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ORGANISATION EUROPEENNE POUR LA RECHERCHE NUCLEAIRE CERN EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH

Angular momentum in quantum mechanics

by

A.R. Edmonds

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Preface

The following lecture notes were originally issued in mimeographed form in Copenhagen in January 1954 (CERN-T/AREI).

I have tried throughout these notes to make clear where arbitrary choices of phase of matrix components have been made, and to follow these choices consistently. I would refer the reader to p.xiii of Condon and Shortley's Theory of Atomic Spectra (1935) for a comment of the importance of these questions of phase. The experiment made in the first edition of these notes, in which unorthodox, but perhaps more logical, choices of phase for the vector-coupling coefficients were made, has been abandoned in favour of orthodoxy. The conservatism of what would appear to be the majority of physicists working in this field has, in this regard at least, been respected. The reader will nevertheless find a few definitions which may be unfamiliar.

This edition contains an outline of the subject of Euler angles and matrix elements of finite rotations, with definitions adhering closely to the common practice of physicists. However this has involved deviating from the familiar formulae of Wigner (1931), since his results were based on a left-handed frame of reference. (cf. Rose (1955) for a different solution of this difficulty).

A number of errors in the first edition have been corrected. I hope that only a few new errors have crept into this one.

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1.1 Definition of angular momentum

In classical mechanics the angular momentum of a particle about a point 0 is

$$(1.1.1) \qquad \qquad \overrightarrow{L} = \overrightarrow{r} \times \overrightarrow{p}$$

where \vec{r} is the position vector and \vec{p} the linear momentum of the particle with respect to 0.

In quantum mechanics we take the well-known commutation relations for the components of position $\overset{\circ}{*}$ momentum and obtain the commutation relations for the components of \vec{L} : -

$$\begin{array}{l} (1.1.2) \\ [L_{_{\boldsymbol{X}}},\ L_{_{\boldsymbol{Y}}}] \ = \ i\hbar L_{_{\boldsymbol{Z}}}\ ;\ [L_{_{\boldsymbol{Y}}},\ L_{_{\boldsymbol{Z}}}] \ = \ i\hbar L_{_{\boldsymbol{X}}};\ [L_{_{\boldsymbol{Z}}},\ L_{_{\boldsymbol{X}}}] \ = \ i\hbar\ L_{_{\boldsymbol{Y}}} \end{array}$$

In the Schrödinger representation we have $p_x = -i\hbar \frac{\partial}{\partial x}$ etc., giving

(1.1.3)
$$L_{x} = -i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

$$L_{y} = -i\hbar \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$$

$$L_{z} = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$

and in spherical polar coordinates

(1.1.4)
$$L_{x} = i\hbar \left(\sin \phi \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right)$$

$$L_{y} = i\hbar \left(-\cos \phi \frac{\partial}{\partial \theta} + \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right)$$

$$L_{z} = -i\hbar \frac{\partial}{\partial \phi}$$

The square of the total angular momentum

(1.1.5)
$$L^2 = L_X^2 + L_Y^2 + L_Z^2$$

commutes with L, L and L, as may be shown by use of (1.1.2). It is given in terms of the spherical differential operators by

$$(1.1.6) \qquad \overset{\rightarrow}{L^2} = - \, h^2 \left[\frac{1}{\sin \theta} \, \frac{\partial}{\partial \theta} \left(\sin \theta \, \frac{\theta}{\partial \theta} \, \right) + \frac{1}{\sin^2 \theta} \, \frac{\partial^2}{\partial \phi^2} \, \right]$$

1.2 The Euler angles

Before we consider the angular momentum of a system of n (n > 1) particles we need to define the Euler Angles, which represent parametrically the displacement of a rigid body due to a rotation about a fixed point.

We suppose a <u>right-handed</u> frame of axes S fixed in the body. A <u>positive</u> rotation about an axis is a rotation undergone by a right-handed screw moving in the positive direction along that axis.

Any displacement about a fixed point may be obtained by performing three rotations successively: -

- (1) a rotation α ($0 \le \alpha < 2\pi$) about the z-axis, bringing the frame S into the position S'.
- (2) a rotation β ($0 \le \beta < \pi$) about the y-axis of the frame S', bringing the frame into the position S".
- (3) a rotation y ($0 \le y < 2\pi$) about the z-axis of the frame S", bringing the body into the final position. The set of three Euler angles $\alpha \beta \gamma$ may frequently be symbolised by ω . This convention for the definition of the Euler angles is the same as that normally used in the theories of molecular spectra (Herzberg 1939) and the collective model of the nucleus (Bohr 1952). It differs, for example, from the conventions of Whittaker(1917), Casimir (1931), and Wigner (1931).

We shall not always adhere to the limits on the values of α β and γ imposed above; we shall however assume that similar limits are imposed such that a 1:1 correspondence between the parameters α β γ and the actual rotations is preserved.

1.3. Angular momentum of a system of particles

This is given classically by

(1.3.1)
$$\vec{L} = \sum_{i=1}^{n} \vec{r}_{i} \times \vec{p}_{i}$$

where \vec{r}_i and \vec{p}_i are the position vector and momentum of the ith particle. Since the operators belonging to different particles commute,

we have in quantum mechanics the same commutation relations for the components of L as those in (1.1.2).

We may choose in some way a frame of axes which moves about its origin and follows the motion of the particles; for example, this frame might be defined by the position vectors of the first and second particles. The system is then described by the (3n-3) coordinates of the particles with respect to the moving frame and by the three Euler angles which give the displacement of the frame from some fixed frame with the same origin.

It may be shown (cf Kemble 1937) that the components of L in the Schrödinger representation are given in terms of the Euler angles by

$$L_{\mathbf{x}} = -i\hbar \left\{ -\cos \alpha \cot \beta \frac{\partial}{\partial \alpha} - \sin \alpha \frac{\partial}{\partial \beta} + \frac{\cos \alpha}{\sin \beta} \frac{\partial}{\partial \gamma} \right\}$$

$$(1.3.2)$$

$$L_{\mathbf{y}} = -i\hbar \left\{ -\sin \alpha \cot \beta \frac{\partial}{\partial \alpha} + \cos \alpha \frac{\partial}{\partial \beta} + \frac{\sin \alpha}{\sin \beta} \frac{\partial}{\partial \alpha} \right\}$$

$$L_z = -i\hbar \frac{\partial}{\partial \alpha}$$

There remains of course the angular momentum of the particles with respect to the moving frame, which is given by expressions containing the previously mentioned 3n - 3 coordinates.

The expression in the scheme (1.3.2) which corresponds to (1.1.6) is

(1.3.3)
$$\overset{\rightarrow}{L^2} = -\frac{\partial^2}{\partial \beta^2} - \cot \beta \frac{\partial}{\partial \beta} - \frac{1}{\sin^2 \beta} \left(\frac{\partial^2}{\partial \alpha^2} + \frac{\partial^2}{\partial \gamma^2} \right) + \frac{2\cos \beta}{\sin^2 \beta} \frac{\partial^2}{\partial \alpha \partial \gamma}$$

1.4 Representations of the angular momentum operators

As is well known, if we start from the commutation relations (1.1.2) as a definition of the angular momentum operators rather than from the classical definition (1.1.1), we obtain the <u>spin</u> représentations as well as those corresponding to the classical or orbital angular momentum. The components of this generalized angular momentum are designated by J_x , J_y and J_z ; we may where necessary use the notation

$$(1.4.1)$$
 $J_{+} = J_{x} + i J_{y}; J_{-} = J_{x} - i J_{y}.$

The representations may be derived by the method given by, for example, Dirac (1947) and Schiff (1949).

The angular momentum eigenvectors are defined as simultaneous eigenvectors of \vec{J}^2 and \vec{J}_z :

$$(1.4.2)$$

$$\overrightarrow{J}^{2} \psi(jm) = \overline{h}^{2} j (j + 1) \psi (jm) ; J_{z} \psi(jm) = \overline{h} m \psi(jm)$$

The quantity j takes the values $\frac{1}{2}$, 1, $\frac{3}{2}$, 2, ...; m takes the values -j, -j+1, j-1, j. j and m are referred to loosely as the eigenvalues of $\psi(jm)$.

In such a representation the matrices of J_+ , J_- , J_x , J_y are not diagonal. They are given by

(1.4.3)
$$J_{\pm} \psi(jm) = e^{i\delta} \hbar [(j + m) (j \pm m + 1)]^{\frac{1}{2}} \psi(j m \pm 1)$$

(1.4.4) The phase e^{iδ} is arbitrary; we shall follow Condon and Shortley* (1935) and take it to be + 1;

^{*} This work will be referred to henceforth as TAS.

the positive value of the square root is assumed throughout.

We have therefore for the non-zero matrix elements of J_x and J_y : -

$$(\gamma \mathbf{jm+1} | J_{\mathbf{x}} | \gamma \mathbf{jm}) = \frac{\hbar}{2} [(\mathbf{j-m}) (\mathbf{j+m+1})]^{\frac{1}{2}}$$

$$(\gamma \mathbf{jm-1} | J_{\mathbf{x}} | \gamma \mathbf{jm}) = \frac{\hbar}{2} [(\mathbf{j+m}) (\mathbf{j-m+1})]^{\frac{1}{2}}$$

$$(\gamma \mathbf{jm+1} | J_{\mathbf{y}} | \gamma \mathbf{jm}) = -\frac{i\hbar}{2} [(\mathbf{j-m}) (\mathbf{j+m+1})]^{\frac{1}{2}}$$

$$(\gamma \mathbf{jm-1} | J_{\mathbf{y}} | \gamma \mathbf{jm}) = \frac{i\hbar}{2} [(\mathbf{j+m}) (\mathbf{j-m+1})]^{\frac{1}{2}}$$

where y symbolises the eigenvalues of a set of operators Γ which forms a complete commuting set with J^2 and J_2 .

In the representation $j = \frac{1}{2}$ we have the Pauli spin matrices:

(1.4.6)

$$J_{x} \sim -\frac{1}{2} + \frac{1}{2} \qquad -\frac{1}{2} + \frac{1}{2} \qquad -\frac{1}{2} + \frac{1}{2}$$

$$J_{y} \sim -\frac{1}{2} \begin{bmatrix} 0 & \hbar/2 \\ +\frac{1}{2} & \hbar/2 & 0 \end{bmatrix} \quad J_{y} \sim -\frac{1}{2} \begin{bmatrix} 0 + i\hbar/2 \\ -i\hbar/2 & 0 \end{bmatrix} \quad J_{z} \sim -\frac{1}{2} \begin{bmatrix} -\hbar/2 & 0 \\ +\frac{1}{2} & 0 & \hbar/2 \end{bmatrix}$$

1.5. The angular momentum eigenvectors

In the integer representations $(j=\ell=0, 1, 2,)$ the eigenvectors $\psi(\ell m)$ are the solutions of the eigenvalue equations

$$-\left[\frac{1}{\sin \theta} \quad \frac{\partial}{\partial \theta} \left(\sin \theta \quad \frac{\partial}{\partial \theta}\right) + \frac{1}{\sin^2 \theta} \quad \frac{\partial^2}{\partial \theta^2}\right] \psi = e(e+1) \psi$$
$$-i \quad \frac{\partial}{\partial \phi} \quad \psi = m \psi$$

They are therefore, apart from normalisation, the spherical harmonics. We write the eigenfunction $\psi(\ell m)$ as

(1.5.1)
$$\psi(e^m) = Y_{e^m}(\theta \phi) = \Theta(e^m) \Phi(m)$$

where θ and Φ are functions of θ and ϕ respectively. The normalisation is such that

(1.5.2)
$$\int_0^{\pi} [\Theta(e^m)]^2 \sin\theta d\theta = 1 \cdot \int_0^{2\pi} \Phi^*(m) \Phi(m) d \phi = 1$$
We have

$$\Theta(e^{\mathbf{m}}) = (-1)^{\ell} \left[\frac{(2e+1)(e+m)!}{2(e-m)!} \right]^{\frac{1}{2}} \frac{1}{2^{\ell}e!} \frac{1}{\sin^{m}\theta} \frac{d^{\ell-m}}{(d\cos\theta)^{\ell-m}} \sin^{2\ell}\theta$$

i.e. in terms of the associated Legendre function (Ferrers' definition)

$$(1.5.4) \qquad \Theta(e^{\mathbf{m}}) = (-1)^{\mathbf{m}} \left[\frac{2e + 1}{2} \frac{(e^{-\mathbf{m}})!}{(e^{-\mathbf{m}})!} \right]^{\frac{1}{2}} P_{e}^{\mathbf{m}} (\cos\theta)$$

Also

$$(1.5.5)$$
 $\Phi(m) = [2\pi]^{-\frac{1}{2}} e^{im\phi}$

The definition of the angular momentum eigenfunction Y involves, in addition to a choice of normalisation, a choice of an arbitrary phase. We have followed above the convention of Condon and Shortley (1935); this implies the symmetry property

(1.5.6)
$$\Theta(em) = (-1)^m \Theta(e-m) \text{ or } Y_{em} = (-1)^m Y_{e-m}^*$$

It is sometimes useful to use another convention (cf. Biedenharn and Rose (1953), namely

$$(1.5.7) \qquad \hat{Y}_{em} = i \quad Y_{em}.$$

The symmetry property is then

(1.5.8)
$$\hat{Y}_{em} = (-1)^{\ell+m} \hat{Y}_{e-m}^*$$

The eigenfunctions corresponding to the representation (1.3.2), (1.3.3) (the spherical top eigenfunctions) are discussed in the chapter of the matrix elements of finite rotations.

2.1 The combination of angular momenta.

Suppose we have a system composed of two parts 1 and 2. It is easily shown that, as in classical mechanics, the angular momentum of the whole system is given in terms of the angular momenta of the parts by $\underline{J} = \underline{J}_1 + \underline{J}_2$, $\underline{J}_K = \underline{J}_{1K} + \underline{J}_{2K}$ where K = X, Y, Z.

 $\frac{J^2}{x} = J_x^2 + J_y^2 + J_z^2 \quad \text{commutes with} \quad J_x, \ J_y$ and J_z , also with J_1^2 and J_2^2 .

Now a state of the system may be given by a linear combination of simultaneous eigenvectors of the complete set of commuting operators Γ , J_1^2 , J_{1Z} , J_{2Z}^2 , J_{2Z} where Γ includes all other operators of the system needed to give a complete set. However, if there is interaction between the parts 1 and 2, the individual angular momenta will not be constants of the motion; but the total angular momentum may be. In this case it is advantageous to go over to the complete set

$$\Gamma, \underline{J_1^2}, \underline{J_2^2}, \underline{J}^2, J_2$$

Suppose we are given the eigenvectors of the set Γ , \underline{J}_1^2 , J_{1_Z} , \underline{J}_2^2 , J_{2_Z} each of which is labelled by the eigenvalues γ j_1 m_1 j_2 m_2 (we shall write always j, m as abbreviations for the eigenvalues $\hbar^2 j$ (j+1), \hbar m). It is of interest to find the unitary transformation which expresses the eigenvectors of Γ , \underline{J}_1^2 , \underline{J}_2^2 , \underline{J}_2^2 , \underline{J}_2^2 , in terms of these given eigenvectors.

(2.1.1)

$$\psi(y \ \mathbf{j_1} \ \mathbf{j_2} \ \mathbf{j_m}) = \Sigma_{\mathbf{m_1}\mathbf{m_2}} (\mathbf{j_1} \ \mathbf{j_2} \ \mathbf{j_m} | \mathbf{j_1} \ \mathbf{j_2} \ \mathbf{m_1}\mathbf{m_2}) \phi(y \ \mathbf{j_1} \ \mathbf{j_2} \ \mathbf{m_1} \ \mathbf{m_2})$$

It may be shown (see TAS p. 58) that any eigenvector ϕ (γ j₁ j₂ m₁ m₂) may be split into a sum of the type

(2.1.2)

$$\phi (\gamma \mathbf{j}_1 \mathbf{j}_2 \mathbf{m}_1 \mathbf{m}_2) = \sum_{\alpha \beta} \phi_1 (\alpha \mathbf{j}_1 \mathbf{m}_1) \phi_2 (\beta \mathbf{j}_2 \mathbf{m}_2)$$

where \underline{J}_1 operates only on ϕ_1 , \underline{J}_2 only on ϕ_2 . We may look at the problem in hand in a different way; namely from the point of view of the transformations of the eigenvectors under rotation of the coordinate system. Let us consider in the original representation all eigenvectors with a given y, j_1 and j_2 . These will span a $(2j_1+1)(2j_2+1)$ -dimensional space, and will form a basis of a product representation of the group SO(3) of proper rotations in 3 dimensions, that is they will be transformed among themselves by rotation of the coordinate system. This representation is however reducible, and may be shown to be the direct sum of a number of irreducible representations $D^{(j)}$, where $|j_1-j_2| \le j \le j_1 + j_2$. That is, the representation space splits up into a number of invariant irreducible subspaces, each corresponding to one of the above values of j and

of dimension 2 j + 1.

