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1976 J. Phys. A: Math. Gen. 9 485

(http://iopscience.iop.org/0305-4470/9/4/005)

J. Phys. A: Math. Gen., Vol. 9, No. 4, 1976. Printed in Great Britain. © 1976

Properties of Cartesian-spherical transformation coefficients

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Received 7 April 1975, in final form 18 July 1975

Abstract. In a previous paper, a standard transformation was proposed for expressing Cartesian tensors and tensor expressions in spherical form, and vice versa. In this paper some properties of the transformation coefficients are derived. A recursion formula is given, which provides a simple means of generating the coefficients from those of the next rank below. The coefficients $\langle\alpha_1\ldots\alpha_n|j_1\ldots j_n;m\rangle$ are tabulated for $n\leq 4$, $m=0$ and for $n=5$, $j_n=0$. Another recursion formula gives the coefficients for $m\neq 0$ in terms of those for $m=0$. A graphical method is used to derive formulae for manipulating the coefficients, and formulae are given for handling products of tensors, contracted or uncontracted.

1. Introduction

It is well-known that a Cartesian tensor of rank greater than one can be reduced into several spherical components (e.g. Fano and Racah 1959). Depending on the nature of a calculation, one or the other of these forms may be more suitable, and it is therefore convenient to have a standard transformation for converting a tensor, or a tensor expression, from one form to the other. In a previous paper (Stone 1975) Cartesian-spherical (CS) transformation coefficients were defined by considering a 'polyadic' $A_{\alpha_1}B_{\alpha_2}\ldots Z_{\alpha_n}$. By transforming each of the vectors in this expression to spherical form, and then coupling the spherical vectors together from left to right, one arrives at a recursive definition for the transformation coefficient:

$$\langle\alpha_1\ldots\alpha_n|j_1\ldots j_n;m\rangle=\sum_{m'm''}\langle\alpha_1\ldots\alpha_{n-1}|j_1\ldots j_{n-1};m'\rangle\langle\alpha_n|1;m''\rangle\langle j_{n-1}1m'm''|j_nm\rangle, \tag{1.1}$$

where $\langle j_{n-1}1m'm''|j_nm\rangle$ is a Clebsch–Gordan coefficient and $\langle\alpha|1;m\rangle$ is the unitary matrix

$$\begin{array}{cc} & \begin{array}{ccc}|1;1\rangle & |1;0\rangle & |1;-1\rangle\end{array}\\ \begin{array}{c}\langle x|\\ \langle y|\\ \langle z|\end{array} & \begin{pmatrix}-\sqrt{\tfrac12}\mathrm{i}\kappa & 0 & \sqrt{\tfrac12}\mathrm{i}\kappa\\ \sqrt{\tfrac12}\kappa & 0 & \sqrt{\tfrac12}\kappa\\ 0 & \mathrm{i}\kappa & 0\end{pmatrix}\end{array}. \tag{1.2}$$

Here κ is a phase factor, which is 1 if Fano and Racah's (1959) phase convention is required, or $-\mathrm{i}$ for Condon and Shortley's (1935). The spherical components $T_{j_1\ldots j_n;m}$

of spherical rank j_n of a Cartesian tensor $T_{\alpha_1\ldots\alpha_n}$ of Cartesian rank n are then given by

$$T_{j_1\ldots j_n;m}=\sum_{\alpha_1\ldots\alpha_n} T_{\alpha_1\ldots\alpha_n}\langle\alpha_1\ldots\alpha_n|j_1\ldots j_n;m\rangle, \tag{1.3}$$

and conversely

$$T_{\alpha_1\ldots\alpha_n}=\sum_{j_1\ldots j_n;m} T_{j_1\ldots j_n;m}\langle j_1\ldots j_n;m|\alpha_1\ldots\alpha_n\rangle, \tag{1.4}$$

where

$$\langle j_1\ldots j_n;m|\alpha_1\ldots\alpha_n\rangle=\langle\alpha_1\ldots\alpha_n|j_1\ldots j_n;m\rangle^*, \tag{1.5}$$

so that the transformation is unitary. The subscripts $j_1, j_2\ldots j_{n-1}$ are (sometimes) required to distinguish between different spherical tensors with the same j_n; they can be dropped where no ambiguity results. j_1 is always 1, but is included in the notation for completeness and for convenience in some formulae.

Some applications of this transformation have been suggested elsewhere (Stone 1975), and in this paper I shall examine some of its mathematical properties. In § 2, two recurrence relations are derived which make the computation of the coefficients somewhat simpler than the direct use of (1.1), while in § 3 a graphical method is described for handling the coefficients. This is used in § 4 to derive some formulae for manipulating the coefficients, particularly in relation to products of tensors, contracted or uncontracted. The need for these can be seen by considering a tensor quantity such as $C_\alpha=A_{\alpha\beta\gamma}B_{\beta\gamma}$. This is a vector, and transforms into a spherical tensor C_{1m} of rank 1; while if we consider the special case where A and B are symmetric and traceless, they transform into spherical tensors $A_{3m'}$ and $B_{2m''}$ of ranks 3 and 2 respectively. However, the tensor C_{1m} is not identical with the tensor $(A_3\times B_2)_{1m}=\langle 32m'm''|1m\rangle A_{3m'}B_{2m''}$, obtained by coupling $A_{3m'}$ and $B_{2m''}$ together, and attempts to make these expressions identical would remove the unitarity of the transformation. The results of § 4 show that in fact

$$C_{1m}=(\tfrac{7}{3})^{1/2}(A_3\times B_2)_{1m}.$$

Previous workers (Coope *et al* 1965, Coope and Snider 1970, Coope 1970) investigated the relationship between Cartesian tensors and their irreducible spherical components, but preferred to work in Cartesian forms throughout. If it is required to follow their approach of projecting out of a Cartesian tensor $A_{\alpha_1\ldots\alpha_n}$ another Cartesian tensor (of the same rank) corresponding to a given spherical component, this can be achieved using the transformation described here:

$$A^{(j_1\ldots j_n)}_{\alpha_1\ldots\alpha_n}=\sum_m\sum_\beta A_{\beta_1\ldots\beta_n}\langle\beta_1\ldots\beta_n|j_1\ldots j_n;m\rangle\langle j_1\ldots j_n;m|\alpha_1\ldots\alpha_n\rangle. \tag{1.6}$$

Indeed the j_n component can be embedded in a Cartesian tensor of any rank $n'\geqslant j_n$:

$$A^{(j_1\ldots j_n)}_{(j'_1\ldots j'_{n'})\alpha_1\ldots\alpha_{n'}}=\sum_m\sum_\beta A_{\beta_1\ldots\beta_n}\langle\beta_1\ldots\beta_n|j_1\ldots j_n;m\rangle\langle j'_1 j'_2\ldots j'_{n'};m|\alpha_1\ldots\alpha_{n'}\rangle, \tag{1.7}$$

where $j'_2\ldots j'_{n'}$ can be chosen in several ways, in general, provided that $j'_{n'}=j_n$. An example is the well-known relationship between the antisymmetric part of a second rank tensor and a vector:

$$A^{(11)}_{(1)\alpha}=\sum_m\sum_\beta A_{\beta_1\beta_2}\langle\beta_1\beta_2|11;m\rangle\langle 1;m|\alpha\rangle=-(\kappa/\sqrt{2})\epsilon_{\alpha\beta_1\beta_2}A_{\beta_1\beta_2}. \tag{1.8}$$

2. Recurrence relations

The definition (1.1) is somewhat inconvenient to use. A little manipulation leads to two recurrence relations: the first provides a formula for obtaining $\langle\alpha_1\ldots\alpha_n|j_1\ldots j_n;m\rangle$ for any m from $\langle\alpha_1\ldots\alpha_n|j_1\ldots j_n;0\rangle$, while the second expresses $\langle\alpha_1\ldots\alpha_{n+1}|j_1\ldots j_{n+1};0\rangle$ in terms of the $\langle\alpha_1\ldots\alpha_n|j_1\ldots j_n;0\rangle$.

