SYMMETRICAL COUPLING OF ANGULAR MOMENTA

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Summary

An expression is given for the integral over the domain of Euler angles of a product of any number of rotation matrices. As a result a scheme has been set up in which any number of angular momenta may be coupled on an equal footing. Explicit algebraic expressions for the coupling coefficients are given. The resulting eigenfunctions, which are degenerate with respect to the total angular momentum, are distinguished by a set of numbers depending symmetrically upon the coupled angular momenta. Although not orthogonal with respect to these labels, this set is complete and several orthogonal sets may be constructed from it.

A simpler derivation of Gaunt's formula and a generating function for $3j$ symbols are obtained as by-products.

I. Introduction

The eigenfunctions of total angular momentum constructed from more than two angular momentum vectors are in general degenerate. In a symmetrical coupling scheme this degeneracy would be resolved in such a way that no angular momentum occupies a privileged position. The usual procedures that depend on coupling two angular momenta at a time are evidently not symmetric. An exposition of such couplings for an arbitrary number of angular momenta has been given by Yutsis, Levinson, and Vanagas (1962). The desirability of symmetrical coupling has been emphasized in a number of works; for example, by Smith (1960), Chakrabarti (1964), Löwden (1964), Dragt (1965), Lévy-Leblond and Lévy-Nahas (1965), Lévy-Leblond and Lurçat (1965), and Shapiro (1965). In such works the problem, approached via group theory or the quantum mechanical operator calculus, is supposed to be to remove the degeneracy not only in a symmetrical way but also in such a way that a complete and *orthogonal* set of basic vectors is obtained. Generally, in this form the problem has been considered intractable. However, some success has been achieved in the works quoted above, particularly with the symmetrical coupling of three angular momenta; although the general calculation of the coupling coefficient, even for this case, is not straightforward.

It is now submitted that the essential part of the problem is to provide a system for distinctly labelling the members of the degenerate sets characterized by given values of the total angular momentum; and to provide explicit formulae for constructing these members from product eigenfunctions of individual angular momenta. Such sets are in general linearly dependent but complete, and therefore, at least in principle, a number of orthogonal sets may be constructed from them.

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The non-uniqueness of the orthogonal sets is inherent in the problem and, perhaps, is to be welcomed, since different sets may be appropriate in different physical contexts. Orthogonality of wavefunctions is not as crucial a requirement as completeness, and once an explicitly defined complete set is available the discussion of physical properties may proceed not only through the use of group theory but also through the more usual analytic procedures of quantum theory. In this connection, non-orthogonal states have already been used by Löwden (1964).

In the present paper a solution of the essential part of the problem is presented.

II. The Coupling Scheme

The scheme is based upon the following resolution of the integral over a product of rotation matrices $\mathfrak{D}^{[j]}{}_{m'm}(R)$

$$\int \mathfrak{D}^{[j_1]}{}_{m_1' m_1}(R)\ \mathfrak{D}^{[j_2]}{}_{m_2' m_2}(R)\ \ldots \mathfrak{D}^{[j_n]}{}_{m_n' m_n}(R)\,\mathrm{d}R$$

$$= \left[\int \mathrm{d}R\right] \sum_{\{\alpha\}} S\begin{pmatrix} j_1\ j_2\ \cdots\ j_n \\ m_1'\, m_2' \ldots m_n' \end{pmatrix}\{\alpha\}\Big) S\begin{pmatrix} j_1\ j_2\ \cdots\ j_n \\ m_1\, m_2 \ldots m_n \end{pmatrix}\{\alpha\}\Big) . \tag{2.1}$$

The details of definitions and the proof of this formula will be given in Section III. At present it is sufficient to note that the symbols S represent real numbers and $\{\alpha\}$ stands for a set of numbers determined by all the j's but independent of the m's. The sum is over all the sets $\{\alpha\}$.

In view of the completeness of the rotation matrices, equation (2.1) is equivalent to the relation

$$\mathfrak{D}^{[j_1]}{}_{m_1' m_1}(R)\, \mathfrak{D}^{[j_2]}{}_{m_2' m_2}(R) \ldots \mathfrak{D}^{[j_n]}{}_{m_n' m_n}(R)$$

$$= \sum_{\{\alpha\}JMM'} \bar{S}(\mathbf{m}_n'|\{\alpha\}JM')\, \mathfrak{D}^{[J]}{}_{M'M}(R)\, \bar{S}(\mathbf{m}_n|\{\alpha\}JM) , \tag{2.2}$$

where

$$\bar{S}(\mathbf{m}_n|\{\alpha\}JM) \equiv (-1)^{J+M}(2J+1)^{\frac{1}{2}}\, S\left(\begin{matrix} j_1\ j_2\ \cdots\ j_n & J \\ m_1\, m_2 \ldots m_n & -M \end{matrix}\{\alpha\}\right) . \tag{2.3}$$

Equation (2.1) in its turn can be recovered from (2.2) by noting that, since $(J+M)$ is always an integer, $(-1)^{2J+M+M'} = (-1)^{M'-M}$ and

$$\mathfrak{D}^{[J]*}{}_{M'M} = (-1)^{M'-M}\, \mathfrak{D}^{[J]}{}_{-M'-M} , \tag{2.4}$$

and using the orthogonality property of the $\mathfrak{D}$'s.

The basic eigenvector $|jm\rangle$ of angular momentum transforms according to the relation (e.g. Rose 1957, p. 52)

$$|jm\rangle_R = \sum_{m'=-j}^{+j} \mathfrak{D}^{[j]}{}_{m'm}(R)\, |jm'\rangle , \tag{2.5}$$

where the subscript R on the left-hand side shows that the eigenvector is expressed in coordinates obtained by rotating the coordinates of $|jm\rangle$ by R.