The problem is thus to find a transformation to a new representation basis so that each basis element (eigenvector) belongs to a definite irreducible representation of SO(3).

This process is known as the finding of the <u>Clebsch-Gordan series</u> (Weyl 1931 p. 123) and the transformation coefficients are called Clebsch-Gordan or vector-coupling coefficients.

There exist many notations for these coefficients; several of these notations are displayed and compared in table I(see p. 61).

2.2 The vector-coupling coefficients

The rules of angular momentum combination in quantum mechanics (cf TAS, Dirac (1935) etc.) tell us that the possible values of j and m arising from the combination of two systems with eigenvalues j_1 , m_1 , j_2 , m_2 are*

$$\mathbf{m} = \mathbf{m}_1 + \mathbf{m}_2$$

(2.2.1)

$$j = |j_1 - j_2|, |j_1 - j_2| + 1, ..., j_1 + j_2 - 1, \text{ or } j_1 + j_2.$$

It follows that the vector coupling coefficients will be zero unless these conditions are satisfied.

The unitary nature of the transformation under consideration is expressed by

^{*} The second equation of (2.2.1) will be referred to frequently as the triangular condition on j_1 , j_2 and j_3 .

(2.2.3)
$$\sum_{\mathbf{m}_{1}\mathbf{m}_{2}} (\mathbf{j}_{1}\mathbf{j}_{2}\mathbf{j}_{1}\mathbf{m}|\mathbf{j}_{1}\mathbf{j}_{2}\mathbf{m}_{1}\mathbf{m}_{2})(\mathbf{j}_{1}\mathbf{j}_{2}\mathbf{m}_{1}\mathbf{m}_{2}|\mathbf{j}_{1}\mathbf{j}_{2}\mathbf{j}'\mathbf{m}') = \delta_{\mathbf{j}\mathbf{j}}, \delta_{\mathbf{m}\mathbf{m}'} \delta(\mathbf{j}_{1}\mathbf{j}_{2}\mathbf{j})$$

$$\mathbf{m}_{1}\mathbf{m}_{2}$$

where $\delta(j_1j_2j) = 1$ if j takes one of the values in (2,2,1)

= 0 otherwise.

The values of the vector-coupling coefficients may be determined by use of the unitary condition and of two recursion relations. These recursion relations are derived from the identities $J_{+} = J_{1+} + J_{2+}$ and $J_{-} = J_{1-} + J_{2-}$ and from the expression (1.4.3). They are:

$$[(j-m)(j+m+1)]^{\frac{1}{2}}(m_1m_2|jm+1) =$$

$$= [(j_1+m_1)(j_1-m_1+1)]^{\frac{1}{2}} (m_1-lm_2|jm) + [(j_2+m_2)(j_2-m_2+1)]^{\frac{1}{2}} (m_1m_2-l|jm)$$
(2.2.5)

$$[(j+m)(j-m+1)]^{\frac{1}{2}}(m_1m_2|jm-1) =$$

=
$$[(j_1-m_1)(j_1+m_1+1)]^{\frac{1}{2}}(m_1+lm_2|jm)+[(j_2-m_2)(j_2+m_2+1)]^{\frac{1}{2}}(m_1m_2+l|jm)$$

The quantum numbers j_1 , j_2 in the V-C coefficients have been omitted for simplicity.

The above relations enable us to compute all the V-C coefficients; we must however make two arbitrary choices of phase in the calculation: -

- (2.2.6) All matrix elements of J_{1Z} in the scheme (γ j₁ j₂ jm) which are non-diagonal are real and non-negative
- (2.2.7) The identical states $\psi(y \ j_1 \ j_2 \ j_m)$ and $\phi(y \ j_1 \ j_2 \ m_1 \ m_2) \text{ have the same phase; i.e.}$ $\psi(y \ j_1 \ j_2 \ j_m) = \phi(y \ j_1 \ j_2 \ m_1 \ m_2)$

These choices are the same as made in TAS. We obtain the result: -

$$(2.2.8)$$
 $(j_1 j_2 m_1 m_2 | j_1 j_2 j_m) =$

$$= \delta(m_1+m_2, m) \left[\frac{(2j+1)(j_1+j_2-j)!(j_1-m_1)!(j_2-m_2)!(j+m)!(j-m)!}{(j_1+j_2+j+1)!(j_1-j_2+j)!(-j_1+j_2+j)!(j_1+m_1)!(j_2+m_2)} \right]^{\frac{1}{2}} \times$$

$$\times \sum_{s} (-1)^{s+j_1-m_1} \frac{(j_1+m_1+s)! (j_2+j-m_1-s)!}{s! (j_1-m_1-s)! (j-m-s)! (j_2-j+m_1+s)!}$$

Note that the coefficient is always real.

We may follow the method of Racah (1942) to get a more symmetric expression: -

$$(2.2.9) \quad (j_1 j_2 m_1 m_2 | j_1 j_2 jm) =$$

2.3. The symmetry properties of the vector-coupling coefficients.

The following properties may be demonstrated by reference to the recursion relations (2.2.4), (2.2.5) or by consideration of the effects of the appropriate replacements on the formula (2.2.9).

$$(2.3.1) \quad (j \ j \ m - m | j \ j \ 0 \ 0) = (-1)^{j-m} (2j+1)^{-\frac{1}{2}}$$

$$(2.3.2)$$
 $(j 0 m 0 | j 0 j m) = 1$

$$(2.3.3) (j_1 j_2 m_1 m_2 | j_1 j_2 j_m) = (-1)^{j_1 + j_2 - j} (j_2 j_1 m_2 m_1 | j_2 j_1 j_m)$$

$$(j_1j_2-m_1m_2|j_1j_2j-m) = (-1)^{j_1+j_2-j} (j_1j_2m_1m_2|j_1j_2jm)$$

$$(j_1 j_2 m_1 m_2 | j_1 j_2 j_3 m_3) = (-1)^{j_2 + m_2} \left(\frac{2j_3 + 1}{2j_1 + 1} \right)^{\frac{1}{2}} (j_2 j_3 - m_2 m_3 | j_2 j_3 j_1 m_1)$$

$$(j_1j_2m_1m_2|j_1j_2j_3m_3) = (-1)^{j_1-m_1}\left(\frac{2j_3+1}{2j_2+1}\right)^{\frac{1}{2}}(j_3j_1m_3-m_1|j_3j_1j_2m_2)$$

2.4. The Wigner 3-j symbol*

This quantity is defined in terms of the vector-coupling coefficient with the chosen phases by

$$\begin{pmatrix} \mathbf{j}_1 & \mathbf{j}_2 & \mathbf{j}_3 \\ \mathbf{m}_1 & \mathbf{m}_2 & \mathbf{m}_3 \end{pmatrix} = (-1)^{\mathbf{j}_1 - \mathbf{j}_2 - \mathbf{m}_3} (2\mathbf{j}_3 + \mathbf{j})^{-\frac{1}{2}} (\mathbf{j}_1 \mathbf{j}_2 \mathbf{m}_1 \mathbf{m}_2 | \mathbf{j}_1 \mathbf{j}_2 \mathbf{j}_3 - \mathbf{m}_3)$$

Its properties are easily deduced from those of the V-C coefficient; its main virtue is the high degree of symmetry exhibited. It is clearly zero unless

$$(2.4.2) m_1 + m_2 + m_3 = 0$$

$$j_a = |j_b - j_e|, |j_b - j_e| + 1, ..., j_b + j_e - 1, \text{ or } j_b + j_e.$$

where a, b, c are any permutation of 1, 2, 3.

^{*} Wigner (1951)

We get the result that an <u>even</u> permutation of the order of j_1 , j_2 and j_3 leaves the value of the symbol unaltered, while an <u>odd</u> permutation has the effect of multiplying the original value by $(-1)^{j_1+j_2+j_3}$.

-That is, we have the relations

$$\begin{pmatrix} \mathbf{j_1} & \mathbf{j_2} & \mathbf{j_3} \\ \mathbf{m_1} & \mathbf{m_2} & \mathbf{m_3} \end{pmatrix} = \begin{pmatrix} \mathbf{j_2} & \mathbf{j_3} & \mathbf{j_1} \\ \mathbf{m_2} & \mathbf{m_3} & \mathbf{m_1} \end{pmatrix} = \begin{pmatrix} \mathbf{j_3} & \mathbf{j_1} & \mathbf{j_2} \\ \mathbf{m_3} & \mathbf{m_1} & \mathbf{m_2} \end{pmatrix}$$

Following from the orthogonality of the V-C coefficients (2.2.2 and 2.2.3) the 3-j symbols satisfy the equations

(2.4.5)
$$\sum_{\mathbf{j}_{3}\mathbf{m}_{3}} (2\mathbf{j}_{3} + 1) \begin{pmatrix} \mathbf{j}_{1} & \mathbf{j}_{2} & \mathbf{j}_{3} \\ \mathbf{m}_{1} & \mathbf{m}_{2} & \mathbf{m}_{3} \end{pmatrix} \begin{pmatrix} \mathbf{j}_{1} & \mathbf{j}_{2} & \mathbf{j}_{3} \\ \mathbf{m}_{1}' & \mathbf{m}_{2}' & \mathbf{m}_{3} \end{pmatrix} = \delta_{\mathbf{m}_{1}\mathbf{m}_{1}'} \delta_{\mathbf{m}_{2}\mathbf{m}_{2}'}$$

$$(2.4.6)$$

$$\sum_{\mathbf{m_1 m_2 m_3}} \begin{pmatrix} \mathbf{j_1} & \mathbf{j_2} & \mathbf{j_3} \\ \mathbf{m_1 m_2 m_3} \end{pmatrix} \begin{pmatrix} \mathbf{j_1} & \mathbf{j_2} & \mathbf{j_3} \\ \mathbf{m_1 m_2 m_3} \end{pmatrix} = (2\mathbf{j_3} + 1)^{-1} \delta_{\mathbf{j_3 j_3}} \delta_{\mathbf{m_3 m_3}} \delta(\mathbf{j_1 j_2 j_3})$$

where $\delta(j_1j_2j_3) = 0$ unless j_1 , j_2 and j_3 satisfy the triangular condition, when it is unity.

The expression corresponding to (2.3.4) is

$$(2.4.7) \qquad \begin{pmatrix} \mathbf{j_1} & \mathbf{j_2} & \mathbf{j_3} \\ \mathbf{m_1} & \mathbf{m_2} & \mathbf{m_3} \end{pmatrix} = (-1)^{\mathbf{j_1} + \mathbf{j_2} + \mathbf{j_3}} \begin{pmatrix} \mathbf{j_1} & \mathbf{j_2} & \mathbf{j_3} \\ -\mathbf{m_1} & -\mathbf{m_2} & -\mathbf{m_3} \end{pmatrix}$$

2.5. Computation of vector-coupling coefficients

It is usually easier to obtain numerical values from tables of the type given in TAS, where j_2 takes a value $\frac{1}{2}$, 1, $\frac{3}{2}$ or 2. The general formula (2.2.9) is too clumsy for most purposes. The greater symmetry of the 3-j symbol is often helpful; formulae for this quantity, similar to those of TAS for the V-C coefficient, are given in Table II. (see p. 63) A table for the V-C coefficient with $j_2 = 3$ has been published by Falkoff et al. (1952). Numerical tables have been given by Alder (1952), and Simon (1954).

Two recursion relations may be useful; the first is due to Wigner (1951).

$$\times \left\{ \begin{pmatrix} \mathbf{j_1} & \mathbf{j_2} & \mathbf{j_3-1} \\ \mathbf{m_1} & \mathbf{m_2-1} & \mathbf{m_3+1} \end{pmatrix} \left[2(\mathbf{j_2-m_2+1})(\mathbf{j_2+m_2})(\mathbf{j_3-m_3-1})(\mathbf{j_3-m_3}) \right]^{\frac{1}{2}} \right\}$$

+
$$\begin{pmatrix} j_1 j_2 j_3 - 1 \\ m_1 m_2 m_3 \end{pmatrix} [8(j_3 + m_3)(j_3 - m_3)m_2^2]^{\frac{1}{2}}$$

$$-\begin{pmatrix} \mathbf{j_1} & \mathbf{j_2} & \mathbf{j_3-1} \\ \mathbf{m_1} & \mathbf{m_2+1} & \mathbf{m_3-1} \end{pmatrix} \begin{bmatrix} 2(\mathbf{j_2-m_2})(\mathbf{j_2+m_2+1})(\mathbf{j_3+m_3})(\mathbf{j_3+m_3-1}) \end{bmatrix}^{\frac{1}{2}} \end{bmatrix}$$

In both expressions $J = j_1 + j_2 + j_3$

The general formula simplifies in certain

cases : -

2.6. Complex conjugate of eigenvectors resulting from vector-coupling

We vector-couple two angular momentum eigenvectors of the type \hat{Y}_{cm} (cf (1.5.7)) to form an allowed eigenvector $\Psi(cm)$:

$$\Psi(e_{\mathbf{m}}) = \sum_{\mathbf{m}_{1}\mathbf{m}_{2}} (e_{1} e_{2} e_{\mathbf{m}} | e_{1} e_{2} \mathbf{m}_{1} \mathbf{m}_{2}) \hat{\mathbf{Y}}_{e_{1}\mathbf{m}_{1}} \hat{\mathbf{Y}}_{e_{2}\mathbf{m}_{2}}$$

It is easy to show from the properties of the V-C coefficients that $\Psi(\mathfrak{e}m)$ also has the symmetry (1.5.8), i.e.

(2.6.2)
$$\Psi(em) = (-1)^{\ell+m} \Psi^*(e-m)$$

On the other hand, a $\Psi(\epsilon m)$ built up from the $Y_{\epsilon m}$ does not have the symmetry (1,5.6)These facts will be of importance when we come to discuss <u>Hermitian tensor operators</u> and the <u>tensor</u> <u>product</u> of tensor operators (see § 5.4)

2.7. Vector-coupling coefficient with two large and one small j-values.

Consider the coefficient $(\kappa \ \mu \ e^{-\tau} \ m^{-\mu} | \kappa \ e^{-\tau} \ e^{-\tau})$ where e, m >> 1 and κ , μ , τ are small with respect to e. Write $\cos\theta = \frac{m}{2}$, so that $\cos\frac{\theta}{2} = \frac{e + m}{2e}^{\frac{1}{2}}$, $\sin\frac{\theta}{2} = \frac{e - m}{2e}^{\frac{1}{2}}$.

Substitution of these into (2.2.9) gives an approximate expression for the V-C coefficient as a matrix element of the finite rotation θ :

(2.7.1)

$$(\kappa \mu e - \tau m - \mu | \kappa e - \tau e m) \approx (-1)^{\kappa - \tau} \mathcal{D}_{\mu \tau}^{(\kappa)}(\theta)$$

(cf. (3.1.7))

 $\underline{N_{\bullet}E_{\bullet}}$ This relation is satisfied more accurately if we take $\cos\theta = \frac{m}{[e(e+1)]^{\frac{1}{2}}}$

3.1 The matrices of finite rotations.

We shall consider the transformations induced on angular momentum eigenvectors due to rotations about the origin of the frame of axes to which these eigenvectors are referred.

The coordinates of a <u>fixed</u> point P in the rotated frame of axes may be expressed in terms of the coordinates of that point in the original frame; in the same way c function of the coordinates of P in the rotated frame may be expressed in terms of functions of

the coordinates of P in the original frame. It is well known that angular momentum eigenvectors with a given j are transformed into eigenvectors with the same j under such transformations. We write in general

(3.1.1)
$$\Psi_{jm'}(\theta'\phi') = \sum_{\mathbf{m}} \Psi_{jm}(\theta\phi) \, \mathcal{D}_{mm'}^{(j)}(\alpha\beta\gamma)$$

where $\Psi_{jm}(\theta\phi)$ is a function of the coordinates $\theta\phi$ of a fixed point P in the original frame, and $\Psi_{jm'}(\theta'\phi')$ is a function of the coordinates θ' ϕ' of the P in the frame obtained by a rotation about the origin described by the Euler angles $\alpha\beta\gamma$ (cf.1.2.). The coefficient $\mathcal{D}_{mm'}^{(j)}(\alpha\beta\gamma)$ are the matrix elements in the j-representation of the finite rotation $\alpha\beta\gamma$.