Consider the expression

$$\begin{aligned}
&[j_n(j_n+1)-m(m+1)]^{1/2}\langle\alpha_1\ldots\alpha_{n-1}\alpha_n|j_1\ldots j_{n-1}j_n;m+1\rangle\\
&\quad=\sum_{m'm''}\langle\alpha_1\ldots\alpha_{n-1}|j_1\ldots j_{n-1};m'\rangle\langle\alpha_n|1;m''\rangle\\
&\qquad\times[j_n(j_n+1)-m(m+1)]^{1/2}\langle j_{n-1}1m'm''|j_nm+1\rangle\\
&\quad=\sum_{m'm''}\langle\alpha_1\ldots\alpha_{n-1}|j_1\ldots j_{n-1};m'\rangle\langle\alpha_n|1;m''\rangle\\
&\qquad\times\{[j_{n-1}(j_{n-1}+1)-m'(m'-1)]^{1/2}\langle j_{n-1}1m'-1m''|j_nm\rangle\\
&\qquad+[1\,.\,2-m''(m''-1)]^{1/2}\langle j_{n-1}1m'm''-1|j_nm\rangle\}.
\end{aligned}\tag{2.1}$$

By replacing m' by $m'+1$ in the first term and m'' by $m''+1$ in the second, we get

$$\begin{aligned}
&\sum_{m'm''}\langle\alpha_1\ldots\alpha_{n-1}|j_1\ldots j_{n-1};m'+1\rangle[j_{n-1}(j_{n-1}+1)-m'(m'+1)]^{1/2}\langle\alpha_n|1;m''\rangle\\
&\qquad\times\langle j_{n-1}1m'm''|j_nm\rangle+\sum_{m'm''}\langle\alpha_1\ldots\alpha_{n-1}|j_1\ldots j_{n-1};m'\rangle\langle\alpha_n|1;m''+1\rangle\\
&\qquad\times[2-m''(m''+1)]^{1/2}\langle j_{n-1}1m'm''|j_nm\rangle.
\end{aligned}\tag{2.2}$$

Now the second term of this expression is like the definition of the cs coefficient except that $\langle\alpha_n|1;m''\rangle$ has been replaced by $\langle\alpha_n|1;m''+1\rangle[2-m''(m''+1)]^{1/2}$. Let us write this last expression as

$$\begin{aligned}
&\sum_{m'''}\langle\alpha_n|1;m'''+1\rangle[2-m'''(m'''+1)]^{1/2}\delta_{m'''m''}\\
&\qquad=\sum_{m'''}\langle\alpha_n|1;m'''+1\rangle[2-m'''(m'''+1)]^{1/2}\langle 1;m'''|1;m''\rangle\\
&\qquad=\langle\alpha_n|\hat{J}_+|1;m''\rangle,
\end{aligned}\tag{2.3}$$

where $\hat{J}_+$ is the usual angular momentum shift operator. It is convenient to introduce new operators $\mathscr{J}_\pm^{(r)}$, defined by

$$\mathscr{J}_\pm^{(r)}\langle\alpha_s|1;m\rangle=\delta_{rs}\langle\alpha_r|\hat{J}_\pm|1;m\rangle.\tag{2.4}$$

($\mathscr{J}_z^{(r)}$ could be defined similarly but will not be needed.) Using (1.2) in the form

$$\begin{aligned}
&\langle\alpha|1;0\rangle=\mathrm{i}\kappa\hat{z}_\alpha,\\
&\langle\alpha|1;\pm1\rangle=\mp\sqrt{\tfrac{1}{2}}\mathrm{i}\kappa(\hat{x}_\alpha\pm\mathrm{i}\hat{y}_\alpha),
\end{aligned}\tag{2.5}$$

where $\hat{x}_\alpha$, $\hat{y}_\alpha$ and $\hat{z}_\alpha$ are unit vectors along the x, y and z axes, it is a straightforward matter to show that

$$\mathscr{J}_a^{(r)}\hat{b}_{\alpha_r}=\sum_c\mathrm{i}\epsilon_{abc}\hat{c}_{\alpha_r},\tag{2.6}$$

where $a=x$ or y; $b,c=x$, y, or z; and $\mathscr{J}_x$, $\mathscr{J}_y$ are defined by $\mathscr{J}_\pm=\mathscr{J}_x\pm\mathrm{i}\mathscr{J}_y$. The effect of

$\mathcal{J}_a^{(r)}$ on expressions such as $\delta_{\alpha_r\alpha_s}$ is now easily found:

$$\mathcal{J}_a^{(1)}\delta_{\alpha_1\alpha_2} = \mathcal{J}_a^{(1)}\sum_b \hat{b}_{\alpha_1}\hat{b}_{\alpha_2} = \sum_{bc} \mathrm{i}\epsilon_{abc}\hat{c}_{\alpha_1}\hat{b}_{\alpha_2}, \tag{2.7}$$

and one finds also that

$$\begin{aligned} &[\mathcal{J}_a^{(1)} + \mathcal{J}_a^{(2)}]\delta_{\alpha_1\alpha_2} = 0, \\ &[\mathcal{J}_a^{(1)} + \mathcal{J}_a^{(2)} + \mathcal{J}_a^{(3)}]\epsilon_{\alpha_1\alpha_2\alpha_3} = 0. \end{aligned} \tag{2.8}$$

One should perhaps emphasize that $\mathcal{J}_a^{(r)}$ is not a respectable quantum mechanical operator but merely a convenient mathematical shorthand.