The corresponding relation for a product of such vectors,

$$|\mathbf{m}_n\rangle \equiv |j_1 m_1\rangle\, |j_2 m_2\rangle \ldots |j_n m_n\rangle\,, \tag{2.6}$$

is

$$|\mathbf{m}_n\rangle_R = \sum_{\mathbf{m}'_n} \mathfrak{D}^{[j_1]}{}_{m'_1\, m_1}(R)\, \mathfrak{D}^{[j_2]}{}_{m'_2\, m_2}(R) \ldots \mathfrak{D}^{[j_n]}{}_{m'_n\, m_n}(R)\, |\mathbf{m}'_n\rangle\,. \tag{2.7}$$

From (2.2)

$$|\mathbf{m}_n\rangle_R = \sum_{\{\alpha\}JMM'} \bar{S}(\mathbf{m}_n|\{\alpha\}JM)\, \mathfrak{D}^{[J]}{}_{M'M}(R) \sum_{\mathbf{m}_n} \bar{S}(\mathbf{m}'_n|\{\alpha\}JM')\, |m'_n\rangle\,. \tag{2.8}$$

One may now define

$$|\{\alpha\}JM\rangle_R \equiv |\{\alpha\}j_1 j_2 \ldots j_n\, JM\rangle_R$$

$$= \sum_{M'} \mathfrak{D}^{[J]}{}_{M'M}(R) \sum_{\mathbf{m}'_n} \bar{S}(\mathbf{m}'_n|\{\alpha\}JM')\, |\mathbf{m}'_n\rangle\,. \tag{2.9}$$

Since

$$\mathfrak{D}^{[J]}{}_{M'M}(0) = \delta_{M'M}\,, \tag{2.10}$$

$$|\{\alpha\}JM\rangle = \sum_{\mathbf{m}_n} \bar{S}(\mathbf{m}_n|\{\alpha\}JM)\, |\mathbf{m}_n\rangle\,. \tag{2.11}$$

Equations (2.9) and (2.11) prove the transformation law for $|\{\alpha\}JM\rangle$ and show that they are the eigenfunctions of total angular momentum J^2 and its z component J_z (see Appendix). The overlap integral of two such eigenfunctions is a number and is therefore equal to its own average under rotations. Hence it follows that

$$\langle\{\alpha'\}J'M'|\{\alpha\}JM\rangle = \sum_{\mathbf{m}_n} \bar{S}(\mathbf{m}_n|\{\alpha'\}J'M')\, \bar{S}(\mathbf{m}_n|\{\alpha\}JM)$$

$$= \delta_{JJ'}\, \delta_{MM'}\, \langle\alpha'|\alpha\rangle^{j_1 j_2 \ldots j_n J}, \tag{2.12}$$

$$\langle\alpha'|\alpha\rangle^{j_1 j_2 \ldots J} = \frac{1}{2J+1} \sum_{\mathbf{m}_n M} \bar{S}(\mathbf{m}_n|\{\alpha'\}JM)\, \bar{S}(\mathbf{m}_n|\{\alpha\}JM)\,. \tag{2.13}$$

In relation (2.12) we have used (2.11) and the orthogonality of $|j_i m_i\rangle$, whereas in (2.13) we have used (2.9) and have averaged over all rotations. It is seen that $|\{\alpha\}JM\rangle$ need not be orthogonal with respect to $\{\alpha\}$, which is the characteristic feature of the problem, whenever $n \geqslant 3$. In coupling n angular momenta one needs an $\bar{S}$ coefficient, which by (2.3) is equivalent to an S coefficient of order $n+1$. The notation (2.3) was chosen to conform to that in transformation theory, as from (2.11) and the orthogonality of $|j_i m_i\rangle$

$$\langle\mathbf{m}_n|\{\alpha\}JM\rangle = \bar{S}(\mathbf{m}_n|\{\alpha\}JM). \tag{2.14}$$

These coefficients are real and occur also in the transformation formula that expresses $|\mathbf{m}_n\rangle$ in terms of $|\{\alpha\}JM\rangle$. By (2.8) and (2.9)

$$|\mathbf{m}_n\rangle = \sum_{\{\alpha\}JM} \bar{S}(\mathbf{m}_n|\{\alpha\}JM)\, |\{\alpha\}JM\rangle\,. \tag{2.15}$$

Since the set $|\mathbf{m}_n\rangle$ is complete, this relation shows the completeness of the new set $|\{\alpha\}JM\rangle$. Using (2.11) on the right-hand side, this gives

$$\sum_{\{\alpha\}JM} \bar{S}(\mathbf{m}_n|\{\alpha\}JM)\,\bar{S}(\mathbf{m}'_n|\{\alpha\}JM) = \delta_{m'_1 m_1}\,\delta_{m'_2 m_2}\ldots\delta_{m'_n m_n}\,. \tag{2.16}$$

Multiplying by $\langle\{\alpha'\}JM|$ and using (2.12),

$$\begin{aligned}\langle\{\alpha'\}JM|\mathbf{m}_n\rangle &\equiv \bar{S}(\mathbf{m}_n|\{\alpha'\}JM)\\ &= \sum_{\{\alpha\}} \bar{S}(\mathbf{m}_n|\{\alpha\}JM)\,\langle\alpha'|\alpha\rangle^{j_1 j_2\ldots j_n J}\,.\end{aligned} \tag{2.17}$$

By using the Schmidt process an orthogonal set $|aJM\rangle$ may be constructed from the $|\{\alpha\}JM\rangle$. The constant coefficients that determine the linear relation between these two sets are in general not unique but depend upon how the orthogonalization is carried out. One can then write

$$|aJM\rangle = \sum_{\{\alpha\}} A_{a\{\alpha\}}\,|\{\alpha\}JM\rangle\,, \tag{2.18}$$

and

$$\langle a'J'M'|aJM\rangle = \delta_{aa'}\,\delta_{JJ'}\,\delta_{MM'}\,. \tag{2.19}$$

One can now select arbitrary numbers $\omega(a)$ and construct the operator

$$\sum_{aJM} |aJM\rangle\omega(a)\langle aJM|\,. \tag{2.20}$$

This operator is diagonal in the new scheme simultaneously with the operators $j_1^2, j_2^2, \ldots j_n^2, J^2$, and J_z. If the numbers $\omega(a)$ are chosen distinct, they may be used to label the eigenfunctions in place of a. The formal problem is thus fully solved.

These relations follow from the form of equation (2.1) and the orthogonality and completeness of the set $|\mathbf{m}_n\rangle$, and give a sufficient indication of how various schemes, orthogonal or non-orthogonal, may be set up and used once the coefficients S are explicitly given.