The effect of a finite rotation may be considered to be equivalent to the effect of the iteration of an infinitesimal-rotation; if we represent by $D(\omega)$ the operator corresponding to a finite rotation of ω of the frame of axes about a given axis, and by J the angular momentum operator corresponding to this axis, it may be shown that

(3.1.2)
$$D(\omega) = \exp - \frac{i\omega}{\hbar} J$$
.

The negative sign follows from the fact that $D(\omega)$ represents a rotation of the frame of coordinates. (Note that our definition differs from those of Wigner (1931), Rose (1955)).

We obtain further for a general rotation . $\alpha\beta\gamma$,

(3.1.3)
$$D(\alpha\beta y) = \exp{-\frac{iy}{\hbar}J_z'' \cdot \exp{-\frac{i\beta}{\hbar}J_y' \cdot \exp{-\frac{i\alpha}{\hbar}J_z}}$$

where J_z , J_y' and J_z'' are defined in the frames S_z , S_z' and S_z'' (cf 1.2). It is convenient to write

 $D(\alpha\beta y)$ in terms of operators defined in the original frame S. Similarity transformations on the J_y' and J_z'' give

(3.1.4)
$$D(\alpha\beta\gamma) = \exp - \frac{i\alpha}{\hbar} J_z \cdot \exp - \frac{i\beta}{\hbar} J_y \cdot \exp - \frac{i\gamma}{\hbar} J_z$$
.

Now the matrices of J_Z are assumed diagonal; we obtain therefore for the matrix elements of $\bar{D}(\alpha\beta\gamma)$

(3.1.5)
$$2) (j) (\alpha \beta y) = e^{-im\alpha} \mathcal{D}_{mm}^{(j)} (\beta) e^{-im'y}$$

where
$$\mathcal{D}_{mm}^{(j)}(\beta) = \mathcal{D}_{mm}^{(j)}(0\beta0) = (jm|\exp - \frac{i\beta}{\hbar} J_y|jm')$$

remains to be computed.

Now it is a straightforward matter to find $\mathcal{D}^{\frac{1}{2}}(\beta)$ from the Pauli matrix for $J_y(1.4.6)$; we have

(3.1.6)
$$\mathcal{D}^{(\frac{1}{2})}(\beta) = -\frac{1}{2} \frac{1}{2} + \frac{1}{2} \frac{1}{2} + \frac{1}{2} + \frac{1}{2} \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} \frac{1}{2} + \frac{1}{2} + \frac{1}{2} - \frac{1}{2} + \frac{1}{2} \frac{1}{2} + \frac{1}{2} + \frac{1}{2} - \frac{1}{2} + \frac{1}{2} \frac{1}{2} + \frac{1}{$$

The angular momentum eigenvectors for general j may be expressed as symmetric functions of spinors (see Weyl(1931) etc.) We may obtain the general matrix elements by consideration of the transformations of such functions when the spinors undergo (3.1.6): -

$$(3.1.7) \ \mathcal{D}_{mm'}^{(j)}(\beta) = \\ = [(j+m)!(j-m)!(j+m')!(j-m')!]^{\frac{1}{2}} \sum_{\sigma} (-1) \frac{j-m'-\sigma[\cos\frac{\beta}{2}]^{2\sigma+m+m'}[\sin\frac{\beta}{2}]^{2j-m+m'-2\sigma}}{\sigma!(j-m-\sigma)!(\sigma+m+m')!(j+m'-\sigma)!}$$

(3.1.7) gives us, for example, in the case j = 1, the matrix $\mathcal{D}^{(1)}(\beta)$:

These matrix elements may be expressed in terms of Jacobi polynomials (cf. Szegő (1939), Erdélyi(1953))

$$\mathcal{D}_{mm'}^{(j)}(\beta) = \frac{(j+m)!(j-m)!}{(j+m')!(j+m')!} \frac{1}{2} \left[\cos \frac{\beta}{2}\right]^{m+m'} \left[-\sin \frac{\beta}{2}\right]^{m-m'} P_{j-m}^{(m-m', m+m')}(\cos \theta)$$

if $m+m' \ge 0$; a similar expression exists for m+m' < 0.

3.2. The symmetries of the matrix elements of finite rotations.

(3.2.1)
$$\mathcal{D}_{\mathbf{mm'}}^{(\mathbf{j})}(-\beta) = \mathcal{D}_{\mathbf{m'm}}^{(\mathbf{j})}(\beta)$$

This follows from the facts (i) $D(-\beta) = D^{-1}(\beta)$; (ii) the matrices are unitary; (iii) the $\mathcal{D}_{mm}^{(j)}(\beta)$ are real.

(3.2.2)
$$\mathcal{D}_{mm'}^{(j)}(\pi) = (-1)^{j+m} \delta_{m,-m'}; \mathcal{D}_{mm'}^{(j)}(-\pi) = (-1)^{j-m} \delta_{m,-m'}$$

- special cases of (3.1.7)*

^{*} Note that $D(\pi) \cdot D(\pi) \neq D(0)$ for the spin $(\frac{1}{2})$ odd integer representations.

$$(3.2.3) \quad \partial_{mm'}^{(j)}(\beta + \pi) = (-1)^{j+m} \, \partial_{-mm'}^{(j)}(\beta)$$

$$(3.2.4) \quad \mathcal{J}_{mm'}^{(j)}(\pi - \beta) = (-1)^{j+m} \quad \mathcal{J}_{m'-m}^{(j)}(\beta)$$

following from the application of (3.2.2) to the relations $D(\beta + \pi) = D(\beta) \cdot D(\pi)$ etc.

In a similar way we may obtain

(3.2.5)
$$\partial_{mm'}^{(j)}(\beta) = (-1)^{m-m'} \partial_{-m-m'}^{(j)}(\beta)$$

$$(3.2.6) \quad \partial_{\mathbf{mm'}}^{(j)}(\beta) = (-1)^{\mathbf{m-m'}} \partial_{\mathbf{m'm}}^{(j)}(\beta)$$

It is easy to extend the symmetry relations to include the complete matrix elements $\mathcal{D}_{mm}^{(j)}(\alpha\beta\gamma)$ by use of (3.1.5). For example, we have

$$\mathcal{D}_{mm'}^{(j)}(\alpha\beta\gamma) = (-1)^{j} \mathcal{D}_{m-m'}^{(j)}(\alpha - \pi, \pi - \beta, \gamma)$$

3.3. Connection of the $\mathcal{O}_{mm}^{(j)}$, with the associated Legendre functions.

The matrix elements are simplified when one or both of m, m' is zero. We may use the properties of the Jacobi polynomials (cf. Szegö loc. cit.) to show that

$$\mathcal{D}_{\text{mo}}^{(\ell)}(\beta) = \left[\frac{(\ell-m)!}{(\ell+m)!} \right]^{\frac{1}{2}} (-1)^{m} P_{\ell}^{m} (\cos\beta)$$

i.e.

$$\mathcal{D}_{\text{mo}}^{\,(e\,)}(\alpha\beta\gamma)\,=\left(\frac{4\,\pi}{2^{\ell}+1}\right)^{\frac{1}{2}}\,Y_{e\,\text{m}}^{*}(\beta,\,\alpha)$$

In particular,

(3.3.3)
$$\mathcal{D}_{00}^{(e)}(\alpha\beta\gamma) = P_{e}(\cos\beta)$$

3.4. The phases of the $\mathcal{D}_{min}^{(j)}(\alpha\beta\gamma)$

The phases depend on (i) the convention adopted in defining the Euler angles; (ii) the nature of the transformation which the \mathcal{D} 's are supposed to represent, i.e. whether one supposes a_rotation of the frame of axes or of the field; (iii) the choice of phases of the non-diagonal matrix elements of J_v .

Our matrix elements differ from those of, for example, Wigner (1931), since he adopted a left-handed frame of axes; however our matrices $\mathcal{D}^{(j)}(\beta)$ are numerically equal to the <u>transpose</u> of the corresponding matrices of Wigner.

3.5. Integrals and other expressions involving the $\mathcal{O}_{mm}^{(j)}(\alpha\beta\gamma)$

The orthogonality and normalisation of the $\mathcal{D}_{mn}^{(j)}$ is easily checked by reference to the properties of the Jacobi polynomials (Szegő 1939). We obtain

(3.5.1)

$$\frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{\pi} \mathcal{J}_0^{(j_1)*}(\alpha\beta\gamma) \mathcal{J}_{m_2m_2}^{(j_2)}(\alpha\beta\gamma) \sin\beta d\beta = d\alpha d\gamma$$

$$= \delta_{\mathbf{m_1m_2}} \delta_{\mathbf{m_1'm_2'}} \delta_{\mathbf{j_1j_2}} \cdot \frac{1}{2\mathbf{j_1}+1}$$

Products of the matrix elements may be reduced

by use of the vector-coupling coefficients; it is easily shown by consideration of the angular momentum eigenvectors implicitly involved that

$$(3.5.2) \quad \partial_{\mathbf{m_1}\mathbf{m'_1}}^{(\mathbf{j_1})}(\omega) \quad \partial_{\mathbf{m_2}\mathbf{m'_2}}^{(\mathbf{j_2})}(\omega) =$$

$$= \sum_{jmm'} (j_1 m_1 j_2 m_2 | j_1 j_2 j_m) \mathcal{D}_{mm'}^{(j)}(\omega) (j_1 j_2 j_m' | j_1 m_1 j_2 m_2')$$

where (ω) symbolises ($\alpha\beta\gamma$). This may be usefully expressed in terms of 3-j symbols (2.4.1): -

(3.5.3)
$$\partial_{\mathbf{m_1}\mathbf{m'_1}}^{(\mathbf{j_1})}(\omega) \partial_{\mathbf{m_2}\mathbf{m'_2}}^{(\mathbf{j_2})}(\omega)$$

$$= \sum_{\mathbf{j},\mathbf{m}'} (2\mathbf{j}+1) \begin{pmatrix} \mathbf{j}_1 \mathbf{j}_2 \mathbf{j} \\ \mathbf{m}_1 \mathbf{m}_2 \mathbf{m} \end{pmatrix} \mathcal{D}_{\mathbf{m}\mathbf{m}'}^{(\mathbf{j})*}(\omega) \begin{pmatrix} \mathbf{j}_1 \mathbf{j}_2 \mathbf{j} \\ \mathbf{m}_1' \mathbf{m}_2' \mathbf{m}' \end{pmatrix}$$

Then (3.5.1) and (3.5.3) give the value of the integral over a product of 3 \mathcal{D} 's:

$$\frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} \int_0^{\pi} \partial_{\mathbf{m_1m_1}}^{(\mathbf{j_1})} (\alpha\beta\gamma) \partial_{\mathbf{m_2m_2}}^{(\mathbf{j_2})} (\alpha\beta\gamma) \partial_{\mathbf{m_3m_3}}^{(\mathbf{j_3})} (\alpha\beta\gamma) \sin\beta d\beta d\alpha d\gamma$$

$$= \begin{pmatrix} j_1 j_2 j_3 \\ m_1 m_2 m_3 \end{pmatrix} \begin{pmatrix} j_1 j_2 j_3 \\ m_1 m_2 m_3 \end{pmatrix}$$

This integral may be specialised by means of (3.3.2) and (3.3.3), giving the useful results:

$$(3.5.5) \int_{0}^{2\pi} \int_{0}^{\pi} Y_{e_{1}m_{1}}(\theta\phi) Y_{e_{2}m_{2}}(\theta\phi) Y_{e_{3}m_{3}}(\theta\phi) \sin\theta d\theta d\phi$$

$$= \left[\frac{(2e_1+1)(2e_2+1)(2e_3+1)}{4\pi}\right]^{\frac{1}{2}} \begin{pmatrix} e_1e_2e_3\\ 0 & 0 \end{pmatrix} \begin{pmatrix} e_1e_2e_3\\ m_1m_2m_3 \end{pmatrix}$$

$$(3.5.6)$$

$$\frac{1}{2} \int_{0}^{\pi} P_{\ell_{1}}(\cos\theta) P_{\ell_{2}}(\cos\theta) P_{\ell_{3}}(\cos\theta) \sin\theta d\theta = \begin{pmatrix} \ell_{1} & \ell_{2} & \ell_{3} \\ 0 & 0 & 0 \end{pmatrix}^{2}$$

The 3-j symbols with $m_1=m_2=m_3=0$ may be evaluated by the formula in table II.

A similar modification of (3.5.2) gives an expression for the product of two spherical harmonics of the same angles: -

$$(3.5.7) \quad Y_{e_1 \mathbf{m}_1}(\theta \phi) \quad Y_{e_2 \mathbf{m}_2}(\theta \phi)$$

$$= \sum_{\ell,m} \left[\frac{(2\ell_1+1)(2\ell_2+1)(2\ell+1)}{4\pi} \right]^{\frac{1}{2}} \begin{pmatrix} \ell_1\ell_2\ell \\ m_1m_2m \end{pmatrix} Y_{\ell,m}^*(\theta\phi) \begin{pmatrix} \ell_1\ell_2\ell \\ 0 & 0 & 0 \end{pmatrix}$$

If the rotation ω is the result of performing successively the rotations ω_1 and ω_2 (in that order), we have

$$\sum_{\mathbf{m'}} \mathcal{Q}_{\mathbf{mm'}}^{(\mathbf{j})} (\omega_2) \mathcal{Q}_{\mathbf{m'm''}}^{(\mathbf{j})} (\omega_1) = \mathcal{Q}_{\mathbf{mm''}}^{(\mathbf{j})} (\omega)$$

We set $j = \ell = integer$ and m = m'' = 0 and obtain the spherical harmonic addition theorem : -

(3.5.8)
$$\frac{4\pi}{2\epsilon+1}\sum_{\mathbf{m}} \mathbf{Y}_{\epsilon \mathbf{m}}^{*} (\theta \phi) \mathbf{Y}_{\epsilon \mathbf{m}} (\theta' \phi') = \mathbf{P}_{\epsilon}(\cos \beta)$$

where $\cos\beta = \cos\theta \cos\theta' + \sin\theta \sin\theta' \cos(\phi - \phi')$

3.6. Recursion relation for the $\mathcal{O}_{mm}^{(j)}(\beta)$.

The relation is obtained from an expression similar to (3,5.2); the 3-j symbols arising are evaluated by use of table II. (see p. 63).

$$(3.6.1) \qquad \qquad \partial_{mn'}^{(j)}(\beta) =$$

$$= \left(\frac{\mathbf{j}-\mathbf{m}}{\mathbf{j}-\mathbf{m'}}\right)^{\frac{1}{2}} \mathcal{O}_{\mathbf{m}+\frac{1}{2}\mathbf{m'}+\frac{1}{2}}^{\left(\mathbf{j}-\frac{1}{2}\right)}(\beta) \cdot \cos\beta/2 - \left(\frac{\mathbf{j}+\mathbf{m}}{\mathbf{j}-\mathbf{m'}}\right)^{\frac{1}{2}} \mathcal{O}_{\mathbf{m}-\frac{1}{2}\mathbf{m'}+\frac{1}{2}}^{\left(\mathbf{j}-\frac{1}{2}\right)}(\beta) \cdot \sin\beta/2$$

The relation is of course useless when m' = j; in this case we evaluate $\partial_{-m-j}^{(j)}(\beta)$, using (3.2.5).

3.7. Computation* of the $\partial_{mm}^{(j)}(\beta)$

A similarity transformation may be employed to express a $D(0 \beta 0)$ in terms of a rotation about the z-axis, i.e. a $D(\beta 0 0)$, which is diagonal in our representations: -

(3.7.1)

$$D(0 \ \beta \ 0) = D(-\frac{\pi}{2} \ 0 \ 0) \ D(0 - \frac{\pi}{2} \ 0) \ D(\beta \ 0 \ 0) \ D(0 \frac{\pi}{2} \ 0) \ D(\frac{\pi}{2} \ 0 \ 0).$$

Thus the problem of computing any matrix $\mathcal{D}^{(j)}(\beta)$ is reduced to the problem of computing the one matrix $\mathcal{D}^{(j)}(\frac{\pi}{2})$, which we symbolise by $\Delta^{(j)}$. These matrices $\Delta^{(j)}$ are easily built up by use of (3.6.1), and a number of them are exhibited in table IV (see p. 69).

