A class of 6-j symbols for SO(2l+1) in terms of rotation matrices for SO(3)

1987 J. Phys. A: Math. Gen. 20 L343

(http://iopscience.iop.org/0305-4470/20/6/001)

J. Phys. A: Math. Gen. **20** (1987) L343–L347. Printed in the UK

LETTER TO THE EDITOR

A class of 6-j symbols for SO($2l+1$) in terms of rotation matrices for SO(3)

B R Judd

Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, Maryland 21218, USA

Received 20 January 1987

Abstract. It is shown that a 6-j symbol for SO($2l+1$) in which four primitive spinor representations $(\frac{1}{2}\frac{1}{2}\ldots\frac{1}{2})$ appear is directly related to an SO(3) rotation matrix possessing a rank of $l+\frac{1}{2}$ and characterised by the Euler angles $(0, \frac{1}{2}\pi, 0)$. An interpretation is given in terms of a rotation operator $\exp(\frac{1}{2}\mathrm{i}\pi T_y)$ acting in the combined spin and quasispin space of an atomic l shell, whose states $|T, M_T)$ are defined in a quasiparticle scheme in which four coupled spinors $(\frac{1}{2}\frac{1}{2}\ldots\frac{1}{2})$ are used.

It was O'Brien (1984) who noticed that some multiplicity-free 6-j symbols for SO(5), calculated numerically by Lister (1983) for an octahedral Jahn–Teller system, could be represented by quite simple algebraic formulae. Several ways of obtaining such formulae have been developed. Racah (1942) originally introduced his W function (an unsymmetrised 6-j symbol) to represent the matrix elements of scalar tensor products of the type $\boldsymbol{C}_{\mathrm{A}}^{(k)} \cdot \boldsymbol{C}_{\mathrm{B}}^{(k)}$, and his equations have been generalised to yield formulae for a variety of multiplicity-free 6-j symbols for SO($2l+1$), G_2, and Sp($2j+1$) (Judd *et al* 1986, Suskin 1987). By elaborating the spinor invariants of Kramers (1930), Judd and Lister (1987) were able to find a large class of multiplicity-free 9-j symbols for Sp($2j+1$) in terms of a generating function similar to that of Schwinger (1965) for SO(3). In the process of searching for methods that might complement such approaches, a striking formula was found for some 6-j symbols for SO($2l+1$) that involve the primitive representation with highest weight $(\frac{1}{2}^l)$ (that is, a weight $(\frac{1}{2}\frac{1}{2}\ldots\frac{1}{2})$ in which l coordinates $\frac{1}{2}$ appear). If we multiply the 6-j symbol by $(D_3D_6)^{1/2}$, where D_3 and D_6 are the dimensions of the representations in its third column, thereby converting it into a U function of the type introduced for SO(3) by Jahn (1951), the formula becomes

$$U_l(m, n) = U\begin{pmatrix} (\frac{1}{2}^l) & (\frac{1}{2}^l) & (1^{l-n}0^n) \\ (\frac{1}{2}^l) & (\frac{1}{2}^l) & (1^{l-m}0^m) \end{pmatrix} = 2^{1/2} d_{MN}^{l+1/2}(\tfrac{1}{2}\pi) \tag{1}$$

where

$$M = (-1)^m(m+\tfrac{1}{2}) \qquad N = (-1)^n(n+\tfrac{1}{2}) \tag{2}$$

and where $d_{MN}^{l+1/2}(\beta)$ is the familiar matrix for a rotation of β about the y axis in ordinary three-dimensional space (Brink and Satchler 1968, p 22). The U function appearing in (1) can be written as the recoupling coefficient

$$\langle((\tfrac{1}{2}^l)(\tfrac{1}{2}^l))(1^{l-n}0^n), (\tfrac{1}{2}^l), (\tfrac{1}{2}^l)|(\tfrac{1}{2}^l), ((\tfrac{1}{2}^l)(\tfrac{1}{2}^l))(1^{l-m}0^m), (\tfrac{1}{2}^l)\rangle \tag{3}$$

0305-4470/87/060343+05\$02.50

without, however, making the rationale for the existence of equation (1) any clearer. For reference purposes, numerical values are set out in table 1 for SO(7), corresponding to $l=3$.