It may also be noted that the calculations, for which the coefficients of fractional parentage were introduced, can be carried out in the present scheme. Consider a many-particle system that is sought to be described on a single-particle basis. The basic wave functions are $|x_i, j_i m_i\rangle$, where x_i are the particle coordinates. The matrix element of any arbitrary operator $\mathcal{O}(x)$ with respect to the many-body eigenfunctions of total angular momentum is then related to the corresponding matrix element in the product basis by means of the coefficients $\bar{S}$. From (2.11)

$$\begin{aligned}\langle\{\alpha'\}J'M'|\mathcal{O}(x)|\{\alpha\}JM\rangle = \sum_{\mathbf{m}_n \mathbf{m}'_n} &\bar{S}(\mathbf{m}'_n|\{\alpha'\}J'M')\,\bar{S}(\mathbf{m}_n|\{\alpha\}JM)\\ &\times\langle\mathbf{x}_n, \mathbf{m}'_n|\mathcal{O}(x)|\mathbf{x}_n, \mathbf{m}_n\rangle\,.\end{aligned} \tag{2.21}$$

In particular $\mathcal{O}(x)$ may contain the permutation operator. Equation (2.21) thus contains calculations with any type of permutation symmetry. Further, since the numbers $A_{a\{\alpha\}}$ (see (2.18)) are also independent of the particle indices, the same argument may be used in evaluating the matrix elements in the basis $|aJM\rangle$.

III. Derivation of the Equation (2.1)

(a) *The Rotation Matrix*

The phase convention and the definition of Euler angles given by Fano and Racah (1959) are used. Accordingly

$$\mathfrak{D}^{[j]}{}_{\mu m} = \mathfrak{D}^{(j)*}{}_{\mu m} = \exp\{-\mathrm{i}(\mu\psi+m\phi)\}$$
$$\times \sum_r (-1)^r \frac{[(j+\mu)!\,(j-\mu)!\,(j+m)!\,(j-m)!]^{\frac{1}{2}}}{(j-\mu-r)!\,(j+m-r)!\,r!\,(r+\mu-m)!}$$
$$\times (\cos\tfrac{1}{2}\theta)^{2j-\mu+m-2r}(\sin\tfrac{1}{2}\theta)^{2r+\mu-m}. \tag{3.1}$$

If we take

$$\mathbf{q} \equiv (q_1, q_2, q_3, q_4); \qquad q^2 \equiv (\mathbf{q}\,.\,\mathbf{q}) = q_1^2+q_2^2+q_3^2+q_4^2, \tag{3.2}$$

$$\mathbf{A} \equiv (A^1, A^2, A^3, A^4),$$

$$A^1 = \mathrm{i}(s+t), \qquad A^2 = (s-t), \qquad A^3 = \mathrm{i}(1-st), \qquad A^4 = (1+st), \tag{3.3}$$

then,

$$\mathbf{A}\,.\,\mathbf{A} \equiv 0. \tag{3.4}$$

Then according to the posthumously published accounts of some work by G. Herglotz (Courant and Hilbert 1953; Erdélyi *et al.* 1953), the rotation matrix (3.1) may be generated from the following relation

$$(\mathbf{q}\,.\,\mathbf{A})^{2j} \equiv \{\mathrm{i}(s+t)q_1+(s-t)q_2+\mathrm{i}(1-st)q_3+(1+st)q_4\}^{2j}$$
$$= q^{2j}(st)^j \sum_{\mu,m=-j}^{+j} s^\mu t^m N^j_{\mu m}\,\mathfrak{D}^{[j]}{}_{\mu m}. \tag{3.5}$$

A binomial expansion of the left-hand side is facilitated by introducing the complex quantities

$$a \equiv |a|\exp\mathrm{i}\rho = (q_2+\mathrm{i}q_1)/q, \tag{3.6}$$

$$b \equiv |b|\exp\mathrm{i}\sigma = (q_4+\mathrm{i}q_3)/q. \tag{3.7}$$

Comparing the coefficients of the powers of s and t, one obtains

$$N^j_{\mu m}\,\mathfrak{D}^{[j]}{}_{\mu m} = \exp\{\mathrm{i}\rho(\mu-m)\}\exp\{-\mathrm{i}\sigma(m+\mu)\}$$
$$\times \sum_r (-1)^r \frac{(2j)!\,|b|^{2j-\mu+m-2r}\,|a|^{2r+\mu-m}}{(j-\mu-r)!\,(j+m-r)!\,r!\,(r+\mu-m)!}. \tag{3.8}$$

The following identifications can be made on comparing with (3.1)

$$N^j_{\mu m} = (2j)!\,[(j+\mu)!\,(j-\mu)!\,(j+m)!\,(j-m)!]^{-\frac{1}{2}}$$
$$= [N^j_{\mu\mu}N^j_{mm}]^{\frac{1}{2}}, \tag{3.9}$$

$$\psi = \sigma-\rho; \qquad \phi = \rho+\sigma; \qquad \theta = 2\tan^{-1}(|a|/|b|) \tag{3.10}$$

Corresponding to the range of Euler angles, the new angles have the ranges

$$0 \leqslant \sigma, \qquad (\rho+\pi) \leqslant 2\pi, \qquad 0 \leqslant \theta \leqslant \pi. \tag{3.11}$$

Since from (3.6) and (3.7)

$$\left.\begin{aligned} q_1 &= q \sin \tfrac{1}{2}\theta \sin \rho, & q_2 &= q \sin \tfrac{1}{2}\theta \cos \rho, \\ q_3 &= q \cos \tfrac{1}{2}\theta \sin \sigma, & q_4 &= q \cos \tfrac{1}{2}\theta \cos \sigma, \end{aligned}\right\} \tag{3.12}$$

it follows that the variables q, σ, $(\rho+\pi)$, and $\frac{1}{2}\theta$ provide an orthogonal system of coordinates in four-dimensional Euclidean space of $\mathbf{q}$. The element of integration over the hypersphere $\mathrm{d}\Omega$ (Courant and Hilbert 1953), however, differs from the corresponding volume element of the rotation group by a factor

$$\begin{aligned} \mathrm{d}R &\equiv \sin\theta \,\mathrm{d}\theta \,\mathrm{d}\psi \,\mathrm{d}\phi = 4\,\mathrm{d}\Omega \\ &\equiv 4 \sin \tfrac{1}{2}\theta \cos \tfrac{1}{2}\theta \,\mathrm{d}(\tfrac{1}{2}\theta)\,\mathrm{d}(\rho+\pi)\,\mathrm{d}\sigma. \end{aligned} \tag{3.13}$$

