral values of t for which the factorials have a meaning, i.e. for which the arguments of the factorials are positive is the smallest of the nine numbers:

$$a \pm \alpha$$
  $b \pm \beta$   $c \pm \gamma$   
 $a+b-c$   $b+c-a$   $c+a-b$ .

# 5. Special Values and Tables

Special values

(i) J and M taking their maximum value:

$$\langle j_1 j_2 j_1 j_2 | j_1 + j_2 j_1 + j_2 \rangle = 1;$$

(ii) one of the j null:  $\langle j0m0|jm\rangle = 1$  or

$$\binom{j}{m-m}\binom{j}{0} = \frac{(-)^{j-m}}{\sqrt{2j+1}};$$

(iii) m1=m2=m3=0:

VECTOR ADDITION COEFFICIENTS, ROTATION MATHICES if  $h_1+h_2+h_3$  is odd, 0. § 5]

1059

$$\begin{pmatrix} l_1 \, l_2 \, l_3 \\ 0 \, 0 \, 0 \end{pmatrix} = 0; \tag{C.23a}$$

if  $2p = l_1 + l_2 + l_3$  is even

$$\begin{pmatrix} l_1 l_2 l_3 \\ 0 0 0 \end{pmatrix} = (-)^p \sqrt{A(l_1 l_2 l_3)} \frac{p!}{(p-l_1)! (p-l_2)! (p-l_3)!}$$
 (C.23b)

(b, b, b integers > 0 verifying the "triangular inequalities"),

Special cases of the Racah formula

The formulae below, or those obtained from them by use of the symmetry relations, give the C.-G. in the following special cases:

(i) 
$$m_1 = \pm j_1$$
 or  $m_2 = \pm j_2$  or  $M = \pm J$ :

$$\langle ijsm_1m_2|JJ \rangle = \langle isj_1 - m_2 - m_1|J - J \rangle$$

$$= (-)^{i_1-m_1} \sqrt{\frac{(2J+1)!(j_1+j_2-J)!}{(j_1+j_2+J+1)!(J+j_1-j_2)!(J+j_2-j_1)!}} \sqrt{\frac{(j_1+m_1)!(j_2+m_2)!}{(j_1-m_1)!(j_2-m_2)!}}$$
 (C.24)

(ii) one of the j is the sum of the two others:

 $(m_1 + m_2 = J);$ 

if J= j1 + j2

$$\langle j_1 j_2 m_1 m_2 | JM \rangle = \sqrt{\frac{(2j_1)! (2j_2)!}{(2J)!}} \sqrt{\frac{(J+M_1)! (J-M_1)! (J-M_1)!}{(j_1+m_1)! (j_1-m_1)! (j_2+m_2)!}} (C.25)$$

$$\langle J j_2 M - m_2 | j_1 m_1 \rangle = (-)^{i_1-m_1} \sqrt{\frac{2j_1+1}{2J+1}} \langle j_1 j_2 m_1 m_2 | JM \rangle. (C.26)$$

Tables of the "3j" symbols

The following tables give expressions for the symbol

$$\begin{pmatrix} j & s & (j+e) \\ m & \mu & (-m-\mu) \end{pmatrix}$$

as a function of j and m for

$$s=0, \frac{1}{2}, 1, \frac{2}{2}, 2$$
  
 $< e < s$   $0 < \mu < s$ .

With these, and with the aid of the symmetry relations, we can easily calculate any of the C.-G. for which one of the j is equal to 0,  $\frac{1}{2}$ , l, 🛊 or.2