Returning to (2.2), we now treat the first term in the same way as the initial expression of (2.1). By repetition we eventually obtain a sum of terms:

$$\begin{aligned} &[j_n(j_n+1) - m(m\pm 1)]^{1/2}\langle \alpha_1 \ldots \alpha_n | j_1 \ldots j_n; m\pm 1\rangle \\ &\qquad = \sum_r \mathcal{J}_\pm^{(r)}\langle \alpha_1 \ldots \alpha_n | j_1 \ldots j_n; m\rangle = \mathcal{J}_\pm \langle \alpha_1 \ldots \alpha_n | j_1 \ldots j_n; m\rangle, \end{aligned} \tag{2.9}$$

where

$$\mathcal{J}_\pm = \sum_{r=1}^{n} \mathcal{J}_\pm^{(r)}.$$

As an example of this formula we may obtain the $\langle \alpha\beta | 12; m\rangle$, $m > 0$, from $\langle \alpha\beta | 12; 0\rangle$, which is shown below to be equal to $-(\kappa^2/\sqrt{6})[3\hat{z}_\alpha\hat{z}_\beta - \delta_{\alpha\beta}]$. We have

$$\begin{aligned} \sqrt{6}\langle \alpha\beta | 12; 1\rangle &= (\mathcal{J}_+^{(\alpha)} + \mathcal{J}_+^{(\beta)})(-\kappa^2/\sqrt{6})[3\hat{z}_\alpha\hat{z}_\beta - \delta_{\alpha\beta}] \\ &= (-\kappa^2/\sqrt{6})[-3(\hat{x}_\alpha + \mathrm{i}\hat{y}_\alpha)\hat{z}_\beta - 3\hat{z}_\alpha(\hat{x}_\beta + \mathrm{i}\hat{y}_\beta)], \end{aligned}$$

so that

$$\langle \alpha\beta | 12; 1\rangle = (\kappa^2/2)[\hat{x}_\alpha\hat{z}_\beta + \hat{z}_\alpha\hat{x}_\beta + \mathrm{i}(\hat{y}_\alpha\hat{z}_\beta + \hat{z}_\alpha\hat{y}_\beta)]. \tag{2.10}$$

Similarly

$$\sqrt{4}\langle \alpha\beta | 12; 2\rangle = (\kappa^2/2)[-2(\hat{x}_\alpha + \mathrm{i}\hat{y}_\alpha)(\hat{x}_\beta + \mathrm{i}\hat{y}_\beta)],$$

so that

$$\langle \alpha\beta | 12; 2\rangle = -(\kappa^2/2)[\hat{x}_\alpha\hat{x}_\beta - \hat{y}_\alpha\hat{y}_\beta + \mathrm{i}(\hat{x}_\alpha\hat{y}_\beta + \hat{y}_\alpha\hat{x}_\beta)]. \tag{2.11}$$

Now we seek a similar formula relating $\langle \alpha_1 \ldots \alpha_n\zeta | j_1 \ldots j_n j; 0\rangle$ and $\langle \alpha_1 \ldots \alpha_n | j_1 \ldots j_n; 0\rangle$. From (1.1) we have

$$\langle \alpha_1 \ldots \alpha_n\zeta | j_1 \ldots j_n j; 0\rangle = \sum_m \langle \alpha_1 \ldots \alpha_n | j_1 \ldots j_n; m\rangle\langle \zeta | 1; -m\rangle\langle j_n 1 m -m | j0\rangle. \tag{2.12}$$

We can use (2.9) in the terms with $m \neq 0$, insert the expressions (2.5) for the $\langle \zeta | 1; m\rangle$, and substitute algebraic expressions for the Clebsch–Gordan coefficients to give

$$\begin{aligned} &\langle \alpha_1 \ldots \alpha_n\zeta | j_1 \ldots j_n j; 0\rangle \\ &\quad = \kappa\{\delta_{j,j_n+1}[(j_n+1)(2j_n+1)]^{-1/2}[\mathrm{i}(j_n+1)\hat{z}_\zeta + \hat{y}_\zeta\mathcal{J}_x - \hat{x}_\zeta\mathcal{J}_y] \\ &\qquad + \delta_{j,j_n-1}[j_n(2j_n+1)]^{-1/2}[-\mathrm{i}j_n\hat{z}_\zeta + \hat{y}_\zeta\mathcal{J}_x - \hat{x}_\zeta\mathcal{J}_y] + \mathrm{i}\delta_{j,j_n}[j_n(j_n+1)]^{-1/2} \\ &\qquad \times [\hat{x}_\zeta\mathcal{J}_x + \hat{y}_\zeta\mathcal{J}_y]\}\langle \alpha_1 \ldots \alpha_n | j_1 \ldots j_n; 0\rangle. \end{aligned} \tag{2.13}$$

Expressions for the $\langle\alpha_1\ldots\alpha_n|j_1\ldots j_n;0\rangle$ for $n\leqslant 4$ and for $n=5$, $j_5=0$ have been derived using this formula, and checked against the results of a computer program which evaluates the coefficients directly using (1.1). The results are given in table 1. For

Table 1.

Cartesian rank 1:

$\langle\alpha|1;0\rangle=\mathrm{i}\kappa\hat{z}_\alpha$

Cartesian rank 2:

$\langle\alpha\beta|10;0\rangle=(\kappa^2/\sqrt{3})\delta_{\alpha\beta}$

$\langle\alpha\beta|11;0\rangle=-(\mathrm{i}\kappa^2/\sqrt{2})[\hat{x}_\alpha\hat{y}_\beta-\hat{y}_\alpha\hat{x}_\beta]$

$\langle\alpha\beta|12;0\rangle=-(\kappa^2/\sqrt{6})[3\hat{z}_\alpha\hat{z}_\beta-\delta_{\alpha\beta}]$

Cartesian rank 3:

$\langle\alpha\beta\gamma|101;0\rangle=(\mathrm{i}\kappa^3/\sqrt{3})\delta_{\alpha\beta}\hat{z}_\gamma$

$\langle\alpha\beta\gamma|110;0\rangle=-(\kappa^3/\sqrt{6})\epsilon_{\alpha\beta\gamma}$

$\langle\alpha\beta\gamma|111;0\rangle=(\mathrm{i}\kappa^3/2)[\hat{z}_\beta\delta_{\alpha\gamma}-\hat{z}_\alpha\delta_{\beta\gamma}]$

$\langle\alpha\beta\gamma|112;0\rangle=12^{-1/2}\kappa^3[3\hat{x}_\alpha\hat{y}_\beta\hat{z}_\gamma-3\hat{y}_\alpha\hat{x}_\beta\hat{z}_\gamma-\epsilon_{\alpha\beta\gamma}]$

$\langle\alpha\beta\gamma|121;0\rangle=-60^{-1/2}\mathrm{i}\kappa^3[2\delta_{\alpha\beta}\hat{z}_\gamma-3\hat{z}_\beta\delta_{\alpha\gamma}-3\hat{z}_\alpha\delta_{\beta\gamma}]$

$\langle\alpha\beta\gamma|122;0\rangle=(\kappa^3/2)[\hat{z}_\alpha\hat{x}_\beta\hat{y}_\gamma-\hat{z}_\alpha\hat{y}_\beta\hat{x}_\gamma+\hat{x}_\alpha\hat{z}_\beta\hat{y}_\gamma-\hat{y}_\alpha\hat{z}_\beta\hat{x}_\gamma]$

$\langle\alpha\beta\gamma|123;0\rangle=-10^{-1/2}\mathrm{i}\kappa^3[5\hat{z}_\alpha\hat{z}_\beta\hat{z}_\gamma-\delta_{\alpha\beta}\hat{z}_\gamma-\hat{z}_\beta\delta_{\alpha\gamma}-\hat{z}_\alpha\delta_{\beta\gamma}]$