We now have from (3.7.1) that

$$\mathcal{D}_{mm'}^{(j)}(\beta) = \sum_{m''} e^{im\pi/2} \Delta_{m''m}^{(j)} e^{-im''\beta} \Delta_{m''m'}^{(j)} e^{-im'\pi/2}$$

$$= \Delta_{om}^{(j)} \Delta_{om'}^{(j)} \kappa(o) + 2 \sum_{m''>o} \Delta_{m''m}^{(j)} \Delta_{m''m'}^{(j)} \kappa(m''\beta)$$

^{*} based on method of Wigner (1951)

3.7 where
$$\kappa(x) = \cos x$$
 if $m-m' \equiv 0 \pmod{4}$

$$= \sin x \qquad \equiv 1 \pmod{4}$$

$$= -\cos x \qquad \equiv 2 \pmod{4}$$

$$= -\sin x \qquad \equiv 3 \pmod{4}$$
.

3.8. The symmetric top in quantum mechanics.

Consider a rigid body with an axis of symmetry, which is free to rotate about a point on this axis, which may be supposed to coincide with the z-axis of the frame of axes fixed in the body. The moment of inertia about the z-axis is represented by I_3 , and that about any axis perpendicular to it by I_4 .

The kinetic energy T is given in terms of the Euler angles describing the orientation of the body by $\overset{\clubsuit}{:}$ -

$$T = \frac{1}{2} \{ I_1(\dot{\beta}^2 + \dot{\alpha}^2 \sin^2 \beta) + I_3(\dot{\gamma} + \dot{\alpha} \cos \beta)^2 \}$$

The Schrödinger equation obtained by replacing the generalised momenta $p_{\alpha} = \frac{\partial T}{\partial \dot{\alpha}}$ etc. in the Hamiltonian by $-i\hbar \frac{\partial}{\partial \alpha}$ etc. is: -

$$(3.8.2)$$

$$-\frac{h^{2}}{2\overline{I}_{1}} \left\{ \frac{\partial^{2}}{\partial \beta^{2}} + \cot \beta \frac{\partial}{\partial \beta} + \left(\overline{I}_{3}^{1} + \cot^{2}\beta \right) \frac{\partial^{2}}{\partial y^{2}} + \frac{1}{\sin^{2}\beta} \cdot \frac{\partial^{2}}{\partial \alpha^{2}} - \frac{2\cos \beta}{\sin^{2}\beta} \cdot \frac{\partial^{2}}{\partial \alpha \partial y} \right\} \Psi(\alpha\beta\gamma) = \mathbb{E} \Psi(\alpha\beta\gamma)$$

If we set $I_1 = I_3$, this equation reduces to the form

^{*} cf. Klein and Sommerfeld (1914), Reiche and Rademacher (1926), Casimir (1931).

$$\begin{array}{ccc}
3.8 & \stackrel{\rightarrow}{L^2} \Psi (\alpha \beta y) = \lambda \Psi (\alpha \beta y)
\end{array}$$

where L^2 is given by (1.3.3).

It may be shown that the eigenfunctions of this equation are in fact the $\mathfrak{D}_{mm'}^{(\mathbf{j})}(\alpha\beta\gamma)$. We may effect a separation of (3.8.2) even when $\mathbf{I}_1\neq\mathbf{I}_3$; we write $\Psi(\alpha\beta\gamma)=\mathrm{B}(\beta)\exp\mathrm{i}(\mathrm{m}\alpha+\kappa\gamma)$. The equation in β still gives us $\mathfrak{D}_{m\kappa}^{(e)}(\beta)$; however the energies corresponding to the triads e, m, κ are now different from the case of $\mathbf{I}_1=\mathbf{I}_3$.

4.1. The compounding of vector-coupling coefficients.

We find frequently in quantum mechanical problems that we have to deal with the addition of a number of angular momenta; this involves the summation of products of vector-coupling coefficients, the summation being over the magnetic quantum numbers m. Now the vector-coupling coefficients are not invariant under rotations of the physical system (we shall see shortly exactly how they transform); but the quantities which we wish to compute -- such as energies and transition probabilities -- are usually scalars. It follows that the vector-coupling coefficients are associated in such a way that they form scalars, and it will be our purpose to describe how this happens. The most important result of this study is that in practice the tedious computation of masses of vector-coupling coefficients is replaced by the evaluation of relatively few invariant quantities.

It is easy to show from the definition of the 3-j symbol (2.4.1) that the expression

$$\sum_{\psi(j_1m_1)\ \psi(j_2m_2)\ \psi(j_3\ m_3)} \begin{pmatrix} j_1j_2j_3\\ m_1m_2m_3 \end{pmatrix}$$

$$m_1m_2m_3$$

is invariant under all rotations of the frame of coordinates.

1960

It follows that the set of $(2j_1+1)(2j_2+1)(2j_3+1)$ 3-j symbols with given values of j_1, j_2 and j_3 and all possible values of m_1, m_2 and m_3 consistent with them may be regarded as a <u>tensor</u> which transforms under rotations <u>contragrediently</u> to the set of products $\psi(j_1m_1)\psi(j_2m_2)\psi(j_3m_3)$. In analogy with the conventional tensor theory, we may define a <u>metric tensor</u> and a corresponding <u>contraction process</u>. The metric tensor is obtained by considering the coupling of two equal angular momenta to give resultant zero: -

$$\sum_{\mathbf{m}} \psi_{1}(\mathbf{jm}) \psi_{2}(\mathbf{j-m}) (-1)^{\mathbf{j-m}} = (2\mathbf{j+1})^{\frac{1}{2}} \Psi(00)$$

(cf. (2.3.1)). Hence if we define

(4.1.1)
$$\binom{j}{m m'} = (-1)^{j+m} \delta_{m_2-m'}$$

we have

$$\sum_{mm'} \psi_1(jm) \psi_2(jm') \begin{pmatrix} j \\ m'm' \end{pmatrix} = invariant.$$

This quantity $\binom{j}{m m'}$ thus behaves as a metric tensor (but only in the (2j+1)-dimensional space of the eigenvectors $\psi(jm)$, $-j \leq m \leq j$). We may use the contragredient tensor (which is identical with $\binom{j}{mm'}$) to carry out contractions of the indices -- the magnetic quantum numbers -- in products of 3-j symbols. We must remember that the contractions may only occur between 3-j symbols which contain the same j values. The simplest process of this kind is the contraction of a 3-j symbol with another identical symbol: -

$$\sum_{\mathbf{m}} \begin{pmatrix} \mathbf{j}_{1} \, \mathbf{j}_{2} \, \mathbf{j}_{3} \\ \mathbf{m}_{1} \, \mathbf{m}_{2} \, \mathbf{m}_{3} \end{pmatrix} \begin{pmatrix} \mathbf{j}_{1} \, \mathbf{j}_{2} \, \mathbf{j}_{3} \\ \mathbf{m}_{1} \, \mathbf{m}_{2} \, \mathbf{m}_{3} \end{pmatrix} = 1$$

Now we ask, what is the next combination of products of 3-j symbols in which contractions may be carried out to give a resultant scalar? We represent a 3-j symbol by

a point which is the vertex of 3 lines, each of which represents a j-value. Each of these j-values must be contracted with a similar j from another 3-j symbol; i.e. each line must terminate at another vertex. It is clear that, apart from the trivial case mentioned above, the simplest diagram satisfying the conditions is a tetrahedron. That is, we may make a sum of products of 4 3-j symbols, which contain among them 6 different j-values, and the summation may be carried out over the possible m-values in such a way that a scalar quantity is the result.

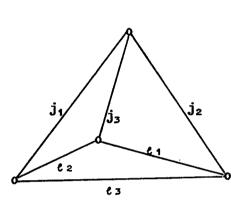


Fig.1

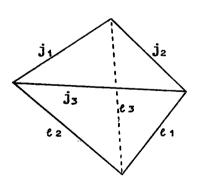


Fig.2

Let us then draw a tetrahedron, and associate with each vertex a 3-j symbol, and with each edge a j-value (Fig. 1). The 3 j-values of each 3-j symbol are the j-values of the edges meeting at the vertex in question.

We may construct an alternative diagram, in which the j-values associated with each 3-j symbol occupy the edges of a face (Fig.2). Since the 3-j symbols are only non-zero when the corresponding j-values form triangles, fig. 2 has a metrical significance; the quantity we are constructing is only non-zero when the 6 j-values chosen correspond to the lengthsof the sides of a tetrahedron. This type of diagram is, however, of no use when we come to consider the 9-j symbol.

The contraction process is

carried out by a definite convention; a different convention would give a similar quantity which might differ by a sign from the one which we construct. The result of this contraction process, which is a scalar quantity, is called a 6-j symbol*, and is defined by

$$= \sum_{\substack{\textbf{c}_{1}\textbf{c}_{2}\textbf{c}_{3}\\\textbf{c}_{1}\textbf{c}_{2}\textbf{c}_{3}\\\textbf{indices}}} \begin{pmatrix} \mathbf{j}_{1}\mathbf{j}_{2}\mathbf{j}_{3}\\ \kappa_{1}\lambda_{2}\mu_{3} \end{pmatrix} \begin{pmatrix} \mathbf{c}_{1}\mathbf{j}_{2}\mathbf{c}_{3}\\ \mu_{1}\kappa_{2}\lambda_{3} \end{pmatrix} \begin{pmatrix} \mathbf{c}_{1}\mathbf{c}_{2}\mathbf{j}_{3}\\ \lambda_{1}\mu_{2}\kappa_{3} \end{pmatrix}$$

$$\times \begin{pmatrix} \mathbf{j_1} \\ \mathbf{c_1} \kappa_1 \end{pmatrix} \begin{pmatrix} \mathbf{j_2} \\ \mathbf{c_2} \kappa_2 \end{pmatrix} \begin{pmatrix} \mathbf{j_3} \\ \mathbf{c_3} \kappa_3 \end{pmatrix} \begin{pmatrix} \mathbf{e_1} \\ \lambda_1 \mu_1 \end{pmatrix} \begin{pmatrix} \mathbf{e_2} \\ \lambda_2 \mu_2 \end{pmatrix} \begin{pmatrix} \mathbf{e_3} \\ \lambda_3 \mu_3 \end{pmatrix}$$

$$=\sum_{\boldsymbol{\ell}\lambda} \begin{pmatrix} \mathbf{j}_1 \mathbf{j}_2 \mathbf{j}_3 \\ \boldsymbol{\iota}_1 \boldsymbol{\iota}_2 \boldsymbol{\iota}_3 \end{pmatrix} \begin{pmatrix} \mathbf{j}_1 \boldsymbol{\ell}_2 \boldsymbol{\ell}_3 \\ -\mathbf{k}_1 \lambda_2 \lambda_3 \end{pmatrix} \begin{pmatrix} \boldsymbol{\ell}_1 \mathbf{j}_2 \boldsymbol{\ell}_3 \\ -\lambda_1 - \boldsymbol{\ell}_2 \lambda_3 \end{pmatrix} \begin{pmatrix} \boldsymbol{\ell}_1 & \boldsymbol{\ell}_2 & \mathbf{j}_3 \\ \lambda_1 - \lambda_2 - \boldsymbol{\iota}_3 \end{pmatrix}$$

$$\times (-1)^{j_1+j_2+j_3+\ell_1+\ell_2+\ell_3+\lambda_1+\lambda_2+\lambda_3}$$

Note the convention by which the contraction is carried out; for half odd integer j the metric tensor is skew-symmetric and the indices may not be permuted without a change of sign.

Use of (2.4.2) and the fact that one of the indices of summation is free makes it possible to replace the summation over 6 indices in (4.1.2) by a summation over 2. The 6-j symbol is then given in terms of the V-C coefficients by means of (2.4.1)

(4.1.3)
$$\begin{cases} j_1 j_2 j_3 \\ e_1 e_2 e_3 \end{cases} =$$

$$= \frac{(-1)^{\frac{1}{3}\frac{1}{1}+\frac{1}{3}2+\ell_{1}+\ell_{2}}}{[(2j_{3}+1)(2\ell_{3}+1)]^{\frac{1}{2}}} \sum_{m_{1}m_{2}} (j_{1}m_{1}j_{2}m_{2}|j_{1}j_{2}|j_{3}m_{1}+m_{2})(j_{3}m_{1}+m_{2}\ell_{1}m-m_{1}-m_{2}|\ell_{1}\ell_{2}m) \times \\ \times (j_{2}m_{2}\ell_{1}m-m_{1}-m_{2}|j_{2}\ell_{1}\ell_{3}m-m_{1})(j_{1}m_{1}\ell_{3}m-m_{1}|j_{1}\ell_{3}\ell_{2}m)$$

^{*} Wigner (1951); with a different phase it is known as a Racah, or W-coefficient (cf.§4.5) (Racah 1942)

where $-\ell_2 \leq m \leq \ell_2$.

4.2 Symmetries of the 6-j symbol.

It follows from the symmetry properties of the 3-j symbols that

I.e. the 6-j symbol is left invariant by any interchange of the columns. We have also that the 6 j symbol is invariant against interchange of the upper and lower arguments in each of any two columns.

E.g.

(4.2.2)
$$\begin{cases} j_1 j_2 j_3 \\ \ell_1 \ell_2 \ell_3 \end{cases} = \begin{cases} j_1 \ell_2 \ell_3 \\ \ell_1 j_2 j_3 \end{cases}$$

In fact there are 24 operations generated by interchanges of type (4.2.1) or (4.2.2) which leave a 6-j symbol invariant, and these form a group isomorphic with the symmetry group of a regular tetrahedron. Any of these operations corresponds to a rotation and/or reflection of the tetrahedron whose sides correspond to the 6 values of j.

4.3 Transformations between different coupling schemes of three angular momenta.

The states of a system built up from two parts

whose states are labelled by quantum numbers y_1 j_1 m_1 and y_2 j_2 m_2 are completely specified by y_1 y_2 j_1 j_2 j m_2 , where j and m are obtained by the usual vector addition process. However if we put together three parts, several states may occur with the same eigenvalues of the operators associated with the total angular momentum of the system, and a complete characterisation of the states requires the specification of the type of coupling carried out, and of the eigenvalues of the intermediate states.

We may for instance couple first j_1 and j_2 giving a resultant j' and couple j_3 to this. The eigenvectors of j, m are then

(4.3.1)

$$\Psi(j_1 j_2(j') j_3 jm) = \sum_{m_3 m'} \Psi(j_1 j_2 j'm') \phi(j_3 m_3) (j' j_3 m'm_3 | j' j_3 jm)$$

$$= \sum_{m_1 m_2 m_3 m'} \phi(j_1 m_1) \phi(j_2 m_2) \phi(j_3 m_3) (j_1 j_2 m_1 m_2 | j_1 j_2 j' m') (j' j_3 m' m_3 | j' j_3 j m)$$

On the other hand we may add j_1 to the resultant j'' of coupling j_2 and j_3 , giving

(4.3.2)

$$\Psi(\mathbf{j}_{1},\mathbf{j}_{2},\mathbf{j}_{3},(\mathbf{j}'')) \mathbf{j}\mathbf{m}) = \sum_{\mathbf{m}_{1},\mathbf{m}_{2},\mathbf{m}_{3},\mathbf{m}''} \phi(\mathbf{j}_{1},\mathbf{m}_{1})\phi(\mathbf{j}_{2},\mathbf{m}_{2})\phi(\mathbf{j}_{3},\mathbf{m}_{3})$$

$$\cdot (j_2 j_3 m_2 m_3 | j_2 j_3 j'' m'') (j_1 j'' m_1 m'' | j_1 j'' jm)$$

These two schemes of eigenvectors are connected by a unitary transformation which is independent of the z-component m of the total angular momentum j:

$$(4.3.3) \quad (j_1 j_2 j_1') j_3 j_1 j_2 j_3 (j'') j) =$$

$$= \sum_{\substack{ (j' j_3 j_m | j' j_3 m' m_3) (j_1 j_2 j' m' | j_1 j_2 m_1 m_2) \\ m_1 m_2 m_3 m' m''}}$$

$$(j_2 j_3 m_2 m_3 | j_2 j_3 j'' m'') (j_1 j'' m_1 m'' | j_1 j'' jm)$$

Use of (2.4.1) and (4.1.2) gives us the transformation coefficients in terms of 6-j symbols.

$$(4.3.4)$$

$$(j_1j_2(j')j_3j|j_4j_2j_3(j'')|j) = (-1)^{j_1+j_2+j+j_3}[(2j'+1)(2j''+1)]^{\frac{1}{2}} \begin{bmatrix} j_1j_2j'\\j_3j|j'' \end{bmatrix}$$

If the order of the angular momenta is changed instead we get in the same way

$$(4.3.5)$$

$$(j_1j_2(j')j_3j|j_1j_3(j'')j_2j) = (-1)^{j_2+j_3+j'+j''}[(2j'+1)(2j''+1)]^{\frac{1}{2}} \begin{bmatrix} j_3j & j' \\ j_2j_1j'' \end{bmatrix}$$

Similar formulae are given by Racah (1943) p. 368.