The above manipulations can be carried out if $(2j)$ is an integer. Thus j itself can take on values $0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$ and, for a given j, m varies in steps of one from $-j$ to $+j$. We further note that

$$\int \mathrm{d}R = 8\pi^2, \tag{3.14}$$

and the normalization is such that

$$\mathfrak{D}^{[0]}{}_{00} = 1 \tag{3.15}$$

and

$$\int \mathfrak{D}^{[j']}{}_{\mu'm'}\, \mathfrak{D}^{(j)}{}_{\mu m}\, \mathrm{d}R = \left\{\frac{8\pi^2}{(2j+1)}\right\} \delta_{jj'}\, \delta_{\mu\mu'}\, \delta_{mm'}. \tag{3.16}$$

(b) *An Integral over Products of* $\mathrm{q_i}$

The following formula is needed in the derivation of the final result

$$\left.\begin{aligned} \int q_{i_1} q_{i_2} \ldots q_{i_n}\, \mathrm{d}R &= 0 && n \text{ odd}, \\ &= \frac{16\pi^2 q^n}{(n+2)!!} \sum_{\text{products}} \left(\prod_{\text{pairs}} \delta_{i_k i_l}\right) && n \text{ even}. \end{aligned}\right\} \tag{3.17}$$

To prove this, note that in view of the completeness of the hyperspherical harmonics $\mathfrak{D}^{[j]}$ we may expand

$$q_{\mathbf{i}_n} \equiv q_{i_1} q_{i_2} \cdots q_{i_n} = \sum_{j\mu m} (j\mu m|\mathbf{i}_n)\, q^n\, \mathfrak{D}^{[j]}{}_{\mu m}. \tag{3.18}$$

From the orthogonality relation (3.16) the coefficients of the expansion become

$$(j\mu m|\mathbf{i}_n) = \left\{\frac{8\pi^2 q^n}{2j+1}\right\}^{-1} \int q_{\mathbf{i}_n}\, \mathfrak{D}^{(j)}{}_{\mu m}\, \mathrm{d}R. \tag{3.19}$$

The integral (3.17) is thus proportional to the constant $(000|\mathbf{i}_n)$, which will now be evaluated using a general property of these coefficients.

From the generating function (3.5) it may be shown that

$$\nabla^2(q^n \mathfrak{D}^{[j]}{}_{\mu m}) = (n-2j)(n+2j+2)q^{n-2}\mathfrak{D}^{[j]}{}_{\mu m}, \tag{3.20}$$

where

$$\nabla^2 \equiv \sum_{i=1}^{4} \partial^2/\partial q_i \partial q_i = \sum_{i,j=1}^{4} \delta_{ij}\partial^2/\partial q_i \partial q_j. \tag{3.21}$$

Applying this relation r times to (3.18) and using the orthogonality relations, the following relation between the coefficients is obtained

$$(j\mu m|\mathbf{i}_n) = \frac{(n-2j-2r)!!\,(n+2j+2-2r)!!}{(n-2j)!!\,(n+2j+2)!!}\sum_{\mathrm{p}}(j\mu m|\mathbf{l}_{n-2r})\,\delta_{k_1 k_2}\delta_{k_3 k_4}\ldots\delta_{k_{2r-1},k_{2r}}, \tag{3.22}$$

where the sum over p is the sum over all arrangements of the indices $\mathbf{i}_n \equiv i_1 i_2 \ldots i_n$, in the indicated manner.

The maximum possible value of $2r$ is $n-2j$. Thus, for $j=0$, the coefficient may be reduced completely to a sum over products of delta functions if n is even. If n is odd, it must naturally vanish. In the former case, the sum over p becomes an unrestricted sum over all permutations of the indices $\mathbf{i}_n$ in which any given product of pairs is repeated $n!!$ times. This is because the same set of $(\frac{1}{2}n)$ pairs occurs $(\frac{1}{2}n)!$ times and each pair itself appears twice in free permutations,

$$2^{\frac{1}{2}n}(\tfrac{1}{2}n)! = n!!. \tag{3.23}$$

Hence finally, from (3.22),

$$\left.\begin{aligned}(000|\mathbf{i}_n) &= \frac{2}{(n+2)!!}\sum_{\text{products}}\Big(\prod_{\text{pairs}}\delta_{i_k i_l}\Big) && n \text{ even},\\ &= 0 && n \text{ odd}.\end{aligned}\right\} \tag{3.24}$$

With (3.19) this proves (3.17).

(c) *An Integral over Products of Generating Functions*

Consider the integral

$$8\pi^2 q^{2J} I_n = \int (\mathbf{q}\,.\,\mathbf{A}_1)^{2j_1}(\mathbf{q}\,.\,\mathbf{A}_2)^{2j_2}\ldots(\mathbf{q}\,.\,\mathbf{A}_n)^{2j_n}\,\mathrm{d}R, \tag{3.25}$$

where*

$$J = \sum_{1}^{n} j_i \tag{3.26}$$

and

$$\mathbf{A}_k \equiv \{\mathrm{i}(s_k+t_k);\,(s_k-t_k);\,\mathrm{i}(1-s_k t_k);\,(1+s_k t_k)\}. \tag{3.27}$$

* Note that the symbol J in this and the subsequent sections has a significance different from that in Section II and the Appendix.