Cartesian rank 4:

$\langle\alpha\beta\gamma\delta|1010;0\rangle=\frac{1}{3}\delta_{\alpha\beta}\delta_{\gamma\delta}$

$\langle\alpha\beta\gamma\delta|1011;0\rangle=-6^{-1/2}\mathrm{i}\delta_{\alpha\beta}[\hat{x}_\gamma\hat{y}_\delta-\hat{y}_\gamma\hat{x}_\delta]$

$\langle\alpha\beta\gamma\delta|1012;0\rangle=-18^{-1/2}\delta_{\alpha\beta}[3\hat{z}_\gamma\hat{z}_\delta-\delta_{\gamma\delta}]$

$\langle\alpha\beta\gamma\delta|1101;0\rangle=-6^{-1/2}\mathrm{i}\epsilon_{\alpha\beta\gamma}\hat{z}_\delta$

$\langle\alpha\beta\gamma\delta|1110;0\rangle=12^{-1/2}[\delta_{\alpha\gamma}\delta_{\beta\delta}-\delta_{\alpha\delta}\delta_{\beta\gamma}]$

$\langle\alpha\beta\gamma\delta|1111;0\rangle=8^{-1/2}\mathrm{i}[(\hat{x}_\alpha\hat{y}_\beta-\hat{y}_\alpha\hat{x}_\beta)\delta_{\gamma\delta}-\epsilon_{\alpha\beta\delta}\hat{z}_\gamma]$

$\langle\alpha\beta\gamma\delta|1112;0\rangle=24^{-1/2}[\delta_{\beta\gamma}(3\hat{z}_\alpha\hat{z}_\delta-\delta_{\alpha\delta})-\delta_{\alpha\gamma}(3\hat{z}_\beta\hat{z}_\delta-\delta_{\beta\delta})]$

$\langle\alpha\beta\gamma\delta|1121;0\rangle=-120^{-1/2}\mathrm{i}[3\epsilon_{\alpha\beta\delta}\hat{z}_\gamma-2\epsilon_{\alpha\beta\gamma}\hat{z}_\delta+3(\hat{x}_\alpha\hat{y}_\beta-\hat{y}_\alpha\hat{x}_\beta)\delta_{\gamma\delta}]$

$\langle\alpha\beta\gamma\delta|1122;0\rangle=8^{-1/2}[\hat{z}_\alpha\hat{z}_\gamma\delta_{\beta\delta}-\hat{z}_\beta\hat{z}_\gamma\delta_{\alpha\delta}-(\hat{x}_\alpha\hat{y}_\beta-\hat{y}_\alpha\hat{x}_\beta)(\hat{x}_\gamma\hat{y}_\delta-\hat{y}_\gamma\hat{x}_\delta)]$

$\langle\alpha\beta\gamma\delta|1123;0\rangle=20^{-1/2}\mathrm{i}[(\hat{x}_\alpha\hat{y}_\beta-\hat{y}_\alpha\hat{x}_\beta)(5\hat{z}_\gamma\hat{z}_\delta-\delta_{\gamma\delta})-\epsilon_{\alpha\beta\gamma}\hat{z}_\delta-\epsilon_{\alpha\beta\delta}\hat{z}_\gamma]$

$\langle\alpha\beta\gamma\delta|1210;0\rangle=180^{-1/2}[3\delta_{\alpha\gamma}\delta_{\beta\delta}-3\delta_{\alpha\delta}\delta_{\beta\gamma}-2\delta_{\alpha\beta}\delta_{\gamma\delta}]$

$\langle\alpha\beta\gamma\delta|1211;0\rangle=120^{-1/2}\mathrm{i}[2\delta_{\alpha\beta}(\hat{x}_\gamma\hat{y}_\delta-\hat{y}_\gamma\hat{x}_\delta)-3\delta_{\alpha\gamma}(\hat{x}_\beta\hat{y}_\delta-\hat{y}_\beta\hat{x}_\delta)-3\delta_{\beta\gamma}(\hat{x}_\alpha\hat{y}_\delta-\hat{y}_\alpha\hat{x}_\delta)]$

$\langle\alpha\beta\gamma\delta|1212;0\rangle=360^{-1/2}[2\delta_{\alpha\beta}(3\hat{z}_\gamma\hat{z}_\delta-\delta_{\gamma\delta})-3\delta_{\alpha\gamma}(3\hat{z}_\beta\hat{z}_\delta-\delta_{\beta\delta})-3\delta_{\beta\gamma}(3\hat{z}_\alpha\hat{z}_\delta-\delta_{\alpha\delta})]$

$\langle\alpha\beta\gamma\delta|1221;0\rangle=-40^{-1/2}\mathrm{i}[\delta_{\alpha\delta}(\hat{x}_\beta\hat{y}_\gamma-\hat{y}_\beta\hat{x}_\gamma)+\hat{z}_\alpha\epsilon_{\beta\gamma\delta}+\delta_{\beta\delta}(\hat{x}_\alpha\hat{y}_\gamma-\hat{y}_\alpha\hat{x}_\gamma)+\hat{z}_\beta\epsilon_{\alpha\gamma\delta}]$

$$\langle\alpha\beta\gamma\delta|1222;0\rangle=-24^{-1/2}[2(\delta_{\alpha\beta}\delta_{\gamma\delta}-\delta_{\alpha\beta}\hat{z}_\gamma\hat{z}_\delta-2\hat{z}_\alpha\hat{z}_\beta\delta_{\gamma\delta})-(\delta_{\alpha\gamma}\delta_{\beta\delta}-\delta_{\alpha\gamma}\hat{z}_\beta\hat{z}_\delta-2\hat{z}_\alpha\hat{z}_\gamma\delta_{\beta\delta})$$
$$-(\delta_{\beta\gamma}\delta_{\alpha\delta}-\delta_{\beta\gamma}\hat{z}_\alpha\hat{z}_\delta-2\hat{z}_\beta\hat{z}_\gamma\delta_{\alpha\delta})]$$

$\langle\alpha\beta\gamma\delta|1223;0\rangle=60^{-1/2}\mathrm{i}[(5\hat{z}_\alpha\hat{z}_\delta-\delta_{\alpha\delta})(\hat{x}_\beta\hat{y}_\gamma-\hat{y}_\beta\hat{x}_\gamma)-\hat{z}_\alpha\epsilon_{\beta\gamma\delta}+(5\hat{z}_\beta\hat{z}_\delta-\delta_{\beta\delta})(\hat{x}_\alpha\hat{y}_\gamma-\hat{y}_\alpha\hat{x}_\gamma)-\hat{z}_\beta\epsilon_{\alpha\gamma\delta}]$

$$\langle\alpha\beta\gamma\delta|1232;0\rangle=210^{-1/2}[\delta_{\alpha\beta}\delta_{\gamma\delta}+\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\beta\gamma}\delta_{\alpha\delta}-5(\hat{z}_\alpha\hat{z}_\beta\delta_{\gamma\delta}+\hat{z}_\alpha\hat{z}_\gamma\delta_{\beta\delta}+\hat{z}_\beta\hat{z}_\gamma\delta_{\alpha\delta})$$
$$+2(\delta_{\alpha\beta}\hat{z}_\gamma\hat{z}_\delta+\delta_{\alpha\gamma}\hat{z}_\beta\hat{z}_\delta+\delta_{\beta\gamma}\hat{z}_\alpha\hat{z}_\delta)]$$