4.4 Algebraic relations between 6-j symbols and between 6-j and 3-j symbols.

We may make use of the defining equation (4.1.2) for the 6-j symbol and the symmetry and orthogonality relations of the 3-j symbols (2.4.3), (2.4.4), (2.4.5) and (2.4.6) to obtain relations between 6-j symbols.

Using the orthogonality of the 3-j symbols, we may write (4.1.2) as

$$(4.4.1) \qquad \sum_{\mathbf{m'}\mu'} = \begin{pmatrix} \mathbf{j}_1 \, \mathbf{j}_2 \, \mathbf{j'} \\ \mathbf{m}_1 \, \mathbf{m}_2 \, \mathbf{m'} \end{pmatrix} \begin{pmatrix} \mathbf{j}_3 \, \mathbf{j}_4 \, \mathbf{j'} \\ \mathbf{m}_3 \, \mathbf{m}_4 \, \mu' \end{pmatrix} \begin{pmatrix} \mathbf{j'} \\ \mathbf{m'} \, \mu' \end{pmatrix} =$$

$$= \sum_{j \neq \mu} (-1)^{2j + 1} (2j + 1) \begin{bmatrix} j_1 j_2 j' \\ j_3 j_4 j \end{bmatrix} \begin{bmatrix} j_3 j_2 j \\ m_3 m_2 m \end{bmatrix} \begin{bmatrix} j_1 j_4 j \\ m_1 m_4 \mu \end{bmatrix} \begin{bmatrix} j \\ m \mu \end{bmatrix}$$

If we interchange the indices 1 and 3 in (4.4.1), we may show by comparison of the original equation and the new one, that

(4.4.2)

$$\sum_{\mathbf{j}} (2\mathbf{j}+1)(2\mathbf{j}''+1) \begin{Bmatrix} \mathbf{j}_1 \mathbf{j}_2 \mathbf{j}' \\ \mathbf{j}_3 \mathbf{j}_4 \mathbf{j}' \end{Bmatrix} \begin{Bmatrix} \mathbf{j}_3 \mathbf{j}_2 \mathbf{j} \\ \mathbf{j}_1 \mathbf{j}_4 \mathbf{j}'' \end{Bmatrix} = \delta_{\mathbf{j}', \mathbf{j}''}$$

It follows from (4.2.2) that

$$(4.4.3) \quad \left[(2j+1)(2j'+1) \right]^{\frac{1}{2}} \left\{ \begin{matrix} j_1 j_2 j' \\ j_3 j_4 j \end{matrix} \right\}$$

forms a real orthogonal matrix, rows and columns being labelled by j and j'.

In a similar way we get the relation

(4.4.4)

$$\sum_{j} (-1)^{j+j'+j''} (2j+1) \begin{Bmatrix} j_1 j_2 j' \\ j_3 j_4 j' \end{Bmatrix} \begin{Bmatrix} j_2 j_3 j \\ j_1 j_4 j'' \end{Bmatrix} = \begin{Bmatrix} j_2 j_1 j' \\ j_3 j_4 j'' \end{Bmatrix}$$

Another useful relation is (cf. Elliott 1953):

(4.4.5)

$$\begin{cases}
j_1 j_2 j_3 \\
\ell_1 \ell_2 \ell_3
\end{cases}
\begin{cases}
j_1 j_2 j_3 \\
\ell_1 \ell_2 \ell_3
\end{cases} = \sum_{\kappa} (-1)^{j_1 + j_2 + j_3 + \ell_1 + \ell_2 + \ell_3 + \ell_1 + \ell_2 + \ell_3 + \ell_4 + \ell$$

Wigner (1951) gives another expression for the product of two 6-j symbols: -

$$(4.4.6) \begin{Bmatrix} j_1 j_2 j_3 \\ e_1 e_2 e_3 \end{Bmatrix} \begin{Bmatrix} j_1 j_2 j_3 \\ e_1 e_2 e_3 \end{Bmatrix} =$$

$$= \sum_{\kappa e} (-1)^{2j_1 + 2e} (2\kappa + 1) (2e + 1) \begin{Bmatrix} j_1 e_2 e_3 \\ \kappa e_2^{j} e_3^{j} \end{Bmatrix} \begin{Bmatrix} e_1 j_2 e_3 \\ \kappa e_2^{j} e_3^{j} \end{Bmatrix} \begin{Bmatrix} e_1 j_2 e_3 \\ \kappa e_2^{j} e_3^{j} \end{Bmatrix} \begin{Bmatrix} e_1 e_2 e_3 \\ e_1 e_2 e_3 \end{Bmatrix}$$

The relation (4.4.1) may be written more conveniently as

$$(4.4.7) \sum_{\mathbf{m'}} (-1)^{\mathbf{j'+m'}} \begin{pmatrix} \mathbf{j}_1 \, \mathbf{j}_2 \, \mathbf{j'} \\ \mathbf{m}_1 \, \mathbf{m}_2 \, \mathbf{m'} \end{pmatrix} \begin{pmatrix} \mathbf{j}_3 \, \mathbf{j}_4 \, \mathbf{j'} \\ \mathbf{m}_3 \, \mathbf{m}_4 \, -\mathbf{m'} \end{pmatrix} =$$

$$= \sum_{\mathbf{jm}} (-1)^{2\mathbf{j}_4 + \mathbf{j} + \mathbf{m}} (2\mathbf{j} + 1) \begin{pmatrix} \mathbf{j}_1 \, \mathbf{j}_2 \, \mathbf{j'} \\ \mathbf{j}_3 \, \mathbf{j}_4 \, \mathbf{j} \end{pmatrix} \begin{pmatrix} \mathbf{j}_3 \, \mathbf{j}_2 \, \mathbf{j} \\ \mathbf{m}_3 \, \mathbf{m}_2 \, \mathbf{m} \end{pmatrix} \begin{pmatrix} \mathbf{j}_1 \, \mathbf{j}_4 \, \mathbf{j} \\ \mathbf{m}_1 \, \mathbf{m}_4 \, -\mathbf{m} \end{pmatrix}$$

We conclude this section with an expression for a certain sum of products of three 3-j symbols:

$$\begin{split} \sum_{\mu_{1}\mu_{2}\mu_{3}} (-1)^{\ell_{2}+\ell_{2}+\ell_{3}+\mu_{1}+\mu_{2}+\mu_{3}} \begin{pmatrix} \mathbf{j}_{1}\ell_{2}\ell_{3} \\ \mathbf{m}_{1}\mu_{2}-\mu_{3} \end{pmatrix} \begin{pmatrix} \ell_{1}\mathbf{j}_{2}\ell_{3} \\ -\mu_{1}\mathbf{m}_{2}\mu_{3} \end{pmatrix} \begin{pmatrix} \ell_{1}\ell_{2}\mathbf{j}_{3} \\ \mu_{1}-\mu_{2}\mathbf{m}_{3} \end{pmatrix} = \\ & = \begin{pmatrix} \mathbf{j}_{1}\mathbf{j}_{2}\mathbf{j}_{3} \\ \mathbf{m}_{1}\mathbf{m}_{2}\mathbf{m}_{3} \end{pmatrix} \begin{pmatrix} \mathbf{j}_{1}\mathbf{j}_{2}\mathbf{j}_{3} \\ \ell_{1}\ell_{2}\ell_{3} \end{pmatrix} \end{split}$$

4.5 Relations between the 6-j symbol and other notations.

(4.5.1)
$$\begin{cases} j_1 j_2 j_3 \\ \ell_1 \ell_2 \ell_3 \end{cases} = (-1)^{j_1 + j_2 + \ell_1 + \ell_2} W(j_1 j_2 \ell_2 \ell_1; j_3 \ell_3)$$
(Racah 1942)

$$(4.5.2) = (-1)^{j_1+j_2+\ell_1+\ell_2} \frac{U(j_1j_2\ell_2\ell_1;j_3\ell_3)}{[(2j_3+1)(2^{\ell_3}+1)]^2} (Jahn 1951)$$

Wigner's choice of phase of the 6-j symbol has the advantage that the resulting quantity has a much greater symmetry than those defined otherwise (cf. Racah, Jahn loc. cit.). A related coefficient, used in angular distribution problems, is defined by Biedenharn, Blatt and Rose (1952). It is

us

Z (abcd; ef) =
$$i^{f-a+e}[(2a+1)(2b+1)(2c+1)(2d+1)]^{\frac{1}{2}}W(abcd;ef)(ac00)$$
 acf0)

4.6 Computation of numerical values of 6-j symbols

6-j symbols occur frequently in the final form of physical calculations. It is therefore important to have methods for numerical computation of these quantities. The general formula may be obtained by substituting the expression (2.2.9) for the V-C coefficients into the defining equation (4.1.2).

A tedious calculation (cf. Racah (1942)) gives

$$(4.6.1) \qquad \begin{cases} j_1 j_2 j_3 \\ e_1 e_2 e_3 \end{cases} =$$

$$= \Delta(\mathbf{j}_1\mathbf{j}_2\mathbf{j}_3)\Delta(\mathbf{j}_1\boldsymbol{e}_2\boldsymbol{e}_3)\Delta(\boldsymbol{e}_1\mathbf{j}_2\boldsymbol{e}_3)\Delta(\boldsymbol{e}_1\boldsymbol{e}_2\mathbf{j}_3) \ \forall \begin{bmatrix} \mathbf{j}_1\mathbf{j}_2\mathbf{j}_3 \\ \boldsymbol{e}_1\boldsymbol{e}_2\boldsymbol{e}_3 \end{bmatrix}$$

where
$$\Delta(abc) = \left[\frac{(a+b-c)!(a-b+c)!(-a+b+c)!}{(a+b+c+1)!}\right]^{\frac{1}{2}}$$

and
$$w \begin{cases} j_1 j_2 j_3 \\ \ell_1 \ell_2 \ell_3 \end{cases} =$$

$$= \sum_{\mathbf{z}} \frac{(-1)^{\mathbf{z}} (\mathbf{z}+1)!}{(\mathbf{z}-\mathbf{j}_{1}-\mathbf{j}_{2}-\mathbf{j}_{3})!(\mathbf{z}-\mathbf{j}_{1}-\epsilon_{2}-\epsilon_{3})!(\mathbf{z}-\epsilon_{1}-\mathbf{j}_{2}-\epsilon_{3})!(\mathbf{z}-\epsilon_{1}-\epsilon_{2}-\mathbf{j}_{3})} \times \\ \times (\mathbf{j}_{1}+\mathbf{j}_{2}+\epsilon_{1}+\epsilon_{2}-\mathbf{z})!(\mathbf{j}_{2}+\mathbf{j}_{3}+\epsilon_{2}+\epsilon_{3}-\mathbf{z})!(\mathbf{j}_{3}+\mathbf{j}_{1}+\epsilon_{3}+\epsilon_{1}-\mathbf{z})!$$

where the sum is over positive integer values of z such that no factorial in the denominator has a negative argument. A recursion relation may be obtained from (4.4.5) by which we may build up 6-j symbols from ones with smaller arguments: -

$$\times \left\{ -2\mathbf{r} \left[(\mathbf{q} + \mathbf{s} + \mathbf{u} + \mathbf{1})(\mathbf{q} + \mathbf{s} - \mathbf{u}) \right]^{\frac{1}{2}} \left\{ \mathbf{p} \cdot \frac{\mathbf{q} - \frac{1}{2}\mathbf{r} - \frac{1}{2}}{\mathbf{s} - \frac{1}{2} \cdot \mathbf{t} \cdot \mathbf{u}} \right\} + \left[(\mathbf{p} + \mathbf{q} - \mathbf{r} + \mathbf{1})(\mathbf{p} + \mathbf{r} - \mathbf{q})(\mathbf{s} + \mathbf{t} - \mathbf{r} + \mathbf{1})(\mathbf{r} + \mathbf{t} - \mathbf{s}) \right]^{\frac{1}{2}} \\ \left\{ \mathbf{p} \cdot \frac{\mathbf{q} \cdot \mathbf{r} - \mathbf{1}}{\mathbf{s} \cdot \mathbf{t} \cdot \mathbf{u}} \right\}$$

Other similar recursion relations may be obtained from the same formula (4.4.5)

(4,6,) If one argument vanishes, we have

If one argument is $\frac{1}{2}$, there are two possibilities: -

(4.6.4)

(4.6.5)

$$\begin{bmatrix} j_1 & j_2 & j_3 \\ \frac{1}{2} & j_3 - \frac{1}{2} & j_2 - \frac{1}{2} \end{bmatrix} = (-1)^{j_1 + j_2 + j_3} \underbrace{ \begin{bmatrix} (j_1 + j_2 + j_3 + 1)(j_2 + j_3 - j_1) \\ 2j_2(2j_2 + 1)2j_3(2j_3 + 1) \end{bmatrix}^{\frac{1}{2}}$$

When one of the triangles becomes a line, e.g. $j_3=\ell_1+\ell_2$ the sum in (4.6.1) reduces to 1 term. We have therefore

$$(4.6.6) \quad \left\{ \begin{matrix} j_1 j_2 \ell_1 + \ell_2 \\ \ell_1 & \ell_2 & \ell_3 \end{matrix} \right\} =$$

$$= (-1)^{j_1+j_2+\ell_1+\ell_2} \underbrace{\frac{(2\ell_1)!(2\ell_2)!(j_1+j_2+\ell_1+\ell_2+1)!(j_1+\ell_1+\ell_2-j_2)!(j_2+\ell_1+\ell_2-j_4)!}{(2\ell_1+2\ell_2+1)!(j_1+j_2-\ell_1-\ell_2)!(j_1+\ell_2-\ell_3)!(\ell_2+\ell_3-j_1)!(j_1+\ell_2+\ell_3+1)!}}_{\underbrace{(j_1+\ell_3-\ell_2)!(j_2+\ell_3-\ell_1)!}{(\ell_1+j_2-\ell_3)!(\ell_1+\ell_3-j_2)!(\ell_1+j_2+\ell_3+1)!}}^{\frac{1}{2}}$$

Formulae are exhibited in Table V (see p. 71) which make possible through the symmetry relations (4.2.1), (4.2.2.) the computation of all 6-j symbols with one argument equal to 1, $\frac{3}{2}$ or 2. Similar expressions are given for the W-coefficients with one argument taking values $\frac{1}{2}$, 1, $\frac{3}{2}$, and 2 by Jahn (1951), Biedenharn

et al. (1952), Biedenharn (1952, and Simon et al.(1954). The case of 5/2 is given by Edmonds and Flowers (1952). Extensive numerical tabulations of the W-coefficients have been made by Biedenharn (1952) and Simon et al. (1954). In the first-mentioned reference the values are given as square roots of fractions (i.e. exactly); in the second they are givento 10 places of decimals. The Z-coefficient (4.5.3) has been tabulated by Biedenharn (1953).

For the case where we have two repeated arguments, Biedenharn (1952) gives a special formula. We put

where the Y are given by the recursion relation:

(4.6.8)

$$Y_{\kappa+1} (j_1 j_2) = \left(\frac{2\kappa+1}{\kappa+1}\right) Y_1(j_1 j_2) Y_{\kappa}(j_1 j_2) - (2\kappa+1) Y_{\kappa}(j_1 j_2) - \frac{\kappa}{\kappa+1} (2j_1+1+\kappa)(2j_2+1+\kappa)(2j_2+1-\kappa) Y_{\kappa-1}(j_1 j_2)$$

We have, for example,

(4.6.9)

$$Y_0 (j_1 j j_2) = 1$$

$$Y_1 (j_1 j j_2) = -2A$$

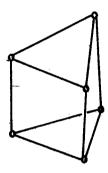
$$Y_2(j_1,j_2) = 6 A(A+1) - 8j_1(j_1+1)j_2(j_2+1)$$

where

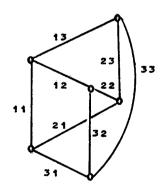
$$(4.6.10) A = j(j+1) - j_1(j_1+1) - j_2(j_2+1)$$

4.7 The 9-j symbol

Let us consider the next most complicated diagram of the type discussed in section 4.1. This would appear to be



However this diagram may be shown to be equivalent to the product of two 6-j symbols encountered in (4.4.5); the next really new invariant corresponds to the diagram



It corresponds to the contraction of products of 6 3-j symbols. There are nine different values of j involved and Wigner has called the invariant formed in this way a 9-j symbol.