By using the summation convention, we may write

$$(\mathbf{q}\,.\,\mathbf{A})(\mathbf{q}\,.\,\mathbf{B}) = A^i B^j q_i q_j, \qquad i,j = 1,2,3,4.$$

Using this repeatedly and applying (3.17), we obtain

$$\left.\begin{aligned} I_n &= \frac{2}{(2J+2)!!} \sum_{\text{products}} \Bigl(\prod_{\text{pairs}} (\mathbf{A}_k\,.\,\mathbf{A}_l)\Bigr), && 2J \text{ even},\\ &= 0, && 2J \text{ odd}. \end{aligned}\right\} \tag{3.28}$$

The products of pairs that are distinct as partitions of the indices $\mathbf{i}_{2J}$ give rise to products of scalar products $(\mathbf{A}_k\,.\,\mathbf{A}_l)$ that are repeated many times in the sum, since the vector $\mathbf{A}_k$ can occur in $(2j_k)!$ ways. Each product of scalar products may be characterized by a set of exponents α_{kl} of the scalar product $(\mathbf{A}_k\,.\,\mathbf{A}_l)$; and is repeated $w(\{\alpha\})$ times in the sum

$$w(\{\alpha\}) = (2j_1)!\,(2j_2)!\dots(2j_n)!\Bigl(\prod_{k<l} (\alpha_{kl})!\Bigr)^{-1}. \tag{3.29}$$

Then for $2J$ even, (3.28) may be written as

$$I_n = \frac{2^{-J}}{(J+1)!} \sum_{\{\alpha\}} \Bigl\{w(\{\alpha\})\Bigl(\prod_{k<l} (\mathbf{A}_k\,.\,\mathbf{A}_l)^{\alpha_{kl}}\Bigr) \prod_{k=1}^{n} \delta\Bigl(\sum_l \alpha_{kl}, 2j_k\Bigr)\Bigr\}. \tag{3.30}$$

The delta functions ensure that the correct number of vectors $\mathbf{A}_k$ occur in the product and the restriction $k<l$ ensures that no pairs are counted twice. The numbers α_{kl} take on all integral values allowed by the delta functions and the factorials. Since $(\mathbf{A}_k\,.\,\mathbf{A}_l) \equiv 0$, we must always have $\alpha_{kk} = 0$, that is, we have

$$\alpha_{kl} \equiv \alpha_{lk}, \qquad \alpha_{kk} \equiv 0, \qquad 0 \leqslant \alpha_{kl} \leqslant \min(2j_k, 2j_l), \tag{3.31}$$

and the restrictions from comparing the powers, i.e. from the delta functions, are

$$\left.\begin{aligned} -2j_1+\alpha_{12}+\alpha_{13}+\alpha_{14}+\dots+\alpha_{1n} &= 0,\\ \alpha_{12}-2j_2+\alpha_{23}+\alpha_{24}+\dots+\alpha_{2n} &= 0,\\ \dots\dots\dots\dots\dots\dots\dots\dots&\\ \alpha_{1n}+\alpha_{2n}+\dots+\alpha_{n-1,n}-2j_n &= 0. \end{aligned}\right\} \tag{3.32}$$

This implies that

$$\sum_{k<l=1}^{n} \alpha_{kl} = \sum_{k=1}^{n} j_k \equiv J \qquad \text{is an integer}. \tag{3.33}$$

Since from (3.27)

$$\mathbf{A}_k\,.\,\mathbf{A}_l = 2(s_k-s_l)(t_k-t_l), \tag{3.34}$$

we may write for (3.29)

$$I_n = [(J+1)!]^{-1} \sum_{\{\alpha\}} \Bigl\{w(\{\alpha\})\Bigl(\prod_{k<l} (s_k-s_l)^{\alpha_{kl}}\,(t_k-t_l)^{\alpha_{kl}}\Bigr) \prod_{k=1}^{n} \delta\Bigl(\sum_l \alpha_{kl}, 2j_k\Bigr)\Bigr\}. \tag{3.35}$$

The number of α's is $\frac{1}{2}n(n-1)$ and hence in general there will be a number of sets of values of α that will satisfy the requirements (3.31) and (3.32). However, for the case $n = 2$ and $n = 3$, all the values of α's are fixed and the sum disappears. For $n = 2$, $2j_1 = \alpha_{12} = 2j_2$ and

$$I_2 = (2j_1+1)^{-1}\,\delta(j_1,j_2)\,(s_1-s_2)^{2j_1}(t_1-t_2)^{2j_2}, \tag{3.36}$$

from which the orthogonality relations (3.16) may be verified.

For $n = 3$, equations (3.32) give

$$\left.\begin{aligned} \alpha_{12} = J-2j_3, \qquad \alpha_{23} = J-2j_1, \qquad \alpha_{13} = J-2j_2,\\ J = j_1+j_2+j_3, \end{aligned}\right\} \tag{3.37}$$

and

$$I_3 = \frac{(2j_1)!\,(2j_2)!\,(2j_3)!}{(J+1)!\,(J-2j_1)!\,(J-2j_2)!\,(J-2j_3)!}$$
$$\times (s_1-s_2)^{J-2j_3}(s_2-s_3)^{J-2j_1}(s_3-s_1)^{J-2j_2}(t_1-t_2)^{J-2j_3}(t_2-t_3)^{J-2j_1}(t_3-t_1)^{J-2j_2}. \tag{3.38}$$

(*d*) *Proof of the Resolution on the Right-hand Side of Equation* (2.1)

From the generating function (3.5), it follows that the integral in equation (2.1) is obtained by picking out the coefficient of

$$s_1^{j_1+m_1'}\,s_2^{j_2+m_2'}\ldots s_n^{j_n+m_n'}\,t_1^{j_1+m_1}\,t_2^{j_2+m_2}\ldots t_n^{j_n+m_n}\,N^{j_1}_{m_1'm_1}\ldots N^{j_n}_{m_n'm_n}$$

in the expression for the integral (3.25). This coefficient is obtained by expanding (3.35) for I_n by the binomial theorem and using delta functions to collect the coefficients of powers. It is

$$\frac{w(\{\alpha\})}{(J+1)!}\sum_{\{\alpha,\beta,\gamma\}}\left\{\left[\prod_{k<l}(-1)^{\beta_{kl}+\gamma_{kl}}\binom{\alpha_{kl}}{\beta_{kl}}\binom{\alpha_{kl}}{\gamma_{kl}}\right]\right.$$
$$\times\prod_{k=1}^{n}\left[\delta\Big(\sum_l \alpha_{kl}, 2j_k\Big).\,\delta\Big(\sum_{l=k+1}^{n}\beta_{kl}+\sum_{l=1}^{k-1}(\alpha_{kl}-\beta_{kl});\,j_k+m_k'\Big)\right.$$
$$\left.\left.\times\,\delta\Big(\sum_{l=k+1}^{n}\gamma_{kl}+\sum_{l=1}^{k-1}(\alpha_{kl}-\gamma_{kl});\,j_k+m_k\Big)\right]\right\}. \tag{3.39}$$

Since the Kronecker deltas used here are idempotent, $\delta(l,k) = [\delta(l,k)]^2$, the summand over $\{\alpha\}$ may be resolved in the product of two factors, one containing all the dependence on the indices m_k' and the other containing all the dependence on the indices m_k; the former being the sum over $\{\beta\}$, the latter that over $\{\gamma\}$. It is clear that these factors are both identical in structure and are real. This is the essence of equation (2.1) and allows the coupling scheme discussed in Section II.