Table 1. *continued*

$$\langle\alpha\beta\gamma\delta|1233;0\rangle = 120^{-1/2}\mathrm{i}[(5\hat{z}_\alpha\hat{z}_\beta-\delta_{\alpha\beta})(\hat{x}_\gamma\hat{y}_\delta-\hat{y}_\gamma\hat{x}_\delta)+(5\hat{z}_\alpha\hat{z}_\gamma-\delta_{\alpha\gamma})(\hat{x}_\beta\hat{y}_\delta-\hat{y}_\beta\hat{x}_\delta)+(5\hat{z}_\beta\hat{z}_\gamma-\delta_{\beta\gamma})$$
$$\times(\hat{x}_\alpha\hat{y}_\delta-\hat{y}_\alpha\hat{x}_\delta)]$$

$$\langle\alpha\beta\gamma\delta|1234;0\rangle = 280^{-1/2}[\delta_{\alpha\beta}\delta_{\gamma\delta}+\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\beta\gamma}$$
$$-5(\delta_{\alpha\beta}\hat{z}_\gamma\hat{z}_\delta+\delta_{\alpha\gamma}\hat{z}_\beta\hat{z}_\delta+\delta_{\alpha\delta}\hat{z}_\beta\hat{z}_\gamma+\delta_{\gamma\delta}\hat{z}_\alpha\hat{z}_\beta+\delta_{\beta\delta}\hat{z}_\alpha\hat{z}_\gamma+\delta_{\beta\gamma}\hat{z}_\alpha\hat{z}_\delta)+35\hat{z}_\alpha\hat{z}_\beta\hat{z}_\gamma\hat{z}_\delta]$$

Cartesian rank 5:

$$\langle\alpha\beta\gamma\delta\epsilon|10110;0\rangle = -18^{-1/2}\kappa\delta_{\alpha\beta}\epsilon_{\gamma\delta\epsilon}$$
$$\langle\alpha\beta\gamma\delta\epsilon|11010;0\rangle = -18^{-1/2}\kappa\epsilon_{\alpha\beta\gamma}\delta_{\delta\epsilon}$$
$$\langle\alpha\beta\gamma\delta\epsilon|11110;0\rangle = -24^{-1/2}\kappa[\epsilon_{\alpha\gamma\epsilon}\delta_{\beta\delta}-\epsilon_{\beta\gamma\epsilon}\delta_{\alpha\delta}-\epsilon_{\alpha\gamma\delta}\delta_{\beta\epsilon}+\epsilon_{\beta\gamma\delta}\delta_{\alpha\epsilon}]$$
$$\langle\alpha\beta\gamma\delta\epsilon|11210;0\rangle = -360^{-1/2}\kappa[4\epsilon_{\alpha\beta\gamma}\delta_{\delta\epsilon}+3(\epsilon_{\alpha\gamma\epsilon}\delta_{\beta\delta}-\epsilon_{\beta\gamma\epsilon}\delta_{\alpha\delta}+\epsilon_{\alpha\gamma\delta}\delta_{\beta\epsilon}-\epsilon_{\beta\gamma\delta}\delta_{\alpha\epsilon})]$$
$$\langle\alpha\beta\gamma\delta\epsilon|12110;0\rangle = -360^{-1/2}\kappa[4\delta_{\alpha\beta}\epsilon_{\gamma\delta\epsilon}+3(\epsilon_{\alpha\gamma\epsilon}\delta_{\beta\delta}+\epsilon_{\beta\gamma\epsilon}\delta_{\alpha\delta}-\epsilon_{\alpha\gamma\delta}\delta_{\beta\epsilon}-\epsilon_{\beta\gamma\delta}\delta_{\alpha\epsilon})]$$
$$\langle\alpha\beta\gamma\delta\epsilon|12210;0\rangle = -120^{-1/2}\kappa[\delta_{\alpha\delta}\epsilon_{\beta\gamma\epsilon}+\delta_{\alpha\epsilon}\epsilon_{\beta\gamma\delta}+\delta_{\beta\delta}\epsilon_{\alpha\gamma\epsilon}+\delta_{\beta\epsilon}\epsilon_{\alpha\gamma\delta}]$$

$n=5$ the number of coefficients becomes rather large, but the six scalars are particularly useful—for example in obtaining spherical averages of tensor properties, which are conveniently expressed in the form

$$\langle T_{\alpha_1\ldots\alpha_n}\rangle = \sum_{j\beta m}\langle\alpha_1\ldots\alpha_n|j_1\ldots j_n;m\rangle\delta_{j_n0}\delta_{m0}\langle j_1\ldots j_n;m|\beta_1\ldots\beta_n\rangle T_{\beta_1\ldots\beta_n}. \qquad (2.14)$$

One can see from these results, as one would expect, that $\langle\alpha_1\ldots\alpha_n|j_1\ldots j_n;0\rangle$ is independent of the axis system if $j_n=0$, and also that a coefficient in which one of the intermediate j_r is zero can be written as a product of simpler coefficients:

$$\langle\alpha_1\ldots\alpha_r\ldots\alpha_n|j_1\ldots j_{r-1}0j_{r+1}\ldots j_n;m\rangle$$
$$=\langle\alpha_1\ldots\alpha_r|j_1\ldots j_{r-1}0;0\rangle\langle\alpha_{r+1}\ldots\alpha_n|j_{r+1}\ldots j_n;m\rangle. \qquad (2.15)$$

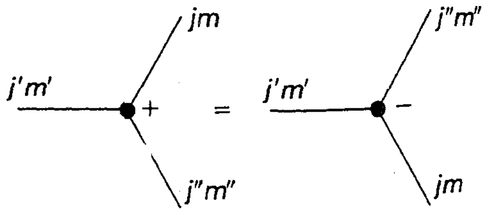
A result which is less apparent, but which is easily proved using the diagram notation of the next section, is that

$$\langle\alpha_1\ldots\alpha_n|j_1\ldots j_{n-1}0;0\rangle = (-1)^n\langle\alpha_n\alpha_{n-1}\ldots\alpha_1|j_{n-1}\ldots j_2j_10;0\rangle. \qquad (2.16)$$

3. Graphical technique

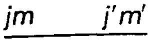
The graphical technique we will use is a simple extension of the one described by Brink and Satchler (1968), which is itself a modification of the scheme given by Yutsis *et al* (1962). Brink and Satchler's technique is based on the representation of the $3j$ symbol by a diagram:

$$\begin{pmatrix} j' & j'' & j \\ m' & m'' & m \end{pmatrix} =$$

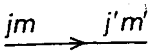


(3.1)

The sign on the node gives the order in which the angular momentum symbols are to be read—counterclockwise if +, clockwise if −. A line by itself represents a delta function, while a line with an arrow on it represents a phase factor:



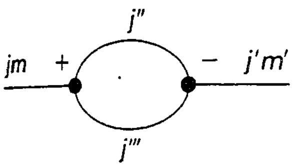
$$= \delta_{jj'}\delta_{mm'}$$



$$= \delta_{jj'}\delta_{m,-m'} \,.\, (-1)^{j-m}. \tag{3.2}$$

Where half-integral angular moments arise, the direction of the arrow is significant, but in the present work it is immaterial.