The 9-j symbol is defined by the equation

4 14

(4.7.1)

$$\begin{cases}
 \mathbf{j}_{11} \mathbf{j}_{12} \mathbf{j}_{13} \\
 \mathbf{j}_{21} \mathbf{j}_{22} \mathbf{j}_{23} \\
 \mathbf{j}_{31} \mathbf{j}_{32} \mathbf{j}_{33}
\end{cases} =$$

$$\begin{array}{c} \sum & \begin{pmatrix} j_{1\,1}j_{1\,2}j_{1\,3} \\ m_{1\,1}m_{1\,2}m_{1\,3} \end{pmatrix} \begin{pmatrix} j_{2\,1}j_{2\,2}j_{2\,3} \\ m_{2\,1}m_{2\,2}m_{2\,3} \end{pmatrix} \begin{pmatrix} j_{3\,1}j_{3\,2}j_{3\,3} \\ m_{3\,1}m_{3\,2}m_{3\,3} \end{pmatrix} \times \\ & \text{all m's} \\ \begin{pmatrix} j_{1\,1}j_{2\,1}j_{3\,4} \\ m_{1\,1}m_{2\,1}m_{3\,1} \end{pmatrix} \begin{pmatrix} j_{1\,2}j_{2\,2}j_{3\,2} \\ m_{1\,2}m_{2\,2}m_{3\,2} \end{pmatrix} \begin{pmatrix} j_{1\,3}j_{2\,3}j_{3\,3} \\ m_{1\,3}m_{2\,3}m_{3\,3} \end{pmatrix} \end{array}$$

It will be seen that the triads of the 3-j symbols correspond to the j-values lying in the same row or the same column of the array.

The 9-j symbol is clearly zero unless all these triads satisfy the triangular condition (2.2.1).

The 9-j symbol has 72 symmetry relations which have been discussed by Jahn and Hope (1954). The operations are generated by (i) an odd permutation of the rows or columns, which multiplies the value of the symbol by $(-1)^{\Sigma}$ where $\Sigma = \Sigma$ j; (ii) a reflection of the symbol in either of the two diagonals, which leaves it invariant.

The expression (4.7.1) for the 9-j symbol in terms of 3-j symbols may be shown to be equivalent to the sum of products of three 6-j symbols:

(4.7.2)

$$\begin{cases}
\dot{J}_{1} & 1 \dot{J}_{1} & 2 \dot{J}_{13} \\
\dot{J}_{2} & 1 \dot{J}_{2} & 2 \dot{J}_{23} \\
\dot{J}_{3} & 1 \dot{J}_{3} & 2 \dot{J}_{33}
\end{cases} =$$

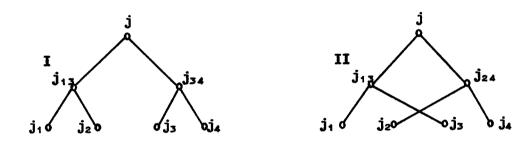
$$\sum_{\kappa} (-1)^{2\kappa} (2\kappa + 1) \begin{bmatrix} j_{11}j_{21}j_{31} \\ j_{32}j_{33} & \kappa \end{bmatrix} \begin{bmatrix} j_{12}j_{22}j_{32} \\ j_{21} & \kappa & j_{23} \end{bmatrix} \begin{bmatrix} j_{13}j_{23}j_{33} \\ \kappa & j_{11}j_{12} \end{bmatrix}$$

If one of the arguments is zero the 9-j symbol reduces essentially to a 6-j symbol; the following relations cover all cases.

(4.7.3)

$$= \begin{pmatrix} \mathbf{b} & \mathbf{a} & \mathbf{e} \\ \mathbf{f} & \mathbf{f} & \mathbf{0} \\ \mathbf{d} & \mathbf{e} & \mathbf{e} \end{pmatrix} = \begin{pmatrix} \mathbf{e} & \mathbf{d} & \mathbf{e} \\ \mathbf{e} & \mathbf{b} & \mathbf{a} \\ \mathbf{0} & \mathbf{f} & \mathbf{f} \end{pmatrix} = \begin{pmatrix} \mathbf{c} & \mathbf{e} & \mathbf{d} \\ \mathbf{a} & \mathbf{e} & \mathbf{b} \\ \mathbf{f} & \mathbf{0} & \mathbf{f} \end{pmatrix} = \frac{(-1)^{\mathbf{b}+\mathbf{c}+\mathbf{e}+\mathbf{f}}}{\left[(2\mathbf{e}+1)(2\mathbf{f}+1)\right]^{\frac{1}{2}}} \quad \begin{pmatrix} \mathbf{a} & \mathbf{b} & \mathbf{e} \\ \mathbf{d} & \mathbf{e} & \mathbf{f} \end{pmatrix}$$

In the same way as the 6-j symbol is related to the transformation between different schemes of coupling three angular momenta, so the 9-j symbol is related to the coupling of four angular momenta.



The transformation coefficient between the two schemes I and II is given in an obvious notation by

(4.7.4)

$$((j_1j_2)j_{12}(j_3j_4)j_{34}j_m|(j_1j_3)j_{13}(j_2j_4)j_{24}j_m) =$$

$$= [(2j_{12}+1)(2j_{34}+1)(2j_{13}+1)(2j_{24}+1)]^{\frac{1}{2}} \begin{cases} j_1 j_2 j_{12} \\ j_3 j_4 j_{34} \\ j_{13} j_{24} j \end{cases}$$

The 9-j symbol calculus is thus useful in the computation, for instance, of transformation coefficients between schemes of LS and jj-coupling (see Edmonds and Flowers 1952).

A function similar to the 9-j symbol was defined by Hope and Jahn (see Hope 1951, Jahn and Hope 1954). Other functions of this type have been considered by Schwinger (1952), Fano (1952) etc. These functions are related to the 9-j symbol by the relations:

(4.7.5)
$$[(2e+1)(2f+1)(2g+1)(2\kappa+1)]^{\frac{1}{2}} \begin{cases} a & b & e \\ e & d & f \\ g & h & \kappa \end{cases} = \begin{cases} \text{(Hope 1952,} \\ \text{Jahn and Hope 1953)} \end{cases}$$

=
$$x$$
 (a b c d; e f; g h; κ)

(4.7.6)
$$(-1)^{j_1+j_4-j_{12}-j_{24}}$$
 $\begin{cases} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13}j_{24}j \end{cases} = S(j_1 j_2 j_3 j_4; \text{ (Schwinger 1952)}$

$$(4.7.7) \quad \begin{cases} \mathbf{j}_1 \mathbf{j}_2 \mathbf{j} \\ \mathbf{j}_3 \mathbf{j}_4 \mathbf{j}' \\ \kappa \kappa' \mathbf{J} \end{cases} = X \quad (\mathbf{j}_1 \mathbf{j}_2 \mathbf{j}_3 \mathbf{j}_4 \mathbf{j}'; \kappa \kappa' \mathbf{J})$$
 (Fano 1952)

A number of relations involving the 6-j and 9-j symbols may be obtained by considering the various coupling schemes of four angular momenta. We may obtain in this way*

^{*} I am grateful to Dr. J.P. Elliott for showing me these results.

4.7

$$(4.7.8) \qquad \sum_{\lambda} (-1)^{\lambda} (2\lambda+1) \begin{pmatrix} b & c & \lambda \\ J_2 a & J_1 \end{pmatrix} \begin{pmatrix} J_2 a & \lambda \\ \kappa_2 d & J \end{pmatrix} \begin{pmatrix} \kappa_2 d & \lambda \\ c & b & \kappa_1 \end{pmatrix} =$$

$$= (-1)^{\kappa_1} \sum_{\lambda} (-1)^{\lambda} (2\lambda+1) \begin{pmatrix} b & d & \lambda \\ a & J & \kappa_2 \\ J_1 J_2 c \end{pmatrix} \begin{pmatrix} d & c & \kappa_1 \\ \kappa_2 b & \lambda \end{pmatrix}$$

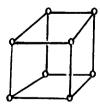
(4.7.9)

$$(-1)^{2\kappa_2} \begin{bmatrix} \mathbf{J_1d} & \kappa_2 \\ \mathbf{J} & \mathbf{c} & \mathbf{J_2} \end{bmatrix} \begin{bmatrix} \mathbf{a} & \mathbf{d} & \kappa_1 \\ \kappa_2 & \mathbf{b} & \mathbf{J_1} \end{bmatrix} = \sum_{\lambda} (2\lambda + 1) \begin{bmatrix} \lambda & \mathbf{c} & \kappa_1 \\ \mathbf{b} & \mathbf{J_1a} \\ \mathbf{J} & \mathbf{J_2d} \end{bmatrix} \begin{bmatrix} \lambda & \mathbf{c} & \kappa_1 \\ \kappa_2 \mathbf{b} & \mathbf{J} \end{bmatrix}$$

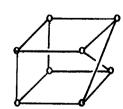
(4.7.90)

$$\sum_{\lambda\mu} (-1)^{\lambda} (2\lambda+1) (2\mu+1) \begin{pmatrix} J_1 b & a \\ e & \lambda & \mu \\ J_2 d & J \end{pmatrix} \begin{pmatrix} \kappa_1 d & a \\ e & \lambda & \mu \\ \kappa_2 b & J \end{pmatrix} = (-1)^{J_2 + \kappa_2 + 2J} \begin{pmatrix} a & d & \kappa_1 \\ b & J & \kappa_2 \\ J_1 J_2 e \end{pmatrix}$$

When we go to coupling schemes of 5 angular momenta we encounter more complex invariants; a 12-j symbol has been defined by Jahn and Hope (1954) and by Ord-Smith (1954). It has been shown however by J.P. Efflictt and by the present author that two distinct 12-j symbols exist; they correspond to diagrams



and



Numerical values of the 9-j symbol are usually obtained most easily by use of (4.7.2) and evaluation of the 6-j symbols by the methods discussed in 4.6. However, formulae have been given for some assignments of numerical values to the arguments by Rose and Osborn (1954).

5.1 Tensor operators.

Quantum mechanical operators are frequently functions of the angular coordinates of the system in which they work. Let us consider such an operator 0, and the effect on it of a rotation ω (see § 1.2) of the frame of coordinates. We have formally, where we consider the transformation $D(\omega)$ as operators on the state vectors,

$$(5.1.1) \quad 0 \to D(\omega) \quad 0 \quad D^{-1}(\omega)$$

An irreducible tensor operator of rank $\kappa(\kappa=0,\frac{1}{2},1,\ldots)$ is a set of $2\kappa+1$ operators $T(\kappa q)$ which are transformed under a rotation ω in the following way:

(5.1.2)
$$D(\omega) T(\kappa q) D^{-1}(\omega) = \sum_{\mathbf{q'} = -\kappa} T(\kappa \mathbf{q'}) \mathcal{D}_{\mathbf{q'}\mathbf{q}}^{(\kappa)}(\omega)$$

where $\mathcal{D}_{\mathbf{q}'\mathbf{q}}^{(\kappa)}(\omega)$ is a matrix element of the $2\kappa+1$ -dimensional irreducible representation $\mathbf{D}^{(\kappa)}$ of the rotation group*; i.e. $\mathbf{T}(\kappa\mathbf{q})$ transform like the angular momentum eigenvectors $\psi(\kappa\mathbf{q})$.

^{*} ef. § 3.1

Thus, a <u>vector</u> operator (see TAS ch. III) is a tensor operator of rank 1 for example, a magnetic moment. A quadrupole moment, on the other hand, is a tensor operator of rank 2.

The concept of tensor operator may be defined in terms of commutation relations with respect to the angular momentum operators (see Racah 1942); the two definitions are equivalent.†

5.2. Factorisation of the matrix elements of tensor operators (Wigner-Eckart theorem)

Consider a tensor operator acting on an eigenvector $\psi(jm)$ of some angular momentum operators \underline{J}^2 , J_z ; under a rotation ω we have

(5.2.1)

$$D(\omega)[T(\kappa q)\psi(jm)] = [D(\omega)T(\kappa q)D^{-1}(\omega)] D(\omega)\psi(jm)$$

From the definition (4.1.2) we see that this is equal to

(5.2.2)

$$\sum_{\mathbf{q'm'}} \mathbf{T}(\kappa \mathbf{q'})_{\psi}(\mathbf{jm'}) \, \mathcal{D}_{\mathbf{q'q}}^{(\kappa)}(\omega) \, \mathcal{D}_{\mathbf{m'm}}^{(\mathbf{j})}(\omega)$$

Thus the vector $T(\kappa q)_{\psi}(jm)$ is transformed by the product representation $D^{(\kappa)} \otimes D^{(j)}$ of the rotation group, and hence (cf.(3.5.2))

(5.2.3)

$$T(\kappa q)\psi(jm) = \sum_{j'm'} (\kappa qjm | \kappa jj'm')\Phi(j'm')$$

t however see A. Simon and T.A. Welton (1953)

where the $\Phi(j'm')$ are eigenvectors of the angular momentum operators \underline{J}^2 , J_z .

The matrix element (where y, y' denote all other quantum numbers)

$$(y'j'm'|T(\kappa q)|yjm) = (\psi (j'm'), T(\kappa q) \psi(jm))$$

is, by orthogonality, equal to

(5.2.4) (
$$\psi$$
 ($j'm'$), Φ ($j'm'$)) ($\kappa q jm | \kappa j j'm'$)

and thus we have factorised the matrix element into a part independent of rotations and a Clebsch-Gordan coefficient.

It is convenient to define the <u>reduced</u> matrix elements, or <u>double-bar</u> matrix elements, by

$$(5.2.5)$$

$$(y'j'm'|T(\kappa q)|yjm) = (-1)^{j'-m'} \begin{pmatrix} j'\kappa & j \\ -m'q & m \end{pmatrix} (y'j'||T^{(\kappa)}||yj)$$

$$(\underline{jm\kappa q}, j\kappa j'm')(y'j'||T(\kappa)||yj)$$

$$(2j'+1)^{\frac{1}{2}}$$

This definition is the same as that given by Racah (1942) and Wigner (1951). Other workers, for example Landau and Lifschitz (1948), Schwinger (1952), Alder (1952) and Biedenharn and Rose (1953) have defined reduced matrix elements with different conventions, and care should be taken because of this (see Table III), p. 66.

The double-bar matrix elements are computed in practice in the obvious way; we choose the easiest to compute of the components $(\gamma'j'm'|T(\kappa q)|\gamma jm)$ and divide it by the appropriate quantity. Is is usually best to take m'=m=q=0 or $m'=m=\frac{1}{2}$, q=0, so that the simpler formulae of table II may be employed.

The integrals evaluated in § 3.5 may also be relevant to the computation - namely in the case of matrix elements of solid or spherical harmonics. (Cf. remarks on matrix elements of two-body interaction in § 5.5.)