IV. The Coefficient of Symmetrical Coupling

In this section some further properties of the coefficients S and an explicit formula for them will be given. It is appropriate to begin with some explanatory remarks.

(a) *Explanation of the Label* $\{\alpha\}$

By comparing (3.39) and (2.1), the symbol $\{\alpha\}$ is seen to stand for a set of values of the $\frac{1}{2}n(n-1)$ numbers α_{kl}; $k, l = 1, 2, 3, \ldots n$. A set of values that satisfies the conditions (3.31) and (3.32) characterizes a non-vanishing coefficient S. The sum in (2.1) is over all such sets of values of $\{\alpha\}$. The coefficients S are symmetric with respect to j_i in the sense that any set of values $\{\alpha\}$ is determined jointly by all the j's. The number of possible sets depends on the numerical values of the j's that are to be coupled. The numbers $\{\alpha\}$ are independent of the m's.*

(b) *Phase Convention, Generating Function, and Explicit Formula*

In equation (3.35) the factor (t_k-t_l) is always associated with (s_k-s_l) so that an interchange of k and l does not produce a change of sign. To obtain an expression for the S coefficients, the s and t parts are to be separated. To fix the sign of the S coefficients and to exhibit their properties under interchange of indices, it is then required to adopt a (phase) convention that specifies the manner in which the indices k, l are to be arranged. It is convenient to associate simple properties with even or odd permutations.

We shall adopt the following convention: if k and l are two numbers out of the sequence $1, 2, 3, \ldots n$ such that the pair sequence k, l can be obtained by an even number of binary interchanges in the sequence, then the negative sign will be associated with l. Thus in the standard arrangement a (t_k-t_l) factor occurs when kl can be brought next to each other, in that order, by an even number of binary interchanges.

* At this point we may note the relation to Löwden's (1964) approach, which also uses non-orthogonal bases, which are obtained by applying an angular momentum projection operator Λ_{JM} to a product wave function. By (2.15), or the resolution of the identity given by (2.16), the matrix elements of this operator are

$$\langle \mathbf{m}'_n | \Lambda_{JM} | \mathbf{m}_n \rangle = \sum_{\{\alpha\}} \bar{S}(\mathbf{m}_n|\{\alpha\}JM)\, \bar{S}(\mathbf{m}'_n|\{\alpha\}JM).$$

Hence, Löwden's non-orthogonal sets may be written as

$$\Theta\mathbf{m}_n(JM) = \sum_{\mathbf{m}'_n} \langle \mathbf{m}'_n | \Lambda_{JM} | \mathbf{m}_n \rangle\, |\mathbf{m}'_n\rangle.$$

For a given JM the degeneracy is here removed by using the sets $\mathbf{m}_n$ themselves as labels. This is adequate, but shows the difference between the two approaches as $\{\alpha\}$ are independent of m's altogether. With the present scheme it is possible to go along very much as with the Wigner coefficients and to express all relations quite generally.

Denoting a product in the standard order by Π^e, we obtain the generating function of S coefficients from equation (3.35) as

$$\left[\frac{w(\{\alpha\})}{(J+1)!}\right]^{\frac{1}{2}}\left[\prod_{k,l}^{e}(t_k-t_l)^{\alpha_{kl}}\right]\prod_{k=1}^{n}\delta\left(\sum_l \alpha_{kl}, 2j_k\right)$$

$$= \sum_{m_1\ldots m_n} t_1^{j_1+m_1}t_2^{j_2+m_2}\ldots t_n^{j_n+m_n}\left[N^{j_1}_{m_1\,m_1}N^{j_2}_{m_2\,m_2}\ldots N^{j_n}_{m_n\,m_n}\right]^{\frac{1}{2}}$$

$$\times S\begin{pmatrix} j_1\; j_2 \cdots j_n \\ m_1\, m_2 \ldots m_n \end{pmatrix}\{\alpha\}\Bigg). \tag{4.1}$$

Hence, or from (3.39),

$$S\begin{pmatrix} j_1\; j_2 \cdots j_n & \{\alpha\} \\ m_1\, m_2 \ldots m_n & \end{pmatrix} = \left[(J+1)!\,N^{j_1}_{m_1\,m_1}N^{j_2}_{m_2\,m_2}\ldots N^{j_n}_{m_n\,m_n}\right]^{-\frac{1}{2}}$$

$$\times\left[w(\{\alpha\})\right]^{\frac{1}{2}}\left[\prod_{k=1}^{n}\delta\left(\sum_l \alpha_{kl}, 2j_k\right)\right]$$

$$\times\sum_{\{\beta_{kl}\}}\left\{\left[\prod_{k,l}^{e}(-1)^{\beta_{kl}}\binom{\alpha_{kl}}{\beta_{kl}}\right]\prod_{k=1}^{n}\delta\left(\sum(\tfrac{1}{2}\alpha_{kl}-\beta_{kl})\epsilon_{kl}\,; m_k\right)\right\}. \tag{4.2}$$

In arriving at the second set of delta functions we have made use of the restrictions implied by the first set. The appearance of the factor ϵ_{kl} is a result of balancing the powers of the t's and the phase convention. If we call a pair even or odd as set out in the convention, then

$$\left.\begin{aligned} \epsilon_{kl} &= +1 \quad \text{for } k,l \text{ even,} \\ \epsilon_{kl} &= -1 \quad \text{for } k,l \text{ odd,} \\ \epsilon_{kl} &= -\epsilon_{lk}\,. \end{aligned}\right\} \tag{4.3}$$