It is not too difficult to derive equation (1). On picking $m=l$, the representation $(1^{l-m}0^m)$ becomes the scalar (0^l), and the U coefficient can be related to a stretched recoupling coefficient that is equal to 1. The intervening factor is proportional to $(D(W))^{1/2}$, where $D(W)$, the dimension of the representation W, is given by

$$D(1^{l-n}0^n)=(2l+1)!/(l+1+n)!(l-n)! \tag{4}$$

in the present case. The entries in the first column of the U table can be immediately written down by dividing $[D(1^{l-n}0^n)]^{1/2}$ by the normalising coefficient 2^l. The third column can be found by generalising Racah's scalar $\boldsymbol{C}_{\mathrm{A}}^{(k)}\cdot\boldsymbol{C}_{\mathrm{B}}^{(k)}$ to $\boldsymbol{T}_{\mathrm{A}}\cdot\boldsymbol{T}_{\mathrm{B}}$, where $\boldsymbol{T}_{\mathrm{A}}$ and $\boldsymbol{T}_{\mathrm{B}}$ are two separate (and commuting) sets of generators for SO($2l+1$). Each set corresponds to the irreducible representation $(110\ldots0)$ of SO($2l+1$), and the eigenvalues of $\boldsymbol{T}_{\mathrm{A}}\cdot\boldsymbol{T}_{\mathrm{B}}$ for the coupled state $|((\frac{1}{2}^l)(\frac{1}{2}^l))(1^{l-n}0^n)\rangle$ are proportional, on the one hand, to $U_l(2,n)[D(1^20^{l-2})D(1^{l-n}0^n)]^{-1/2}$ (the dimensional factor taking into account the difference between the U coefficient and the 6-j symbol), and, on the other hand, to the combination $G_{\mathrm{A+B}}-G_{\mathrm{A}}-G_{\mathrm{B}}$ of Casimir's operators, a combination whose eigenvalues are themselves proportional to

$$(l-n)(l+n+1)-\tfrac{1}{4}l(2l+1)-\tfrac{1}{4}l(2l+1) \tag{5}$$

that is, to $N^2-\frac{1}{4}(2l+1)$. The appropriate coefficient connecting $U_l(2,n)$ to (5) can be found by insisting that $U_l(2,0)=U_l(0,2)$. Orthogonality between $U_l(2,n)$ and $U_l(0,n)$ provides a check. Passing now to the fifth column, we note that $(\boldsymbol{T}_{\mathrm{A}}\cdot\boldsymbol{T}_{\mathrm{B}})^2$ contains parts of the form $\boldsymbol{V}_{\mathrm{A}}^{(W)}\cdot\boldsymbol{V}_{\mathrm{B}}^{(W)}$ for which $W=(2^20^{l-2})$, (21^20^{l-3}), and (20^{l-1}). (See, for example, Wybourne (1970, tables D-6 and D-7).) Operators $\boldsymbol{V}_{\mathrm{A}}^{(W)}\cdot\boldsymbol{V}_{\mathrm{B}}^{(W)}$ with such labels are ineffective because all three W do not occur in the Kronecker square $(\frac{1}{2}^l)^2$, and hence have null matrix elements. We are left with $W=(0^l)$, (1^20^{l-2}), and (1^40^{l-4}), some mixture of which must yield the square of the expression (5). It is now obvious that an operator $\boldsymbol{V}_{\mathrm{A}}^{(11110\ldots0)}\cdot\boldsymbol{V}_{\mathrm{B}}^{(11110\ldots0)}$ has matrix elements proportional to some linear combination $A+BN^2+CN^4$. Orthogonality between the fifth column and the first and third yields the relative values of A, B, and C. We can proceed in this way to calculate all the values of $U_l(m,n)$ for which $m=l$, $l-2$, $l-4,\ldots,1$ or 0. Having found the entries in the odd columns (and, from the imposed symmetry of $U_l(m,n)$,

Table 1. The functions

$$U\begin{pmatrix}(\frac{1}{2}\frac{1}{2}\frac{1}{2}) & (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & W\\ (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & W'\end{pmatrix}$$

for SO(7). Values of the corresponding 6-j symbols can be found by dividing by $[D(W)D(W')]^{1/2}$.