A simple example of a tensor operator of rank l is the radius vector \vec{r} ; this has the components (cf Table VI p. 69).

$$(5.2.6)$$
 $\mathbf{r}_{0} = \mathbf{z}$; $\mathbf{r}_{\pm} = \pm \frac{1}{\sqrt{2}} (\mathbf{x} \pm i\mathbf{y})$

Similarly in the spherical scheme the angular momentum to has components

$$(5.2.7) \quad \epsilon_o = \epsilon_z \quad \epsilon_{\pm} = \mp \frac{1}{\sqrt{2}} (\epsilon_x \pm i\epsilon_y) ;$$

we have corresponding expressions for the components of s

Reference to (5.2.5) and table II shows that

(5.2.8)
$$(e||\vec{t}||e') = \hbar \delta_{ee}, [(2e+1)(e+1)e]^{\frac{1}{2}}$$
 and $(\frac{1}{2}||\vec{s}||\frac{1}{2}) = \hbar \sqrt{\frac{3}{2}}$

(we consider $(\epsilon \mathbf{m} | \epsilon_o | \epsilon' \mathbf{m}') = \delta_{\epsilon \epsilon'} \delta_{\mathbf{mm}} \hbar \mathbf{m}$ and the corresponding 3-j symbol). We use (3.5.6) to obtain in the same way the double-bar matrix elements for the spherical harmonics. $Y_{\kappa G}(\theta \phi)$, where \mathbf{r}, θ , ϕ are the particle coordinates.

$$(5.2.9) \qquad (\epsilon | | Y_{\kappa} | | \epsilon') = \frac{(-1)^{\epsilon}}{2\pi^{\frac{1}{2}}} \left[(2\epsilon + 1)(2\kappa + 1)(2\epsilon' + 1) \right]^{\frac{1}{2}} \begin{pmatrix} \epsilon & \kappa & \epsilon' \\ 0 & 0 & 0 \end{pmatrix}$$

(cf. Racah (1942))

5.3 Tensor product of tensor operators.

We define the tensor product of two tensor operators T (κ_1q_1) and U (κ_2q_2) by

(5.3.1)
$$X(\kappa \mathbf{q}) = \sum_{\mathbf{q}_1 \mathbf{q}_2} T(\kappa_1 \mathbf{q}_1) U (\kappa_2 \mathbf{q}_2) (\kappa_1 \mathbf{q}_1 \kappa_2 \mathbf{q}_2 | \kappa_1 \kappa_2 \kappa \mathbf{q})$$

It is easy to show that this product is also a tensor operator, being transformed under rotations as a basis element of the representation $D^{(\kappa)}$. Use of the orthogonality of the C-G coefficients gives the decomposition of a simple product of two tensor operator components:

(5.3.2)
$$T(\kappa_1 q_1) U(\kappa_2 q_2) = \sum_{\kappa q} X(\kappa q) (\kappa_1 \kappa_2 \kappa q | \kappa_1 q_1 \kappa_2 q_2)$$

The <u>sealar product</u> of two tensor operators of the same rank is, however defined not as X(00) but as

$$(5.3.3) \qquad (T(\kappa) \cdot U(\kappa)) = \sum_{\mathbf{q}} (-1)^{\mathbf{q}} T(\kappa \mathbf{q}) U(\kappa - \mathbf{q})$$

5.4 Definition of Hermitian tensor operators.

We have to alter our conception of a Hermitian operator, since evidently the eigenvalues of the components $T(\kappa q)$ of a tensor operator will not all be real. We required in § 1.5 that the complex conjugate of the spherical harmonic Y should be given by Y* = $(-1)^m$ Y however we remember from §2.6 that this property is not preserved under vector-coupling. The alternative convention gives a spherical harmonic $\hat{Y}_{\epsilon m}$ (1.5.7) in which the corresponding

property is preserved under vector-coupling : -

$$(5.4.1) \quad \mathring{\Upsilon}_{em}^{*}(\theta\phi) = (-1)^{e+m} \quad \mathring{\Upsilon}_{e-m}(\theta\phi)$$

Now in the ordinary quantum theory a Hermitian operator 0 (satisfying $0^{\dagger}=0$) has real eigenvalues (satisfying $a^*=a$). It is easy to see that we have a consistent system when we extend the concept of a Hermitian operator and require that a Hermitian tensor operator should satisfy*

(5.4.2)
$$T^{\dagger}(\kappa q) = (-1)^{\kappa+q} T(\kappa-q)$$

It is clear from (5.1.2) that this property is preserved under rotations. Tensor operators of half odd integer rank cannot be Hermitian in this sense, and are therefore not of physical significance. This is discussed by Wigner (1951) p. 48 and Schwinger (1952) p. 57.

If $T(\kappa q)$ is a Hermitian tensor operator, then the double-bar matrix elements must satisfy the condition

$$(5.4.3) \quad (j||T(\kappa)||j') = (-1)^{j-\kappa-j'}(j'||T(\kappa)||j)*$$

It may be shown (cf. §2.6) that if two tensor operators $T(\kappa_1q_1)$ and $T(\kappa_2q_2)$ are Hermitian, then, provided that they commute, their tensor product (5.3.1) is also Hermitian. Tensor products of certain tensor operators which do not commute have been discussed by Rose and Osborn (1954).

5.5 Matrix elements of products of tensor operators.

Suppose that two tensor operators $T(\kappa_1q_1)$ and $U(\kappa_2q_2)$ operate upon parts 1 and 2 respectively of a

^{*} This definition differs from that of Racah (1942), who takes (-1)\(^2\). With Racah's definition tensor products of Hermitian tensor operators are not Hermitian.

quantum mechanical system (i.e. they commute). The angular momentum quantum numbers of parts 1 and 2 and of the whole system are denoted by j_1m_1 , j_2m_2 and jm respectively.

Then by use of (2.4.1), (2.4.6), (4.7.1), (5.2.5) and (5.3.1) we may compute the double-bar matrix element of the tensor product $X(\kappa q)$, in the seheme $(\gamma j_1 j_2 j_m)$.

We first express the matrix element $(\gamma j_1 j_2 j_m | X(\kappa q) | \gamma' j_1' j_2' j'm')$ by a Clebsch-Gordan transformation in terms of matrix elements in the scheme $(\gamma j_1 j_2 m_1 m_2)$:

(5.5.1)

 $(\gamma j_1 j_2 jm | X(\kappa q) | \gamma' j_1 j_2 j'm') =$

$$\sum_{\substack{m_1m_1'\\m_2m_2'}} (j_1j_2jm|j_1j_2m_1m_2)(\gamma j_1j_2m_1m_2|X(\kappa q)|\gamma'j_1'j_2'm_1'm_2')$$

In the scheme $(yj_1j_2m_1m_2)$ the matrix element of $X(\kappa q)$ may be written in terms of products of the matrix elements of $T(\kappa_1q_1)$ and $U(\kappa_2q_2)$:

(5.5.2)

 $(\gamma \mathbf{j}_1 \mathbf{j}_2 \mathbf{m}_1 \mathbf{m}_2 | \mathbf{X}(\kappa \mathbf{q}) \gamma' \mathbf{j}_1 \mathbf{j}_2 \mathbf{m}_1 \mathbf{m}_2) =$

$$\sum_{\substack{q_1q_2\\ (\kappa_1q_1\kappa_2q_2) | \kappa_1\kappa_2\kappa q_1}} |T(\kappa_1q_1)| y' j_1'm_1') (y j_2m_2 | U(\kappa_2q_2) | y' j_2'm_2')$$

Now we combine (5.5.1) and (5.5.2), substituting the double-bar matrix elements of $X(\kappa q)$, $T(\kappa_1 q_1)$ and

 $U(\kappa_2 q_2)$ by use of (5.2.5).

Reference to the orthogonal property of the 3-j symbols (2.4.5.) and the definition of the 9-j symbols (4.7.1) shows that the double-bar matrix element of $X(\kappa q)$ in the scheme $(\gamma j_1 j_2 j_m)$ may be expressed in terms of the double-bar matrix elements of $T(\kappa_1 q_1)$ and $U(\kappa_2 q_2)$ and a 9-j symbol. Thus we have removed all quantities which depend on the particular coordinate system.

$$(yj_1j_2j||X(\kappa)||y'j_1j_2j') =$$

$$= [(2j+1)(2j'+1)(2\kappa+1)]^{\frac{1}{2}} \begin{cases} \kappa' j j' \\ \kappa_1 j_1 j_1' \\ \kappa_2 j_2 j_2' \end{cases} \sum_{\gamma'''} (\gamma j_1 || T(\kappa_1) || \gamma'' j_1') \\ \times (\gamma'' j_2 || U(\kappa_2) || \gamma' j_2')$$

where y,y',y'', denote all quantum numbers not associated with angular momentum. This formula is applied, for example, to the computation of the matrix elements of tensor and spin-orbit forces in nuclei by Elliott(1953) and to β -decay problems by Rose and Osborn (1954).

The formula for the matrix element of the scalar product of two commuting tensor operators (5.3.3) in the scheme $(\gamma j_1 j_2 j_m)$ is obtained by setting $\kappa=0$ and applying (4.7.3). We get

$$(\gamma j_1 j_2 jm | (T(\kappa) \cdot U(\kappa)) | \gamma' j_1 j_2 j'm')$$

If we have only an operator $T(\kappa q)$ operating on part 1 and we want the matrix element in the scheme

 (yj_1j_2jm) we get it by putting $\kappa_2=0$ in $(5.5.3)(substituting <math>U(\kappa_2q_2)=1$) and applying (4.7.3). The result is

(5.5.5)

 $(\gamma j_1 j_2 j | T(\kappa) | \gamma' j (j_2 j') =$

$$= (-1)^{j_1 + j_2 + j' + \kappa} \left[(2j+1)(2j'+1) \right]^{\frac{1}{2}} \left\{ \begin{matrix} j_1 j_1 j_2 \\ j' j'_1 k \end{matrix} \right\} (\gamma j_1 || T(\kappa) || \gamma' j'_1)$$

the computation of the matrix element of the scalar product of two vector quantities. An application of (5.5.5) is found in the use of the spherical harmonic addition theorem (3.5.8) in the calculation of the matrix elements of a two-body interaction (electrostatic interaction or Wigner force). Cf. Racah (1942). When $j_1=j_1'$, $j_2=j_2'$ the matrix elements may be obtained by the well-known method (see, for example, Kopfermann (1940)). A quantity enters into the calculation which in the limit of large j_1 and j_2 becomes the cosine of the angle (j_1, j_2) between the two angular momentum vectors j_1 , j_2 . This quantity is

$$(5.5.6) \qquad \frac{j(j+1) - j_1(j_1+1) - j_2(j_2+1)}{2j_1j_2}$$

The corresponding 6-j symbol has the value

(5.5.7)

Hence in the limit of large j_1 and j_2 , $\begin{cases} j_2 j_1 \\ l_1 j_1 j_2 \end{cases}$ approaches the value $(-1)^{j_1+j_2+j}[(2j_1+1)(2j_2+1)]^{-\frac{1}{2}}\cos(j_1, j_2)$

For $\kappa_1 = 2$ the Legendre function

$$P_2(\cos(j_1,j_2)) = \frac{1}{2} \left(\frac{3}{2} \cos^2(j_1,j_2) - \frac{1}{2} \right)$$

takes the place of $\cos(\underline{j_1},\underline{j_2})$ (see again Kopfermann loc.cit.) and we may write a similar asymptotic value

for
$$\begin{bmatrix} \mathbf{j} & \mathbf{j_2} \, \mathbf{j_1} \\ 2 & \mathbf{j_1} \, \mathbf{j_2} \end{bmatrix} .$$

In general, for $\kappa_1 = \kappa$ we have, as has been remarked by Racah (1951),

$$\begin{cases}
\mathbf{j} \ \mathbf{j}_{2} \mathbf{j}_{1} \\
\kappa \ \mathbf{j}_{1} \mathbf{j}_{2}
\end{cases} \rightarrow (-1)^{\mathbf{j}_{1} + \mathbf{j}_{2} + \mathbf{j}} [(2\mathbf{j}_{1} + 1)(2\mathbf{j}_{2} + 1)]^{-\frac{1}{2}} P_{\kappa}(\cos(\mathbf{j}_{1}, \mathbf{j}_{2}))$$

for large j_1 and j_2 , and small κ . (see §4,6 for recursion relation for this type of 6-j symbol).

Table 1

(i) Unsymmetrised C-G coefficients.

These are all numerically equal (insofar as the authors have stated their assumptions about phases) to the C-G coefficient defined by Condon and Shortley. The symbols used for the angular momentum quantum numbers are the same throughout for ease of comparison, and in some places are different from those used by the authors mentioned.

a)	Biedenharn	(1952)		CJ1 J2 J m ₁ m ₂ m
b)	Blatt and W	le isskop f	(1952)	C _{j,j2} (jm;m,m ₂)

e) Condon and Shortley (1935)
$$\begin{cases} (j_1 j_2 j_2 | j_1 j_2 m_1 m_2) \\ (j_1 j_2 j_2 | j_1 m_1 j_2 m_2) \\ (j_2 | m_1 m_2) \end{cases}$$

d) Eckart (1930)
$$A_{\text{HM}_1 \text{m}_2}^{\text{jj}_1 \text{j}_2}$$

e) Fano (1952)
$$\langle j_1 m_1, j_2 m_2 | (j_1 j_2) j m_2 \rangle$$

f) Jahn (1951), Alder (1952)
$$c_{j_1m_1j_2m_2}^{j_m}$$

g) Rose (1953)
$$C(j_1 j_2 j; m_1 m_2)$$

i) Wigner (1931)
$$S_{jm_1m_2}^{j_1j_2}$$

j) Boys (1951)
$$X(j,m,j_{1},j_{2},m_{1})$$

(ii) Symmetrised C-G coefficients.

These are given relative to Wigner's 3-j symbol, which is given in terms of the C-G coefficient by (2.4.1).

a) Fano (1952):
$$\langle j_1 m_1, j_2 m_2, j_3 m_3 | 0 \rangle (-1)^{j_1 - j_2 + j_3} = \begin{pmatrix} j_1 j_2 j_3 \\ m_1 m_2 m_3 \end{pmatrix}$$
.

b) Landau and Lifschitz (1948):

$$S_{j_1m'_1;j_2m_2;j'_3m'_3}^{(-1)^{j_1-j_2+j_3}} = - - -$$

- e) Racah (1942) $\forall (j_1 j_2 j_3; m_1 m_2 m_3) (-1)^{j_3 + j_2 j_1} - -$
- d) Sehwinger (1952) $X(j_1 j_2 j_3; m_2 m_2 m_3) = " -$

Table II

$$\begin{pmatrix} j_1 j_2 j_3 \\ 0 0 0 \end{pmatrix} = (-1)^{\frac{1}{2}J} \left[\frac{(j_1 + j_2 - j_3)!(j_1 + j_3 - j_2)!(j_2 + j_3 - j_1)!}{(j_1 + j_2 + j_3 + 1)!} \right]^{\frac{1}{2}} \times$$

$$\times \frac{(\frac{1}{2}J)!}{(\frac{1}{2}J-j_1)!(\frac{1}{2}J-j_2)!(\frac{1}{2}J-j_3)!}$$

if J is even

$$\begin{pmatrix} \mathbf{j}_1 \, \mathbf{j}_2 \, \mathbf{j}_3 \\ 0 \, 0 \, 0 \end{pmatrix} = 0 \quad \text{if} \quad \mathbf{J} \quad \text{is odd} \qquad \text{where} \quad \mathbf{J} = \mathbf{j}_1 + \mathbf{j}_2 + \mathbf{j}_3$$

$$\begin{pmatrix} J + \frac{1}{2} & J & \frac{1}{2} \\ M - M - \frac{1}{2} & \frac{1}{2} \end{pmatrix} \quad (-1)^{J - M - \frac{1}{2}} \begin{bmatrix} J - M + \frac{1}{2} \\ (2J + 2)(2J + 1) \end{bmatrix}^{\frac{1}{2}} \qquad \qquad \underline{J + \frac{1}{2}, J, \frac{1}{2}}$$

$$\begin{pmatrix} J+1 & J & 1 \\ M & -M+1 & 1 \end{pmatrix} (-1)^{J-M-1} \begin{bmatrix} (J-M)(J-M+1) \\ \hline (2J+3)(2J+2)(2J+1) \end{bmatrix}^{\frac{1}{2}}$$

$$\begin{pmatrix} J+1 & J & 1 \\ M & -M & 0 \end{pmatrix} (-1)^{J-M-1} \begin{bmatrix} (J+M+1)(J-M+1) \cdot 2 \\ \hline (2J+3)(2J+2)(2J+1) \end{bmatrix}^{\frac{1}{2}}$$

$$\begin{pmatrix} J & J & 1 \\ M & -M-1 & 1 \end{pmatrix} \quad (-1)^{J-M} \quad \begin{bmatrix} (J-M)(J+M+1) \cdot 2 \\ (2J+2)(2J+1)(2J) \end{bmatrix}^{\frac{1}{2}}$$

$$\begin{pmatrix} J & J & 1 \\ M & -M & 0 \end{pmatrix} \quad (-1)^{J-M} \quad \frac{M}{[(2J+1)(J+1)J]^{\frac{1}{2}}}$$

$$\frac{J,J,1}{[(2J+1)(J+1)J]^{\frac{1}{2}}}$$

$$\begin{pmatrix} J + \frac{3}{2} & J & \frac{3}{2} \\ M & -M - \frac{3}{2} & \frac{3}{2} \end{pmatrix} \qquad (-1)^{J - M + \frac{1}{2}} \begin{bmatrix} \frac{(J - M - \frac{1}{2})(J - M + \frac{1}{2})(J - M + \frac{3}{2})}{(2J + 4)(2J + 3)(2J + 2)(2J + 1)} \end{bmatrix}^{\frac{1}{2}}$$

$$\begin{pmatrix} J + \frac{3}{2} & J & \frac{3}{2} \\ M & -M - \frac{1}{2} & \frac{1}{2} \end{pmatrix} \qquad (-1)^{J - M + \frac{1}{2}} \begin{bmatrix} \frac{3(J - M + \frac{1}{2})(J - M + \frac{3}{2})(J + M + \frac{3}{2})}{(2J + 4)(2J + 3)(2J + 2)(2J + 1)} \end{bmatrix}^{\frac{1}{2}}$$

$$\begin{pmatrix} J + \frac{1}{2} & J & \frac{3}{2} \\ M & -M - \frac{3}{2} & \frac{3}{2} \end{pmatrix} \qquad (-1)^{J - M - \frac{1}{2}} \begin{bmatrix} \frac{3(J - M - \frac{1}{2})(J - M + \frac{1}{2})(J + M + \frac{3}{2})}{(2J + 3)(2J + 2)(2J + 1)2J} \end{bmatrix}^{\frac{1}{2}}$$

$$\begin{pmatrix} J + \frac{1}{2} & J & \frac{3}{2} \\ M & -M - \frac{1}{2} & \frac{1}{2} \end{pmatrix} \qquad (-1)^{J - M - \frac{1}{2}} \begin{bmatrix} \frac{J - M + \frac{1}{2}}{(2J + 3)(2J + 2)(2J + 1)2J} \end{bmatrix}^{\frac{1}{2}} \times$$

$$\times (J + 3M + \frac{3}{2})$$

$$\begin{pmatrix} J+2 & J & 2 \\ M & -M-2 & 2 \end{pmatrix} \qquad (-1)^{J-M} \begin{bmatrix} (J-M-1)(J-M)(J-M+1)(J-M+2) \\ (2J+5)(2J+4)(2J+3)(2J+2)(2J+1) \end{bmatrix}^{\frac{1}{2}}$$

$$\begin{pmatrix} J+2 & J & 2 \\ M & -M-1 & 1 \end{pmatrix} \qquad 2(-1)^{J-M} \begin{bmatrix} (J+M+2)(J-M+2)(J-M+1)(J-M) \\ (2J+5)(2J+4)(2J+3)(2J+2)(2J+1) \end{bmatrix}^{\frac{1}{2}} \qquad \underline{J+2,J,2}$$

$$\begin{pmatrix} J+1 & J & 2 \\ M & -M-2 & 2 \end{pmatrix} \quad 2(-1)^{J-M+1} \left[\frac{(J-M-1)(J-M)(J-M+1)(J+M+2)}{(2J+4)(2J+3)(2J+2)(2J+1)2J} \right]^{\frac{1}{2}}$$

$$\begin{pmatrix} J+1 & J & 2 \\ M & -M & 0 \end{pmatrix} \quad (-1)^{J-M+1} 2M \left[\frac{6(J+M+1)(J-M+1)}{(2J+4)(2J+3)(2J+2)(2J+1)2J} \right]^{\frac{1}{2}}$$