The restrictions on the β's may be written more explicitly as

$$\left.\begin{array}{l} -m_1 \qquad +(\tfrac{1}{2}\alpha_{12}-\beta_{12})-(\tfrac{1}{2}\alpha_{13}-\beta_{13})+\ldots+\epsilon_{1n}(\tfrac{1}{2}\alpha_{1n}-\beta_{1n}) = 0, \\ -(\tfrac{1}{2}\alpha_{12}-\beta_{12})-m_2 \qquad +(\tfrac{1}{2}\alpha_{23}-\beta_{23})+\ldots+\epsilon_{2n}(\tfrac{1}{2}\alpha_{2n}-\beta_{2n}) = 0, \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \epsilon_{n1}(\tfrac{1}{2}\alpha_{1n}-\beta_{1n})+\epsilon_{n2}(\tfrac{1}{2}\alpha_{2n}-\beta_{2n})+\ldots+\tfrac{1}{2}(\alpha_{n-1,n}-\beta_{n-1,n})-m_n = 0. \end{array}\right\} \tag{4.4}$$

The appearance of $\frac{1}{2}\alpha_{kl}$ corresponds to the fact that, although α_{kl}, β_{kl}, and $(j_k \pm m_k)$ are all required to be integers, both j_k and m_k by themselves can either be integers or half of odd integers.

Also,

$$0 \leqslant \beta_{kl} \leqslant \alpha_{kl}\,. \tag{4.5}$$

If for a given set of m's no β's in this range satisfy the equations (4.4), then the corresponding coefficient must vanish.

(c) *Some Further Properties of the Coupling Coefficients*

In Section II some properties of the S coefficients were derived that are consequences of equation (2.1) and the properties of rotation matrices. Properties to be mentioned here are related to their explicit form.

The coefficient vanishes unless, from (3.33),

$$J \equiv \sum_1^n j_k = \sum_{k<l}^n \alpha_{kl} \qquad \text{is a positive integer;} \tag{4.6a}$$

hence, from (3.32),

$$j_k \leqslant \sum_{l \neq k} j_l \tag{4.6b}$$

and, from (4.4),

$$\sum_1^n m_k = 0. \tag{4.7}$$

From the generating function (4.1) it is seen that an interchange of any two columns, say, (j_k, m_k) and (j_l, m_l) is equivalent to interchanging t_k and t_l. This can at most alter the sign of the expression, since $\{\alpha\}$ are determined by all the j's in a symmetric fashion. Because of the phase convention and (3.32)

$$S\begin{pmatrix} j_1 \cdots j_k \cdots j_l \cdots j_n \\ m_1 \ldots m_k \ldots m_l \ldots m_n \end{pmatrix}\{\alpha\} = (-1)^{2(j_k+j_l)-\alpha_{kl}} S\begin{pmatrix} j_1 \cdots j_l \cdots j_k \cdots j_n \\ m_1 \ldots m_l \ldots m_k \ldots m_n \end{pmatrix}\{\alpha\}. \tag{4.8}$$

By (4.5), reversing the signs of all the m's is equivalent to changing the sign in all pairs $(t_k - t_l)$ in the generating function. Hence by (4.6)

$$S\begin{pmatrix} j_1\ j_2 \cdots j_n \\ m_1\, m_2 \ldots m_n \end{pmatrix}\{\alpha\} = \left(-1\right)^{\sum_1^n j_k} S\begin{pmatrix} j_1 & j_2 & \cdots j_n \\ -m_1 & -m_2 \ldots & -m_n \end{pmatrix}\{\alpha\}. \tag{4.9}$$

For $n = 3$, because of (3.37) both operations have the same parity $(-1)^J$, which is a known property of the $3j$ symbols and is now seen to be peculiar to that case only.

Recursion relations and summation properties involving coefficients of different orders can be derived using the known relations involving the rotation matrices.

V. Some Applications

(a) *The Case* n = 3

From equation (4.1), or by factorizing (3.38), one obtains a generating function for $3j$ symbols

$$\Big[(J+1)!\,(J-2j_1)!\,(J-2j_2)!\,(J-2j_3)!\Big]^{-\frac{1}{2}} (t_1-t_2)^{J-2j_3}\,(t_2-t_3)^{J-2j_1}\,(t_3-t_1)^{J-2j_2}$$

$$= \sum_{m_1, m_2, m_3} \left\{ \prod_{i=1}^3 \Big[(j_i+m_i)!\,(j_i-m_i)!\Big]^{-\frac{1}{2}} t_i^{j_i+m_i} \right\} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \tag{5.1}$$

Other generating functions for the $3j$ symbols have been obtained and discussed by Schwinger (1952), Regge (1958), Bargmann (1962), and Ansari (1965).

On using the relation between the spherical harmonics and the rotation matrices, equation (2.1) provides an expression for an integral over a product of spherical harmonics. For the special case $n = 3$, the integral may be obtained by collecting the appropriate coefficients in (3.38). The formula for an integral over three spherical harmonics was derived by Gaunt (1929) using recursion relations for associated Legendre polynomials and partial integrations over θ. Another derivation was given by Racah (1942), who used completeness relations and the Wigner–Eckart theorem.

(b) *An Extension of the Wigner–Eckart Theorem*

For the quantum mechanical expectation value of a product of n-tensor operators, a formula analogous to the Wigner–Eckart theorem may be derived by using the argument that led to (2.12).

The transformation law for a tensor operator is

$$T_R{}^{(j)}{}_{m'} = \sum_{m=-j}^{+j} \mathfrak{D}^{(j)}{}_{m'm}(R)\, T^{(j)}{}_m . \tag{5.2}$$