The joining of two lines implies that the m values are set equal and summed over, so that for example



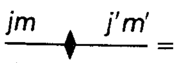
$$= \sum_{m''m'''} \begin{pmatrix} j & j''' & j'' \\ m & m''' & m'' \end{pmatrix} \begin{pmatrix} j' & j''' & j'' \\ m' & m''' & m'' \end{pmatrix}$$

$$= (2j+1)^{-1}\delta_{jj'}\delta_{mm'}. \tag{3.3}$$

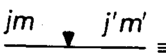
Any distortion of a graph leaves its value unchanged, provided that a change of the orientation of lines at a node is accompanied by a change of sign at that node.

Let us now extend this notation a little. First, the factor $(2j+1)^{1/2}$ which occurs in many formulae is represented by a solid triangle with its base attached to a line. More than one factor may occur, while negative powers are represented by attaching the point of the triangle to the line:

$$\equiv (2j+1)^{1/2}\delta_{jj'}\delta_{mm'}, \tag{3.4}$$

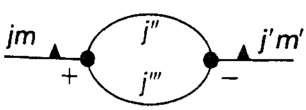


$$= (2j+1)\delta_{jj'}\delta_{mm'}, \tag{3.5}$$



$$\equiv (2j+1)^{-1/2}\delta_{jj'}\delta_{mm'}. \tag{3.6}$$

Using this notation we may for example write (3.3) as



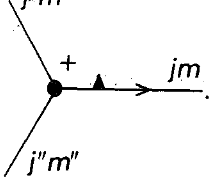
$=$

. (3.7)

The Wigner coefficient is now easily represented:

$$\langle j'j''m'm''|jm\rangle = (-1)^{j'-j''+m}(2j+1)^{1/2}\begin{pmatrix} j' & j'' & j \\ m' & m'' & -m \end{pmatrix}$$

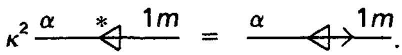
$$= (-1)^{j'-j''+j}$$



. (3.8)

Next we need symbols for the basic Cartesian-spherical transformation (1.2), and we shall take

to represent $\langle\alpha|1;m\rangle$ and $\langle 1;m|\alpha\rangle$ respectively. The star can be added or removed by the rule

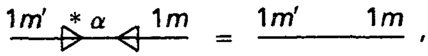


(3.9)

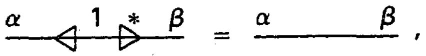
This corresponds to the equation

$$\kappa^2\langle 1;m|\alpha\rangle=(-1)^{1-m}\langle\alpha|1;-m\rangle.$$

A line with two triangles and one star is equal to a line with no triangles:



(3.10)



(3.11)

corresponding to

$$\langle 1;m'|\alpha\rangle\langle\alpha|1;m\rangle=\delta_{mm'}$$

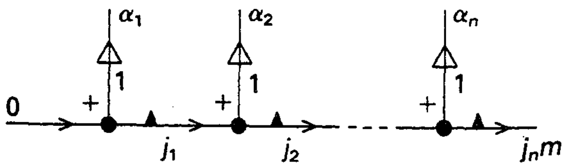
and

$$\sum_m\langle\alpha|1;m\rangle\langle 1;m|\beta\rangle=\delta_{\alpha\beta}.$$

We see that joining two Cartesian lines corresponds to setting the Cartesian subscripts equal and summing. Clearly the joining of a Cartesian to an angular momentum line is meaningless.

Then remembering that all quantum numbers are integral, we find that the cs transformation coefficient can be represented by

$\langle\alpha_1\ldots\alpha_n|j_1\ldots j_n;m\rangle=$

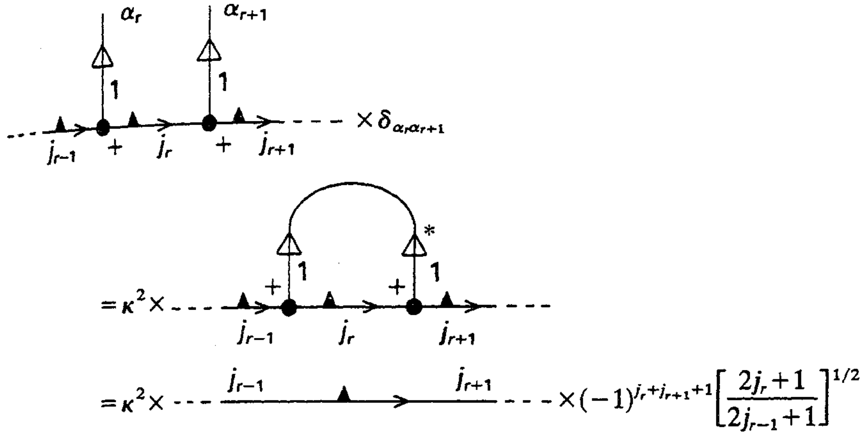


(3.12)

4. Manipulation of cs coefficients

Now we can use the notation introduced in § 3 to derive some formulae for the manipulation of cs coefficients.

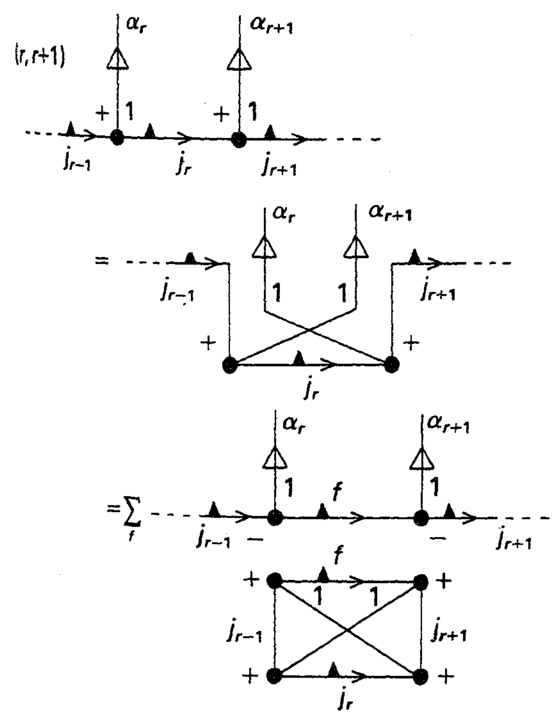
4.1. *Contraction of adjacent suffixes*



whence

$$\langle \alpha_1 \ldots \alpha_n | j_1 \ldots j_n; m\rangle \delta_{\alpha_r \alpha_{r+1}}$$
$$= \langle \alpha_1 \ldots \alpha_{r-1}\alpha_{r+2} \ldots \alpha_n | j_1 \ldots j_{r-1} j_{r+2} \ldots j_n; m\rangle \kappa^2 (-1)^{j_r + j_{r+1} + 1}$$
$$\times\ \delta_{j_{r-1} j_{r+1}} [(2j_r + 1)/(2j_{r-1} + 1)]^{1/2}. \quad (4.1)$$