		M	$-\frac{7}{2}$	$\frac{5}{2}$	$-\frac{3}{2}$	$\frac{1}{2}$
		W	(000)	(100)	(110)	(111)
N	W'	$D(W)$	1	7	21	35
$-\frac{7}{2}$	(000)		1/8	$7^{1/2}/8$	$(21)^{1/2}/8$	$(35)^{1/2}/8$
$\frac{5}{2}$	(100)		$7^{1/2}/8$	$-5/8$	$(27)^{1/2}/8$	$-5^{1/2}/8$
$-\frac{3}{2}$	(110)		$(21)^{1/2}/8$	$(27)^{1/2}/8$	1/8	$-(15)^{1/2}/8$
$\frac{1}{2}$	(111)		$(35)^{1/2}/8$	$-5^{1/2}/8$	$-(15)^{1/2}/8$	3/8

the odd rows as well), we are left with the entries in the simultaneously even rows and columns to work out. The linear independence of the odd columns makes it clear that the orthogonality conditions alone are enough to lead to unambiguous solutions for the remaining entries that we need. If a solution can be guessed for the even–even sites of the U matrix, and if all the orthogonality conditions are satisfied, the solution is correct. Since the odd columns involve even powers of N it is natural to try odd powers of N for the even columns; and this is indeed how things work out. For example, the second column of table 1 is proportional to $N[D(W)]^{1/2}$ and the fourth to $(N^3-\frac{19}{4}N)[D(W)]^{1/2}$. Having established the general structure of the table of U coefficients, we can turn to standard mathematical procedures to find explicit algebraic forms for the entries. This involves converting the orthogonality conditions to recurrence relations, expressing the latter in terms of generating functions, and then finding the differential equation satisfied by these functions. It was only when the last stages of this work was being carried out that the close connection of the U matrices to the rotation matrices of SO(3), as represented by equation (1), was recognised.

The connection between such dissimilar quantities as $U_l(m, n)$ and $d^{l+1/2}_{MN}(\frac{1}{2}\pi)$ must lead to parallelisms between the various relations that they separately satisfy. The orthogonality of the matrix $U_l(m, n)$ corresponds to that of each quarter of the matrix $d^j_{MN}(\beta)$ when j is half-integral and $\beta=\frac{1}{2}\pi$. More interesting is the so-called Racah back-coupling relation (Brink and Satchler 1968, equation 3.21, Edmonds 1957, equation 6.2.11) which, for our U functions, is

$$\sum_n (-1)^{p(k)+p(m)+p(n)} U_l(m, n) U_l(k, n) = U_l(m, k) \tag{6}$$

where $p(n)=0$ (1) if $(1^{l-n}0^n)$ occurs in the symmetric (antisymmetric) part of the Kronecker square $(\frac{1}{2}^l)^2$. The parity function $p(n)$ does not simply alternate as n increases in unit steps: it turns out that $p(n)=0$ for $n=0, 3, 4, 7, \ldots$, and $p(n)=1$ for $n=1, 2, 5, 6, \ldots$ That is,

$$(-1)^{p(n)}=2^{1/2}\,\mathrm{Re}[\exp(\tfrac{1}{2}\mathrm{i}N\pi)].$$

The introduction of the exponential function does not complicate matters too much because we can incorporate it into the analysis by means of such equations as

$$\exp(\tfrac{1}{2}\mathrm{i}N\pi)d^{l+1/2}_{KN}(\tfrac{1}{2}\pi)=\mathscr{D}^{l+1/2}_{NK}(-\tfrac{1}{2}\pi, -\tfrac{1}{2}\pi, 0) \tag{7}$$

where $\mathscr{D}^j_{NK}(\alpha, \beta, \gamma)$ is the full three-dimensional rotation matrix corresponding to the Euler angles α, β, and γ (Brink and Satchler 1968, § 2.4). On substituting the d functions for the U functions in equation (6), we get after some manipulation (in which the evenness of $M-K$ and oddness of $M+K$ is used) the result

$$\sum_N \mathscr{D}^{l+1/2}_{MN}(0, \tfrac{1}{2}\pi, 0)\mathscr{D}^{l+1/2}_{NK}(-\tfrac{1}{2}\pi, -\tfrac{1}{2}\pi, 0)=\mathscr{D}^{l+1/2}_{MK}(-\tfrac{1}{2}\pi, -\tfrac{1}{2}\pi, \tfrac{1}{2}\pi). \tag{8}$$

Thus Racah's back-coupling relation for SO($2l+1$) corresponds to the statement that two successive rotations in SO(3) characterised by the Euler triads $(-\frac{1}{2}\pi, -\frac{1}{2}\pi, 0)$ and $(0, \frac{1}{2}\pi, 0)$ are equivalent to a single rotation for which $(\alpha, \beta, \gamma)\equiv(-\frac{1}{2}\pi, -\frac{1}{2}\pi, \frac{1}{2}\pi)$.