Since the expectation value is an average of itself over rotations, we have

$$\begin{aligned}&\langle \beta' J' M' |\, T^{(j_1)}{}_{m_1} T^{(j_2)}{}_{m_2} \ldots T^{(j_n)}{}_{m_n} | \beta J M \rangle \\ &= \sum_{\{\alpha\}} (-1)^{J+M} S\begin{pmatrix} J' & j_1 & j_2 & \ldots & j_n & J \\ M' & m_1 & m_2 & \ldots & m_n & -M \end{pmatrix}\{\alpha\}\, \langle \beta' J' || T^{(j_1)} T^{(j_2)} \ldots T^{(j_n)} || \beta J \rangle^{\{\alpha\}},\end{aligned} \tag{5.3}$$

where the second factor in the summand is independent of m indices, in fact,

$$\begin{aligned}&\langle \beta' J' || T^{(j_1)} T^{(j_2)} \ldots T^{(j_n)} || \beta J \rangle^{\{\alpha\}} \\ &= \sum_{M \mathbf{m}_n M'} (-1)^{J+M} S\begin{pmatrix} J' & j_1 & j_2 & \ldots & j_n & J \\ M' & m_1 & m_2 & \ldots & m_n & -M \end{pmatrix}\{\alpha\}\, \langle \beta' J' M |\, T^{(j_1)}{}_{m_1} \ldots T^{(j_n)}{}_{m_n} | \beta J M \rangle .\end{aligned} \tag{5.4}$$

In deriving this, the transformation laws (5.2) and (2.5) have been used to express the effect of rotations on the individual factor and the average is performed by using (2.1). The appearance of a factor independent of the m's in (5.3) is a consequence of the separation of the two types of m indices in (2.1). The Wigner–Eckart theorem concerns the case $n = 3$, in which there is no sum over $\{\alpha\}$.

In closing it may be remarked that the greater facility provided by the use of the generating function (3.5) for the rotation matrix may be used in the investigations concerning other objects associated with the rotation group, e.g. the Racah coefficients. The calculations involving spherical harmonics are also simplified by using the corresponding three-dimensional generating functions.

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Appendix

The argument of Section II is restated here in a different form to bring out a point on which caution is needed in using the non-orthogonal sets.

Let the rotation R be represented by a vector $\boldsymbol{\varepsilon}$ such that $|\boldsymbol{\varepsilon}|$ is the angle of rotation and $\boldsymbol{\varepsilon}$ is in the direction of the axis of rotation. Then the rotation operator is explicitly given by

$$\mathrm{D}(R) \equiv \exp(-\mathrm{i}\boldsymbol{\varepsilon}\,.\mathbf{J})\,, \tag{A.1}$$

$$\mathbf{J} = \mathbf{j}_1+\mathbf{j}_2+\ldots+\mathbf{j}_n\,. \tag{A.2}$$

As $R \to 0$; $\boldsymbol{\varepsilon} \to 0$ and $\mathrm{D}(R) \to 1$. Also,

$$[\mathbf{J}^2, \mathrm{D}(R)] = 0\,, \tag{A.3}$$

$$\nabla_\varepsilon \mathrm{D}(R) = -\mathrm{i}\mathbf{J}\,\mathrm{D}(R)\,, \tag{A.4}$$

$$\mathbf{J}^2\,\mathrm{D}(R) = \mathrm{D}(R)\,\mathbf{J}^2 \equiv -\nabla_\varepsilon^2\,\mathrm{D}(R)\,. \tag{A.5}$$

The product of rotation matrices in (2.2) is the matrix element,

$$\langle \mathbf{m}'_n|\,\mathrm{D}(R)|\mathbf{m}_n\rangle \equiv \mathfrak{D}^{[j_1]}{}_{m'_1\,m_1}\ldots\mathfrak{D}^{[j_n]}{}_{m'_n\,m_n}\,. \tag{A.6}$$

Then the following identifications can be consistently made

$$\langle \mathbf{m}'_n | \mathrm{D}(R) | \{\alpha\} JM \rangle = \sum_{M'} \mathfrak{D}^{[J]}{}_{M'M}(R) \, \bar{S}(\mathbf{m}'_n | \{\alpha\} JM') \,, \tag{A.7}$$

$$\langle \{\alpha\} JM | \mathbf{m}_n \rangle = \bar{S}(\mathbf{m}_n | \{\alpha\} JM) \,. \tag{A.8}$$

From the completeness of the system $|\mathbf{m}_n\rangle$, equation (A.7) gives

$$\mathrm{D}(R) | \{\alpha\} JM \rangle = \sum_{M'} \mathfrak{D}^{[J]}{}_{M'M}(R) \sum_{\mathbf{m}_n} \bar{S}(\mathbf{m}_n | \{\alpha\} JM') \, |\mathbf{m}_n\rangle \,. \tag{A.9}$$

This is equation (2.9) with the left-hand side written differently.

To show that $|\{\alpha\} JM\rangle$ are eigenfunctions of $\mathbf{J}^2$, we recall (e.g. Fano and Racah 1959, Appendix E) that

$$\nabla_{\varepsilon}^2 \mathfrak{D}^{[J]}{}_{M'M}(R) = -J(J+1) \, \mathfrak{D}^{[J]}{}_{M'M}(R) \,. \tag{A.10}$$

Then by (A.5) and (A.9)

$$\begin{aligned} \mathbf{J}^2 \mathrm{D}(R) \, | \{\alpha\} JM \rangle &= -\nabla_{\varepsilon}^2 \mathrm{D}(R) \, | \{\alpha\} JM \rangle \\ &= J(J+1) \, \mathrm{D}(R) \, | \{\alpha\} JM \rangle \,. \end{aligned} \tag{A.11}$$

Since the operator $\mathbf{J}^2$ can act only on $|\mathbf{m}_n\rangle$ in (A.9), the coefficient $\bar{S}$ must have the correct properties in J and M to ensure (A.11). It now appears that equations (2.9) and (A.9) are the basic defining equations, and that the functions $|\{\alpha\} JM\rangle$ defined by (2.11) must always be understood as a limit

$$|\{\alpha\} JM\rangle = \lim_{R \to 0} \left(\mathrm{D}(R) \, | \{\alpha\} JM \rangle \right) . \tag{A.12}$$

This is of importance if we apply the rotation operator a second time. Thus

$$\mathrm{D}(R_2) \; | \{\alpha\} JM \rangle = \lim_{R_1 \to 0} \mathrm{D}(R_2) (\mathrm{D}(R_1) \, | \{\alpha\} JM \rangle) \,. \tag{A.13}$$

If the left-hand side is evaluated directly by using (2.11), then it may not be compared with $\mathrm{D}(R_2) \, |\{\alpha\} JM\rangle$ as given by (2.9). Rather the connection with (2.9) is seen by using it on the right-hand side and taking the limit. This inconvenience can be eliminated only by changing to another basis that is orthogonal with respect to all the indices.