4.2. *Permutation of adjacent suffixes*



(see Brink and Satchler, equation (7.37)) whence

$$(r, r+1)\langle \alpha_1 \ldots \alpha_n | j_1 \ldots j_n; m\rangle$$
$$= \sum_f (-1)^{j_r+f}[(2j_r+1)(2f+1)]^{1/2} \begin{Bmatrix} 1 & j_{r-1} & j_r \\ 1 & j_{r+1} & f \end{Bmatrix}$$
$$\times \langle \alpha_1 \ldots \alpha_n | j_1 \ldots j_{r-1} f\, j_{r+1} \ldots j_n; m\rangle. \qquad (4.2)$$

This result is to be expected, since the transposition involves a simple recoupling of the basis vectors of the polyadic $A_{\alpha_1}B_{\alpha_2} \ldots Z_{\alpha_n}$.

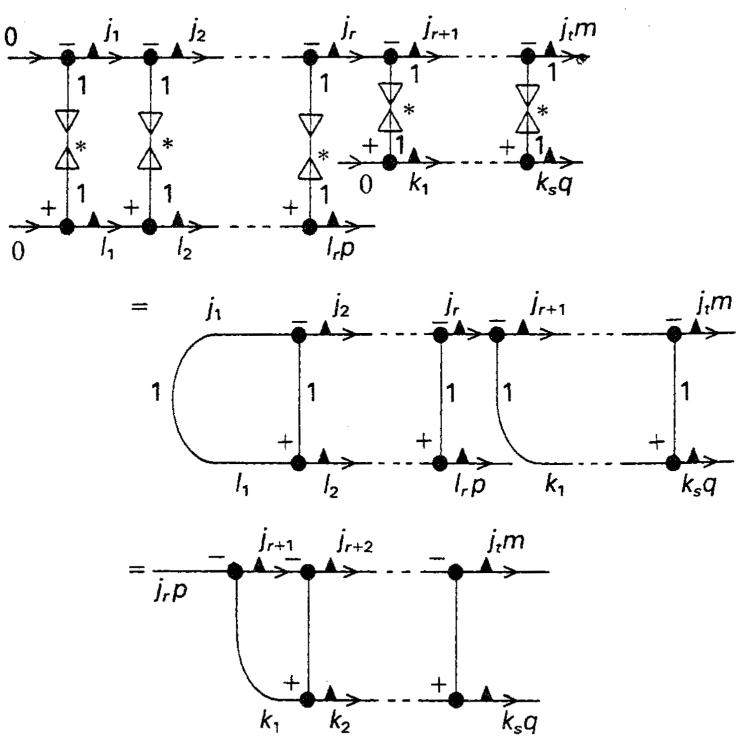
A discussion of the implications of this formula to the symmetry of the cs coefficients with respect to permutation of Cartesian subscripts may be found in Stone (1975).

4.3. *Inner and outer products*

Consider the following expression:

$$\sum_{\alpha_1\ldots\alpha_r} \sum_{\beta_1\ldots\beta_s} \langle l_1 \ldots l_r; p | \alpha_1 \ldots \alpha_r\rangle \langle k_1 \ldots k_s; q | \beta_1 \ldots \beta_s\rangle \langle \alpha_1 \ldots \alpha_r \beta_1 \ldots \beta_s | j_1 \ldots j_t; m\rangle \qquad (4.3)$$

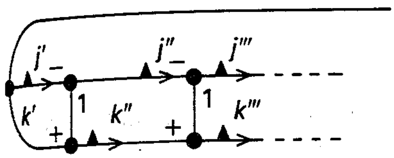
where $t = r + s$. In graphical notation, this expression is:

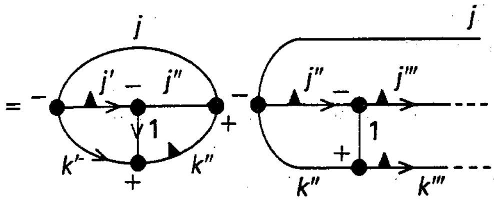


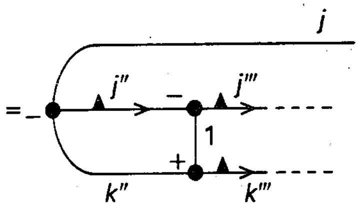
$$\times\, \delta_{j_1 l_1} \delta_{j_2 l_2} \ldots \delta_{j_r l_r} \qquad (4.4)$$

by repeated use of the orthogonality of $3j$ symbols, equation (3.7).

Now we require the following relation, which is obtained using Brink and Satchler's equation (7.34):







$$\times[(2j'+1)(2k''+1)]^{1/2}W(k'1jj''; k''j'). \tag{4.5}$$

Use of this formula $(s-1)$ times, and finally (3.8), yields:

$$\sum\langle l_1\ldots l_r; p|\alpha_1\ldots\alpha_r\rangle\langle k_1\ldots k_s; q|\beta_1\ldots\beta_s\rangle\langle\alpha_1\ldots\alpha_r\beta_1\ldots\beta_s|j_1\ldots j_t; m\rangle$$
$$=\prod_{\sigma=2}^{s}\{[(2k_\sigma+1)(2j_{r+\sigma-1}+1)]^{1/2}W(k_{\sigma-1}1j_rj_{r+\sigma}; k_\sigma j_{r+\sigma-1})\}$$
$$\times\delta_{j_1l_1}\ldots\delta_{j_rl_r}\langle j_rk_spq|j_tm\rangle. \tag{4.6}$$

The special cases $s=0$ and $s=1$ are covered by (4.6) if we interpret the null product as unity and write $k_s=q_s=0$ when $s=0$. The equation for $s=0$ merely expresses the unitarity of the transformation.

Using (4.6) we can now derive the following:

4.3.1. *Inner products*

$$R_{\alpha_1\ldots\alpha_t}T_{\alpha_1\ldots\alpha_t}=\sum\langle\alpha_1\ldots\alpha_t|l_1\ldots l_t; p\rangle\langle\alpha_1\ldots\alpha_t|j_1\ldots j_t; m\rangle R_{l_1\ldots l_t;p}T_{j_1\ldots j_t;m}. \tag{4.7}$$

Since

$$\langle\alpha_1\ldots\alpha_t|l_1\ldots l_t; p\rangle=\langle l_1\ldots l_t; p|\alpha_1\ldots\alpha_t\rangle^*=\kappa^{2t}(-1)^{l_t-p}\langle l_1\ldots l_t; -p|\alpha_1\ldots\alpha_t\rangle, \tag{4.8}$$

(as can be shown inductively from equation (1.1)) this becomes

$$R_{\alpha_1\ldots\alpha_t}T_{\alpha_1\ldots\alpha_t}=\sum \delta_{l_1j_1}\delta_{l_2j_2}\ldots\delta_{l_tj_t}\delta_{-p,m}\kappa^{2t}(-1)^{l_t-p}R_{l_1\ldots l_t;p}T_{j_1\ldots j_t;m}$$

$$=\sum_{j_1\ldots j_t}(\kappa^2)^{t+j_t}R_{j_1\ldots j_t}\cdot T_{j_1\ldots j_t}, \qquad (4.9)$$

where the phase factor in the last term arises from the different definitions of the scalar product used by Fano and Racah and by Condon and Shortley.