It is interesting to note that for SO(3) Edmonds (1957, equation A2.2) has given the approximate formula

$$U\begin{pmatrix} J & S & L \\ j & L-\delta & S+\varepsilon \end{pmatrix} \simeq (-1)^{J+S+L} d^j_{\delta\varepsilon}(\phi)$$

where J, S, $L \gg |\delta|$, $|\varepsilon|$, and where ϕ satisfies the equation

$$\cos\phi=[J(J+1)-S(S+1)-L(L+1)]/2[S(S+1)L(L+1)]^{1/2}.$$

In this case the Racah back-coupling relation for SO(3) turns out to be equivalent to the non-controversial statement that the interior angles of a plane triangle whose sides are approximately $J+\frac{1}{2}$, $S+\frac{1}{2}$, and $L+\frac{1}{2}$ add up to π.

New 6-j symbols for SO($2l+1$) can be produced by generalising the Biedenharn–Elliott sum rule (Edmonds 1957, equation 6.2.12). Writing W_x for $(1^{l-x}0^x)$, we have

$$\sum_n [D(W_n)]^{-1/2} U_l(m,n) U_l(r,n) U_l(t,n)$$
$$= [D(W_m)D(W_r)D(W_t)]^{1/2} \begin{Bmatrix} W_m & W_r & W_t \\ (\frac{1}{2}^l) & (\frac{1}{2}^l) & (\frac{1}{2}^l) \end{Bmatrix}^2 . \qquad (9)$$

The 6-j symbol in this equation vanishes unless $W_m \times W_r \times W_t$ contains the identity (0^l). For example, the entries in table 1 for SO(7) can be used to show that

$$\begin{Bmatrix} (110) & (110) & (100) \\ (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & (\frac{1}{2}\frac{1}{2}\frac{1}{2}) \end{Bmatrix} = 0 \qquad (10)$$

a result that must follow because $(110)^2 \times (100)$ does not contain (000) (see Wybourne 1970, table D-4). The substitution of d functions for the U functions in equation (9) leads to previously unsuspected relations satisfied by rotation matrices for which $(\alpha, \beta, \gamma) = (0, \frac{1}{2}\pi, 0)$.

Having said all this, the problem remains as to why equation (1) has the form it does. The derivation given above, although not particularly intricate, gives no clue as to the final outcome. Why, in particular, should the d function have a rank of $l+\frac{1}{2}$? Although there is nothing in the recoupling coefficient (3) to suggest such a rank, we note that the maximum spin S occurring in the electronic configurations l^u $(0 \leq u \leq 4l+2)$ is precisely $l+\frac{1}{2}$. For example, ^{8}S is the term of maximum multiplicity in the atomic f shell. However, the relevant angular momentum vector for us is not $\boldsymbol{S}$ but rather the sum $\boldsymbol{S}+\boldsymbol{Q}$ $(=\boldsymbol{T}$, say), where $\boldsymbol{Q}$ is the quasispin (Judd 1967). Since ^{8}S occurs only once in the f shell it is a quasispin singlet, so $T = S = \frac{7}{2}$ in this case. It is known that the states of the atomic l shell can be formed by factorising both the spin-up and spin-down spaces into two parts, each labelled by $(\frac{1}{2}^l)$ (Armstrong and Judd 1970). Thus an S state belonging to (0^l) can be written in the coupled form

$$|((\tfrac{1}{2}^l)_\lambda(\tfrac{1}{2}^l)_\mu)(1^{l-n}0^n), ((\tfrac{1}{2}^l)_\nu(\tfrac{1}{2}^l)_\xi)(1^{l-n}0^n), (0^l)\rangle \qquad (11)$$