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$$\begin{pmatrix} J & J & 2 \\ M & -M-2 & 2 \end{pmatrix} \qquad (-1)^{J-M} \left[\frac{6(J-M-1)(J-M)(J+M+1)(J+M+2)}{(2J+3)(2J+2)(2J+1)(2J)(2J-1)} \right]^{\frac{1}{2}}$$

$$\begin{pmatrix} J & J & 2 \\ M & -M-1 & 1 \end{pmatrix} \qquad (-1)^{J-M} (1+2M) \left[\frac{6(J+M+1)(J-M)}{(2J+3)(2J+2)(2J+1)(2J)(2J-1)} \right]^{\frac{1}{2}} \qquad J,J,2$$

$$\begin{pmatrix} J & J & 2 \\ M & -M & 0 \end{pmatrix} \qquad (-1)^{J-M} \quad \frac{2[3M^2-J(J+1)]}{[(2J+3)(2J+2)(2J+1)(2J)(2J-1)]^{\frac{1}{2}}}$$

Table III

Notations relating to tensor operators and reduced matrix elements.

N.B. We assume throughout the usual convention, that

$$(\mathbf{a} \mid \mathbf{0} \mid \mathbf{b}) = \int \psi_{\mathbf{a}}^{*} 0 \psi_{\mathbf{b}} d\tau$$

The q component of a tensor operator of rank κ is written in these notes as $T(\kappa q)$, and the matrix elements between the states α jm and α' j'm' as $(\alpha \text{ j m } |T(\kappa q)|\alpha'\text{ j'm'})$. This is identical with the notation of Schwinger (1952). Other notations, which are equivalent to those already mentioned, are given below.

Racah (1942): q component of tensor operator of rank $\kappa:=T_{\mathbf{q}}^{(\kappa)}$. Matrix element of this operator :— $(\alpha \mathbf{jm}|T_{\mathbf{q}}^{(\kappa)}|\alpha'\mathbf{j'm'})$

Wigner (1951): τ component of tensor operator of rank t: — t_{τ} . Matrix element of this operator between states with angular momenta e κ , $e'\lambda$: — $(\psi_{\kappa}^{e}, t_{\tau}, \psi_{\lambda}^{e'})$.

Landau and Lifschitz (1948): m component of tensor operator of rank $j := f^{(jm)}$.

Matrix element of this operator between states with angular momenta $j_1m_1, j_2m_2 := (f^{(jm)})_{j_2m_2}^{j_1m_2}$

Biedenharn and Rose (1953): μ componant of tensor operator of rank L, with parity $\pi(=\pm 1):$ — $T(L \mu,\pi)$. Matrix element of this operator between states with angular momenta j_1m_1 , $j_m:$ — $\langle j_1m_1 | T(L \mu,\pi) | j_m \rangle$.

Fano (1951): q component of tensor operator of rank $\kappa: -T_{\kappa \mathbf{Q}} . \text{ Matrix element of this operator between states with angular momenta}$ $\mathbf{j'm'} \text{ and } \mathbf{jm}: - <\mathbf{j'm'} \mid T_{\kappa \mathbf{Q}} \mid \mathbf{jm}>.$

The <u>double-bar</u> matrix element, or reduced matrix element, is defined in these notes as follows:

$$(\alpha j m | T(\kappa q) | \alpha' j' m') = (-1)^{j-m} (\alpha j | |T(\kappa)| | \alpha' j') \begin{pmatrix} j & \kappa j' \\ -m & q & m' \end{pmatrix}$$

This is identical with the definition of Racah (1942); however in his notation the relation is:

Racah (1942)

$$(\alpha \mathbf{j} \mathbf{m} | \mathbf{T}_{\mathbf{Q}}^{(\kappa)} | \alpha' \mathbf{j}' \mathbf{m}') = (-1)^{\mathbf{j}+\mathbf{m}} (\alpha \mathbf{j} | | \mathbf{T}^{(\kappa)} | | \alpha' \mathbf{j}') \times \mathbf{V}(\mathbf{j} \mathbf{j}' \kappa; -\mathbf{m}\mathbf{m}' \mathbf{Q})$$

The definition of Wigner (1951) is also equivalent to ours:

$$(\psi_{\kappa}^{\ell}, \mathbf{t}_{\tau} \psi_{\lambda}^{\ell}) = (-1)^{\ell-\kappa} \begin{pmatrix} e & \mathbf{t} & e' \\ -\kappa & \tau & \lambda \end{pmatrix} \mathbf{t}_{e \ell}$$

Other notations, which are <u>not</u> equivalent to ours, are given below; reference should be made to Table I for the notations for Clebsch-Gordan coefficients.

<u>Schwinger</u> (1952):

$$(y \mathbf{j} \mathbf{m} | \mathbf{T}(\kappa \mathbf{q}) | y' \mathbf{j}' \mathbf{m}') = (-1)^{\kappa - \mathbf{j}' + \mathbf{m}} [y \mathbf{j} | \mathbf{T}^{(\kappa)} | y' \mathbf{j}'] \mathbf{X} (\mathbf{j} \kappa \mathbf{j}'; -\mathbf{m} \mathbf{q} \mathbf{m}')$$

Biedenharn and Rose (1953):

$$\langle \mathbf{j}_1 \mathbf{m}_1 | \mathbf{T}(\mathbf{L} \mu, \pi) | \mathbf{j} \mathbf{m} \rangle = \mathbf{C}(\mathbf{j}_1 \mathbf{L} \mathbf{j}; \mathbf{m}_1 \mathbf{m} - \mathbf{m}_1)(\mathbf{j}_1 | \mathbf{T}(\mathbf{L}\pi) | \mathbf{j}) \delta(\pi, \pi_1 \pi_2)$$

Landau and Lifschitz (1948)

$$(f^{(jm)})_{j_2m_2}^{j_1m_1} = (f^{(j)})_{j_2}^{j_1}(-1)_{j_2}^{m_2} \sqrt{2j_2+1} S_{j_1m_1}, j_m; j_2, -n_2$$

Fano (1951):

$$\sum_{\mathbf{m'm}} \langle (\mathbf{j'j}) \overline{\kappa \mathbf{q}} | \mathbf{j'm'}, \mathbf{j-m} \rangle (-1)^{\mathbf{j-m}} \langle \mathbf{j'm'} | \mathbf{T}_{\kappa \mathbf{q}} | \mathbf{j} \mathbf{m} \rangle = \langle \mathbf{j'j} | \mathbf{T}_{\kappa} \rangle \times \delta_{\overline{\kappa}\kappa} \delta_{\overline{\mathbf{q}}\mathbf{q}}$$

Condon and Shortley (1935): We relate the analogous notation of TAS for vector operators to our own by quoting equations (30) of Racah (1942):

$$(\alpha \ j | | T^{(1)} | | \alpha' j') = [j(j+1)(2j+1)]^{\frac{1}{2}} (\alpha \ j \ \vdots \ T \ \vdots \ \alpha' j)$$

$$(\alpha \ j | | T^{(1)} | | \alpha' j-1) = [j(2j-1)(2j+1)]^{\frac{1}{2}} (\alpha \ j \ \vdots \ T \ \vdots \ \alpha' j-1)$$

$$(\alpha \ j | | T^{(1)} | | \alpha' j+1) = -[(j+1)(2j+1)(2j+3)]^{\frac{1}{2}} (\alpha \ j \ \vdots \ T \ \vdots \ \alpha' j+1)$$

Table IV

$$\mathcal{D}_{mm'}^{(j)} \left(0 \ \frac{\pi}{2} \ 0\right) = \Delta_{mm'}^{(j)} \quad (cf. \S 3.7)$$

$$\frac{\mathbf{j} = \frac{1}{2}}{-\frac{1}{2}} \quad \frac{\mathbf{m}' \quad -\frac{1}{2}}{\frac{1}{\sqrt{2}}} \quad \frac{+\frac{1}{2}}{\frac{1}{\sqrt{2}}} \\
-\frac{1}{2} \quad \frac{1}{\sqrt{2}} \quad \frac{1}{\sqrt{2}} \\
+\frac{1}{2} \quad -\frac{1}{\sqrt{2}} \quad \frac{1}{\sqrt{2}}$$

$$= \frac{\mathbf{j} = 1}{\mathbf{m}} \quad -1 \quad 0 \quad +1 \\
-1 \quad \frac{1}{2} \quad \frac{1}{\sqrt{2}} \quad \frac{1}{2}$$

$$= 0 \quad -\frac{1}{\sqrt{2}} \quad 0 \quad \frac{1}{\sqrt{2}}$$

$$+ 1 \quad \frac{1}{2} \quad -\frac{1}{\sqrt{2}} \quad \frac{1}{2}$$

j = 2 m'	- 2	- 1	0	+ 1	+ 2
- 2	1/4	1 2	√3 2√2	<u>1</u>	1 Z
- 1	$-\frac{1}{2}$	- 1 /2	0	1 2	1 2
0	√3 2√2	0	- 1 2	0	$\frac{\sqrt{3}}{2\sqrt{2}}$
+ 1	- 1	1 2	0	$-\frac{1}{2}$	1 2
+ 2	1 4	- 1 /2	$\frac{\sqrt{3}}{2\sqrt{2}}$	- 1 2	1 Z

:

Table V

Formulae for the 6-j symbol

$${ a b e 1 e b } = (-1)^{s+1} \frac{2\{b(b+1) + c(c+1) - a(a+1)\}}{[2b(2b+1)(2b+2)2e(2c+1)(2c+2)]^{\frac{1}{2}}}$$

s = a + b + c

$$\begin{bmatrix} a & b & c \\ \frac{3}{2} & c - \frac{3}{2} & b + \frac{1}{2} \end{bmatrix} = (-1)^{8} \begin{bmatrix} \frac{3(s+1)(s-2a)(s-2b-1)(s-2b)(s-2c+1)(s-2c+2)}{2b(2b+1)(2b+2)(2b+3) \cdot (2c-2)(2c-1)2c(2c+1)} \end{bmatrix}^{\frac{1}{2}}$$

$$\begin{cases} a & b & e \\ \frac{3}{2} & e^{-\frac{1}{2}} & \frac{1}{b^{-\frac{1}{2}}} \end{cases} = (-1) \frac{s\{2(s-2b)(s-2e)-(s+2)(s-2a-1)\}[(s+1)(s-2a)]^{\frac{1}{2}}}{[(2b-1)2b(2b+1)(2b+2)\cdot(2e-1)2e(2e+1)(2e+2)]^{\frac{1}{2}}}$$

$$\begin{cases} a & b & e \\ \frac{3}{2} & e^{-\frac{1}{2}} & b^{\frac{1}{2}} \end{cases} = (-1) \frac{s[(s-2b-1)(s-2e) - 2(s+2)(s-2a)][(s-2b)(s-2e+1)]^{\frac{1}{2}}}{[2b(2b+1)(2b+2)(2b+3) \cdot 2e(2e+1)(2e+2)(2e+3)]^{\frac{1}{2}}}$$

s = a + b + e

$$\begin{bmatrix} a & b & e \\ 2 & c-2 & b+1 \end{bmatrix} = (-1) \cdot 2 \cdot \begin{bmatrix} (s+1)(s-2a)(s-2b-2)(s-2b-1)(s-2b)(s-2c+1)(s-2c+2)(s-2c+3) \\ \hline (2b+1)(2b+2)(2b+3)(2b+4) \cdot (2e-3)(2c-2)(2e-1)2e(2e+1) \end{bmatrix}^{\frac{1}{2}}$$

where
$$s = a+b+c$$
, $X = b(b+1) + c(c+1) - a(a+1)$

Table VI

Spherical and solid harmonics

$$y_{em}(\mathbf{r}) = \mathbf{r}^e y_{em} (\theta \phi)$$

e, m	Y _{em} (†)	Υ _{ε m} (θ,φ)
0 0	$\frac{1}{2\sqrt{\pi}}$	$rac{1}{2\sqrt{\pi}}$
1 0	$\frac{1}{2}\sqrt{\frac{3}{\pi}}$ z	$\frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta$
1±1	$-\frac{1}{2}\sqrt{\frac{3}{2\pi}} (x \pm iy)$	$-\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin \theta e^{\pm i\phi}$
2 0	$\frac{1}{4} \sqrt{\frac{5}{\pi}} (2z^2 - x^2 - y^2)$	$\frac{1}{4}\sqrt{\frac{5}{\pi}}\left(2\cos^2\theta-\sin^2\theta\right)$
2±1	$\frac{-1}{+2}\sqrt{\frac{15}{2\pi}} z (x \pm iy)$	$-\frac{1}{2}\sqrt{\frac{15}{2\pi}}\cos\theta\sin\theta e^{\pm i\phi}$
2±2	$\frac{1}{4}\sqrt{\frac{15}{2\pi}} (x \pm iy)^2$	$\frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta \ e^{\pm 2i\phi}$
3 0	$\frac{1}{4} \sqrt{\frac{7}{\pi}} (2z^2 - 3x^2 - 3y^2)z$	$\frac{1}{4}\sqrt{\frac{7}{\pi}}\left(2\cos^3\theta-3\cos\theta\sin^2\theta\right)$
3±1	$-\frac{1}{+8}\sqrt{\frac{21}{\pi}} (4z^2-x^2-y^2)(x\pm iy)$	$\frac{1}{18}\sqrt{\frac{21}{\pi}}\left(4\cos^2\theta\sin\theta-\sin^3\theta\right)e^{\pm i\phi}$
3±2	$\frac{1}{4}\sqrt{\frac{105}{2\pi}}z (x\pm iy)^2$	$\frac{1}{4}\sqrt{\frac{105}{2\pi}}\cos\sin^2\theta e^{\pm 2i\phi}$
3±3	$-\frac{1}{+8}\sqrt{\frac{35}{\pi}}\left(\mathbf{x}\pm\mathbf{i}\mathbf{y}\right)^{3}$	$\frac{1}{+8}\sqrt{\frac{35}{\pi}}\sin^3\theta e^{\pm 3i\phi}$

Irreducible tensors containing in addition the components of some other vector $\vec{\mathbf{r}}'$ may be constructed by polarization of the solid harmonics with the operator $\vec{\mathbf{r}}' \cdot \nabla \equiv \mathbf{x}' \frac{\partial}{\partial \mathbf{x}} + \mathbf{y}' \frac{\partial}{\partial \mathbf{y}} + \mathbf{z}' \frac{\partial}{\partial \mathbf{z}}$. Cf. Rose (1954)

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CERN Theoretical Study Division Blegdamsvej 17, Copenhagen, Denmark