4.3.2. Non-scalar inner products. If $R_{\alpha_1\ldots\alpha_r}=T_{\alpha_1\ldots\alpha_r\beta_1\ldots\beta_s}S_{\beta_1\ldots\beta_s}$, the spherical components of R are given in terms of those for T and S by

$$R_{l_1\ldots l_r;p}=\sum_{jkmq}\langle l_1\ldots l_r;p|\alpha_1\ldots\alpha_r\rangle\langle\alpha_1\ldots\alpha_r\beta_1\ldots\beta_s|j_1\ldots j_t;m\rangle$$

$$\times\langle\beta_1\ldots\beta_s|k_1\ldots k_s;q\rangle T_{j_1\ldots j_t;m}S_{k_1\ldots k_s;q}$$

$$=\sum_{jkmq}\prod_{\sigma=2}^{s}\{[(2k_\sigma+1)(2j_{r+\sigma-1}+1)]^{1/2}W(k_{\sigma-1}1l_rj_{r+\sigma};k_\sigma j_{r+\sigma-1})\}$$

$$\times\kappa^{2s}(-1)^{k_s-q}\langle l_rk_sp-q|j_tm\rangle T_{l_1\ldots l_rj_{r+1}\ldots j_t;m}S_{k_1\ldots k_s;q} \qquad (4.10)$$

(using (4.6) and (4.8)) and since

$$\langle ab\alpha-\beta|c\gamma\rangle=[(2c+1)/(2a+1)]^{1/2}(-1)^{2b-\beta+c-a}\langle cb\gamma\beta|a\alpha\rangle, \qquad (4.11)$$

we get

$$R_{l_1\ldots l_r;p}=\kappa^{2s}\sum_{jk}(-1)^{j_t-k_s-l_r}[(2j_t+1)/(2l_r+1)]^{1/2}$$

$$\times\prod_{\sigma=2}^{s}\{[(2k_\sigma+1)(2j_{r+\sigma-1}+1)]^{1/2}W(k_{\sigma-1}1l_rj_{r+\sigma};k_\sigma j_{r+\sigma-1})\}$$

$$\times(T_{l_1\ldots l_rj_{r+1}\ldots j_t}\times S_{k_1\ldots k_s})_{l_rp}. \qquad (4.12)$$

An equivalent expression is

$$R_{l_1\ldots l_r;p}=\kappa^{2s}\sum_{jk}(-1)^{j_t-k_s-l_r}(T_{l_1\ldots l_rj_{r+1}\ldots j_t}\times S_{k_1\ldots k_s})_{l_rp}$$

$$\times\prod_{\sigma=1}^{s}\{[(2k_\sigma+1)(2j_{r+\sigma}+1)]^{1/2}W(k_{\sigma-1}1l_rj_{r+\sigma};k_\sigma j_{r+\sigma-1})\} \qquad (4.13)$$

since

$$W(01l_rj_{r+1};1j_r)=\delta_{j_rl_r}[3(2l_r+1)]^{-1/2}.$$

Similarly, if $S_{\beta_1\ldots\beta_s}=R_{\alpha_1\ldots\alpha_r}T_{\alpha_1\ldots\alpha_r\beta_1\ldots\beta_s}$, then

$$S_{k_1\ldots k_s;q}=\sum_{jlmp}\langle k_1\ldots k_s;q|\beta_1\ldots\beta_s\rangle\langle\alpha_1\ldots\alpha_r|l_1\ldots l_r;p\rangle$$

$$\times\langle\alpha_1\ldots\alpha_r\beta_1\ldots\beta_s|j_1\ldots j_t;m\rangle R_{l_1\ldots l_r;p}T_{j_1\ldots j_t;m}$$

(where $t=r+s$)

$$=\kappa^{2r}\sum_{j}(-1)^{j_r-p}\langle j_r k_s -pq|j_t m\rangle R_{j_1\ldots j_r;p}T_{j_1\ldots j_t;m}$$

$$\times\prod_{\sigma=2}^{s}\{[(2k_\sigma+1)(2j_{r+\sigma-1}+1)]^{1/2}W(k_{\sigma-1}1j_rj_{r+\sigma};k_\sigma j_{r+\sigma-1})\}$$

$$=\kappa^{2r}\sum_{j}(-1)^{j_r+k_s+j_t}(R_{j_1\ldots j_r}\times T_{j_1\ldots j_t})_{k_s q}$$

$$\times\prod_{\sigma=2}^{s}\{[(2k_\sigma+1)(2j_{r+\sigma-1}+1)]^{1/2}W(k_{\sigma-1}1j_rj_{r+\sigma};k_\sigma j_{r+\sigma-1})\}. \tag{4.14}$$

4.3.3. Outer products. If $T_{\alpha_1\ldots\alpha_r\beta_1\ldots\beta_s}=R_{\alpha_1\ldots\alpha_r}S_{\beta_1\ldots\beta_s}$, then

$$T_{j_1\ldots j_t;m}=\sum_{klpq}\langle j_1\ldots j_t;m|\alpha_1\ldots\alpha_r\beta_1\ldots\beta_s\rangle\langle\alpha_1\ldots\alpha_r|l_1\ldots l_r;p\rangle$$

$$\times\langle\beta_1\ldots\beta_s|k_1\ldots k_s;q\rangle R_{l_1\ldots l_r;p}S_{k_1\ldots k_s;q}$$

$$=\sum_{k}(R_{j_1\ldots j_r}\times S_{k_1\ldots k_s})_{j_t m}$$

$$\times\prod_{\sigma=2}^{s}\{[(2k_\sigma+1)(2j_{r+\sigma-1}+1)]^{1/2}W(k_{\sigma-1}1j_rj_{r+\sigma};k_\sigma j_{r+\sigma-1})\}. \tag{4.15}$$

References

Brink G M and Satchler G R 1968 *Angular Momentum* (Oxford: Clarendon Press)
Condon E U and Shortley G H 1935 *The Theory of Atomic Spectra* (Cambridge: University Press)
Coope J A R 1970 *J. Math. Phys.* **11** 1591–612
Coope J A R and Snider R F 1970 *J. Math. Phys.* **11** 1003–17
Coope J A R, Snider R F and McCourt F R 1965 *J. Chem. Phys.* **43** 2269–75
Fano U and Racah G 1959 *Irreducible Tensorial Sets* (New York: Academic Press)
Stone A J 1975 *Molec. Phys.* **29** 1461–71
Yutsis A P, Levinson I B and Vanagas V V 1962 *The Theory of Angular Momentum* (Jerusalem: Israel Program for Scientific Translations)