where $(\frac{1}{2}^l)_\theta$ is the primitive spinor representation of the group SO$_\theta(2l+1)$ whose generators $(\boldsymbol{\theta}^\dagger\boldsymbol{\theta})^{(k)}$ (with k odd) are built from the quasiparticle creation and annihilation operators $\boldsymbol{\theta}^\dagger$. From their definition in terms of the standard annihilation and creation operators ($\boldsymbol{a}$ and $\boldsymbol{a}^\dagger$) for the electrons (Armstrong and Judd 1970, equation 1), it is straightforward to show that, under the action of $\exp(\frac{1}{2}i\pi T_y)$, we have $\boldsymbol{\lambda} \to -\boldsymbol{\nu}$, $\boldsymbol{\mu} \to \boldsymbol{\mu}$, $\boldsymbol{\nu} \to \boldsymbol{\lambda}$ and $\boldsymbol{\xi} \to \boldsymbol{\xi}$. The interchange of λ and ν in the ket(11) can be accomplished by an expansion that involves a generalised 9-j symbol with one argument equal to (0^l). With the help of an analogue of equation (6.4.14) of Edmonds (1957), this reduces to precisely the U function of equation (1). On the other hand, we can apply $\exp(\frac{1}{2}i\pi T_y)$ directly to the ket (11). It is not difficult to show that the states of the atomic l shell belonging to (0^l) of SO($2l+1$) (and formed as in the ket (11)) possess both T and M_T (the eigenvalue of T_z) as good quantum numbers. We have already seen that $T = \frac{7}{2}$ for the f shell: in general it is $l+\frac{1}{2}$. The first representation $(1^{l-n}0^n)$ in the ket (11) corresponds to either $l-n$ or $l+n+1$ spin-up electrons; the second to either $l-n$ or $l+n+1$ spin-down electrons (a quadruple ambiguity originating in table I of Racah

(1949)). Since M_Q (the eigenvalue of Q_z) is given in terms of the total number of electrons u by $-\frac{1}{2}(2l+1-u)$ (Judd 1967, p 41), we get

$$M_T = M_S + M_Q$$
$$= \tfrac{1}{2}(l-n) - \tfrac{1}{2}(l-n) - \tfrac{1}{2}(2l+1-2l+2n) = -(n+\tfrac{1}{2}) \tag{12}$$

together with three other possibilities, all of which are of the form $\pm(n+\frac{1}{2})$, that is, $\pm(-1)^n N$, from equations (2). The effect of the operator $\exp(\frac{1}{2}\mathrm{i}\pi T_y)$ on the kets of the type $|T, M_T\rangle$ is represented by $d^T_{M_T M_T'}(\frac{1}{2}\pi)$, which, in view of equation (12) and its three companions, corresponds precisely to the d function of equation (1). The factor $2^{1/2}$ appearing there is related to the fact that two independent kets of the type (11) correspond to a specified $|T, M_T\rangle$. The ambiguities in sign in the connections $M_T \leftrightarrow N$ and $M_T' \leftrightarrow M$ lead at most to overall phase changes since $d^T_{MN}(\frac{1}{2}\pi) = (-1)^{T-N} d^T_{-MN}(\frac{1}{2}\pi)$, etc. Different choices of phase could have been made at many points of the above analysis, but such distractions have been avoided for the sake of simplicity. As a final remark, it should be noted that equation (1) presumably exists in its own right and not as a consequence of the existence of electrons in atoms with angular momentum quantum numbers l; but the insight that such an interpretation affords is very gratifying.

Partial support of the above work by the United States National Science Foundation is acknowledged.

References

Armstrong L and Judd B R 1970 *Proc. R. Soc.* A **315** 27-37
Brink D M and Satchler G R 1968 *Angular Momentum* (Oxford: Clarendon)
Edmonds A R 1957 *Angular Momentum in Quantum Mechanics* (Princeton: Princeton University Press)
Jahn H A 1951 *Proc. R. Soc.* A **205** 192-237
Judd B R 1967 *Second Quantization and Atomic Spectroscopy* (Baltimore: The Johns Hopkins Press)
Judd B R and Lister G M S 1987 *J. Phys. A: Math. Gen.* **20** at press
Judd B R, Lister G M S and O'Brien M C M 1986 *J. Phys. A: Math. Gen.* **19** 2473-86
Kramers H A 1930 *Proc. K. Ned. Akad. Wet.* **33** 953-8
Lister G M S 1983 *DPhil Thesis* University of Oxford
O'Brien M C M 1984 private communication
Racah G 1942 *Phys. Rev.* **62** 438-62
—— 1949 *Phys. Rev.* **76** 1352-65
Schwinger J 1965 *Quantum Theory of Angular Momentum* ed L C Biedenharn and H van Dam (New York: Academic)
Suskin M A 1987 *PhD Thesis* The Johns Hopkins University
Wybourne B G 1970 *Symmetry Principles and Atomic Spectroscopy* (New York: Wiley Interscience)